

W.E.Nagel · W.Jäger
M.Resch (Eds.)

High Performance Computing in Science and Engineering '05



H L R I S

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High Performance Computing in Science and Engineering '05

Wolfgang E. Nagel · Willi Jäger · Michael Resch
Editors

High Performance Computing in Science and Engineering '05

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Editors

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Front cover figure: Vortex system of a helicopter main rotor in decent flight. Vortex-adapted grids allow for an improved vortex conservation.

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Preface

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The year 2005 has been a great year for high performance computing in Baden-Württemberg, and even beyond for all local states. In July, the new building for the HLRS as well as Stuttgart's new NEC supercomputer – which is leading edge in Germany for quite some time – have been inaugurated in an impressive celebration. Almost simultaneously, the SSC Karlsruhe is finalizing the installation of a very large high performance system complex from HP, built from many hundreds of Intel Itanium processors. Additionally, a fast network connection has been opened. With a bandwidth of 40 Gbit/s it is not only the first installation of this kind in Germany, but it also brings the machine rooms of HLRS and SSC Karlsruhe very close together. Finally, the University Heidelberg – especially the WiR – has joined the Center for Competence in

High-Performance Computing in Baden-Württemberg (HKZ-BW) to further strengthen the aspects of computational science. With the investment of more than 60 Million Euro, we – as the users of such a valuable infrastructure – are not only thankful to science managers and politicians, but also to the people running these components as part of their daily business, on a 24-7 level. Most of the time, operating leading edge technology is a challenge and requires more personal dedication and commitment than usually can be expected.

All support from government, politics, and people is driven by the knowledge that the high performance computing infrastructure – together with the innovative computational algorithms, methods and tools – are driving the long time success of our country. These components will strongly influence the development of new technologies and industrial products; beyond that, this will finally determine if Germany will be an accepted partner among the leading technology and research nations.

Currently, there are lots of activities on all scientific, advisory, and political levels to decide if Germany will install an even larger European supercomputer, where the hardware costs alone will be around 100 to 150 Million Euro. There are many good reasons to invest in such a program because – beyond the infrastructure – such a scientific research tool will attract the best brains to tackle the problems related to the software and methodology challenges. What will additionally be required is, therefore, a related research program to support Computational Science and Engineering on that level of expertise and performance. We do not only need competitive hardware but also excellent software and methods to approach – and solve – the most challenging problems in science and engineering.

Since 1996, the HLRS is supporting the scientific community as part of its official mission. Like in the years before, the major results of the last 12 months were reported at the Eighth Results and Review Workshop on High Performance Computing in Science and Engineering, which was held October 13-14, 2005 at Stuttgart University. This volume contains the written versions of the research work presented. The papers were selected in an internal review from all projects processed at the HLRS and at the SSC Karlsruhe during the time period beginning October 2004. Overall, 25 papers have been chosen from Physics, Solid State Physics, Computational Fluid Dynamics, Chemistry, and other topics. The largest number of contributions, as in many other years, came from CFD with 11 papers. To a certain extend, the selected papers demonstrate the state of the art in high-performance computing in Germany. The authors were encouraged to emphasize computational techniques used in solving the problems examined. The importance of the newly computed results for the specific disciplines, as interesting as they may be from the scientific point of view, were not the major focus of this volume.

We gratefully acknowledge the continued support of the Land Baden-Württemberg in promoting and supporting high-performance computing. Grateful acknowledgement is also due to the Deutsche Forschungsgemeinschaft (DFG): many projects processed on the machines of the HLRS and

the SSC could not have been carried out without the support of the DFG. Also, we thank the Springer Verlag for publishing this volume and thus helping to position the local activities into an international frame. We hope that this series of publications is contributing to the global promotion of high performance scientific computing.

Stuttgart, September 2005

Wolfgang E. Nagel

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Michael Resch

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Physics

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High performance computing has become a matter of routine in physical research. Complex theoretical models generally can only be fully analysed with assistance of numerical simulations, while also experimental research more and more has been complemented and even replaced by scientific computing, in particular in those fields where experiments are dangerous, difficult or unfeasible. The articles in this section, which present a selection of projects related to physical research currently running at the HLRS, exemplify this nicely.

It is of the intrinsic nature of research in Astrophysics and Cosmology that experiments are impossible. Thus it is not astonishing that applications in those fields have comprised a major contribution to all projects in 2004. A particular highlight is the work by M. Krause, V. Gaibler, and M. Camenzind, which deals with high-resolution simulations of astrophysical jets in dense environments. In particular, they continued to analyse the interactions of jets emanating from galactic cores with a galactic wind, especially with regards to differences between purely hydrodynamic and magneto-hydrodynamic effects. Furthermore they were able to increase the performance of the finite-differences code (NIRVANA) which they use for their simulations by a factor of three.

Another example for a cosmological application consists in the simulations of host galaxies of Gamma-ray bursts by G. Björnsson, S. Courty, and E.H. Gudmundsson. Because Gamma-ray bursts are among the most energetic events in the universe, they are generally considered to be able to give insight into fundamental galaxy formation processes. In this project, the properties of certain populations of galaxies were investigated distinguishing between absolute star formation rate and star formation rate per galaxy mass, adopting a particle-mesh algorithm.

On a much smaller length scale focus the interests of C. Dahnken, M. Potthoff, E. Arrigoni, and W. Hanke, who study the doping dependence of the quasiparticle band of electron-doped cuprates, in particular comparing their simulation results with experimental data. Using variational cluster-perturbation theory to calculate the spectral function they were able to show

that the evolution of the Fermi surface can be well described by the unapproximated one-banded Hubbard model.

A more computer science related direction has the contribution by M. Hipp et al. They report on the improvements of a parallel Smoothed Particle Hydrodynamics (SPH) code, focusing on enhancements for hybrid parallel architectures and on optimized I/O. SPH is a numerical method for simulating hydrodynamics and continuum mechanics problems. Accordingly, M. Hipp et al. additionally present briefly some examples for applications, ranging again from Astrophysics, where the simulation of a so called accretion disc, a gas disc rotating around a compact star, is shown, to simulations of brittle fraction of a solid body and of two-phase flows during the injection of diesel into a combustion chamber.

All these projects demonstrate the high scientific level that high performance computing has reached. Striking is however the particularly small number of projects that were available this time – does this indicate a decreasing demand for computing time? Are local computing resources meanwhile powerful enough to suffice for most of the problems? Or does the development of algorithms encounter special difficulties for the application on current supercomputers?

Simulations of Astrophysical Jets in Dense Environments

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Summary. We have simulated the interaction of jets with a galactic wind at high resolution using the magnetohydrodynamics code NIRVANA on the NEC SX-6 at the HLRS. This setup may describe a typical situation for the starbursting radio galaxies of the early universe. The results show a clear resolution dependence in the expected way, but the formed clumps are denser than expected from linear extrapolation. We also report our recent progress in the adaptation of the magnetic part of NIRVANA to the SX-6. The code is now fully tuned to the machine and reached more than 3 Gflops. We plan to use this new code version to extend our study of magnetized jets down to very low jet densities. This should be especially applicable to the conditions in the young universe.

1 Introduction

Extragalactic jets emerge from the cores of bright elliptical galaxies (1). This is the result of extensive observations on nearby radio galaxies (e.g. 2). Radio galaxies have, however, been found up to redshifts in excess of five and are associated with an enormous release of energy, exceeding 10^{40} watts (3, 4).

Many characteristic properties of these progenitors are not known of in any detail. According to our present understanding of the formation of galaxies, present-day bright ellipticals are not the product of a late normal merging sequence of fainter galaxies. Indeed, results obtained by the Hubble Space Telescope (HST) suggest that early radio galaxies, which still consist of individual gas clumps, are the progenitors of the bright ellipticals (in the sense of proto-cD galaxies).

As observations show, the external medium is rapidly cooling by line emission. One of our main goals is the study of the influence of cooling mechanisms on the evolution of magnetized jets. We are especially interested in the structural differences between purely hydrodynamic jets and magnetized jets and

the differences in the emission properties of the shock-heated ambient gas (Fig. 3). An accurate jet model is important to achieve an understanding of the observational data from the early universe (high redshifts) and to find out, whether the observed emission line regions can be explained solely by shock excitation or whether another source of energy is needed.

Supermassive Black Holes with masses up to a few billion solar masses have been found in the centers of such bright ellipticals. These dark masses are probably formed in the early evolution of the core region of these galaxies at redshifts > 6 . The Black Holes are thought to be the main drivers for the jets which are the sources of the radio emission.

The radio emission is polarized which reveals the synchrotron nature of the emission. This is evidence for the presence of magnetic fields. We have started a parameter study for magnetized jets of differing density. Preliminary results indicate that the magnetic field is especially important for low jet densities. Low jet densities have been favoured for the studied systems, also on the grounds of our hydrodynamic simulations (e.g. 4), and for other reasons. For the first time we use a zero gradient boundary condition at the jet's nozzle. This results in good numerical behaviour down to a density contrast of at least 10^{-3} . We plan to augment this parameter study at least with 10^{-4} density contrast simulations, and also 3D studies. But for this, high performance computing is essential, since the computational power requirement increases dramatically when lowering the jet density. Due to the SX-6 installation, code adaptation became necessary. We report on our recent vectorization success in section 3.

At redshifts of $z > 0.6$ extended optical continuum and emission line regions, aligned with the radio structures, become prominent companions (5). Beyond a redshift of $z \approx 2$, most of the optical emission originates from the Lyman α transition of hydrogen. Huge Ly α halos have been observed in the young universe (6). Their size often exceeds the radio size. Only for radio extents smaller than 50 kpc^4 , the Ly α emission, that has turbulent velocities of typically 1000 km/s , is totally absorbed with a velocity width of several 10 km/s (7). The absorbers are typically blue-shifted (8, 7).

We have recently proposed a scenario that is able to explain this observation (9, 10). The model postulates a galactic wind with a radiative bow shock. The jet starts inside the galactic wind shell about 100 million years after the onset of the wind. The associated Ly α emission is absorbed by the cooled wind shell as long as the jet remains inside. When the jet reaches the shell, it increases the pressure in the bubble which accelerates, and then fragments due to the Rayleigh–Taylor instability. The mechanism was demonstrated by high performance simulations on the NEC SX-5 (10). Meanwhile we were able to study the process at higher resolution, and report the new findings in section 4.

⁴ $\text{kpc} = 3260 \text{ light years} = 3 \times 10^{19} \text{ m}$

PROG.UNIT	FREQUENCY	EXCLUSIVE TIME[sec](%)	AVER.TIME [msec]	MOPS	MFLOPS	V.OP RATIO	AVER. V.LEN	BANK CONF
ct	30	16.868(55.1)	562.253	2252.0	629.4	99.73	256.0	1.1183
lorentz	30	6.816(22.3)	227.200	3465.8	1026.6	99.67	255.8	0.1290
advect	30	2.934(9.6)	97.791	7344.1	2634.6	99.46	254.9	0.1362
data	4	1.821(6.0)	455.215	276.4	152.8	2.95	205.0	0.0046
scr	30	0.680(2.2)	22.665	5878.3	3093.3	99.40	255.6	0.0123

Fig. 1. Performance results from a short test run of the *non-optimized* code on the SX-6. Output from **sftrace** profiler is shown for the five most time-consuming routines

2 Computational Technique

We use the non-relativistic finite-difference code NIRVANA, developed by Udo Ziegler (11) and adapted to jet simulations by M. Thiele (12) at the Landessternwarte Königstuhl to solve the magnetohydrodynamic equations in two or three dimensions for density, velocity, internal energy and magnetic field. NIRVANA has been modified in our group to include cooling effects, which are important for the propagation of jets (12) and has already been used with this modification in our project. While up to now, the hydrodynamic parts have extensively been used and optimized for the SX-6, it is now important for our computations to improve the performance of the magnetic parts of the code.

Because of large loops with lots of temporary variables and conditional expressions for the array indices, the vector performance initially was very disappointing. Figure 1 shows the results of a performance measurement with **sftrace** for a short test run. Our first goal was to improve the performance on a single CPU.

The most important change was splitting the loops into three different cases which made it possible to move conditionals outside of the loop. It was now possible to completely eliminate minimum/maximum expressions for the array indices or at least improve performance by calculating two possible results for conditional expressions and selecting the needed one afterwards – similar to the approach called “masking” which the compiler would choose in simpler cases.

This yields a performance better by a factor of 3 and with 2.6 Gflops of the same order as the advection routine, which is the most time-consuming part for pure hydrodynamics. Figure 2 shows the results of a test run. The production performance will be higher without profiling overhead and 3 Gflops should be achievable. Parallelization with SX-specific OpenMP-like methods works very well for the hydrodynamic parts (10). We do not expect specific problems for the magnetic subroutines, but this was not tested so far.

PROG.UNIT	FREQUENCY	EXCLUSIVE TIME[sec](%)	AVER.TIME [msec]	MOPS	MFLOPS	V.OP RATIO	AVER. V.LEN	BANK CONF
ct	30	4.679(33.8)	155.954	6487.5	2560.4	99.64	256.0	0.0276
advect	30	2.893(20.9)	96.422	7452.4	2676.6	99.60	254.9	0.1357
lorentz	30	2.552(18.4)	85.070	7612.3	2718.4	99.61	255.8	0.0218
data	4	1.826(13.2)	456.512	275.6	152.3	2.95	205.0	0.0063
scr	30	0.545(3.9)	18.172	6746.7	3902.8	99.38	255.6	0.0071

Fig. 2. Performance results as in Fig. 1, but for the code version with *optimized* vectorization

3 Planned Simulations of Magnetized Jets

We already found suitable initial conditions for the magnetic fields for setups with less extreme density contrast. The jets should be simulated up to a length of several hundred times the jet radius. This will enable us to compare the results with the already done parameter study for very light and pure hydrodynamic jets and examine the influence of the magnetic field on the jet evolution.

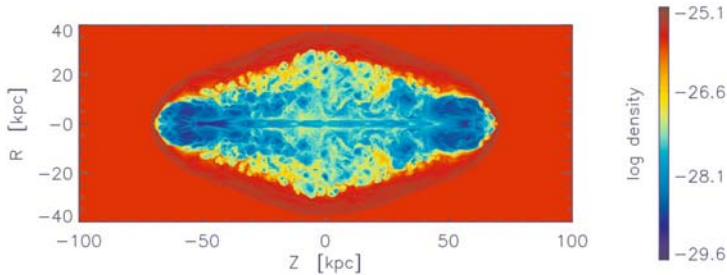


Fig. 3. Density of a magnetic jet with density contrast $\eta = 10^{-2}$ propagating into an environment with constant density after 10 million years. The structure is very similar to pure hydrodynamic jets, but the contact surface near the head region is more stable. The jets quickly adjust their magnetic field according to jet pressure and density contrast to an equilibrium structure.

We are especially interested in the following questions:

- Is the shape and propagation law of the bow shock changed by the magnetic fields or is it rather unchanged?
 - What emission would we see from the gas?
- With a model for the electron distribution, radio maps and spectra as well as “power at frequency vs. size” diagrams are to be computed and compared with literature data and observations.

- How do magnetic fields influence the entrainment rate into the jet cocoon? Here, sufficient resolution is crucial.
- What velocity distribution do we find?
Is there equipartition of kinetic and magnetic energy? How do kinetic and magnetic energy decrease against position and jet size? What about the velocity components? How does all this depend on the field strength and resolution? This has to be compared to emission line kinematics.

Another aim is to explore the interaction of the jet with structured background media, e.g. clouds or galaxies along the jet. Interaction with a real clumpy medium is not possible because we would need a resolution that is way too high to be feasible. But interaction with galaxy-sized clumps at different positions relative to the jet is possible and would shed light upon the effects of galaxy collisions. The evolution of Ly α emission and the intensity and spectrum of bremsstrahlung gives information about observable consequences. What would happen with the gas and how does the result depend on the resolution of the simulation?

4 A Highly Resolved Jet-in-Wind Simulation

4.1 Setup

Again, NIRVANA was used for the computation. The axisymmetric computational domain ($[Z \times R] = [200 \text{ kpc} \times 50 \text{ kpc}] = [4092 \text{ cells} \times 1022 \text{ cells}]$) was initialized with a King atmosphere ($\varrho = 0.3 m_p \text{ cm}^{-3} / (1 + r^2/100 \text{ kpc}^2)$, $r^2 = R^2 + Z^2$, ϱ is the density) at a temperature of 10^6 K . In order to break the symmetry, random fluctuations on the percent level have been added to the density. The galactic wind was simulated by a distributed energy and mass density increase, $\propto \exp(-r/3 \text{ kpc})$, $3 \times 10^{43} \text{ erg/s}$, and $10 M_\odot/\text{yr}$ in total. With these parameters, both cold gas due to a cooling flow and a radiative bow shock by the galactic wind can be expected. After 80 Myr, a bipolar jet with a radius of 1 kpc, a density of $10^{-5} m_p \text{ cm}^{-3}$, a Mach number of 13, a velocity of 2/3 the speed of light, and a total power of $4 \times 10^{45} \text{ erg/s}$ was injected in the centre of the grid. This simulation is compared to an earlier simulation at half resolution (10).

4.2 Results

The time evolution of density and temperature is shown in Figs. 4 and 5. Magnifications of the head and sideways bow shock regions are shown in Figs. 6 and 7.

The beam is stuck for some time after reaching the shell. During this time the jet's cocoon fills the wind bubble, and accelerates the shell sideways. The shell destruction is different at the jet head and towards the sides. The simulation shows that the direct impact heats the bow shock in the head region,

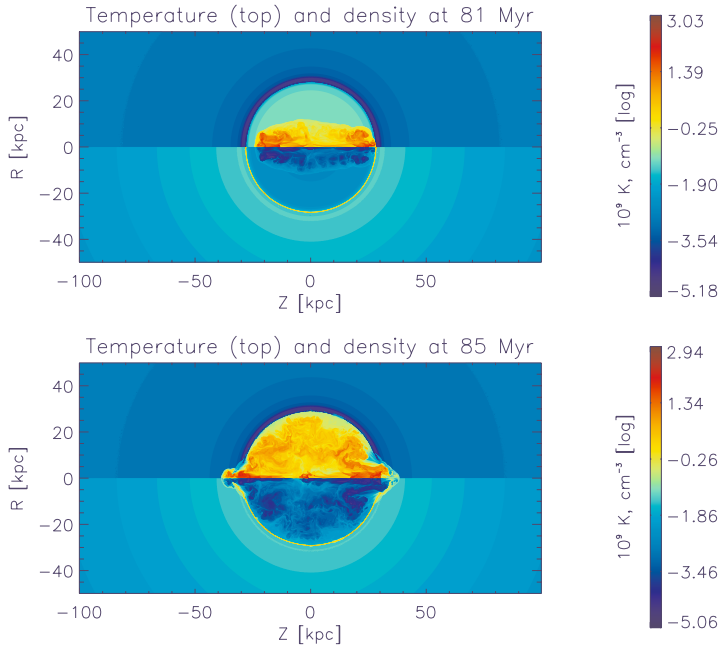


Fig. 4. Density and temperature for the full grid at different times. It takes some time for the jet to pierce the shell. While the shell is filled by the jet cocoon, it gets accelerated and starts to fragment.

which then expands and bends sideways, allowing for the passage of the beam (Fig. 6). Sideways, the acceleration causes compression and then Rayleigh-Taylor instabilities, leading to fragmentation and entrainment of dense gas into the cocoon.

The compression in this simulation is about twice as high as in an earlier simulation at half the resolution, for early times (Fig. 8). In this phase, the shell is intact, and only one dimension (the spherical radius) is additionally compressed. Later, the gas gets up to four times denser, reflecting the change, to a more cloud-like distribution. Since the process is driven by the Rayleigh-Taylor instability, it starts earlier at higher resolution, because smaller instable wavelengths are resolved. Therefore, the fragmentation may happen even faster in nature.

We have computed the covering fraction of neutral hydrogen over time (Fig. 8). After about 7 Myr of jet activity, it drops quickly to 50%, and keeps falling. The drop appears slightly later than in the earlier simulation at half resolution. The number has to be squared, to compare to observations, since an equal reduction in the (not simulated) azimuthal direction can be expected.

This is therefore in excellent agreement with the observed disappearance of the absorption in the bigger sources.

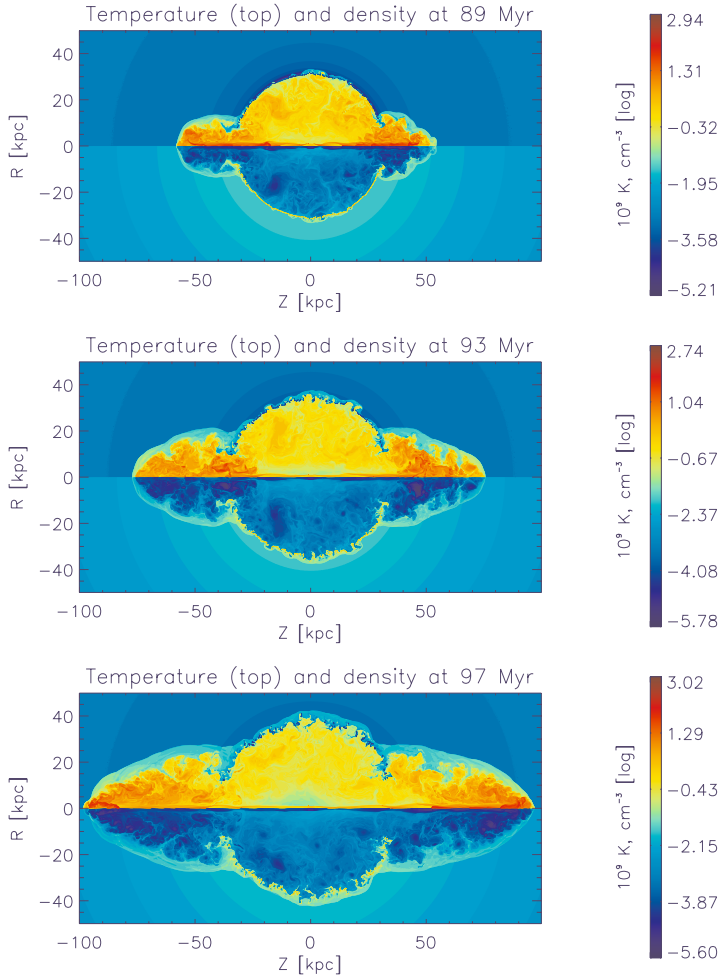


Fig. 5. Continuation of Fig. 4

5 Summary

We could confirm our earlier results on the jet-in-wind scenario by a higher resolution simulation. The compression starts earlier and the covering fraction decreases later. Hence, the observed absorption in the smaller sources can be explained by the proposed galactic wind shell.

Also, we could reach a performance increase by a factor of three for the SX-6 version of the magnetic part of the code (NIRVANA). The code now reaches about 3 Gflops, and is ready for the proposed magnetized jet simulations on the NEC SX-8.

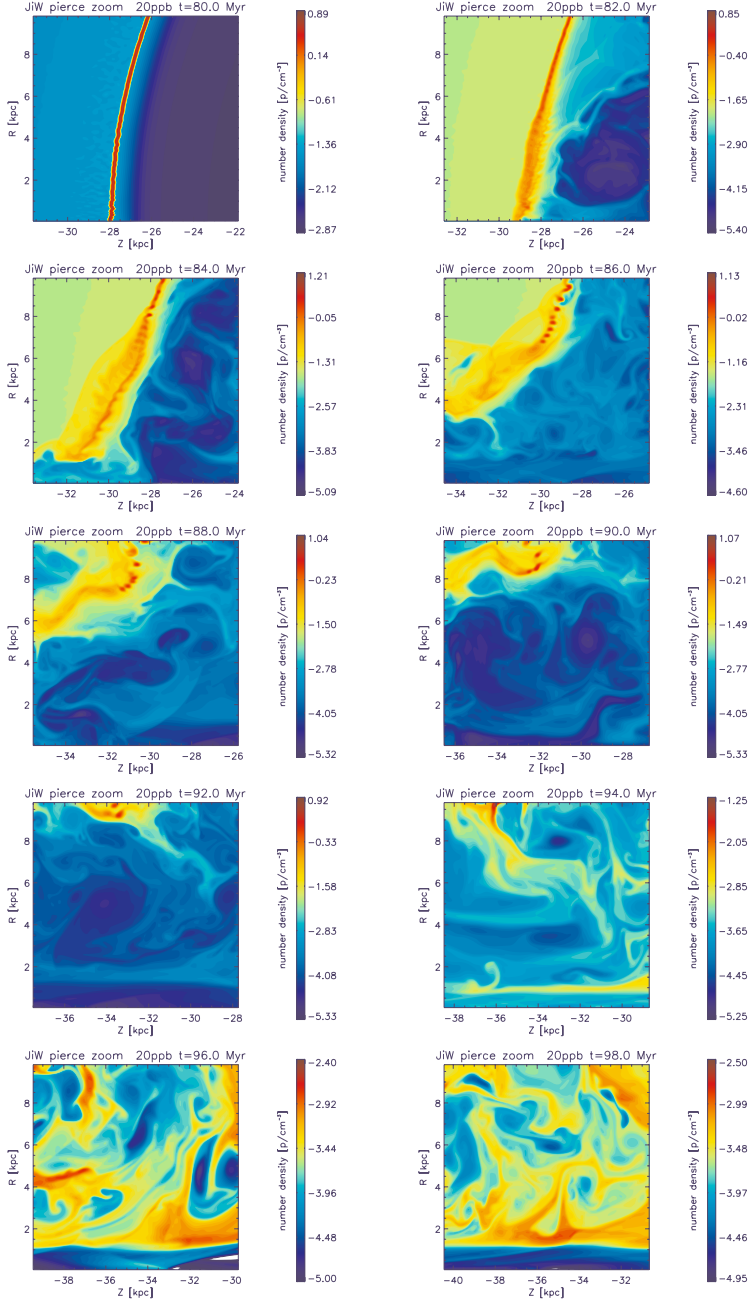


Fig. 6. Density at the jet head, magnified. The direct impact of the jet heats the shell, which first expands, and then bends to allow the jet's passage. Note the leftward shift.

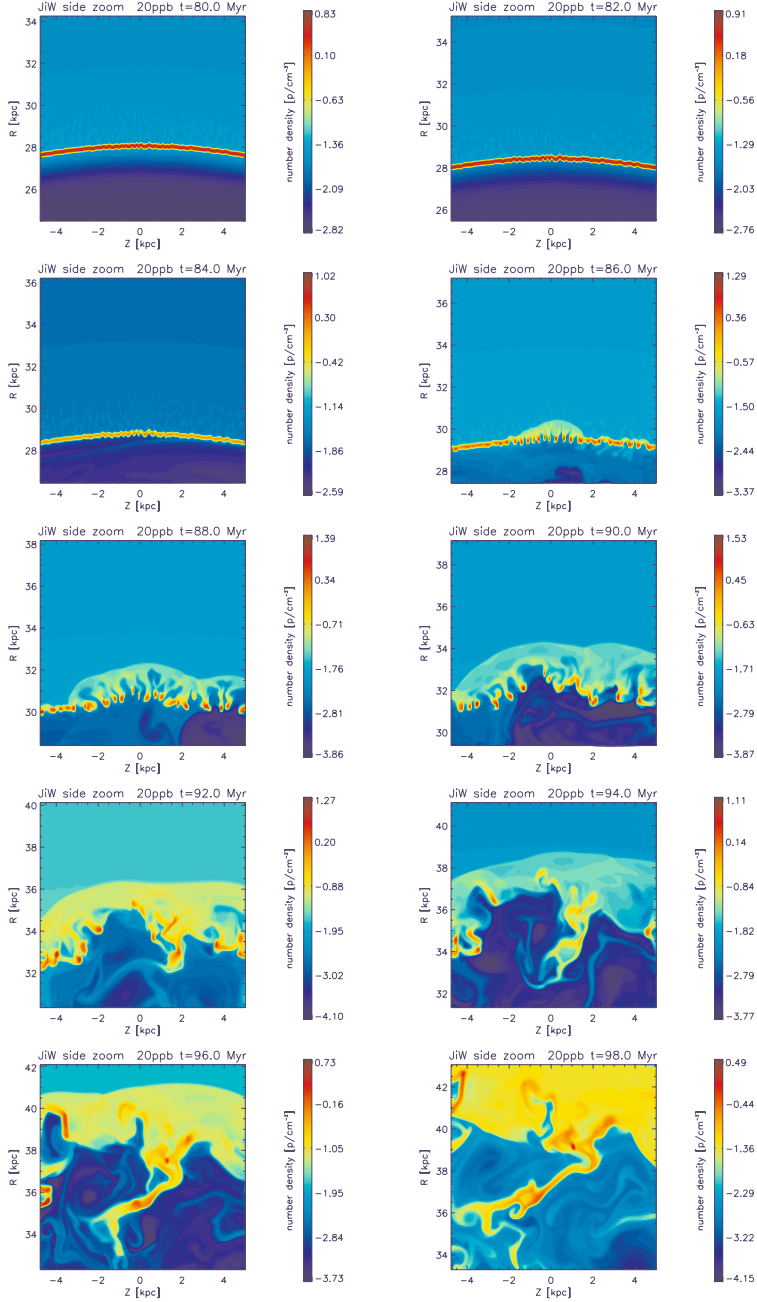


Fig. 7. Density at the sideways bow shock, magnified. The shell is compressed and fragments. Note the upward shift.

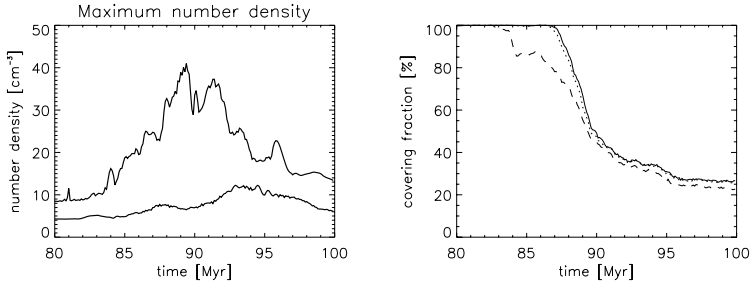


Fig. 8. Left: Maximum number density in this simulation compared to a simulation with half the resolution. Right: Covering fraction of neutral hydrogen over time for a column in excess of 10^{18} cm^{-2} (solid), 10^{19} cm^{-2} (dotted), and 10^{20} cm^{-2} (dashed)

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Numerical Simulations of Host Galaxies of Gamma-Ray Bursts

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Summary. In this project we address the nature of host galaxies of gamma-ray bursts (GRBs) through numerical simulations of galaxy formation. GRBs are the most energetic events in the universe and those longer than about 2 seconds are thought to result from the core collapse and explosion of massive stars [Pir05]. Because of the cosmologically short lifetime of the massive progenitors, GRBs are generally considered to be powerful tracers of the massive star formation history of the universe. They can therefore also be expected to provide useful insights into the understanding of the galaxy formation process. The current interest in GRB research started in 1997 with the discovery of their optical afterglow emission. To date over 40 optical detections have been made, but the number of GRB host galaxy observations is still rather limited with only about 20 positive detections.

1 Research project

Our group is the first to use numerical simulations of galaxy formation as an approach to investigate the properties of GRB host galaxies. The numerical code we use is a 3D N-body/hydrodynamical code following the cosmological evolution of the dark matter and the baryonic matter components in a self-consistent way. A cosmological scenario is specified to describe the expansion of the universe. The growth of structures is determined by gravitational instability: any inhomogeneity in the initial field will accrete matter and eventually collapse to form structures. The initial conditions are given by the density fluctuation power spectrum, taking inflation into account as an origin for the density fluctuations, and the non-relativistic nature of the dark matter. The model includes a number of physical processes: gravitation, hydrodynamical shocks, radiative cooling processes, photoionization, thermal non-equipartition between the ions, neutrals and electrons of the cosmological plasma. The cooling rates are explicitly computed from the evolution of the six species of the hydrogen-helium primordial composition plasma. At this stage, such a code is able to reproduce the large scale structure of the universe: the

formation of dark matter potential wells located along a network of filaments. Gas is accreted, cools and settles into dark matter over-densities.

Although simulations of large scale structure formation in the universe do not have sufficient resolution to follow the formation of individual stars, galaxy formation is followed through phenomenological prescriptions, motivated by physical criteria. Indeed a necessary condition for the formation of a galaxy is that the cooling time-scale of a gas region must be less than its dynamical time-scale. Advantage is then taken of the simulated gas distribution and in each cell satisfying the appropriate criteria, a part of the gas is turned into a stellar particle. The evolution of these particles is then followed in a similar way as the evolution of the dark matter. After the simulation run is complete, stellar particles are grouped together to form a galaxy-like object at the different simulation outputs. These are saved at different cosmic times that is most often expressed in terms of the corresponding redshift. The galaxy-like objects have statistical properties that are very similar to observed galaxies. One of the most striking and important results of these simulations was to reveal a significant population of low mass galaxies [AC04]. The observational counterparts of these galaxies, although difficult to detect, are however a crucial key to the understanding of galaxy formation and evolution. A comprehensive understanding of the properties and nature of host galaxies of gamma-ray bursts is therefore highly relevant in this context.

We started our project a few months before submitting an application to the HLRS. At that time we had available few outputs of an earlier numerical simulation computed for a different purpose, and could distinguish in there different populations of galaxies, especially if we considered the specific star formation rate. The star formation rate (SFR) is computed from the amount of gas that is turned into stellar particles in 10^8 years, conventionally expressed in solar masses per year ($M_{\odot}/\text{year}$). The specific star formation rate is then defined as the ratio between the SFR of a galaxy and its mass (SFR/M). It turned out that for a given SFR, some of the low-mass galaxies had as low specific star formation rate as the high-mass galaxies. The few existing observations of GRB host galaxies seemed to suggest that the hosts were dwarf-like, blue, sub-luminous galaxies [Cha02, LeF03, Jau03] with low-metallicity and although we had limited information regarding their colors and luminosities, we could show that identifying hosts with galaxies of high *specific* SFR is more consistent with the observations than identifying hosts with galaxies of high SFR [Cou04].

We are now carrying out a detailed investigation into the GRB host galaxy properties using simulations performed on the NEC-SX6 of the High Performance Computing Center in Stuttgart.

2 Description of the method

Cosmological galaxy formation is a highly complex phenomenon, requiring the solution of non-linear equations to follow the evolution of the dark matter as well as the baryonic matter. A number of physical processes must also be included and a model of galaxy formation must be introduced, making the resulting numerical codes highly memory-demanding as well as computationally intensive. Our simulations requires vector architectures that are not available in Iceland.

The numerical code we use follows the two components of matter, dark and baryonic, whose dynamical evolutions are coupled through the gravitational potential. The dynamical equations are solved in the Newtonian approximation and written in comoving coordinates to take into account the expansion of the universe. Details of the numerical method are given in [Tey98]. The computational volume is a cube with the comoving size of each side of the box denoted by L_{box} . Periodic boundary conditions are adopted.

The dark matter is treated as a non-collisional fluid and sampled with N_p^3 particles. The particles are displaced using a particle mesh-scheme algorithm, according to the following approach. During each time-step the dark matter density field is obtained by distributing each particle mass on the eight surrounding nodes of the grid. The gravitational potential is then computed by solving the Vlasov-Poisson equation using the fast Fourier transformation method, enabling the determination of the new velocity components and positions. The equation of motion is solved with a predictor-corrector time scheme. The gravitational potential is computed for the total matter density field, dark matter plus baryonic gas, and is used in the equation of motion that is solved for the gas component.

The baryonic matter is discretized on a grid with N_g^3 cells. The motion and energy equations are solved in their Lagrangian form, using a predictor-corrector time integration scheme (second-order time integration scheme inspired by the implicit method). Hydrodynamical quantities are then projected from the perturbed Lagrangian grid onto the fixed Eulerian grid. The advection scheme is the donor cell method and shock heating is treated using the artificial viscosity method. If no additional dissipative terms are included, the code runs in its adiabatic version. However, following galaxy formation in the simulations requires cooling processes to be taken into account. Collisional ionization equilibrium is not assumed, thus cooling rates are explicitly derived from the evolution of the six densities of the primordial composition hydrogen-helium plasma. The densities are then computed cell by cell and this dissipative step is very time consuming. In its non-adiabatic version, the code computes 17 quantities: 3 coordinates of position and 3 velocity components for the dark matter; 3 gas velocity components, the mass, the energy, and the 6 chemical densities. In addition to the two components of matter, galaxy formation is also followed and at each time-step, new stellar particles are formed

Table 1. Typical run on the NEC-SX6

Real Time (sec)	17031.666776
User Time (sec)	15692.228593
Sys Time (sec)	121.224510
Vector Time (sec)	10919.597701
Inst. Count	2229565577340.
V. Inst. Count	374150200665.
V. Element Count	50081359629770.
FLOP Count	15934488051897.
MOPS	3309.713130
MFLOPS	1015.438181
VLEN	133.853622
V. Op. Ratio (Memory Size (MB)	12912.031250
MIPS	142.080876
I-Cache (sec)	72.651039
O-Cache (sec)	1430.652979
Bank (sec)	655.907607

Computational information for a typical run on the NEC-SX6 at the HLRS in Stuttgart. The numbers correspond to first 300 timesteps for a typical run. A typical simulation may require 300 timesteps at redshift $z = 1.13$ and 600 timesteps at redshift $z = 0$.

and contribute to the gravitational potential. Their evolution is treated as a non-collisional fluid, using the same approach as for the dark matter.

The numerical code has been optimized and widely used for several years on vector architectures such as the CRAY and NEC-SX5 computers at the Institut du Développement et des Ressources en Informatique Scientifique (I.D.R.I.S.) in France. The code is written in Fortran90 and is fully vectorized. The resolutions used typically requires 256^3 dark matter particles and 256^3 gas cells, giving the following characteristic masses for a comoving size of the computational volume, $L_{box} = 32 h^{-1} Mpc$: A dark matter particle with mass $2.01 \times 10^8 M_\odot$, and a gas mass initially enclosed in each grid cell $3.09 \times 10^7 M_\odot$. In the case of $L_{box} = 16 h^{-1} Mpc$, a dark matter particle has a mass of $2.51 \times 10^7 M_\odot$, and the gas mass is $3.87 \times 10^6 M_\odot$. Table 1 lists the computational information for a typical run on the NEC-SX6 at the HLRS.

3 Results

The simulations we have run at the HLRS over the past year were mainly of two different kinds:

i) In the $L_{box} = 32 h^{-1} Mpc$ configuration, we ran the same simulation as described in the first step of our project (section 2 above), but saving numerous outputs (every fifteen timesteps) in order to follow the evolution in

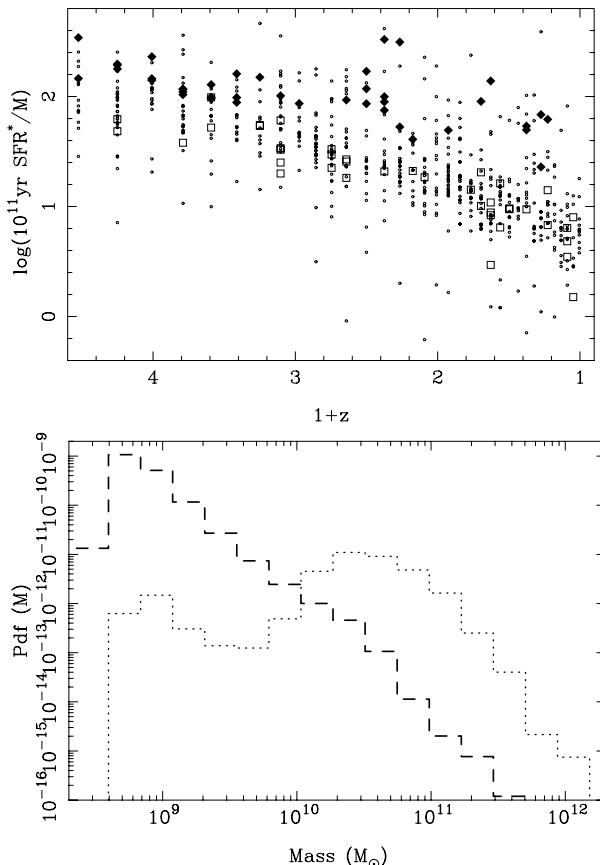


Fig. 1. Top panel: Galaxies with high SFRs (open squares) or high specific SFRs (filled squares) compared to a randomly selected galaxy population (dots). Bottom panel: Probability density functions of having a mass in the range $[M, M+dM]$ for the high SFR population (dotted histogram) and the high specific SFR population (dashed histogram).

redshift of galaxy properties. This procedure is time consuming and the high performance of the NEC-SX6 was a huge benefit.

We have then compared three simulated galaxy populations: at any given redshift we select a population of galaxies with high star formation rates, another population with high specific SFRs, and finally a population consisting of galaxies selected at random from our catalog at this redshift. The top panel of Fig. 1 shows the cosmological evolution of the specific SFR of the first two populations. The distinction between the three populations and the increase of this quantity as a function of redshift is clearly seen. The probability density functions of the mass for the same populations (bottom panel of Fig. 1) are quite different. Selecting high specific SFRs tends to select a larger popu-

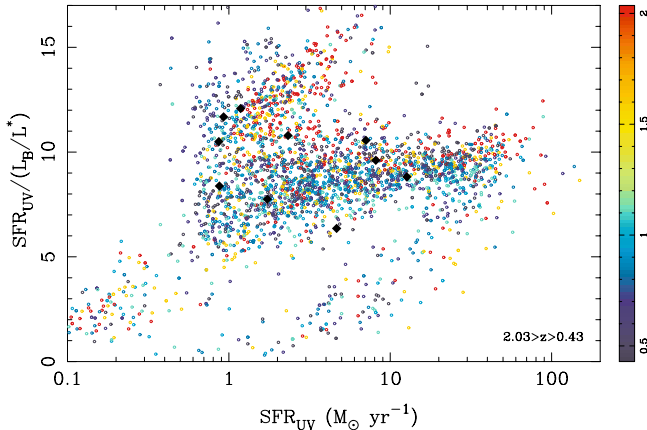


Fig. 2. The specific SFR as a function of SFR for 3000 simulated galaxies randomly selected in ten galaxy catalogs between the redshifts 2.03 and 0.43 (redshifts are color-coded). The star formation rate is estimated from the UV part of the synthesized spectrum. The diamond symbols are observations of host galaxies in the same redshift range [Chr04].

lation of low-mass galaxies. This may suggest that host galaxies, if faint and blue, are not galaxies with the highest star formation rates.

Moreover comparing directly our conclusions with observations requires properties of the simulated populations to be similar to those observed in the hosts. The primary output of a simulation is the galaxy mass and to obtain luminosities, magnitudes and colors requires the use of a stellar population synthesis model. The several outputs obtained for this single simulation allowed us to compare the simulated galaxies with observations of host galaxies *at similar redshifts*. In Fig. 2 we overplot ten catalogs of simulated galaxies in a given range of redshifts as well as the observationally derived values for 10 GRB hosts [Chr04]. The diagram shows observational-like quantities: the star formation rate estimated from the UV part of the spectrum of the simulated galaxy and the ratio between this UV star formation rate and the galaxies B-band luminosity. Remarkably, the simulation is able to reproduce numerical counterparts to the observed hosts. The black diamond symbols indicate that the observed hosts clearly belong to the population of faint, high specific SFR galaxies. These results are currently being written up for publication.

ii) The second set of simulations concerns an on-going project focusing on the thermodynamics of the gas involved in the galaxy formation process. These simulations differ from the previous one by the fact that photoionization processes are taken into account and we use the $L_{box} = 16 h^{-1} Mpc$ configuration. As before we saved numerous outputs. This project requires us first to determine the “history” of each galaxy: starting at a final redshift with a catalog of galaxies, we search for the main progenitor of each galaxy by looking through the catalogs at earlier redshifts. We can therefore follow

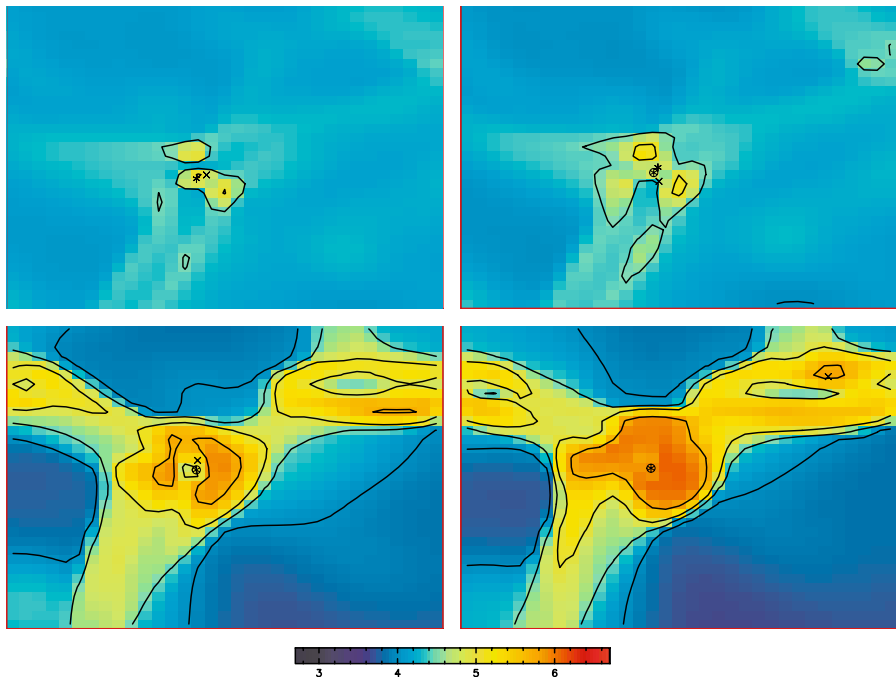


Fig. 3. Temperature distribution of the surroundings of a particular galaxy at four different redshifts. Each slice is 2 comoving h^{-1} Mpc on a side with one-cell thickness. The isocontours are $T = 10^4, 3.10^4, 10^5, 5.10^5$ K. The circled star symbol (and the star in the top-left panel) marks the center of mass of the galaxy. From top-left and clockwise: $z = 4.7, z = 4.2, z = 2.3, z = 2$.

the cosmological evolution of the properties of a given galaxy: each redshift is an evolutionary phase in its history.

As an example, Fig. 3 shows temperature maps at different redshifts of an area surrounding the center of mass of a particular galaxy. As the evolution proceeds and the potential well deepens, the accreted gas is heated to higher temperatures, slowing down the quantity of cold gas available and any increase in mass of the galaxy. After some time the surrounding gas is even too hot to allow any further stellar formation. Figure 4 shows clearly that the increase in mass decreases with time. A direct consequence of that is that the specific SFR is clearly highest in the early phases of the evolution of the galaxy. This pattern is well reproduced for a number of galaxies. This suggests, and should be quantified statistically, that if high specific SFRs are found in the early phases of galaxy evolution, high SFRs occur at later epochs.

This description gives us important insight into GRB host galaxy properties. The idea that the hosts could at the same time be young galaxies with low metallicities and high specific SFR galaxies (rather than with high SFRs), may be a consequence of this behavior.

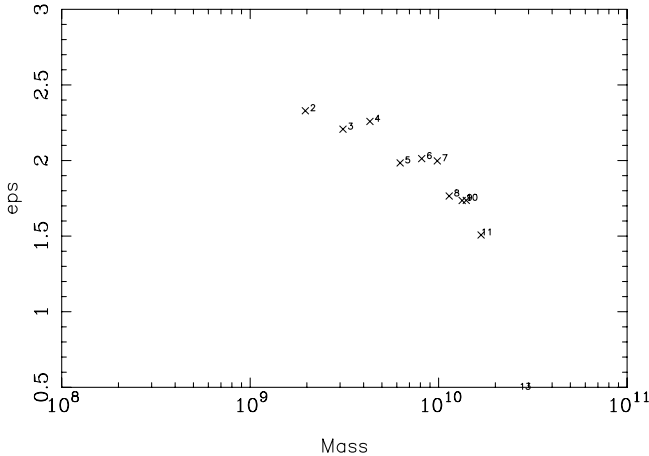


Fig. 4. Cosmological evolution of the specific star formation rate as a function of mass for the same galaxy as in Fig. 3. The numbers represent the different evolutionary phases, from the earliest epoch (2) to the latest epoch (11).

4 Future of the project

A number of interesting topics have come up during the course of this work. We list a few of the below.

- It appears that metallicity may play an important role in determining if a galaxy is likely to host a GRB event. A model for the evolution of the metallicity will therefore be included in the numerical code. We will use cooling functions dependent on the metallicity that are available in the literature. The aim is, first to confirm if a correlation between high specific SFRs and low-metallicity exists, and then to constrain our population of candidate GRB host galaxies. In the second round of this work we will be able to follow the cosmological evolution of the metallicity in galaxies and in particular in host galaxies.

- The properties of hosts at very high redshift may be crucial in cosmological applications of GRBs. We plan to pursue the same kind of analysis as discussed in this report, but in higher redshift ranges ($z > 5$), that requires lower computational volume and higher resolution. These kinds of simulations are only possible for us with the platforms available at the HLRS.

- In our group a strong emphasis has been on the issue of the GRB phenomenon and the physics involved in it. We plan to introduce models of GRB events, or rather their outputs, in the simulations to follow in-situ the GRB formation. Here again high-performance computers are required since such a computational procedure would be very time consuming.

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Electron-doping Evolution of the Quasiparticle Band of the Cuprates

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Summary. We present a numerical study of the doping dependence of the spectral function of the n-type cuprates. Using cluster-perturbation theory and the self-energy-functional approach, we calculate the spectral function of the Hubbard model with next-nearest neighbor electronic hopping amplitude $t' = -0.35t$ and on-site interaction $U = 8t$ at half filling and doping levels ranging from $x = 0.077$ to $x = 0.20$. We show that a comprehensive description of the single particle spectrum of the electron doped cuprates is only possible within a strongly correlated model. Weak coupling approaches that are based upon a collapse of the Mott gap by vanishing on-site interaction U are ruled out.

1 Introduction

Angular resolved photoemission spectroscopy (ARPES) has greatly contributed to our current understanding of systems of strongly correlated electrons, in particular high-temperature superconductors (HTSC). The most prominent parent materials usually investigated in ARPES experiments, e.g. $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ (SCOC) and $\text{Ca}_2\text{CuO}_2\text{Cl}_2$ (CCOC), have hole-doped descendants. Since only the part of the spectral function that is occupied by electrons can be seen by ARPES, only a fraction of the interesting region around the insulating gap can be investigated upon doping. Although the observation of the unoccupied parts of the spectral function is in principle possible (inverse photoemission), the process is highly involved and does not yield the desired resolution. An opportunity for a more comprehensive study of the doping dependence of the spectral function is offered by electron doped cuprates. Not only the excitations below the Fermi level in the *lower* Hubbard band, but also those below the Fermi level in the *upper* Hubbard band can be studied and thus a large part of the important low energy excitations is covered. The investigation of such n-type cuprates by ARPES is highly desirable.

Recently, an ARPES study of the doping dependence of the electron-doped cuprate $\text{Nd}_{2-x}\text{Ce}_x\text{CuOCl}_{4\pm\delta}$ (NCCO) has been published [1]. The low energy

excitations of $\text{Nd}_2\text{CuOCl}_{4\pm\delta}$ (NCO) were shown to essentially coincide with SCOC and CCOC at half filling, thus demonstrating the universality of the electronic structure of the (single layer) cuprates. Upon doping a particularly interesting Fermi surface (FS) evolution is found. In the heavily electronically underdoped region the regions spectral weight are limited to an area close around $\mathbf{k} = (\pi, 0)$. This has been interpreted as the formation of hole pockets. With increasing doping level, these hole pockets connect by patches and finally form a large LDA-like FS closed around $\mathbf{k} = (\pi, 0)$.

The spectral function and FS data presented in [1] gave rise to several theoretical interpretations which also include the collapse of the Mott gap by a strongly reduced local Coulomb repulsion[14]. This conclusion was based on mean field calculations which employ a self-consistent determination of the on-site repulsion U_{eff} of the Hubbard model by keeping the experimental value of the antiferromagnetic order parameter fixed at each considered doping level.

Using both standard cluster-perturbation theory (CPT) [11, 24, 23] and a variationally improved version in addition, i.e. variational cluster-perturbation theory (V-CPT) [3], we calculate the spectral function of the Hubbard model with next-nearest neighbor hopping amplitude $t' = -0.35t$ and fixed on-site interaction $U = 8t$ at half filling and doping levels ranging from $x = 0.077$ to $x = 0.20$. It is shown that the salient features of the recent ARPES experiments for electron-doped cuprates can be reproduced with one-and-the-same extended Hubbard model without the necessity to resort to any (rather arbitrary) change of the U -values as used in previous theoretical studies. So our challenge here is to reproduce the global (i.e. n- and p-doped phase diagram by one universal choice of the model parameters, starting from a Mott-Hubbard physical picture.

2 Model

The widely used model for the HTSC compounds is certainly the one-band Hubbard model [13] H_{1b} , i.e.

$$H_{1b} = -t \sum_{\langle i,j \rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + h.c. \right) + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1)$$

Here, $c_{i\sigma}^\dagger$ ($c_{i\sigma}$) creates (annihilates) an electron on site i with spin σ , $\langle \dots \rangle$ denotes nearest neighbors and U is the on-site part of the Coulomb repulsion. It has been shown [26, 5] that the pure Hubbard model is not sufficient to describe the dispersion of the quasiparticle band of the cuprates. Although the $t - U$ Hubbard model at low temperature develops a quasiparticle band of the appropriate width [9, 10], the dispersion shows a degeneracy between $\mathbf{k} = (\pi, 0)$ and $\mathbf{k} = (\pi/2, \pi/2)$. From ARPES experiments, however, we know that the quasiparticle peak at $\mathbf{k} = (\pi, 0)$ is shifted to higher binding energies. Actually, the dispersion of the quasiparticle peak shows two parabola with

lowest binding energy at $\mathbf{k} = (\pi/2, 0)$ and $\mathbf{k} = (\pi, \pi/2)$. It is, thus, indispensable to add at least one additional term, which – for simplicity – is taken to be the hopping between next-nearest neighbors ($\langle\langle\ldots\rangle\rangle$), i.e.

$$-t' \sum_{\langle\langle i,j \rangle\rangle} (c_{i\sigma}^\dagger c_{j\sigma} + h.c.). \quad (2)$$

Even longer range hopping (t'') elements have been proposed to achieve consistency with experiment [25]. However, for the purpose of a qualitative analysis, it is sufficient to lift the degeneracy between $\mathbf{k} = (\pi, 0)$ and $\mathbf{k} = (\pi/2, \pi/2)$ and, thus, create the indirect gap as observed in experimentally.

3 Numerical Technique

Despite the considerable simplification arising from the use of an effective single band model, the calculation of the spectral function of the Hubbard model is a difficult task. The exact calculation of such quantities is possible only up to 4×4 sites, if periodic boundary conditions are used. Larger lattice sizes can only be calculated by stochastic methods, such as the quantum Monte Carlo (QMC) technique [12] or the density matrix renormalization group algorithm (DMRG) [18]. These techniques certainly represent powerful approaches to strongly correlated electron systems. For the present problem, however, they are known to be problematic. In case of QMC, doping and low temperatures lead to the well-known sign problem, i.e. the computation time increases exponentially with T and system size [8, 10]. DMRG, in contrast, is a ground state technique and insensitive to doping, but displays convergence problems when it comes to two-dimensional systems.

Recently, a strong coupling perturbation theory has been developed where the infinite lattice is subdivided into sufficiently small clusters such that these can be treated exactly, followed by an infinite-lattice expansion in powers of the hopping between the clusters [11, 23, 24]. The expansion in the inter cluster hopping can be formally carried out up to arbitrary order following the diagrammatic method of Refs. [17, 19, 20]. The lowest order of this strong-coupling expansion in the inter-cluster hopping has been termed “cluster perturbation theory” (CPT). The CPT Green’s function is given by

$$\mathbf{G}_\infty = \mathbf{G}_0 + \mathbf{G}_0 \mathbf{T} \mathbf{G}_0 + \mathbf{G}_0 \mathbf{T} \mathbf{G}_0 \mathbf{T} \mathbf{G}_0 \dots = [\mathbf{G}_0^{-1} - \mathbf{T}]^{-1}, \quad (3)$$

where the $\mathbf{G}_\infty$ is the Green’s function of the infinite system, $\mathbf{G}_0$ the cluster Green’s function and $\mathbf{T}$ the inter-cluster hopping. All quantities are matrices with indices referring to a particular cluster and to the sites within that cluster. The CPT can be viewed as a systematic approach with respect to the cluster size, i.e. it becomes exact in the limit $N_c \rightarrow \infty$, where N_c is the number of sites within a cluster. Moreover, CPT provides results for an infinitely

extended system: The CPT Green’s function is defined for any wave vector $\mathbf{k}$ in the Brillouin zone, contrary to common “direct” cluster methods, like QMC or ED, for which only a few momenta are available.

CPT results for static quantities as well as for the single-particle spectral function have been shown to agree very well with different exact analytical and numerical results [23, 24]. On the other hand, there is also a serious disadvantage of the CPT at this level: Namely, the method does not contain any self-consistent procedure which implies that symmetry-broken phases cannot be studied. We have recently proposed a variational approach (V-CPT) to this problem which is based on the self-energy-functional approach (SFA). This method is in detail explained elsewhere[3]. We use the V-CPT to calculate the Green’s function of the half-filled Hubbard model with long-range antiferromagnetic order.

For a reasonable approximation to the full many-body problem, CPT and V-CPT calculations for comparatively large clusters are required. In particular for underdoped systems this implies the need for numerically rather demanding techniques. Here, we have calculated $\mathbf{G}$ for half filling and doping $x = 0.07$ to 0.2. To achieve the smallest doping level, we used clusters consisting of 13 sites. The calculation of $\mathbf{G}$ requires the diagonalization $n_{\text{sites}} \times n_{\text{sites}}$ matrices of sidelength L of at most $30 \cdot 10^6$ for each photoemission and inverse photoemission spectrum. Of course, this cannot be achieved by standard diagonalization techniques, e.g. the Householder algorithm. Instead, we use the Lanczos algorithm in order to perform the necessary diagonalizations[15]. This method allows for the computation of the smallest eigenvalues and their eigenvectors within an iterative scheme. Convergence is typically reached in 50-100 steps. The large vector length makes this problem ideal for vector processors. The algorithm reaches as much as 90% percent of the peak performance on suitable vector machines as the NEC SX5.

4 Results and Discussion

We have performed V-CPT (electron filling $\langle n \rangle = 1.0$) and CPT ($\langle n \rangle > 1.0$) calculations of the single-band Hubbard model at zero temperature. Useful parameterizations of the $t - t' - U$ Hubbard model can be taken from the literature [5, 2]. We choose $t' = -0.35t$ and $U = 8t$ here, which yields a sufficiently accurate ratio for the Mott gap $\Delta \approx 4t$ and the width of the quasiparticle band $W \approx 1t$, and fits the experimental dispersion of the quasiparticle band.

Figure 1 shows the spectral function $A(\mathbf{k}, \omega)$ of the half-filled ($x := 0.0$, panel A) and overdoped $t - t' - U$ Hubbard model ($x := 0.2$, panel B). The plots show $A(\mathbf{k}, \omega)$ along the momenta $\Gamma = (0, 0) \rightarrow X = (\pi, 0) \rightarrow M = (\pi, \pi) \rightarrow \Gamma = (0, 0)$ through the Brillouin zone.

The half-filled system in panel A shows a narrow quasiparticle band, roughly between $\omega = -3t$ and $\omega = -2t$. A more detailed plot is given in panel C. One notices the characteristic parabolic dispersion close to $\mathbf{k} = (\pi/2, 0)$,

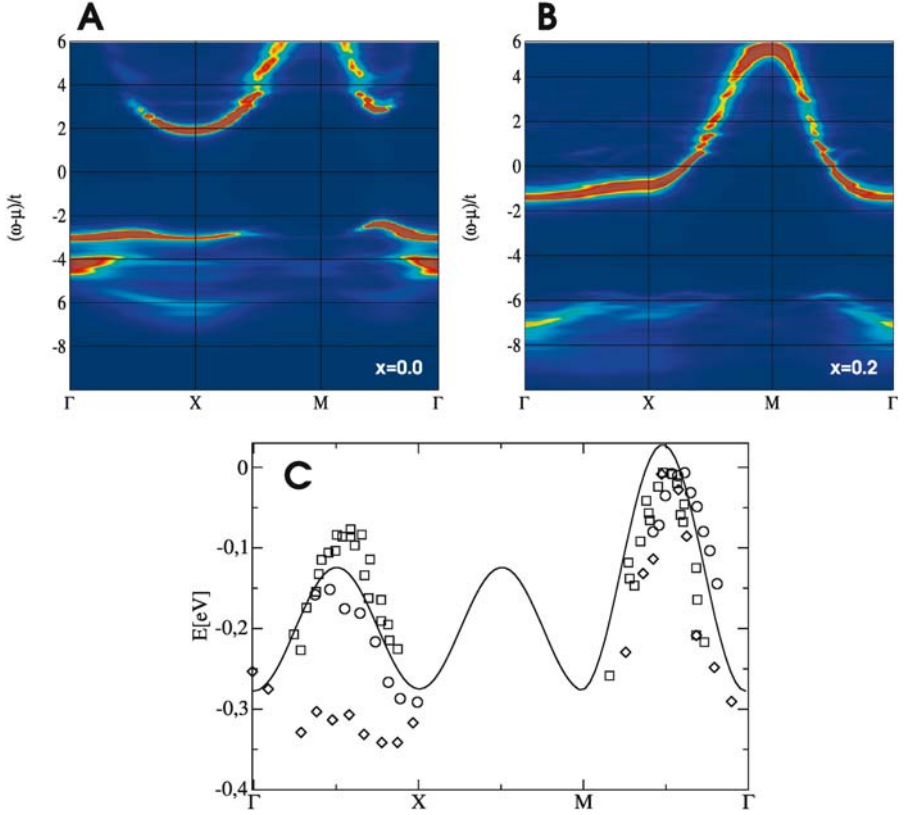


Fig. 1. Spectral function of the $t - t' - U$ Hubbard model with $t' = -0.35t$ and $U = 8t$. Panel A: half filling. Panel B: overdoped system with $x = 0.2$. Panel C: Detailed dispersion of the quasiparticle band of panel A for $t = 0.5$ eV. Symbols represent the experimentally determined dispersion for $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ (squares [6], circles [16], diamonds [27]). Both spectra were obtained by a CPT calculation using a 10 site cluster.

$\mathbf{k} = (\pi, \pi/2)$ and $\mathbf{k} = (\pi/2, \pi/2)$. Assuming $t \approx 0.5$ eV, this dispersion is practically identical with the ARPES data [1, 6, 16, 22]. The indirect single particle gap between $\mathbf{k} = (\pi, 0)$ and $\mathbf{k} = (\pi/2, \pi/2)$ is about $4t$, which is the maximum this is still compatible with the experiments. Separated by about $1t$ at higher binding energies, one finds another feature with maximal spectral weight around $\mathbf{k} = (0, 0)$. The classification of the feature varies, since the resolution of many methods is limited at larger distances from the Fermi level. From older QMC simulations [21], exact diagonalizations of the t -J model [7] and approximate methods as the self-consistent Born approximation (SCBA), this spectral weight has mostly been perceived as “incoherent” and featureless. Newer QMC simulations [9] and V-CPT calculations [3] of the $t - U$ Hubbard

model indicate that one may also interpret this as a second band. This is also supported by analytical considerations [4].

For the time being, we contrast the half-filled insulating system in panel A with the overdoped ($x=0.2$) system. One finds a metallic quasiparticle band with a flat dispersion just below the Fermi level at $\mathbf{k} = (\pi, 0)$. The band pushes through the Fermi level at $\mathbf{k} = (\pi/2, \pi/2)$ and $\mathbf{k} = (\pi, \pi/2)$ and therefore creates a large Fermi surface closed around $\mathbf{k} = (\pi, \pi)$ in the Brillouin zone. The quasiparticle band shows almost the same dispersion as the tight-binding ($U = 0$) model with the same parameterization. At some distance between $\omega = -6t$ and $\omega = -10t$, one finds the remainder of the lower Hubbard band at half filling, i.e. the area between $\omega = -2t$ and $\omega = -6t$ in panel A.

Figure 2 considers the area around the Fermi level at doping levels of $x = 0.077$ (panel A), $x = 0.091$ (panel B) and $x = 0.200$ (panel C) in more detail. For $x = 0.077$, the Fermi level is now shifted into the upper Hubbard band with only slight modifications of the spectral weight. Most important, the arc at $\mathbf{k} = (\pi, 0)$ in the upper Hubbard band of the half-filled spectrum is virtually unchanged and now forms an electron pocket around $\mathbf{k} = (\pi, 0)$ in panel A. The Fermi level is not yet shifted deep enough into the upper Hubbard band to touch the parabola at $\mathbf{k} = (\pi/2, \pi/2)$ of the half-filled system. Some new spectral weight is created between $\omega = -1t$ and $\omega = -0.5t$ at $\mathbf{k} = (0, 0)$ and between $\omega = -0.5t$ and $\omega = 0t$ at $\mathbf{k} = (\pi/2, \pi/2)$. These features are slightly gapped from the rigidly shifted band structure of the half-filled insulator. For $x = 0.091$ (panel B), this new spectral weight becomes more pronounced and mimics the branches at $\mathbf{k} = (0, 0) \rightarrow (\pi, 0)$ and $\mathbf{k} = (0, 0) \rightarrow (\pi/2, \pi/2)$ below the Fermi level of the overdoped system in panel C.

The results described above provide much insight in the doping process of the $t - t' - U$ Hubbard model, as it is generally used for the HTSC. Nevertheless, one must keep in mind that we have silently assumed that the parameters of the model do not change upon doping. Although this assumption is widely believed to be true for the doping range considered here, it is all but clear that the on-site repulsion U is constant over a broader doping range.

The possibility of a varying on-site repulsion was considered recently on basis of a spin-density wave (SDW) mean field calculation of the $t - t' - t'' - U$ Hubbard model to describe the experimental data on NCCO [14, 1]. Contrary to the usual SDW calculation, where one self-consistently determines the single particle gap Δ_{mf} under the assumption that U is a fixed parameter, the authors of Ref. [14] assumed the experimentally measured antiferromagnetic order parameter, i.e. the staggered magnetization

$$m = \frac{1}{N} \sum_{\mathbf{r}} (-1)^{|\mathbf{r}|} (\langle n_{\mathbf{r}, \uparrow} \rangle - \langle n_{\mathbf{r}, \downarrow} \rangle) \quad (4)$$

to be fixed and self-consistently determined the on-site repulsion U_{eff} instead. This scheme was termed uniformly doped antiferromagnet (UDAF). The value of U_{eff} drops sharply upon doping from $U_{\text{eff}} = 6t$ at half filling to $U_{\text{eff}} \approx 3t$ at $x \approx 0.15$. The results from this procedure show excellent agreement

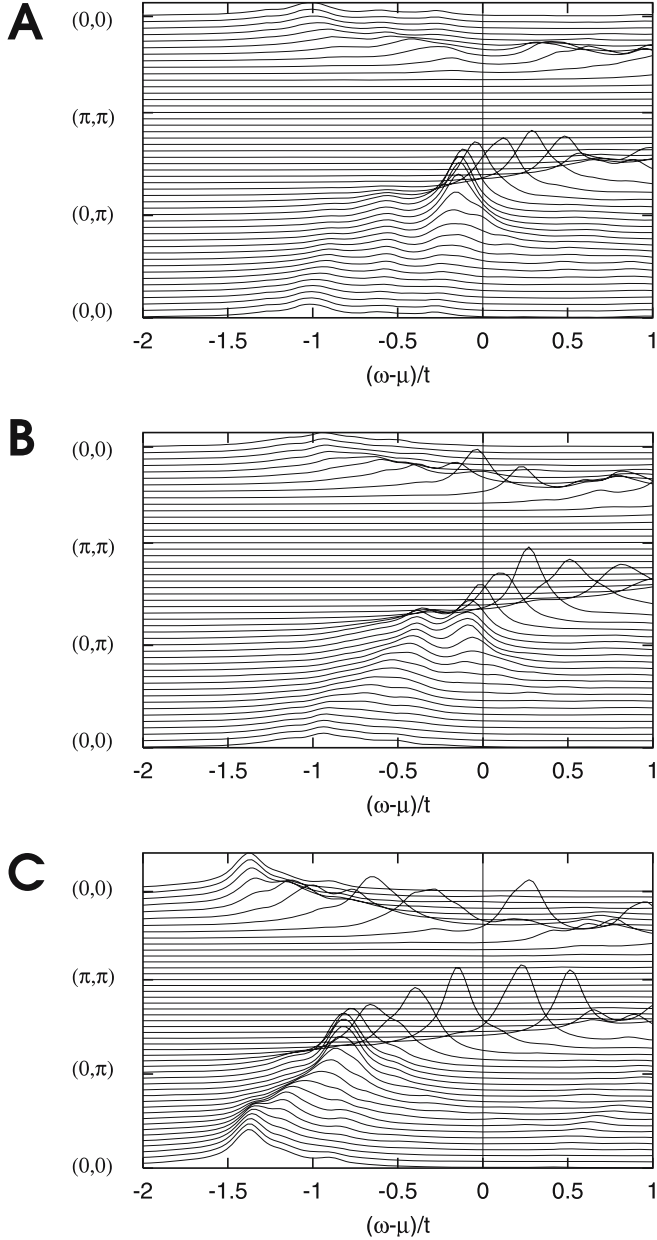


Fig. 2. Detailed plot of the spectral function of the $t - t' - U$ Hubbard model with $t' = -0.35t$ and $U = 8t$. Panel A: $x=0.077$, obtained from a 13 site cluster. Panel B: $x=0.091$, obtained from a 11 site cluster. Panel C: $x=0.200$, obtained from a 10 site cluster.

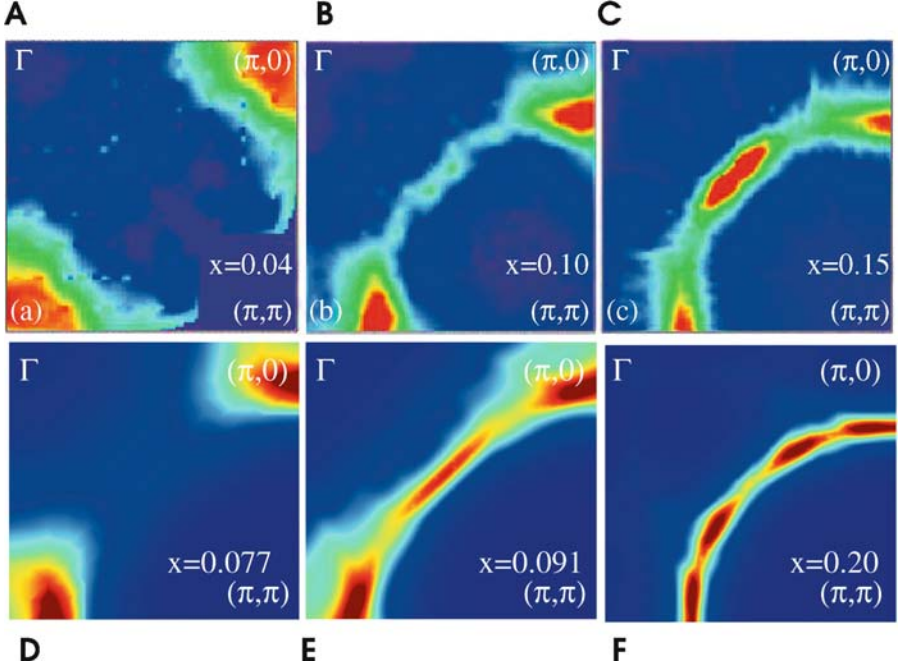


Fig. 3. Panels A through C: Experimentally determined Fermi surfaces for indicated doping levels (taken from [1]). Panels D through F: CPT Fermi surface for doping levels close to the ARPES results above. The CPT FS correspond to the line plots in Fig. 2.

with the doping evolution of the experimentally observed Fermi surface. The whole scenario, however, is based upon the assumption that a varying U_{eff} is indispensable for the reproduction of the experimental results.

Let us compare our results with the experimentally observed Fermi surface. The upper row of Fig. 3 (panels A through C) are the ARPES data taken from [1], whereas the lower row (panels D through F) are the Fermi surfaces obtained by taking $A(\mathbf{k}, 0)$ in the CPT calculation.¹

Although we only used a minimal set of standard parameters and did not change the parameterization with doping, the CPT Fermi surface of the fully correlated Hubbard model qualitatively reproduces the experimental result. In particular, we observe hole pockets, a FS patch at $\mathbf{k} = (\pi/2, \pi/2)$ for about $x = 0.10$ and a large FS for overdoping. All these features have been also found in [1] and [14]. Figure 2 indicates a mechanism that is very similar to the closing gap of the UDAF is also found in the Hubbard model, but appears naturally here, as a consequence of the large U .

¹ Note that the doping levels are, of course, not identical since the available fillings in CPT are determined by the cluster sizes.

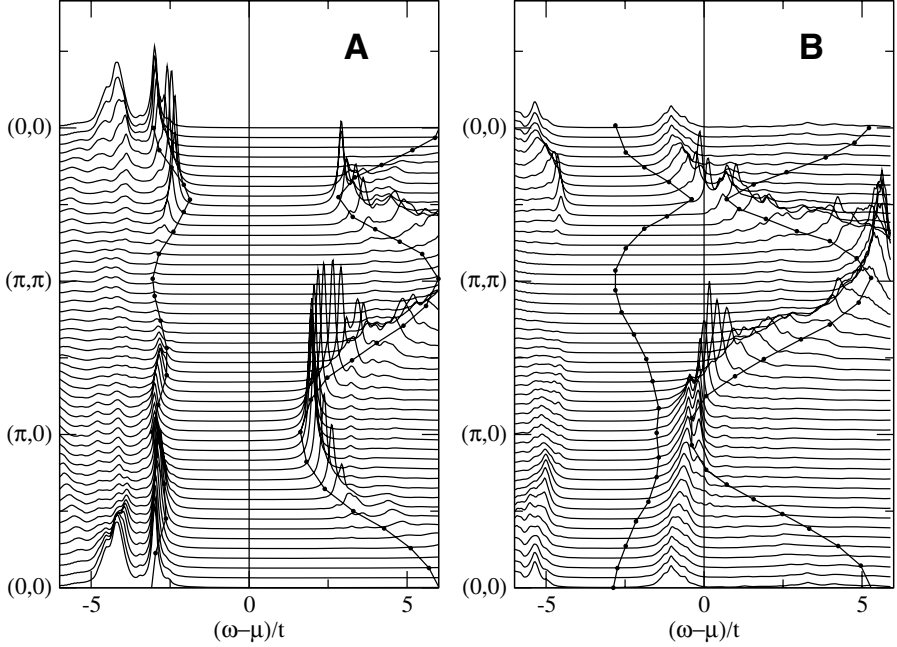


Fig. 4. Direct comparison between CPT and UDAF results. The UDAF dispersion is indicated by the solid line. In order to obtain compatible energy scales, the UDAF hopping t has been normalized to 1. A: half-filling; B: $x = 0.10$ (CPT $x = 0.091$)

Figure 4 directly compares the CPT and UDAF quasiparticle dispersion at half filling and $x = 0.10$ (CPT $x = 0.091$). The intensity of the UDAF results is suppressed and the dispersion is indicated by the solid line. In order to have compatible energy scales, we normalized the hopping t in [14] to 1.

For half filling (Panel A) both methods show almost identical dispersions for the excitation of lowest energy, since both methods have been fitted to the experimental observation. As a SDW-type mean field method, the UDAF results cannot describe the full lower Hubbard band and is exclusively fitted to the low-energy excitations. Hence, the whole part of the spectrum at about $\omega = -3t$ to $\omega = -4t$ is ignored in this technique.

Upon doping the gap closes in both techniques. Although the CPT dispersion is much weaker and the small gap at $\mathbf{k} = (\pi/2, \pi/2)$ is almost closed, the qualitative development is very similar. In contrast to the UDAF, the CPT spectrum provides information on spectral weight at higher binding energies in addition. Particularly, a remainder of the parabolic dispersion at $\mathbf{k} = (\pi/2, \pi/2)$ is found at $\omega \approx -5t$. This feature does not appear in the mean field calculation, but can be clearly identified in the experimental data [1].

5 Conclusion

In conclusion, we have shown that the evolution of the Fermi surface of the electron doped cuprates is well described within the framework of the unapproximated one-band Hubbard model. In particular, we have provided indications that a vanishing on-site repulsion is not necessary to describe the doping dependence of the experimental data.

Acknowledgments

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Libraries and Methods for Parallel Particle Simulations [★]

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Summary. We used the high performance systems at HLRS in the last year for two different works. One was the hybrid implementation and optimization of ParaSPH a library for the parallel computation of particle simulations. We give details of the parallelization of ParaSPH for hybrid architectures (clustered SMPs) using MPI and OpenMP and discuss performance results for single node and speedups of the code on the Opteron Cluster and the NEC SX-6. The other work we present is the enhancement of an object-oriented framework for messages passing called TPO++ to support object-oriented parallel I/O.

The range of applications using our libraries and methods is extended continuously. At present it covers many different astrophysical phenomena, basically accretion procedures, impact simulations, the simulation of brittle material and the simulation of separated two phase flows, for example the injection of diesel jets. Recently we work on a solution to simulate granular media with SPH.

1 Introduction

In the Sonderforschungsbereich 382 (SFB 382) scientists work on methods for the simulation of astrophysical problems. A major focus are particle simulations and the Smoothed Particle Hydrodynamics method (SPH) in particular. We address several problems to increase the performance of our numerical codes. For the increasing number of hybrid architectures, the parallelization of ParaSPH combining threads and message passing is a promising way to reduce the parallel overhead. A more general aspect is the work on TPO++ to exploit a simple way for performant I/O for object oriented codes.

In the second chapter we present a comparison of ParaSPH on NEC SX-6 and the Cray Opteron cluster at HLRS. The third chapter explains parallel I/O in TPO++ together with several performance results. The last chapter presents applications on top of the libraries together with physical results.

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2 Hybrid ParaSPH

2.1 Motivation

The majority of parallel machines in the TOP500 list are so called hybrid parallel architectures, a combination of N-way shared memory nodes with message passing communication between the nodes.

Hybrid parallelization is the combination of a thread based programming model for parallelization on the shared memory nodes together with message-passing based parallelization between the nodes. The standard library for message passing is MPI [3]. OpenMP [5] has become the standard for thread based programming for scientific applications. The annotation of parallel sections in existing codes makes an incremental parallelization possible and keeps the code portable, since non-OpenMP compilers ignore the directives.

A hybrid implementation reduces the amount of message passing communication, since domains inside a SMP node are combined to one large domain.

One can also see a big difference between the MPI-inter communication (comparable to the hybrid programming model with implicit intra node communication) and the MPI-intra/inter *pure MPI* communication model with explicit MPI intra node communication.

The communication of a 200 MB data array between 32 nodes on a Hitachi SR8000 with 8 CPUs per node is a simple test. In a pure MPI programming model 256 MPI processes contribute 800 kB of the array. In the hybrid programming model 32 MPI processes contribute 6400 kB. The communication takes 200 seconds for the pure MPI communication compared to only 25 seconds for hybrid communication (while the other non-master threads are idle). Thus the hybrid programming model is about a factor of 8 faster.

2.2 Implementation

The hybrid implementation is an extension of the ParaSPH library for particle simulations. ParaSPH is written in C and parallelized with MPI. The library separates the parallelization from the physics and numerics code. The interface between the library and the application is optimized for particle simulations. The library provides an iterator concept to step through all particles and their neighbours and later communicates the results.

In parallel mode, the library transparently distributes the work amongst all processors. Every local iterator processes only a subset of all particles. The code performs well on machines with a fast message-passing network. An extension to this pure message-passing implementation is to use OpenMP for the inner intra-node parallelization, while MPI is still used for inter-node communication. To achieve better portability only the master thread calls the MPI library, since not all MPI implementations are thread safe.

We provide two different load-balancing strategies. The standard load balancer for distributed memory is still used for a coarse load balancing between

the nodes. For the fine balancing on the node we provide two load balancers. The user can choose between a fixed load balancing and a dynamic master-worker load balancing. The master-worker algorithm promises the best load balancing, especially for inhomogeneous problems but has disadvantages in cache utilization. Hence, the static load balancing is usually faster.

2.3 Performance results

Our standard test application is a two dimensional SPH particle simulation. For the 1 CPU test we had a small setup with 30 000 particles and for parallel tests we used a medium size simulation with 300 000 particles. Every particle was configured to have 80 interaction partners. On one cpu, the small problem requires about 120 MB memory on a x86 system (32 Bit mode) and about 250 MB on the NEC SX-6. The test application makes one time step. Real production runs in three dimensions and with more particles need hours or days of computation time.

Single CPU performance

First we compare the performance of the application on a single CPU for the Opteron cluster and the NEC SX-6 with different compile options for the small problem with 30 000 particles and 80 interaction partners (see Table 1). **Total** is the total time, **kNN** is the time for the nearest neighbor search and **ArtVisc** is the computation of the artificial viscosity. This is a typical example of the SPH computation of a physical quantity. The times are given in seconds.

Table 1. Performance on a single CPU for Opteron cluster and NEC SX-6

System	Compiler and options	Total	kNN	ArtVisc
NEC SX-6	ssafe	206	16	105
	hopt	24	15	2
	aopt	24	15	2
Opteron	pgcc 5.2.4 -O2 32bit	10.4	2.9	2.5
	pgcc 5.2.4 -O2 64bit	10.9	2.9	2.8
	gcc 3.3.1 -O2 32bit	13.4	3.5	3.8
	gcc 3.3.1 -O2 64bit	13.6	3.5	3.9

The first result is, that the vectorization significantly increases the performance for the physical quantity on the NEC SX-6, but can not exploit vectorization for the nearest neighbour search. Another interesting point is, that the less aggressive optimizations **vsafe** and **vopt** generate wrong code.

The overall performance of the NEC SX-6 is still poor compared to much cheaper systems like the Opteron cluster. The fairly short vector lengths together with inhomogeneous computations in SPH code makes the code better suited for general purpose processors like the Opteron CPUs.

Table 2. NEC SX-6 aopt results

Real Time (sec)	:	28.240938
User Time (sec)	:	24.440779
System Time (sec)	:	2.077101
Vector Time (sec)	:	5.037796
Instruction Count	:	3375883204
Vector Instruction Count	:	142651913
Vector Element Count	:	14060339645
FLOP Count	:	5033377101
MOPS	:	707.570366
MFLOPS	:	205.941762
Average Vector Length	:	98.563975
Vector Operation Ratio (\%)	:	81.303854
Memory size used (MB)	:	223.779770

Table 2 shows the NEC SX-6 aopt run results.

Although 81% (14.1 of total 17.3 billion operations) of the operations are vector operations, only about 20% of the time is spent in vectorized code segments. The average vector length is a little better than the expected 80 for our simulation setup with 80 interaction partners, since the compiler also vectorizes some longer loops, f.ex. loops over all particles.

We recommend to use the Opteron Cluster for SPH simulation and therefore concentrate on the Opteron Cluster for further performance results. We also recommend to use the Portland Group Compiler (PGI) on the Cluster. While Version 5.0 of the PGI Compiler showed similar performance results compared to the Gnu C Compiler (GCC), the newer Version 5.2.4 generates significantly better code. The difference between 32bit and 64bit code is very small.

Single node performance

For the single node runs for all further parallel runs we use the larger problem with 300000 particles. The performance results are given in Table 3. The notation NxMxT in brackets means N nodes with M MPI processes per node and T threads per MPI process.

Increasing the number of CPUs from one to two shows a super linear speedup for all compilers. The pgcc is still a little faster. The gcc does not support OpenMP so, we can give only numbers for *pure MPI*. The OpenMP and Hybrid version is always a little slower compared to *pure MPI* for two CPUs.

First reason is the not fully OpenMP annotated code. There is a small serial part (about 2%), which is not present in the pure MPI version. The serial part is a fixed overhead over the *pure MPI* parallelization.

Table 3. Performance on a single node for Opteron cluster

Configuration	N=1	N=2
gcc MPI 32	136	59
gcc MPI 64	139	60
pgcc 32 OpenMP (1x1xN)	106	58
pgcc 64 OpenMP (1x1xN)	109	60
pgcc 32 Hybrid (1x1xN)	119	65
pgcc 64 Hybrid (1x1xN)	112	62
pgcc 32 MPI (1xNx1)	106	Err
pgcc 64 MPI (1xNx1)	112	47

Similar to the serial part is the OpenMP overhead itself (thread creation, locking of critical sections) together with some additional parallelization work (difference between Hybrid and MPI for the pgcc binary).

The second reason is a lesser efficient cache utilization. The parts computing the physical quantities have a near perfect hybrid parallelization together with a near perfect load balancing. Only the neighbour search is a little unbalanced, but this is no disadvantage over the *pure MPI* version.

When we monitor the number of data load/stores and the data cache misses we get an almost equal number of load/stores but a higher data cache miss rate. The reason for this is not yet investigated. There is no simple reason, since the intra-node load balancer tries to schedule the same load to the same thread for successive runs over the particle list and concurrent memory accesses of the same data exist only for reading causing no cache trashes. Only data writes from different threads may fall into the same cache line resulting in a higher cache miss rate.

Parallel Speedup

Next we compare the speedup of the *pure MPI* and the hybrid parallelization for different processor numbers (see Fig. 1). The speedup is compared to the best single CPU run.

On an Opteron node with only 2 CPUs the speedup shows only little difference between the *pure MPI* and the Hybrid version even for larger node numbers. The reason why the hybrid version is a little faster than the *pure MPI* version for large node numbers is the reduced communication. The time consuming calls in the communication part are a MPI_Allgather and (after a code change) several calls to MPI_Allgather_v together with some post processing to reorganize the received data. One can see a small difference in the communication inside the parallelization module ("Para") for 32 nodes. The difference in the communication of the physical quantities ("Communication") is about 0.4 seconds for 32 nodes and difficult to see in the plot.

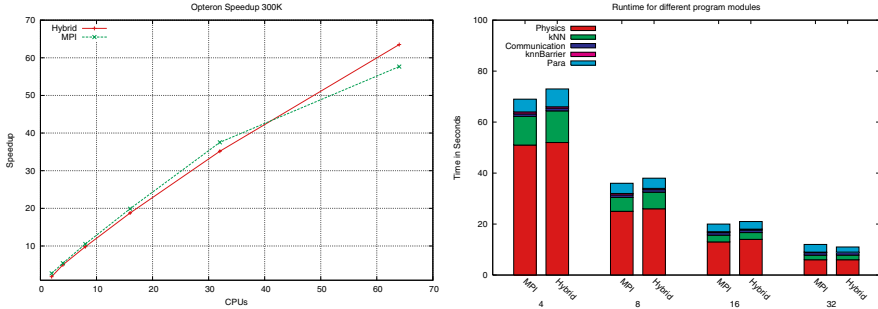


Fig. 1. Speedup for different node numbers on Opteron Cluster

3 Object-oriented Parallel I/O

3.1 Motivation

The computations of our massive parallel applications show a lack in performance due to sequential I/O. The I/O bottleneck limits the scalability of the parallelization significantly. The constantly growing gap between processor and hard disk performance during the last decades makes this problem even worse and requires the use of parallel I/O systems. Distributed hard disks in special I/O nodes, which use the underlying communication network for data exchange are the most common way in massive parallel systems to overcome the problem. Thus, the application can profit from the aggregated performance of all hard disks available in the system.

However, special parallel I/O interfaces have to be implemented and used by the application to benefit from the whole hard disk performance. The most often used interface for parallel I/O is MPI-IO [4]. One implementation of this part of the widely accepted and used standard MPI 2 is ROMIO [13], which is setup on top of the file system using an abstract device interface for I/O (ADIO) to achieve high portability.

In implementing parallel I/O two major problems arise: First, the application has to be ported on the parallel I/O interface of MPI 2 to enable the use of higher hard disk throughput. Second, besides a parallel implementation sequential I/O also has to be implemented for keeping the portability of the interface. Both leads to a more complex and larger implementation. Moreover, MPI 2 only supports procedural interfaces for parallel I/O, which makes it hard to be used in object-oriented applications. To close the gap between object-oriented software development and procedural communication we developed a communication library for parallelizing object-oriented applications called TPO++. Its concepts for mapping objects on simpler communication structures were reused for the implementation of an object-oriented parallel I/O interface.

3.2 MPI-IO

To keep a high portability and efficiency, the interface was implemented on top of MPI-IO and integrates all of its powerful features. The two most important are **File Views** and collective I/O calls.

File views are a powerful functionality of MPI-IO, allowing the user to access noncontiguous data from a file into memory with only one single I/O call. Therefore the user has to create a **file view** and commit it to the system [3]. The view then represents the data which can be accessed by each process. Since noncontiguous accesses are very common in parallel applications [11], TPO++ has to provide this feature, too.

Another key feature of MPI-IO are **collective** I/O functions, which allow the user to partition a file between several processors with one single call. All processes that opened the file have to make this call simultaneously. This enables the MPI-IO implementation to analyze and merge small noncontiguous requests of different processes into one large contiguous request, leading to a significant improvement in performance [12].

3.3 Implementation

In an object-oriented parallel I/O system one would ideally like to have a simple interface providing a single write and a single read method to which every object could be passed in a type-safe manner and without having the user to give any information about the objects to be transferred. TPO++ already preserves this functionality for sending and receiving objects. Therefore, on extending the library to parallel I/O we reuse the serialization and deserialization mechanisms already implemented in TPO++ to make objects and containers persistent. The new implemented class **File** represents the interface to object-oriented writing and reading. All data transfer methods provide the same orthogonal interface for specifying the data objects to read or write. The user has two options: provide a single data type (basic or object) or a range of data elements by using a pair of STL iterators.

Predefined C++ types are library and basic types and can be read and written very simple (see Fig. 2 left, **read** analog). STL containers can be transferred using the same overloaded method (see Fig. 2 right, **read** analog). The STL conventions require two iterators specifying begin and end of a range, which also allows to transfer sub-ranges of containers.

The same overloaded methods can be used to specify an offset in the file. The user simply has to add a third parameter in the call containing the offset.

Views are implemented in TPO++ by defining a STL vector containing Boolean values. The conformity of object-oriented concepts demands extending the granularity from a single concatenation of data types to object level. Therefore, it is only possible to select or deselect the whole object by setting

<code>double d;</code>	<code>vector<double> vd;</code>
<code>File fh;</code>	<code>File fh;</code>
<code>fh.open(...);</code>	<code>fh.open(...);</code>
<code>fh.write(d);</code>	<code>fh.write(vd.begin(), vd.end());</code>
<code>fh.close();</code>	<code>fh.close();</code>

Fig. 2. Example code for writing a basic type (left) and a STL container (right)

the Boolean value **TRUE** or **FALSE**. Accessing single members of an object is not possible since breaking up the structure of the object would violate object-oriented principles.

Using the combination of serialize and deserialize mechanisms and the implementation of views enables collective I/O to TPO++. The view on the object is internally transformed into a byte stream view using `MPI_BYTE` as elementary data type within the `set_view` command of MPI-IO. Then, collective TPO++ calls can profit from the MPI-IO internal optimization of noncontiguous collective accesses.

3.4 Performance Results

The performance of the interface is measured using a synthetic benchmark, which includes two test sets. The first test is about reading and writing different sizes ($2^0 - 2^{27}$ bytes) of data to and from the parallel file system by one single process measuring the average transfer rates. The second test uses collective operations to perform reading and writing operations by several processes to and from a single file in the parallel file system at the same time. Again, the average transfer rates for different data sizes ($2^0 - 2^{27}$ bytes) are measured.

The measurements were made on the Cray Opteron Cluster. Its architecture consists of 128 nodes with dual AMD Athlon processors with 2 GHz and 2 GB memory each. The I/O architecture consists of two I/O servers connected to external RAID systems through a 2 Gbit/s Fibre-Channel network. Each computing node is connected to the I/O server through a 1 Gbit/s Ethernet network for I/O purposes leading to a bottleneck at the I/O server. This bottleneck limits the aggregated I/O transfer rate to about 1 Gbit/s.

Figure 3 shows the performance results of the first (above) and second (below) test set. The lines at 1 Gbit/s and 1/32 Gbit/s indicate the overall limit of the system in the corresponding test set. The results show nearly no differences between MPI-IO and TPO++ when reading data. Since TPO++ saves the structure of an object into a small meta file, the system can cache this structure, leading to almost no overhead compared to MPI-IO.

However, writing some data leads to an overhead due to the object-oriented abstraction of TPO++. This overhead increases when using collective calls, since TPO++ additionally has to process internal computations like offsets or

generating file views out of object-oriented structures. However, this lack in performance disappears when using file sizes of more than 256 kB - a small size in scientific computing. Therefore, object-oriented parallel I/O using TPO++ achieves almost the same bandwidth as MPI-IO.

Measurements on other platforms like the Kepler Cluster in Tübingen [7] or the Hitachi SR8000 at HLRB in Munich show comparable results and prove the efficiency and portability of the library on different platforms.

Besides the synthetic benchmarks, we already implemented the interface into several applications out of different scientific areas. F.ex. in simulating the injection of diesel into a combustion chamber with our particle framework SPH2000 or in searching motifs with structural and biochemical properties in biological sequences like DNA with a software tool called ParSeq [10]. Due to the complexity of the search, we incorporated an object-oriented parallel search which uses our parallel I/O interface and implemented it on the Kepler Cluster in Tübingen, increasing the performance significantly [8].

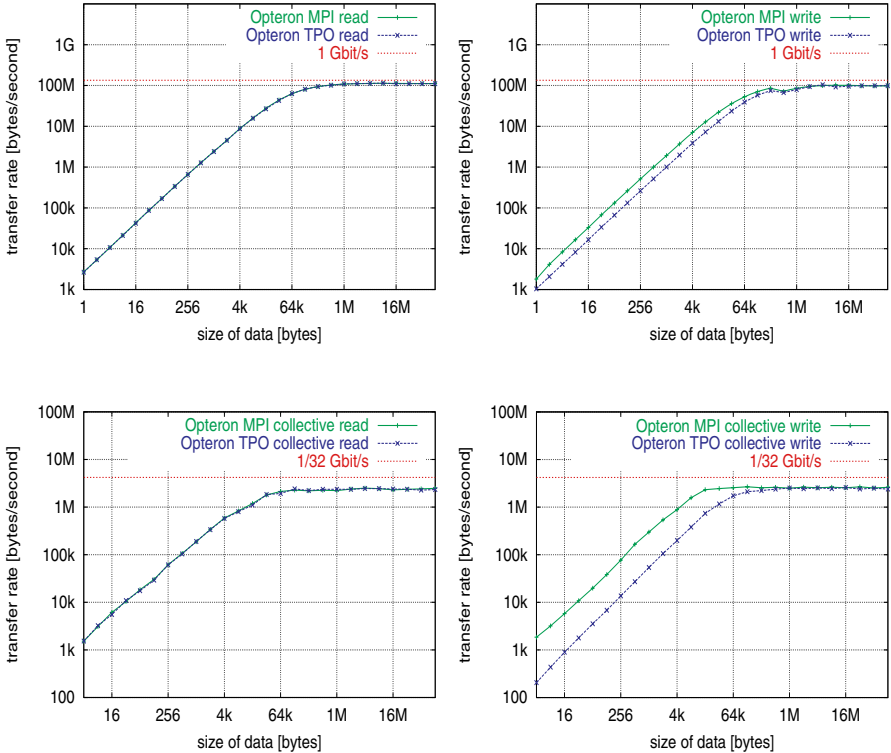


Fig. 3. Single read/write performance (above) and collective read/write performance on the Cray Opteron Cluster (below)

4 Applications

4.1 Application in Astrophysics: Early Humps of WZ Sge

Dwarf Novae are close binary star systems where a low mass main sequence star transfers matter via the inner Lagrangian point to its compact companion, a white dwarf. Due to its intrinsic angular momentum, the in-falling matter cannot be accreted directly by the white dwarf, instead a thin gaseous accretion disk is formed. The accretion disk is subject to two instabilities. A thermal instability, connected to the ionization of hydrogen, can lead to repetitive brightening of the disk. These “dwarf nova outbursts” last several days, have amplitudes of 2 to 5 mag and occur on timescales of weeks to months. The second instability is due to the tidal forces of the secondary star and can distort the accretion disk to an eccentric shape, precessing slowly prograde. This can happen only in systems with extreme mass ratio $M_2/M_1 < 0.3$. During an outburst, the outer disk rim can reach the critical 3:1 resonance radius (a particle at this radius makes exactly 3 orbits around the white dwarf during one orbit of the secondary), and the resonant tidal forces induce an eccentricity in the disk, the disk starts to precess. The precession leads to a higher dissipation of energy, making the outburst brighter (“superoutburst”). Also, an additional modulation of the brightness with a period a few percent longer than the orbital period can be observed.

WZ Sge is a dwarf nova with very a peculiar outburst behavior. Its rare outbursts, every 2 to 3 decades, are all superoutbursts of high amplitude and long duration. In the early stages of the superoutburst of WZ Sge, a peculiar type of photometric humps can be observed, occurring with the orbital period and double-peaked in profile. The “ordinary” superhumps develop only after about 10 to 20 days into superoutburst, after the early humps (sometimes referred to as early superhumps) have vanished. WZ Sge has an extremely low mass ratio, $q \approx 0.1$. In this case also the 2:1 resonance lies within the truncation radius. When the superoutburst sets in, the disk rim expands and reaches the 2:1 resonance region. A strong two-armed spiral dissipation pattern at the disk rim appears. As the growth rate of the 3:1 resonance is very slow for small q , ordinary superhumps appear only later, when the 2:1 resonance pattern has already died away. For the simulation shown in Fig. 4 the following parameters were chosen: $M_1 = 0.7M_\odot$, $M_2 = 0.056M_\odot$, corresponding to $q = 0.08$. The simulations started with an empty disk, and matter was fed into the Roche lobe of the White Dwarf via the inner Lagrangian point at a rate of $10^{-9}M_\odot\text{yr}^{-1}$. A physical viscosity of $\nu = 10^{-8}R_\odot^2\text{s}^{-1}$ and a polytropic equation of state were assumed. After 50 orbital periods the disk has expanded well into the area of the 2:1 resonance, and the expected stationary two-armed spiral pattern developed (Fig. 4 left). The simulation had about 50 000 particles at that time. Assuming that half of the tidally dissipated energy in the spiral arms is radiated away radially, and assuming an edge-on view on the disk, one can extract a phase-resolved pseudo light curve from

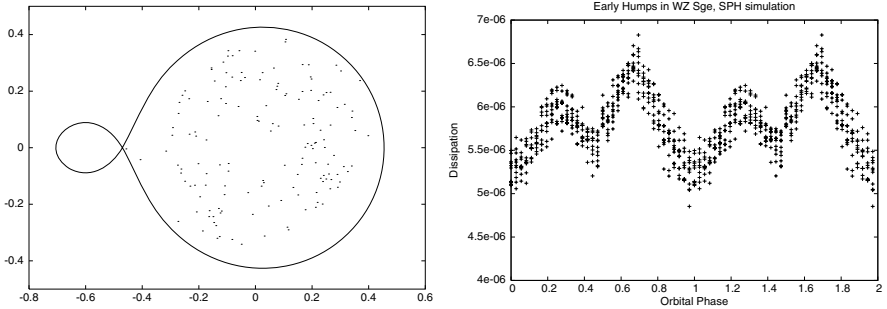


Fig. 4. SPH simulation of the disk of WZ Sge during the early superhump phase. Left: snapshot of the disk, the two-armed spiral is clearly visible. Right: phase-resolved pseudo light curve

the simulation data (Fig. 4 right). It shows a strong peak at phase 0.7 and a less prominent peak at phase 0.2, very similar to the observations. This is a good indication that indeed the 2:1 resonance is responsible for the early (super)hump phenomenon in WZ Sge stars. As the simulation continued, the disk became excentric and started to precess, leading to superhumps.

4.2 Simulation of brittle material

The SPH method was extended to the simulation of elastic and plastic solid bodies in the beginning of the nineties. This work was mainly pioneered by researches at the Los Alamos National Laboratory and improved later on by many other scientists ([2, 9]). In order to simulate brittle fracture, [1] added a damage model to the SPH method. Their damage model follows a statistical approach, which is based on two assumptions: Firstly, brittle materials contain flaws that are sources of weakness leading to the activation and growth of cracks under tensile loading, and secondly, the dynamic fracture depends on the rate of tensile loading.

Damage is defined as a scalar parameter $0 \leq D \leq 1$, such that, $D = 0$ represents an undamaged and intact material, whereas $D = 1$ corresponds to a fully damaged material which does not feel any stress or tensile forces. The damage parameter D expresses the reduction in strength under tensile loading. The elastic stress σ is decreased by the factor $(1 - D)$. Actually, the reduction of elastic stress may be interpreted as a reduction of the elastic parameters, the bulk and shear moduli K and μ . Hence, a damaged material has elastic parameters, that are reduced by the factor $(1 - D)$, resulting in $K_{\text{damaged}} = (1 - D)K$ and $\mu_{\text{damaged}} = (1 - D)\mu$. The distribution of flaws in a brittle material is given by the Weibull distribution which reads $n(\varepsilon) = k\varepsilon^m$, where $n(\varepsilon)$ is the most likely number of flaws per unit volume that have activation thresholds (or failure strains) lower than ε . The Weibull distribution

has two material parameters k and m . The parameter k has the unit 1/volume, and defines the number of flaws per unit volume.

As an example of the implementation in our parallel SPH code **ParaSPH**, we present the simulation of a brittle rod. The initial setup is as follows: A rectangular plate with a length of 3 and a height of 1 cm is taken under tensile loading by pulling both ends either by a constant velocity.

Physically, fracture is expected to occur as soon as the local strain of one region exceeds its activation threshold strain, that is when the microscopic bonds between the atoms break and fail and little flaws accumulate. If only certain bonds between atoms break plastic flow occurs resulting in planes of atom layers sliding over each other. Plastic flows lead to permanent deformation. As soon as the ends of the plate are torn apart elastic waves will travel through it. As the volume of the plate is conserved the plate decreases its height if it is pulled apart. What follows depends on the material properties of the plate. If it is a rocky like brittle plate, the plate will break first where the lowest activation threshold strain is located. If the plate consists of flaw-less ductile material, the height will continue decreasing, leading to so-called necking, until fracture occurs. The simulation outcome for three different strain rates is shown in Fig. 5. The dependence of the damage pattern is investigated in this simulations. Higher strain rates are expected to lead to more damaged material. The faster the rod is pulled apart, the higher the damage, or the larger and longer are the cracks. Though stress is released by the formation of cracks, the relief is coupled to the finite crack growth velocity

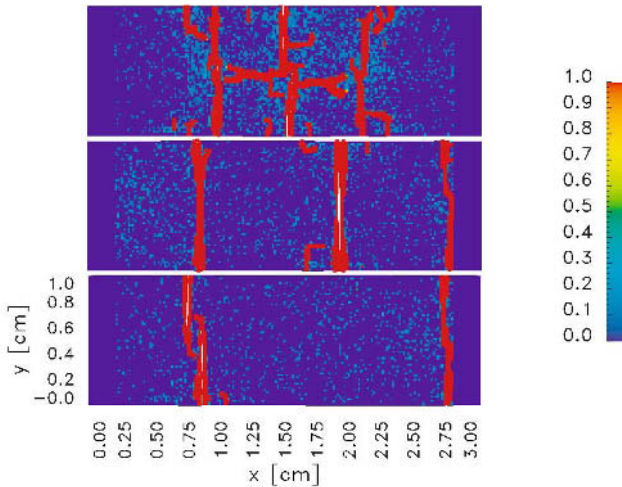


Fig. 5. Outcome of the simulation of the tensile rod at three different strain rates, $\dot{\epsilon}_0 = 3.33 \times 10^{-3}$, 6.67×10^{-4} , 3.33×10^{-4} , from top to bottom.

c_g , and a single crack might not release stress fast enough to prevent further crack formation by the activation of more flaws. Thus, higher strain rates result in smaller sized fragments. Figure 5 shows the outcome of the three simulations for three different times, namely at the end of each simulation when the damage pattern remains the same. Clearly, the simulation results obey the tendency that higher strain rates lead to more damage. The SPH method can be applied successfully to the simulation of brittle materials such as basaltic rocks.

4.3 Simulation of diesel injection

Approaches made for the simulation of free surfaces were already introduced in 1994 by Monaghan. The SPH method is able to describe the breakup of diesel jets [6]. Examinations on the influence of inflow boundary conditions on the jet breakup at the beginning of the injection revealed that a realistic breakup behavior can only be achieved by stochastic disturbance at the inlet. The viscous stress tensor was implemented in the SPH formalism to be able to simulate the complete Navier-Stokes equations. The SPH method has been enhanced to simulate flows of two separated phases such as occur in the primary jet breakup. The main problem is caused by the huge density leap at the boundary layer of the different fluids. Due to discontinuous functions generating large errors during the smoothing process, which the numerical deviation is based on, an alternative formulation of the continuity equation and density calculation had to be implemented. This enhancement has been examined by several test problems and proved stable even for huge density variations. Since the SPH method is able to simulate compressible flows the method is highly applicative to simulate the processes at extremely high injection pressures.

Figure 6 shows a pressure distribution. The field quantities are interpolated on a Cartesian grid whose lattice parameter is of the same order of magnitude as the smoothing length. In the pictured simulation the inflowing diesel and the air inside the chamber have the same pressure of 50 bar. The illustration below reveals the compressional wave precursory to the diesel jet which flows in at about 60% of the sound-propagation velocity of the system.

A basic region of interest is the implementation of surface tension within the SPH method. Still fundamental research has to be done in this field. Injection pressures are increasing quickly. The current pressures in diesel engines generate sprays with a drop size distribution which is so small, that a large contingent of the injection energy dissipates into surface energy. The surface energy causes a lower limit for drop sizes. While in literature the semi-analytic description prevails it is inapplicable to set up discretizable hydrodynamic equations. A fundamental derivation of the strain tensor for surface tension was developed and its relevance for energy conservation was verified. The chosen description results in a representation for the surface tension as a singular force density on the boundary layer.

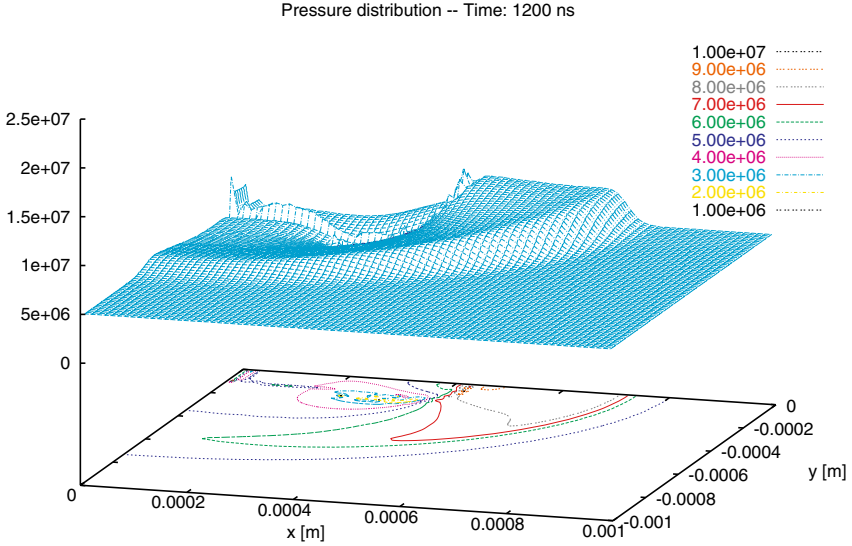


Fig. 6. Pressure distribution after 1200 ns at 50 bar and $400 \frac{m}{s}$ fluid jet speed.

Future simulations including heat transfer, surface tension and turbulence will require much more computing time and much higher I/O performance. The limitation of I/O performance is not only a problem during the simulation run but also during the evaluation. For the analysis of the data records the files have to be processed several times with comparatively low calculating time.

5 Summary

For massive parallel applications, scalability is always an issue. Besides improving the parallel algorithms, we currently follow two other approaches to reduce the serial parts: A hybrid parallelization promises to reduce the communication cost, because intra-node data can be shared, and parallel I/O can reduce the time spent for persistency. However, the studies of ParaSPH on the architectures available at HLRS show that improving the performance with an hybrid parallelization is not trivial. The main obstacle for the use of parallel I/O is the lack of an object-oriented interface in current standards.

For this reason, we extended our object-oriented message passing library TPO++ by an interface to parallel I/O. It exploits object-oriented and generic programming concepts, allows easy reading and writing objects and makes use of advanced C++ techniques and features as well as supporting these features, most notably it supports STL data types. The system introduces

object-oriented techniques while preserving MPI-IO semantics and naming conventions as far as possible and reasonable. This simplifies the transition from existing code.

Several applications using our libraries and methods prove the efficiency, usability and portability of our efforts in optimizing parallel applications.

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Solid State Physics

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The unifying theme of the computer applications in the area of solid-state physics at the HLRS is the contribution to the many-body aspects of interacting particles. The simulations of the Stuttgart group around A. Muramatsu are concerned with strongly correlated quantum gases, magnetic and correlated electron systems. The program of the Jena group around W. G. Schmidt deals with the understanding of surface optical spectra in weakly correlated systems, such as semi-conductors like silicon. On the other hand, the University of Konstanz project of P. Nielaba and co-workers is concerned with nano-systems in reduced geometry, which contain typically 10 to 10,000 interacting particles. The corresponding implications of strong or weak correlations on the one side and the influence of nano-physics in reduced geometry on the other side, can be dealt with very effectively using modern supercomputing, based simultaneously on sophisticated algorithmic tools. This will be discussed in detail in what follows:

The Stuttgart project of Dr. C. Lavalle and the group of Prof. A. Muramatsu studies a variety of different many-body systems with relevance to topics such as magnetism and high-temperature superconductivity. The basic aim there is to understand systems such as the high- T_C superconducting cuprates and the manganites, which, in principle, have the possibility of very important technological applications, such as high-transition temperatures in superconductivity or magnetic data recording in manganites. However, in these systems there still exists a major obstacle in obtaining a basic understanding of the complicated phase diagram:

The central issue, for example in the field of high-temperature superconductivity (HTSC), is the connection of the microscopic interactions at the level of electrons and ions, which are at high energy and temperature T with the “emerging phenomena” at $T = 0$, i.e. competing and nearly degenerate orders - antiferromagnetism (AF), d-wave superconductivity (d-SC), etc. Ideally speaking, we should start at the several eV-physics of interacting electrons and ions, and then, bridge high to low energies and, eventually, go to $T = 0$ and solve the ground-state problem. There, different competing orders

appear (AF, d-SC, heterogeneous phases, etc.), which are not separated by distinct energies in the remaining problem. So, it is not obvious how one can systematically apply the renormalization-group idea (for the strong correlation case realised in the HTSC) to integrate out the irrelevant degrees of freedom. What is required is a kind of “magnifying lens”, which allows resolving the competing orders. For this “magnifying lens”, the Stuttgart group has used a variety of Quantum-Monte-Carlo algorithms, complimented with a new exact numerical method. Several strongly correlated systems, which are presently the subject of intense research in the solid-state community, have specifically been simulated by the Stuttgart group, namely degenerate quantum gases, a quantum antiferromagnet on a quasi-crystal and the celebrated t-J model for high-temperature superconductivity. The degenerate quantum gases have been treated in the framework of so-called hard-core-boson algorithms, revealing an interesting variety of new results, which, in particular, may be realised in atom lasers. In the case of the quantum antiferromagnet on a quasi-crystal, a non-trivial magnetic structure has been established, which is a pure quantum effect not produced in the classical limit. The t-J model, on the other hand, relevant for the HTSC, has been compared with exact Bethe-Ansatz solutions. This comparison achieves the above-mentioned transition to $T = 0$ by finding that the Bethe-Ansatz reproduces the major features of the t-J Model spectra.

The project of the Jena group dealing with the detailed simulation of surface optical spectra of semi-conductors has concentrated on clean, oxidized as well as organically modified Si (001) surfaces. It uses the density functional theory in the local approximation (LDA) and the corresponding (Kohn-Sham) equations. In this Jena work, the emphasis is placed on obtaining an accurate description of the single-electron approximation achieved within the density-functional scheme. The optical properties are then calculated in the independent particle-approximation, which neglects many-body effects such as local-field and excitonic effects. This is a reasonable first step, in that the density functional implementation for the Si (001) surfaces is already a very demanding computational project. However, it is known that the above many-body effects, which describe repeated interactions between electrons and holes created in the optical response, are introducing qualitative changes. On the other hand, already the single particle electronic properties reveal valuable information on the structural properties of the surfaces and interfaces considered. For example, an oxide layer directly above the Si (001) interface was found to be disordered, the oxidation proceeds layer by layer and there exists a one-to-one correspondence between the layer oxidation and the interface optical anisotropy. Hopefully, this calculation of the non-interacting optical susceptibility will be supplemented in the future with the corresponding inclusions of the many-body effects. It is clear that then a valuable wealth of information on surface optical properties in semi-conductors can be obtained from state of the art numerical simulations.

The last project deals with the computer simulations at the HLRS by the P. Nielaba's group of the University of Konstanz. Nanostructures in reduced geometry have become, in context with a large variety of solid state materials, an interesting research in the last few years. One major obstacle in connecting the wealth of experimental information on these systems with a first-principle understanding from theory is that these systems with their 10 to 10,000 particles are lying just in between the few-particle limit of a very small cluster, which can be dealt with with numerical and even exact numerical techniques, and the thermodynamic limit (with infinitely many particles). Many new results have been obtained for these systems employing state of the art numerical techniques and algorithms at the HLRS in Stuttgart and the SSC in Karlsruhe. In the HLRS/SSC project, classical molecular dynamical simulations (Car-Parrinello-Simulations), for example, of the breaking of nano-contacts have been combined with conductance calculations based on a tight-binding model. These classical and quantum physics combinations have given access to crucial information such as contact geometries, forces, total conductance and transmission coefficients of nano-wires. For example, for the specific case of gold wires, the results suggest that the low-temperature conductance histograms are a consequence of a subtle interplay between mechanical and electrical properties of these nano-contacts. An interesting project concerns Car-Parrinello studies, which are performed for clusters and surfaces, where in particular the cluster stability and their usefulness as building blocks as a "cluster material" will be analysed. This aims at explaining, from a theoretical point of view experimental data, which show that Si_4 and Si_7 clusters are possible candidates for a "cluster material". Another highly topical theme is simulations of soft-matter systems by Monte-Carlo simulations. This concerns the crystallisation and melting of colloidal suspensions, both in two and three dimensions. There, the melting transition is a theoretical challenge, which, seems to be entirely controlled by the elastic constants. However, both experimental and theoretical studies of elastic constants are quite rare. Therefore, the development of tools for the determination of the elastic properties (in colloidal model systems) is important.

In summary, then, the three solid-state projects carried out at the HLRS and partly at the SSC in Karlsruhe, have profited enormously from the supercomputing possibilities and facilities at these two topical locations. Substantial progress was achieved in the understanding of so-called strongly correlated electron systems such as high-temperature superconductors and other oxide systems displaying magnetic phases in competition with superconductivity and charge order. These systems are of great interest for technological applications. Similarly, the HLRS simulations performed by the Jena group on the optical properties of semi-conductor surfaces have achieved a first understanding of the interplay between structural properties and the electronic physics at interfaces and surfaces. These two solid-state groups have considered interacting fermions of solid-state materials from a purely quantum mechanical point of view. The Konstanz group, on the other hand, has combined classical

molecular dynamic simulations of interacting atoms with quantum mechanical (conductance) calculations. The common denominator of all these successful computer projects was and is that they aim at replacing the still mostly carried out “empirical search” for improved material properties by a first-principle “guidance”, namely understanding the materials properties from the point of view of ions and electrons interacting in the solid or liquid, respectively.

Numerical Simulations of Quantum Gases, Magnetic, and Correlated Electronic Systems

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Summary. A variety of quantum Monte Carlo algorithms are used to study the equilibrium properties of strongly correlated quantum systems relevant to the fields of high- T_c superconductivity and magnetism. Furthermore, a new exact numerical method was developed and applied to strongly correlated quantum gases to unveil their universal properties in equilibrium and new states of matter out of equilibrium.

1 Introduction

Strongly correlated many-body quantum systems are becoming an active common subject of research for a number of fields in physics, like ultra-cold atoms, magnetic, and electronic systems. Such a development is leading presently to an interdisciplinary convergence among the communities of quantum optics, atomic, and condensed matter physics.

Along the lines of such an exciting development in physics, we present a number of numerical studies performed with different algorithms, each optimized for the problem at hand. In all these problems, the use of numerically exact methods is imperative due to the absence of reliable analytical tools.

In Sec. 2 we discuss first universal properties of strongly interacting bosons (hard-core bosons - HCB) in one dimension [RIGO04A], a system that has been recently realized experimentally [PARE04, KINO04]. We then analyze the non-equilibrium dynamics of pure Fock states of HCB when they are let to evolve freely. Although initially there are no correlations between the particles, they build up dynamically during the evolution of the system leading to the emergence of quasi-condensates at finite momentum [RIGO04B]. Such a propagating coherent matter wave offers a new realization of an atom laser.

In Sec. 3 we study the effects of quantum fluctuations on a two-dimensional quantum antiferromagnet defined on a quasiperiodic lattice-structure, that explicitly lacks translational symmetry. Our results are a first step towards understanding recent neutron diffraction studies on the recently discovered

Zn-Mg-Ho icosahedral quasicrystals [SATO00], which show an onset of anti-ferromagnetic correlations at low temperatures.

Finally, we present in Sec. 4 new results for the so called t - J model, that is the simplest model for high temperature superconductors (HTS). Although treated in one dimension, several features of charge inhomogeneities appear, a subject of much discussion in HTS.

2 Hard-core bosons in 1D

Recent experiments with ultra-cold atoms have opened a new possibility for studying systems where quantum fluctuations play a key important role. Even the noninteracting case presents unusual features [RIGO04D]. The superfluid–Mott-insulator transition in 1D [BATR02] has been observed experimentally by Stöferle *et al.* [STOF03]. The fermionic case displays local quantum criticality [RIGO03, RIGO04C, RIGO04E]. In addition, 1D geometries have allowed the observation of the strongly correlated hard-core boson (HCB) limit with [PARE04] and without [KINO04] a lattice along the 1D tubes.

In a 1D lattice, the HCB Hamiltonian can be written as

$$H_{HCB} = -t \sum_i (b_i^\dagger b_{i+1} + h.c.) + V_\alpha \sum_i x_i^\alpha n_i, \quad (1)$$

with the addition of the on-site constraints $b_i^{\dagger 2} = b_i^2 = 0$, $\{b_i, b_i^\dagger\} = 1$, where $b_i^\dagger$ and b_i denote the creation and annihilation operators, respectively. $n_i = b_i^\dagger b_i$ is the particle number operator, and t is the hopping parameter. The last term in (1) depicts an arbitrary confining potential, with power α and strength V_α .

We then use the Jordan-Wigner transformation (JWT) [JORD28], which maps the HCB Hamiltonian into the one of noninteracting fermions

$$H_F = -t \sum_i (f_i^\dagger f_{i+1} + h.c.) + V_\alpha \sum_i x_i^\alpha n_i^f, \quad (2)$$

with $f_i^\dagger$ and f_i being creation and annihilation operators for spinless fermions, and $n_i^f = f_i^\dagger f_i$.

The Green's function for the HCB can be expressed using the JWT as

$$G_{ij} = \langle \Psi_{HCB}^G | b_i b_j^\dagger | \Psi_{HCB}^G \rangle = \langle \Psi_F^G | \prod_{\beta=1}^{i-1} e^{i\pi f_\beta^\dagger f_\beta} f_i f_j^\dagger \prod_{\gamma=1}^{j-1} e^{-i\pi f_\gamma^\dagger f_\gamma} | \Psi_F^G \rangle. \quad (3)$$

$|\Psi_{HCB}^G\rangle$ is the ground state for the HCB and $|\Psi_F^G\rangle$ is the ground state for the noninteracting fermions. The latter is a Slater determinant, i.e., a product of single particle states $|\Psi_F^G\rangle = \prod_{\delta=1}^{N_f} \sum_{\sigma=1}^N P_{\sigma\delta} f_\sigma^\dagger |0\rangle$, with N_f the number of fermions ($N_f = N_b$), N the number of lattice sites and $\mathbf{P}$ is the matrix of the

components of $|\Psi_F^G\rangle$. It can be seen that the action of $\prod_{\gamma=1}^{j-1} e^{-i\pi f_\gamma^\dagger f_\gamma}$ on the fermionic ground state in (3) generates only a change of sign on the elements $P_{\sigma\delta}$ for $\sigma \leq j-1$, and the further creation of a particle at site j implies the addition of one column to $\mathbf{P}$ with the element $P_{jN_f+1} = 1$ and all the others equal to zero [the same applies to the action of $\prod_{\beta=1}^{i-1} e^{i\pi f_\beta^\dagger f_\beta} f_i$ on the left of (3)]. Then the HCB Green's function can be calculated exactly as

$$G_{ij} = \langle 0 | \prod_{\delta=1}^{N_f+1} \sum_{\beta=1}^N P'_{\beta\delta}{}^A f_\beta \prod_{\sigma=1}^{N_f+1} \sum_{\gamma=1}^N P'_{\gamma\sigma}{}^B f_\gamma^\dagger | 0 \rangle = \det \left[\left(\mathbf{P}'^A \right)^\dagger \mathbf{P}'^B \right], \quad (4)$$

where $\mathbf{P}'^A$ and $\mathbf{P}'^B$ are the new matrices obtained from $\mathbf{P}$ when the required signs are changed and the new columns added. A proof of the last step in (4) can be found in [MURA99]. As shown by (4), the evaluation of G_{ij} can be done very efficiently numerically, allowing for the study of systems with up to 10^4 lattice sites. The approach above can be easily generalized to study the non-equilibrium dynamic of HCB on 1D lattices [RIGO04B].

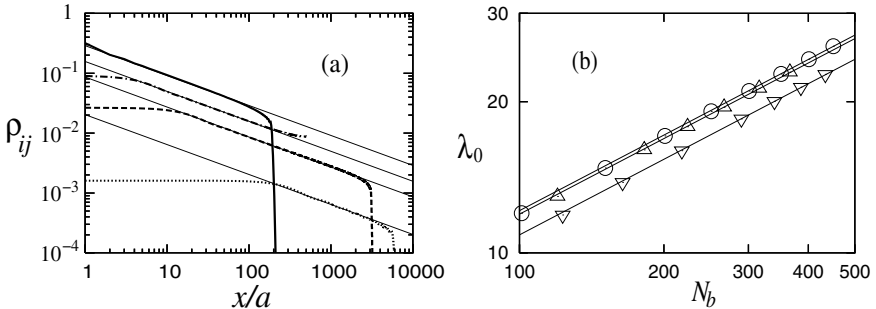


Fig. 1. (a) OPDM vs x/a ($x = |x_i - x_j|$) for a periodic system with $\rho = 9.1 \times 10^{-2}$, $N_b=91$ (dashed-dotted line), harmonic traps with $\tilde{\rho} = 4.5 \times 10^{-3}$, $N_b=100$ (dashed line) and $\tilde{\rho} = 2.7$, $N_b=501$ (thick continuous line, a $n_i = 1$ region is present), and a trap with power $\alpha = 8$, $\tilde{\rho} = 7.6 \times 10^{-4}$, $N_b=11$ (dotted line). In the trapped cases the abrupt reduction of ρ_{ij} occurs when $n_j \rightarrow 0, 1$, for $n_i \neq 0, 1$. Thin continuous lines correspond to power laws $\sqrt{x/a}$. (b) Lowest NO occupation vs N_b for periodic systems with $\rho = 0.5$ ($\circ$), harmonic traps with $\tilde{\rho} = 1.0$ ($\triangle$), and traps with $\alpha = 8$ and $\tilde{\rho} = 1.0$ (∇). Thin continuous lines correspond to power laws $\sqrt{N_b}$.

We first focus on the large- x behavior of the OPDM. For the periodic case ($V_\alpha = 0$), we obtain that for any density $\rho \equiv N_b/N \neq 0, 1$ the OPDM decays as a power law $\rho_{ij} \sim (x/a)^{-1/2}$ for large x [Fig. 1(a)], with a the lattice constant. This behavior is known from exact analytical treatments [KITA02]. In the presence of a confining potential, the system loses the translational invariance and no analytical results are available. We first analyze the case where $n_i < 1$ all over the system. We find, remarkably, that in this case

the OPDM decays as a power law $\rho_{ij} \sim (|x_i - x_j|/a)^{-1/2}$ for large x , i.e., independently of the local changes of the density. (They become relevant only when $n_i, n_j \rightarrow 0$.) Moreover, the exponent of the OPDM power-law decay does not depend on the power α of the confining potential, i.e., it is universal [Fig. 1(a)]. A drastic difference between the continuous case and the one with a lattice is the possibility to build up regions with densities $n_i = 1$, so that such sites are not any more coupled to the rest. Even in this case we find that the OPDM decays as a power law $\rho_{ij} \sim (|x_i - x_j|/a)^{-1/2}$ in the regions away from $n_i, n_j \neq 0, 1$ [Fig. 1(a)].

The universal behavior of the power-law decay of the OPDM above has important consequences in the coherent properties of the system. For their understanding, we have studied how the lowest NO occupation λ_0 (which would be the condensate in higher dimensions) scales with an increasing number of particles in the system, keeping the characteristic density $\tilde{\rho} = N_b a / \zeta$ [RIGO04C, RIGO04D, RIGO04E] constant. $\zeta = (V_\alpha/t)^{-1/\alpha}$ is a length scale of the trap in the presence of the lattice [RIGO04C, RIGO04D, RIGO04E]. In Fig. 1(b) we show results for periodic systems, harmonic traps, and traps with $\alpha = 8$. They show that the scaling of the lowest NO occupation is also universal $\lambda_0 \sim \sqrt{N_b}$. As expected HCB systems do not exhibit Bose-Einstein condensation in 1D $\lambda_0/N_b \rightarrow 0$ for $N_b \rightarrow \infty$, but $\lambda_0 \rightarrow \infty$ so that one can speak about quasi-condensation in these systems.

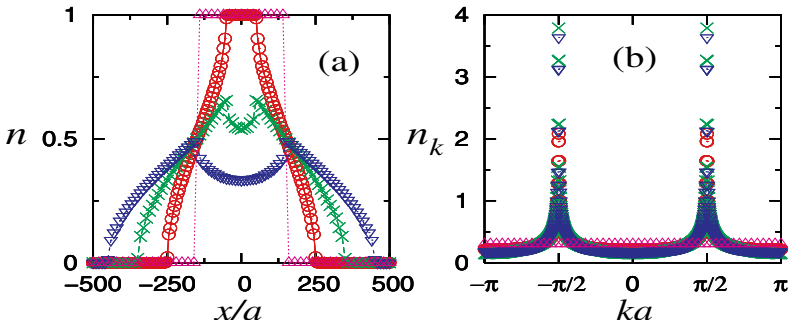


Fig. 2. Evolution of density profiles (a) and n_k (b) of 300 HCB in 1000 lattice sites. The times are $\tau = 0$ ($\triangle$), $50/t$ ($\circ$), $100/t$ ($\times$), and $150/t$ (∇).

Next we study the free time evolution of Fock states of HCB with one particle per lattice site [Fig. 2(a)]. In such states [Fig. 2(a)] at $\tau = 0$ all the particles are totally uncorrelated since the one-particle density matrix is just a delta function $\rho_{ij} = \delta_{ij}$ for the occupied lattice sites, and zero everywhere else. The corresponding momentum distribution function n_k is totally flat, as shown in [Fig. 2(b)] at $\tau = 0$. Surprisingly, we find that when the system is allowed to evolve two peaks appear in n_k at $k = \pm\pi/2$ [Fig. 2(b)].

The peaks in n_k reflect the onset of quasi-long range correlations in the system. This can be seen in Fig. 3(a) as a power-law decay of the form $|\rho_{ij}| = 0.25 |(x_i - x_j)/a|^{-1/2}$, that remains almost unchanged during the evolution of the system. The above power law is exactly the same observed previously in the ground state. In order to know if the appearance of such quasi-long range correlations led to the emergence of quasi-condensates, we have studied the scaling of the lowest NO wave function and its occupation with increasing the number of particles in the initial Fock state. In Fig. 3(b) we show that a scaled NO ($|\varphi_0| = N_b^{1/2} |\phi^0|$) exists when its size is normalized by $N_b a$. Results for the maximum occupation of the lowest NO as a function of the number of particles in the initial Fock state are shown in the inset in Fig. 3(a). The $\sqrt{N_b}$ power-law behavior is evident and a fit allowed us to obtain the constant $A = 0.72$. Since the above quasi-condensates move with momenta $k = \pm\pi/2a$ [RIGO04B], they cause the appearance of the peaks in n_k observed in Fig. 2(b).

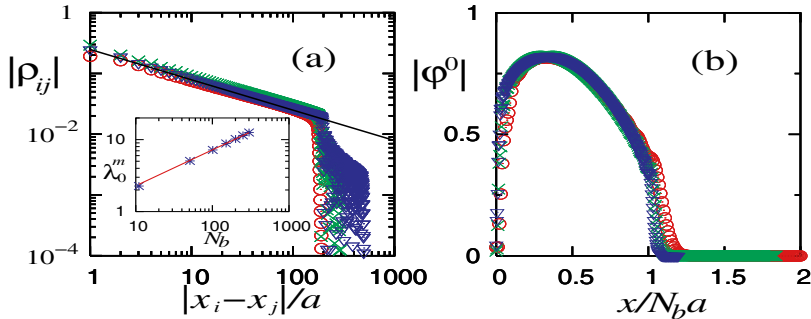


Fig. 3. (a) OPDM for: $\tau=50/t$ ($\circ$), $100/t$ ($\times$), and $150/t$ (∇), the straight line is $0.25 |(x_i - x_j)/a|^{-1/2}$. (b) Scaled lowest NO right lobe's vs $x/N_b a$ for $N_b = 101$ ($\circ$), 201 ($\times$), and 301 (∇). The inset in (a) shows the maximum occupation of the lowest NO vs N_b of the initial Fock state, the line is $0.72 N_b^{1/2}$.

In summary, we have developed an exact approach that allows to study ground state properties and the non-equilibrium dynamics of HCB on 1D lattices. This approach has been used to study the off-diagonal behavior of the one-particle density matrix where universal quasi-long-range correlations $\rho_{ij} \sim |(x_i - x_j)/a|^{-1/2}$ are observed, and the lowest NO occupation has been found to scale $\lambda_0 \sim \sqrt{N_b}$. We have also studied the non-equilibrium dynamics of pure Fock states of HCB when they are allowed to evolve. We find that in this case quasi-long range correlations develop in the system, and they lead to the emergence of quasi-condensates at finite momentum.

3 Quasiperiodic Antiferromagnets

Low-dimensional quantum antiferromagnetism has become an intense field of solid state research in recent years. Quantum fluctuations, disorder and geometric frustration add to a large variety of new, exotic quantum phases in such systems [SCHO04]. In certain cases, they lead to a complete destruction of long-ranged magnetic order. In general, the systems under consideration share the translational invariance of the underlying lattice structure - assuming sufficient self averaging in the case of quenched disorder.

Quasiperiodic antiferromagnets were believed to not allow for long-ranged magnetic order. We show that on non-frustrated quasiperiodic lattices they actually develop strong magnetic correlations, and indeed order at zero temperature. Using a combination of quantum Monte Carlo simulations and finite-size spin-wave theory, we study the static and dynamical properties of the antiferromagnetically ordered ground state.

We analyzed the magnetic ground state and the excitation spectrum of the nearest-neighbor antiferromagnetic Heisenberg model,

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j, \quad J > 0, \quad (5)$$

on the octagonal tiling. Here, the $\mathbf{S}_i$ denote spin- $S = 1/2$ degrees of freedom on the sites of the octagonal tiling, and J denotes the antiferromagnetic exchange along its bonds. The octagonal tiling is a bipartite quasiperiodic crystal system, and possesses an overall eightfold rotational symmetry, allowing for simple two-sublattice antiferromagnetism [LIFS04]. Sites in this tiling have coordination numbers z ranging from 3 to 8. A further important property of the octagonal tiling, in the absence of translational invariance, is its self-similarity under inflation transformations [DUNE89]. This operation refers to a well-defined decimation of a subset of vertices of the tiling, followed by a re-connection of the new vertices. Aside from a trivial rescaling of the length scale, the infinite quasicrystal is left unchanged by this transformation. For our numerical study we consider finite square approximants of the octagonal tiling [DUNE89] with up to 5572 sites (Fig. 4). We employ the stochastic series expansion quantum Monte Carlo (SSE-QMC) algorithm [SAND97, ALET05], to study ground state properties of the approximants [WESS02, WESS05A]. From our quantum Monte Carlo simulations, we found that the octagonal tiling allows for long-ranged antiferromagnetic correlations. In particular, the value of the staggered magnetic moment, obtained from a finite size scaling analysis, is $m_s = 0.337 \pm 0.002$ [WESS02]. This makes a semiclassical description of the antiferromagnetic ground state feasible. We developed a numerical finite size linear spin-wave theory (LSWT) for quasiperiodic systems [WESS05B]. In both the SSE-QMC and the LSWT approach, the magnetic ground state on the octagonal tiling was found to exhibit a nontrivial local structure reflecting the self-similarity of the underlying quasiperiodic

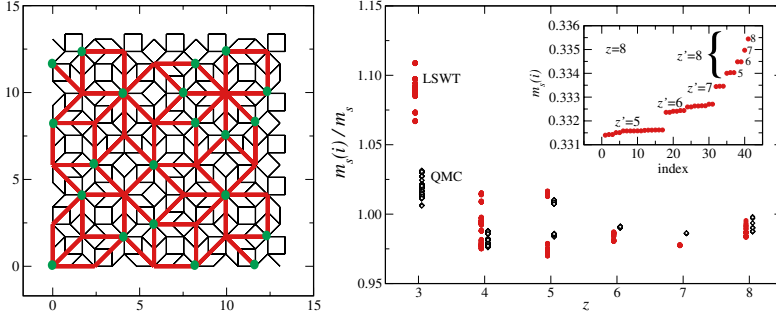


Fig. 4. (Left) Superimposed finite approximant of the octagonal tiling, exhibiting its selfsimilar and bipartite nature. (Right) Local staggered magnetization grouped according to the coordination number z . Numbers next to symbols in the inset give the value of z'' for $z' = 8$ sites under a further deflation.

lattice structure: In Fig. 4 the value of the local staggered magnetization, $m_s(i)$, are shown for the largest approximant, grouped according to the coordination number z of the various sites. We observe (i) a wide spread of the moments, in particular for small values of z , (ii) a prominent bimodal splitting of the moments for $z = 5$ and (iii) hierarchical structures in the splitting of the moments for sites with $z = 8$, shown in the inset of Fig. 4. These splittings in the local staggered moments can be accounted for by the properties of inequivalent sites under deflation transformations, reflecting their different local environments [WESS02]. We also find the semi-classical theory to indeed provide a qualitative, and even quantitative account on the magnetic ground state properties of the Heisenberg model on the octagonal tiling, with limitations at low values of z , as expected from its mean-field character.

We then analyzed spectral properties of this quasiperiodic antiferromagnet. In particular, we studied the dynamical spin structure factor, accessible experimentally by inelastic neutron scattering,

$$S^\perp(\mathbf{k}, \omega) = \frac{1}{2N} \sum_{i,j=1}^N e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle S_i^+(t) S_j^-(0) + S_i^-(t) S_j^+(0) \rangle \quad (6)$$

In the elastic limit of $S^\perp(\mathbf{k}, \omega \rightarrow 0)$, shown in the left of Fig. 5, we can identify the magnetic Bragg peak positions. For energies up to $\omega/JS \approx 2$, similar patterns as in $S^\perp(\mathbf{k}, \omega = 0)$ are observed, albeit with the width of the peaks increasing upon increasing the energy. Eventually, these peaks evolve into ring-like structures, centered around the magnetic Bragg peaks [WESS05B]. This is a clear indication for magnetic soft-modes at low energies, which dominate the magnetic response in this energy regime.

We also find the plots of $S^\perp(\mathbf{k}, \omega)$ at higher frequencies to exhibit an eight-fold symmetry, as expected for the octagonal tiling. However, the positions of the dominant peaks are different from the magnetic Bragg peaks found below

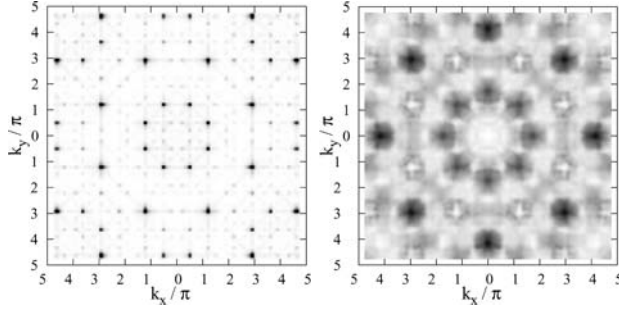


Fig. 5. Intensity plot of the dynamical spin structure factor, $S(\mathbf{k}, \omega)$, for fixed $\omega/JS = 0$ (left) and $\omega/JS = 3.0$ (right). For both panels, the relative intensity is denoted by a linear grayscale ranging between zero (white) and maximum intensity (black).

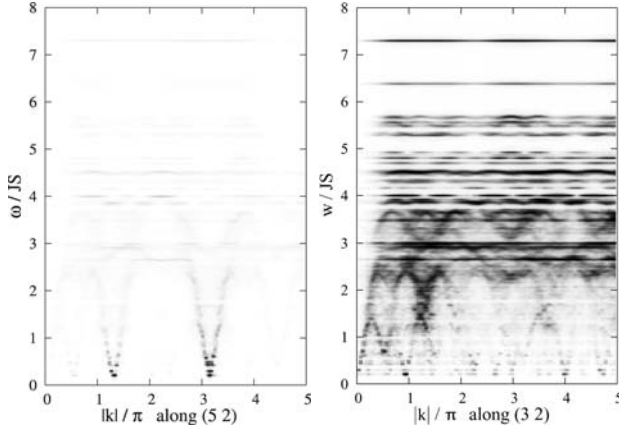


Fig. 6. Intensity plot of the dynamical spin structure factor, $S(\mathbf{k}, \omega)$, along the $(5, 2)$ momentum space direction (left) and along the line $(3, 2)$ (right). For both panels, the relative intensity is denoted by a linear grayscale ranging between zero (white) and maximum intensity (black).

$\omega/JS \approx 2$. For example, for $\omega/JS = 3.0$ (right of Fig. 5), most spectral weight is located at $\mathbf{k} \approx (0, 1.3\pi)$, and $\mathbf{k} \approx (0, 4.3\pi)$, as well as symmetry-related momenta. Peaks at these momenta are absent in the nuclear Bragg scattering (Fig. 5 (a) of Ref. [WESS02]). In fact, we do not observe pronounced spectral weight at nuclear Bragg peak positions for any finite energy cut [WESS05B].

In order to analyze the momentum dependence of the dominant peaks in the dynamical spin structure factor, we choose representative directions in momentum space, and analyze $S^\perp(\mathbf{k}, \omega)$ along such cuts (Fig. 6). The cut in the left of Fig. 6 passes through two of the major magnetic Bragg peaks.

In the low-energy region, below $\omega/JS \approx 2$, most spectral weight is located along straight lines, emerging from the magnetic Bragg peaks, with spectral weight that increases for decreasing energy, characteristic of magnetic soft-modes. Near the magnetic Bragg peaks, $\mathbf{k}_B$, we thus observe linear dispersion relations of the magnetic excitations, $\omega = c|\mathbf{k} - \mathbf{k}_B|$, with an estimated spin-wave velocity $c/JS \approx 2.1$, which is of similar order of magnitude than the linear spin-wave result for the square lattice ($c/JS = \sqrt{8} \approx 2.83$). In spite of the absence of translational symmetry, the dynamical spin structure factor of the antiferromagnetic quasicrystal thus exhibits linear soft-modes near the magnetic Bragg peak positions of the quasiperiodic crystal. We expect such a generic feature of magnetic long-range order to be present also in other magnetically ordered quasicrystals. At high frequencies, $\omega/JS > 5.5$, we do not observe any significant dispersion of the spectral weight. In particular, the flat bands seen in the right of Fig. 6 are due to localized states [WESS05B]. In the intermediate energy regime, the distribution of spectral weight can be accounted for by band-like segments, which recur at different energies and with varying bandwidths, as shown in the right of Fig. 6. Furthermore, bifurcations emerge as branches of these band-segments extending towards lower energies. Such self-similar structures might have been expected to dominate the dynamical spin structure factor, due to the geometric properties of the octagonal tiling, reflecting its inflation symmetry. Nevertheless, we find them well separated in energy from more conventional low-energy features, that reflect the magnetic order in this system.

Summarizing, we have shown that nonfrustrated quasiperiodic antiferromagnets allow for pronounced long-ranged magnetic order. The quantum fluctuations exhibit the self-similarity of the underlying lattice structure, leading to a non-trivial magnetic structure. This is a pure quantum effect, not reproduced in the classical limit. The broken $SU(2)$ symmetry of the ordered ground-state leads to the emergence of low-energy soft-modes with a linear dispersion near the magnetic Bragg-peaks. These are well separated in energy from multifractal excitations and localized states in high-energy regions.

4 The one-dimensional nearest-neighbor t - J model at finite doping

The nearest-neighbor (n.n.) t - J model in one dimension reads:

$$H_{t-J} = -t \sum_{i,\sigma} \left(\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{i+1,\sigma} + h.c. \right) + J \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{4} \tilde{n}_i \tilde{n}_{i+1} \right). \quad (7)$$

Here, $\tilde{c}_{i,\sigma}^\dagger$ are fermion operators in the subspace without doubly occupied sites $\tilde{c}_{i,\sigma}^\dagger = (1 - c_{i,-\sigma}^\dagger c_{i,-\sigma}) c_{i,\sigma}^\dagger$, $\tilde{n}_i = \sum_\alpha \tilde{c}_{i,\alpha}^\dagger \tilde{c}_{i,\alpha}$ and $\mathbf{S}_i = (1/2) \sum_{\alpha,\beta} c_{i,\alpha}^\dagger \boldsymbol{\sigma}_{\alpha,\beta} c_{i,\beta}$.

Since analytical approaches can deal only with few special cases ($J/t = 2$ [BARE91], $J/t \rightarrow 0$ [PENC96]) and do not provide definitive insight, numerical methods constitute then a fundamental tool to study the t - J model as shown by exact diagonalization [DAGO94], or recent advances in density matrix renormalization group (DMRG) [BENT04], and quantum Monte Carlo (QMC) simulations [LAVA03]. We apply a newly developed QMC algorithm that is able to deliver accurate results for static and dynamical observables for the t - J model. Although there are a number of algorithms dealing with the t - J model, like the ones deriving from the Green Function Monte Carlo [BEMM94, HAAF95, SORE99], ours is the only one able to calculate dynamical correlation functions.

Our algorithm is inspired by an alternative formulation of the t - J model where the degrees of freedom are expressed in terms of spinless fermions and pseudospins [KHAL90]

$$\tilde{H}_i = +t P_{i,i+1} \left(f_i^\dagger f_{i+1} + h.c. \right) + \frac{J}{2} \Delta_{i,i+1} (P_{i,i+1} - 1), \quad (8)$$

where $P_{i,j} = (1 + \sigma_i \cdot \sigma_j)/2$, $\Delta_{i,j} = (1 - n_i - n_j)$, and $n_i = f_i^\dagger f_i$. This Hamiltonian is bilinear in the fermion fields, i.e. after a canonical transformation a system of interacting spinfull fermions, is described by free spinless fermions interacting with a quantum pseudospin background. The constraint to avoid doubly occupied states transforms into a conserved quantity.

In this formulation it is possible to simulate the t - J model via a QMC evolution treating the fermionic degrees of freedom with the determinantal algorithm [SUGI86],[BLAN81] and the spin degrees of freedom with the loop algorithm [EVER03] (hence, the name *hybrid-loop algorithm*).

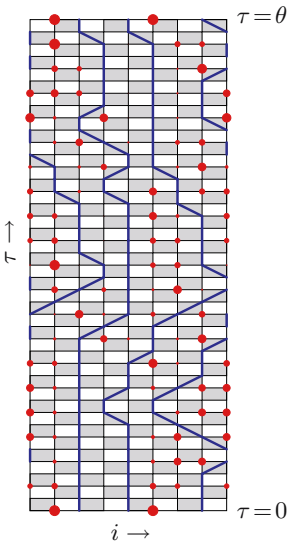


Fig. 7. One realization of the pseudospin background σ , over which the spinless fermions are evolved in imaginary time τ exactly. The system shown has $N = 8$ sites and periodic boundary conditions. Discretizing imaginary time into small slices, here $N_\theta = 20$ slices, and performing a Trotter-Suzuki decomposition leads to a checkerboard pattern of shaded plaquettes, on which two-site interactions may take place. The blue worldlines connect sites with pseudospin state $|\downarrow\rangle$. The radius of the red circles indicates the local spinless fermion density, which is just the hole density unless it is non-zero on a blue worldline, where it would indicate double occupancy. Here, the trial wavefunction $|\Psi_T\rangle$ at $\tau = 0, \theta$ consists of two holes, and, as can be seen, no doubly occupied sites are generated during their evolution.

Within the *hybrid-loop algorithm* one calculates the expectation value of an arbitrary observable $\hat{\mathcal{O}}$ at $T = 0$,

$$\langle \hat{\mathcal{O}} \rangle = \lim_{\Theta \rightarrow \infty} \frac{\sum_{\{\sigma_0\}} \langle \sigma_0 | \otimes \langle \Psi_T | \mathcal{P} e^{-\frac{\Theta}{2} \mathcal{H}} \hat{\mathcal{O}} e^{-\frac{\Theta}{2} \mathcal{H}} \mathcal{P} | \Psi_T \rangle \otimes | \sigma_0 \rangle}{\sum_{\{\sigma_0\}} \langle \sigma_0 | \otimes \langle \Psi_T | \mathcal{P} e^{-\Theta \mathcal{H}} \mathcal{P} | \Psi_T \rangle \otimes | \sigma_0 \rangle}, \quad (9)$$

($\{|\sigma_0\rangle\}$) is a complete set of spin states, $|\Psi_T\rangle$ a trial wavefunction for the spinless fermions (see Fig. 7) and $\mathcal{P}$ is a projector ensuring the constraint against double occupancy), as

$$\langle \hat{\mathcal{O}} \rangle = \lim_{\Theta \rightarrow \infty} \frac{\sum_{\{\sigma_0, \dots, \sigma_L\}} P(\sigma) D_f(\sigma) \langle \mathcal{O} \rangle(\sigma)}{\sum_{\{\sigma_0, \dots, \sigma_L\}} P(\sigma) D_f(\sigma)} \quad (10)$$

where $P(\sigma)$ corresponds to the probability distribution of a Heisenberg anti-ferromagnet for the spin field configuration σ given by the loop algorithm and $D_f(\sigma)$ is the fermions contribution to the weight of the spin field realization σ [LAVA03, LAVA05].

This algorithm has several advantages. For a given pseudospin realization, fermions are evolved exactly in a quantum mechanical way (see Fig. 7). Due to the determinantal part it is possible to measure static and in particular dynamical observables that are not accessible with other techniques. The loop-algorithm with its global update for the pseudospin lead to short autocorrelation-times and avoids metastability problems compared to algorithms based on local updates. As a drawback in principle the fermionic contribution $D_f(\sigma)$ should be calculated from scratch for each pseudospin realization. An important recent improvement was to be able to speed up the algorithm by an order of magnitude by carefully analyzing the structure of the loops in order to avoid unnecessary calculation of the fermionic weight, i.e. updating only the parts that were actually affected by the change of the pseudospin realization. Dynamical data is obtained from the imaginary time Green's function and analytically continued using stochastic analytic continuation [BEAC04].

The one-dimensional t - J model is highly interesting for the understanding of correlated electron systems. In fact due to its rich phase diagram, where it is possible to find a Luttinger liquid phase, a superconducting phase, a spin gap phase and a phase separation regime, it is possible to study in a lower dimension all the phases that are suspected in the 2D high temperature superconductors.

First we concentrate on the Luttinger liquid (LL) phase. One of the most striking properties of the LL is that the low energy elementary excitations do not act like a coherent electron but they split into two independent elementary excitations one of pure spin (*spinon*) and one of pure charge (*holon*), i.e. what is called *spin-charge separation* takes place. To study the elementary excitations of the 1D nearest-neighbor (n.n) t - J model we have studied some dynamical properties like the spectral function (Fig. 8).

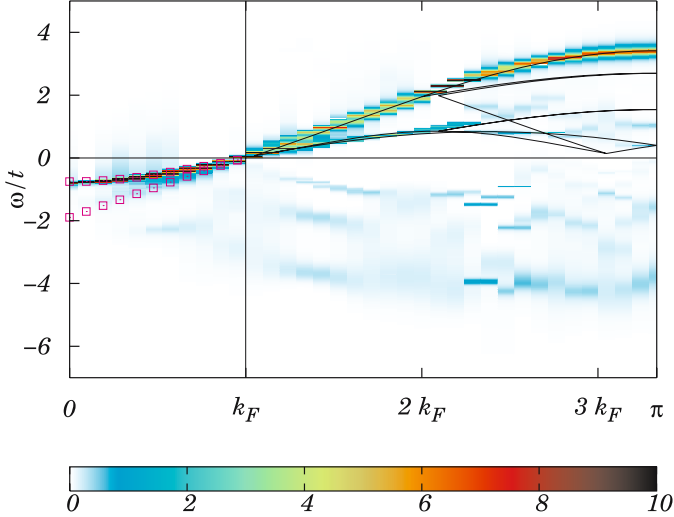


Fig. 8. Spectral function, $A(k, \omega)$, at $J/t = 2$ for $N = 70$ sites and density $n_e = 0.6$ from hybrid-loop algorithm calculation. Solid lines: dispersion curves obtained from Bethe Ansatz equations.

We have already with success realized that it is possible to have a better understanding of the n.n. model via a comparison with another type of t - J model in which both the hopping and the interaction term scale like $1/r^2$ and which, thanks to its high symmetry, is at $J/t = 2$ mostly analytically solvable [LAVA03]. In the $1/r^2$ t - J model it has been proved that only a small number of elementary excitations contribute to the spectral functions and that *spin-charge separation* takes place at all energies and in the form of three free excitations: a spinon with charge $Q = 0$ and spin $S = 1/2$, a holon with charge $Q = -e$ and spin $S = 0$, and an antiholon with charge $Q = 2e$ and spin $S = 0$. Here e is the charge of the electron. Now we use that the n.n. and the $1/r^2$ t - J model are two different singular limits of a more general integrable model [INOZ90]. For this reason we expect that excited states expressed by the same configuration of Bethe-Ansatz quantum numbers are adiabatically connected between the two models and that the elementary excitations of the $1/r^2$ model provide the main contribution to those of the n.n. model. We have performed the Bethe-Ansatz calculation for the n.n. model using these ingredients and in Fig. 8 we show that this procedure makes sense since all major features of the spectral function calculated with the *hybrid-loop algorithm* are well described by the Bethe-Ansatz calculation [LAVA05].

We have a clear sign of *spin-charge separation* in the photoemission sector of the spectral function ($\omega < 0, 0 \leq k \leq k_F$). At $k = 0$ we see a single δ peak as expected [SORE98]. The main spectral weight is on the lines coming from the elementary excitations of the $1/r^2$ model.

Let us consider the phase separated regime. For large values of J/t the homogeneous Luttinger liquid phase becomes unstable and the large effective attraction between the electrons favors the system to separate into electron-rich and a hole-rich droplets [EMER90]. Shortly before phase separation sets in superconducting correlations become dominant [OGAT91], making this region of the phase diagram particularly interesting, especially as real materials most probably lie in the corresponding region of the phase diagram of the 2D t - J model [DAGO94]. Hence for subsequent studies of the behavior close to the boundary an accurate determination of the boundary between the Luttinger liquid and phase separated regimes is important.

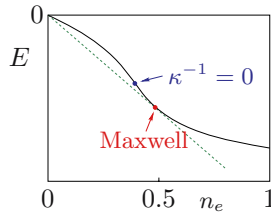


Fig. 9. Schematic behavior of $E(n_e)$ in one dimension.

In the canonical ensemble, for a finite system the instability towards phase separation is signaled by the ground state energy $E(n_e)$ becoming concave, as shown schematically for the 1D case in Fig. 9. With the inverse compressibility given by

$$\kappa^{-1} = \frac{n_e^2}{N} \frac{\partial^2 E}{\partial n_e^2} \quad (11)$$

this corresponds to $\kappa^{-1} = 0$ at the boundary n_e^c . Alternatively one can use a Maxwell construction as also shown in Fig. 9, where the boundary n_e^c is given by the point, where the tangent touches $E(n_e)$. In the thermodynamic limit both the Maxwell construction and the divergence of the compressibility should lead to the same results. On a finite system we may therefore regard them as upper and lower bounds on the $N \rightarrow \infty$ phase separation boundary $n_e^c(J/t)$.

In Fig. 10 our results for a 40-site system are shown along with the boundaries obtained by exact diagonalization of a 16-site system ($\kappa^{-1} = 0$) [OGAT91] and from a DMRG study of a 100-site system using a different method [ROMM00]. The DMRG boundary consistently lies well in between our two boundaries.

In summary, we have studied the nearest-neighbor t - J model at finite doping for different values of the interaction parameter J/t , i.e. in the Luttinger liquid region and in the phase separated regime using the *hybrid-loop* QMC algorithm which we were able to speed up by an order of magnitude. We have calculated the spectral function of the n.n. t - J model in the Luttinger liquid region and we have shown via Bethe-Ansatz calculation that the contribution

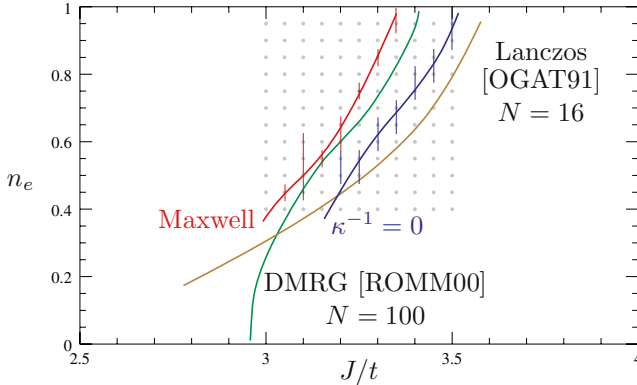


Fig. 10. Boundaries between the Luttinger liquid and phase separated regime obtained by different methods. The grey dots indicate the points, where the energy has been calculated ($N = 40$, $\theta t = 80$, $\Delta\tau = 0.1$).

to the spectrum from the $1/r^2$ model exhausts the major features of the n.n. model spectrum. We have shown a clear sign of *spin-charge separation* over all energy scales. The boundary the phase separated regime has been determined and compared to previous results obtained using different techniques.

5 Conclusions

We have presented studies for three strongly correlated systems that are the subject of current active research. For degenerate quantum gases we developed an exact algorithm for both equilibrium and nonequilibrium properties of hard-core bosons, revealing universalities and the emergence of a quasi-condensate with finite momentum, a state that offers a new realization of an atom laser.

For a quantum antiferromagnet on a quasicrystal, we have shown that the quantum fluctuations exhibit the self-similarity of the underlying lattice structure, leading to a non-trivial magnetic structure. This is a pure quantum effect, not reproduced in the classical limit. Here an efficient algorithm for quantum magnets was used (Stochastic Series Expansion), allowing for the simulation of systems with up to ~ 10000 sites.

For the t - J model that serves as a paradigm for high temperature superconductors, we have shown via a comparison with Bethe-Ansatz the major features of its spectrum. Furthermore we have started a study of charge inhomogeneous phases by determining the boundary to the phase separated regime.

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Large-Scale Simulations for Understanding Surface Optical Spectra

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Summary. Surface optical spectroscopies are non-destructive and capable of operation within a wide range of environments. Their potential for materials characterization can only be exploited fully, however, when the physical mechanisms giving rising to optical features are well understood. Here we use large-scale numerical simulations to investigate two highly relevant and at the same time prototypical cases from *first principles*: (i) the origin of the optical anisotropy oscillations accompanying the thermal oxidation of Si(001) and (ii) the modification of the Si(001) surface optical response upon adsorption of 9,10-phenanthrenequinone. It is demonstrated to what extent strain, molecular transitions and adsorption-modified Si bulk wave functions contribute to the surface optical anisotropy.

1 Introduction

Optical spectroscopies are extremely valuable for the *in situ*, non-destructive and real-time surface monitoring under challenging conditions as may be encountered, e.g., during epitaxial growth. Reflectance anisotropy spectroscopy (RAS) is one of the plethora of surface sensitive spectroscopies probing linear optical coefficients which has been particularly successful in exploring surface structures. However, reliable calculations of the surface optical response are needed to fully exploit its diagnostic potential. The anisotropy of the reflectivity R of light polarized in two perpendicular directions in the surface plane, x and y , is given by [1, 2]

$$\frac{\Delta R}{R}(\omega) \equiv 2 \frac{R_x - R_y}{R_x + R_y}(\omega) = \frac{16\pi\omega}{c} \Im \left\{ \frac{\alpha_{xx}^{hs}(\omega) - \alpha_{yy}^{hs}(\omega)}{\epsilon_b(\omega) - 1} \right\}. \quad (1)$$

Here $\alpha_{ii}^{hs}(\omega)$ with $i = x, y$ is the diagonal tensor component of the averaged half-slab polarisability and $\epsilon_b(\omega)$ denotes the bulk dielectric function.

In this article we compare measured and calculated (according to Eq. 1) RAS spectra in order to better understand the physics and optical fingerprints

of Si oxidation and the influence of thin organic layers on the optical properties of semiconductors.

2 Computational Method

The calculations are based on density functional theory (DFT) [3] which states that the ground-state energy E_0 of a N -electron system in an external potential $v_{ext}(\mathbf{r})$ is an unique functional of the ground-state electron density $n(\mathbf{r})$:

$$E_0[n] = T_s[n] + \int d^3r v_{ext}(\mathbf{r})n(\mathbf{r}) + \frac{1}{2} \iint d^3r d^3r' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + E_{xc}[n]. \quad (2)$$

The functionals $T_s[n]$ and $E_{xc}[n]$ give the single-particle kinetic and the exchange-correlation energy of a N -electron system of density $n(\mathbf{r})$, respectively. The two other contributions to E_0 are the energy of the electrons in the external potential and the Hartree energy.

For a given external potential $v_{ext}(\mathbf{r})$ the functional $E_0[n]$ is minimized at the density $n_0(\mathbf{r})$ of the correct ground state. This variational property leads to an one-particle equation, the Kohn-Sham equation, that maps the many-electron problem onto a system of non-interacting electrons $\{\psi_i\}_i^N$ that has the same ground state density [4]:

$$\left\{ -\frac{\hbar^2}{2m} \nabla^2 + v_{ext}(\mathbf{r}) + v_H(\mathbf{r}) + v_{xc}(\mathbf{r}) \right\} \psi_i(\mathbf{r}) = \varepsilon_i \psi_i(\mathbf{r}), \quad (3)$$

$$n(\mathbf{r}) = \sum_{i=1}^N |\psi_i(\mathbf{r})|^2. \quad (4)$$

The terms $v_H(\mathbf{r})$ and $v_{xc}(\mathbf{r}) = \delta E_{xc} / \delta n(\mathbf{r})$ represent the Hartree and the exchange-correlation potential, respectively. By solving equations (3) and (4) self-consistently, one obtains the exact ground state density $n_0(\mathbf{r})$ and thus all physical properties that are functionals of this density.

For the numerical solution we expand the wave functions and potentials into plane waves $\psi_i(\mathbf{r}) \equiv \psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{G}} c_{n\mathbf{k}}(\mathbf{G}) e^{i(\mathbf{k}+\mathbf{G})\mathbf{r}}$. This leads to very efficient algorithms for periodic systems, because it renders the kinetic energy operator diagonal and symmetries in reciprocal space can be exploited. The convergence is easily controlled by adjusting the energy cutoff of the plane-wave components in the basis.

The representation of the rapid oscillations of the wave functions near the nuclei demands many plane waves. However, it is the interstitial region that determines most of the interesting physical properties. There the wave functions are rather smooth and can be described by comparatively few plane waves. We therefore employ the Projector Augmented Wave (PAW) method [5], which establishes a one-to-one relation between the exact wave functions

and a set of smooth pseudo wave functions, that match the exact ones outside a certain radius around each nucleus. The connection is mediated by a set of one-center projector functions $\{|p_j\rangle\}$. The Kohn-Sham equations for the plane wave coefficients $c_{n\mathbf{k}}(\mathbf{G})$ then read [6]

$$\sum_{\mathbf{G}'} \left\{ \frac{2(\mathbf{k} + \mathbf{G})^2}{2m} \delta_{\mathbf{G}\mathbf{G}'} + V_{eff}(\mathbf{G} - \mathbf{G}') + \sum_{ij} p_{i\mathbf{k}}(\mathbf{G}) D_{ij} p_{j\mathbf{k}}^*(\mathbf{G}') \right\} c_{n\mathbf{k}}(\mathbf{G}') \\ = \sum_{\mathbf{G}'} \varepsilon_{n\mathbf{k}} \langle \mathbf{k}\mathbf{G} | S | \mathbf{k}\mathbf{G}' \rangle c_{n\mathbf{k}}(\mathbf{G}') \quad (5)$$

whith

$$V_{eff}(\mathbf{G} - \mathbf{G}') = \langle \mathbf{k}\mathbf{G} | V_{eff} | \mathbf{k}\mathbf{G}' \rangle, \quad p_{j\mathbf{k}}(\mathbf{G}) = \langle \mathbf{k}\mathbf{G} | p_j \rangle. \quad (6)$$

Here V_{eff} are the Fourier components of the effective local potential (containing v_{ext} , v_H and v_{xc}), $|p_j\rangle$ the projector functions and D_{ij} are the components of the non-local potential localized around the nuclei.

$$S = 1 + \sum_{ij} |p_i\rangle Q_{ij} \langle p_j| \quad (7)$$

is the overlap operator of the projector functions. The Kohn-Sham equations are thus rewritten as a generalized eigenvalue problem. Since the non-local parts of the Hamilton operator and the overlap operator have the same structure, the problem at hand can be solved very efficiently using iterative methods. The diagonalization of equation (5) can be efficiently parallelized, since it is diagonal in the index n of the eigenstate (“inter-band distribution”); furthermore, if there are enough nodes available, the diagonalization for the n -th state may be parallelized as well (“intra-band distribution”). However, each node must provide enough memory to store the total charge density given on a real-space mesh and the calculated wave functions. Since the orthogonalization of the eigenstates requires redistribution of the wave functions between all nodes, communication and latency become issues.

We use the DFT-PAW implementation in the Vienna Ab-initio Simulation Package (VASP) [7], together with the gradient-corrected parametrization of the exchange-correlation energy [8, 9]. The Kohn-Sham matrix is diagonalized using the Residual Minimization Method with Direct Inversion in Iterative Subspace (RMM-DIIS) [10]. This scheme is preferred over the more common Conjugate Gradient (CG) method, since the latter requires explicit orthonormalization of the search vector for each wave function with respect to all other wave functions during each iteration step, an $\mathcal{O}(N^3)$ operation. The RMM-DIIS scheme reduces the number of $\mathcal{O}(N^3)$ operations to a minimum [7]. Parallelization is done using the Message Passing Interface (MPI).

The surface systems are modeled using periodically repeated slabs. Each slab consists of 12 layers of Si covered with oxygen or an organic layer on

both sides, and at least 10 Å of vacuum to avoid direct interaction of adjacent slabs. Within the surface plane we use a $p(4 \times 2)$ surface supercell. Brillouin zone integrations are performed on regular meshes in reciprocal space [11], corresponding to 64 k points in the (1×1) surface Brillouin zone. Wave functions are expanded into plane waves up to a cutoff energy of 400 eV (340 eV) for oxidized (organic adlayer covered) surfaces. Relaxations of ionic positions are carried out using conjugate gradient or quasi-Newton algorithms, until the Hellmann-Feynman forces fall below 5 meV/Å (10 meV/Å). For optical properties we calculate the transition matrix elements from all-electron wave functions at an equivalent of 256 k points in the (1×1) surface Brillouin zone. The half-slab polarizabilities are then calculated in independent-particle approximation, but applying a scissors operator shift of $\Delta E = 0.5$ eV to account for the DFT band gap underestimation.

A large part of our calculations were carried out on a Cray T3E or a Cray Opteron cluster. Figure 1 shows the scaling behavior of our code on both systems. The efficiency is slightly better on the Opteron cluster than on the T3E, but both show significant loss due to overhead when using more than 16 processors. The systems we treat are rather large. The T3E has only 128 MB memory per processor, so we are forced to use more than 32 processors to handle our systems. The Opteron cluster, on the other hand, comes with 2 GB memory per processor, so we can exploit its good scaling behavior by using 4 to 8 processors per job. Typical job run times are 12 to 48 wall clock hours.

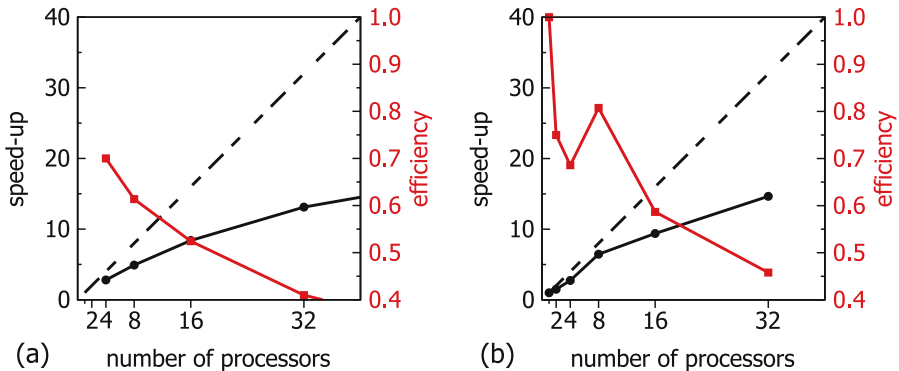


Fig. 1. Speedup and efficiency for (a) Cray T3E, and (b) Cray Opteron cluster.

3 Results

3.1 Optical anisotropy of oxidized Si(001) surfaces

Despite decades of effort, the mechanism of the Si(001) surface oxidation as well as the microscopic structure of the silicon/silicon oxide interface are still under discussion, see, e.g., Ref. [12]. Photons penetrate deeply into the substrate, of the order of 10^3 Å, and could thus be helpful to explore the oxidation process, even far below the surface. RAS spectra measured during thermal oxide growth show oscillations, i.e., repeated changes of the optical anisotropy polarity, for photon energies around the E_1 and E_2 critical points (CPs) of bulk Si as well as above 5 eV [13, 14]. Scanning reflection electron microscopy [15] and total-energy calculations [16] indicate that the thermal oxidation of Si(001) proceeds layer-by-layer. This suggests to relate the optical anisotropy oscillations to the layer oxidation. However, previous numerical simulations based on ordered oxidized Si(001) surfaces [17, 18, 19, 20] failed to explain the measured data and their relation to the interface structure.

Figures 2 (iv) and (iii) show schematically the clean Si(001) surface and an energetically favored geometry used to model the oxidation of the first Si layer [21], respectively. The bottom curve in Fig. 2 shows the reflectance anisotropy calculated for the clean Si(001) $c(4\times 2)$ surface. It is characterized by a strong, dimer-state related minimum at 1.7 eV. An additional minimum/maximum structure slightly below/above the E_1/E_2 CP energy of bulk Si at 3.5/4.3 eV results from surface-modified bulk states. The calculated spectrum agrees with the data measured for highly oriented, single-domain Si(001) surfaces [22, 23].

Upon oxidation, the reflectance anisotropy of the clean surface changes strongly. The 1.7 eV feature is quenched, due to the saturation of the Si-dimer states. In Fig. 2 we show the measured RAS data assigned to the complete oxidation of the first atomic monolayer [13]. It is positive for all photon energies considered, with maxima close to the E_1 and E_2 CPs and at about 5.3 eV. RAS calculations based on translationally invariant models of oxidized Si(001) surfaces only explain part of the measured features. The oxidation model shown in Fig. 2 (iii) gives rise to an optical anisotropy that is positive throughout the energy range probed. However, there are clear deviations between experiment and theory. The discrepancies between experiment and theory are even more pronounced for RAS calculations based on ordered surface structures different from the model shown in Fig. 2 (iii) [18, 19, 20].

The top curve in Fig. 2 shows experimental data assigned to the oxidation of the second monolayer [13]. Nearly an inversion of the signal is observed, compared to the spectrum assigned to the oxidation of the first monolayer (this inversion occurs repeatedly during the progression of the oxidation, see Ref. [14]). Negative anisotropies occur for photon energies close to the Si bulk CPs and above 4.5 eV. We failed completely to reproduce this spectrum using any of the structural models proposed for oxidation of the uppermost two atomic layers of Si(001) [21]. Strong deviations from experiment occur in all cases.

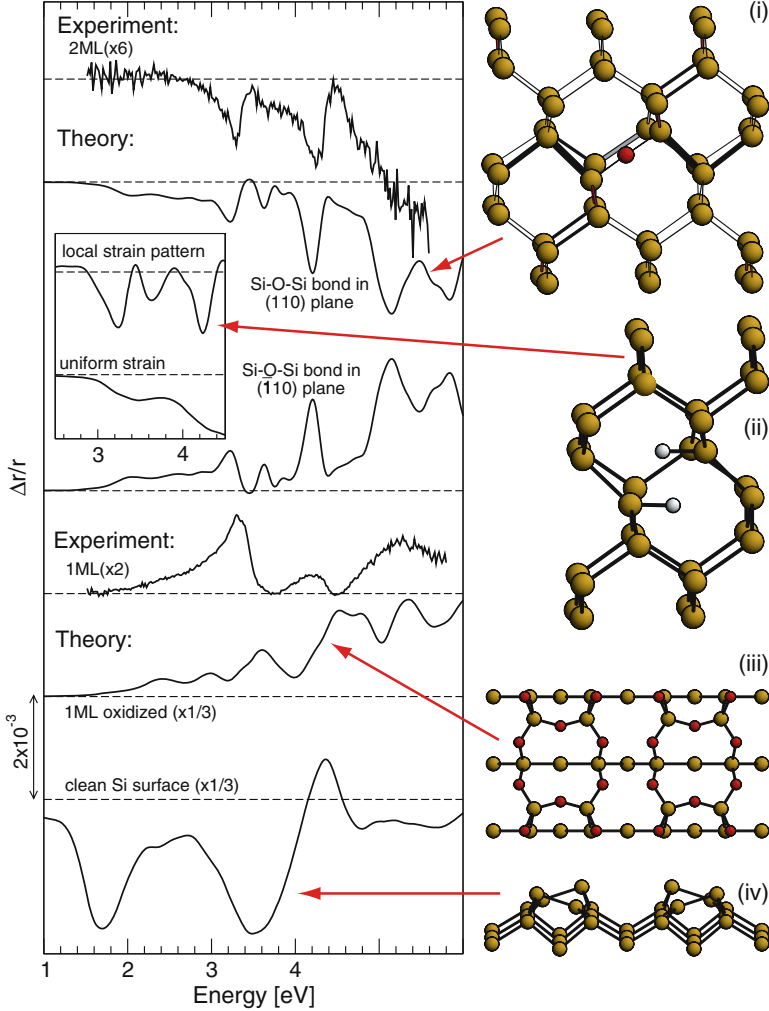


Fig. 2. RAS spectra $[Re\{(r_{[110]} - r_{[110]})/\langle r \rangle\}]$ calculated for the clean and oxidized Si configurations shown in the right panel (see text) are compared with measured data [13]. Dark yellow (red, white) symbols indicate Si (O, H) atoms.

Surface disorder not contained in the translationally invariant oxidation models could possibly explain the failure of the calculations. That oxidation causes considerable surface disorder is in accord with high-energy electron diffraction data [15] and scanning tunneling microscopy images of Si(001) surfaces exposed to oxygen [24]. Bulk Si is optically isotropic. If the disorder of the oxide film above the interface renders this film optically isotropic too, the only source of optical anisotropy are oxygen atoms inserted into Si-Si bulk bonds directly at the interface. Therefore, the optical anisotropy induced

by oxygen inserted into bulk Si bonds is investigated, using an orthorhombic supercell with $2 \times 2 \times 20$ periodicities along the $[\bar{1}10]$, $[110]$, and $[001]$ directions, respectively. The difference of the $[\bar{1}10]$ and $[110]$ bulk polarizability components is normalized such as to compare with the surface reflectance anisotropy. The results for Si-O-Si bonds in $(\bar{1}10)$ and (110) planes (shown in Fig. 2) reproduce the major features measured after oxidation of the first and second monolayer, respectively. Given the simplicity of this idealized model, the agreement between calculation and measurement is impressive. The measured RAS oscillations are thus explained naturally by assuming that (i) the oxidation occurs layer-by-layer and (ii) the silicon oxide directly above the abrupt interface is disordered and therefore optically isotropic.

After having reproduced the experimental data by calculations for oxidized Si bulk, we investigate the origin of the optical anisotropies in more detail. Earlier measurements of the Si-SiO₂ interface optical properties have often been interpreted in terms of strain-induced shifts of the Si bulk CP energies. We perform model calculations for bulk Si uniformly strained by 2% along $[110]$, a value that roughly accounts for the lattice compression around an oxygen atom inserted into a Si(001)(2×2) interface unit cell. As seen in the inset of Fig. 2 (left panel), the optical anisotropy induced by such a macroscopic strain accounts for the sign and roughly for the magnitude of the measured signal, but does not reproduce the line shape. Therefore, either the Si-O bond-related electronic states or the complicated local deformation pattern must cause the peculiar features at E_1 and E_2 . Based on a detailed analysis of the transition matrix elements contributing to the total RAS signal, we can exclude the first possibility: The optical anisotropies are caused by a multitude of perturbed Si bulk states. To corroborate the second hypothesis we perform calculations using the frozen lattice deformation pattern around an inserted oxygen, but replacing the O atom with two H atoms for Si dangling bond termination (see Fig. 2 (ii) and “local strain pattern” curve). Indeed, a line shape is obtained that agrees well with the oxygen inserted case, at least around E_1 and E_2 . This shows that the strain is indeed causing the optical anisotropy. However, it is important to account for the *local* deformation pattern around the defect. A uniform compression is not sufficient to model the measured RAS. Figure 2 (i) illustrates the complexity of the Si bulk deformation around an oxidized Si bond. Here compressive and tensile strain is indicated by dark and light gray bonds, respectively, with the thickness of the bonds indicating the amount of local strain.

3.2 Si(001) surface optical anisotropies induced by PQ molecules

In the last years, an increasing amount of work has been dedicated to the grafting of organic molecules on the Si(001) surface. Such hybrid systems open the way for integrating the electronic, optical or biological properties of organic layers in classical silicon-based devices. The structural investigation of these systems by the usual laboratory surface techniques using electrons is difficult,

because the direct access to the interface is prevented by the presence of the organic adlayer. In contrast, techniques based on photons can be used to study the interface through the adsorbed thin film. Presently, however, the contribution of organic thin films to the semiconductor surface optical response is essentially unknown, hindering the efficient use of optical spectroscopies for organic layer and interface characterization.

Recently, Hacker and Hamers [25] studied the optical anisotropy of 9,10-phenanthrenequinone (“PQ”, $C_{14}O_2H_8$) adsorbed on Si(001) as a prototype for a π -conjugated overlayer system. PQ has two highly reactive carbonyl groups assumed to bond to the surface (“bonding group”), a delocalized π -electron system (“functional group”), and forms a large variety of derivatives. The π -conjugation, likely to remain intact upon adsorption, should allow for direct observation of intramolecular as well as interface- and substrate-related transitions in the experimentally accessible photon energy range. Indeed, a pronounced RAS feature was measured for photon energies of about 5.2 eV and assigned to intramolecular $\pi - \pi^*$ transitions. Here we use the adsorption of PQ to analyze in detail the optical response of an organic monolayer on Si(001).

Experiment [26] and total-energy calculations [27] indicate that the molecules bond via their carbonyl groups to the Si dimer, forming a [4+2] Diels-Alder product. The optimized geometry is shown in Fig. 3 (i). It features PQ molecules that arrange in zig-zag chains on the surface and co-adsorbed hydrogen at the remaining Si dimer atoms. This configuration is used below for optical-response calculations.

The reflectance anisotropy calculated for PQ molecules adsorbed on Si(001) (solid curve in Fig. 3) is in good agreement with the measured data [25]. Compared to the spectrum of the clean surface (see, e.g., Refs. [22, 23]), new optical anisotropies show up. Among these, the B_1 feature at about 5.2 eV is the most pronounced one.

In order to determine the origin of these interface optical anisotropies, the valence orbitals of the supercell are classified with respect to their localization either below or above the Si surface. This decomposition allows for the separation of the substrate and organic layer contributions to the total optical signal. The respective RAS spectra are shown by the dashed lines in Fig. 3. Obviously, bulk contributions dominate the optical signal. The RAS features at the E_1 and E_2 Si bulk critical points as well as the B_1 and B_2 features arise from transitions involving Si bulk states. This is in clear contrast to the interpretation of the B_1 feature as due to molecular $\pi - \pi^*$ transitions [25]. Therefore, we perform additional calculations: The adsorbed PQ molecules are replaced by two OH groups each (cf. Fig. 3 (ii)). By keeping the slab geometry (including the O atoms) fixed, the RAS contribution of the strained and rebonded substrate can be calculated. The obtained spectrum (bottom curve in Fig. 3) reproduces all main features of the Si substrate signal, i.e., the E_1/E_2 features as well as B_1 and B_2 . Evidently, B_1 and B_2 do not arise from molecular transitions but are clearly due to adsorption-induced distortions of

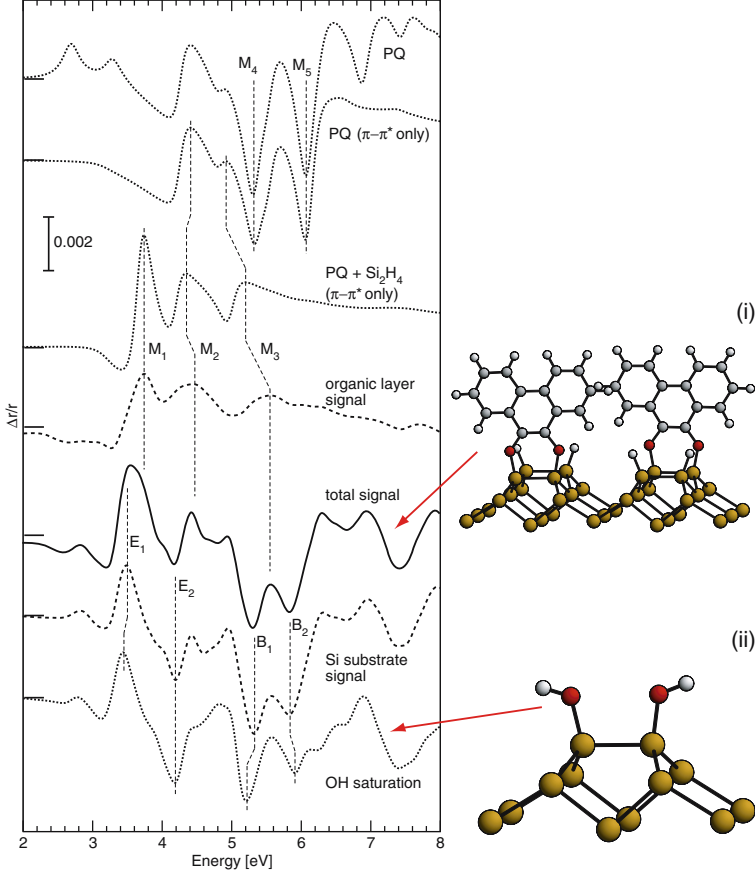


Fig. 3. Total calculated RAS spectrum $[Re\{(r_{[\bar{1}10]} - r_{[110]})/\langle r \rangle\}]$ and its decomposition into overlayer and bulk contributions (see text). The side panel shows (i) the structural model for PQ adsorption on Si(001) and (ii) a model where PQ molecules have been substituted by OH groups (see text). Large (dark, grey, light) circles denote Si (O, C, H) atoms, respectively.

the substrate. We find that both the adsorption-induced strain in the silicon lattice and the formation of Si-O bonds contribute to these anisotropies.

Although less pronounced than expected, there are also RAS contributions to the total signal that originate in the organic layer as shown in Fig. 3: The total signal is modified by molecular transitions denoted M_1 , M_2 , and M_3 . What is the origin of these features? To answer this question we simulate the RAS response of an organic overlayer on top of optically isotropic Si by using the three-layer model shown in the inset of Fig. 4. This model allows for simulating the optical response as a function of the organic layer constituents.

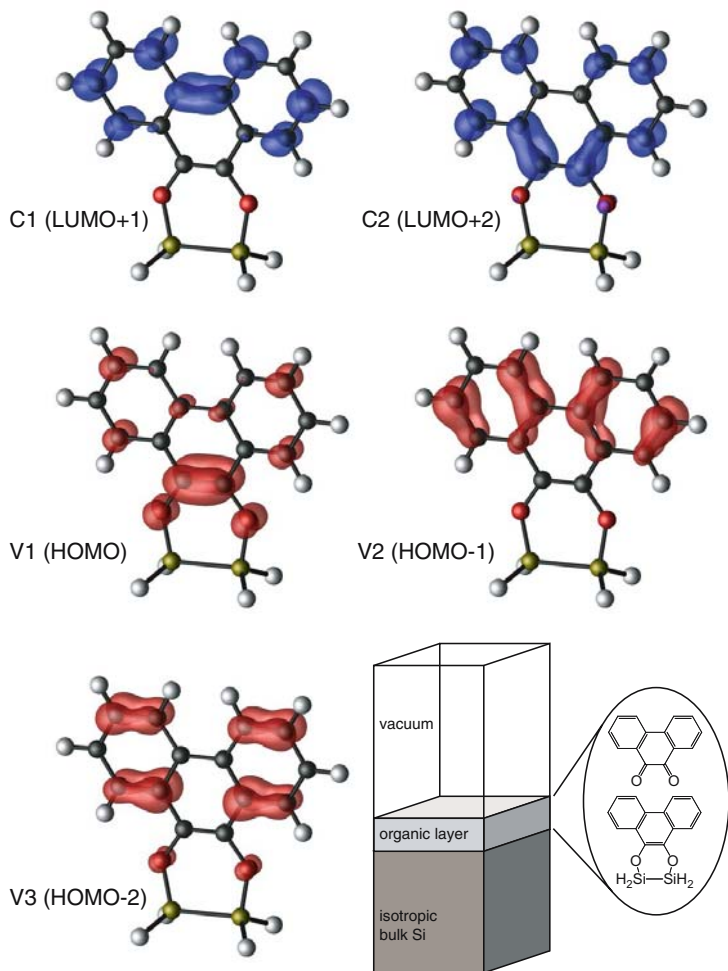


Fig. 4. Relevant molecular orbitals of the PQ+Si₂H₄ molecule (see text). The three-layer model for simulating "simplified" RAS spectra is shown as inset.

The topmost RAS curve in Fig. 3 is obtained by assuming the organic layer to consist of PQ molecules that have an optical absorption equal to their gas-phase spectrum. Interestingly, the calculated RAS spectrum shows pronounced π - π^* transition-related M_4 and M_5 features that nearly coincide in energy with the B_1 and B_2 peaks measured by Hacker and Hamers [25]. However, the RAS obtained from the fictitious layer of gas-phase PQ molecules clearly fails to reproduce the calculated organic layer contribution to the total signal (upper dashed curve in Fig. 3). This is expected: The carbonyl group-related transitions will vanish or at least be shifted to much higher energies upon molecular adsorption.

Therefore, in a second step, we calculate the RAS as above, but restrict the optical response to π - π^* transitions of the gas-phase molecule. The result, however, agrees only slightly better with the organic layer contribution to the total RAS.

To model the bonding with the Si substrate, we therefore construct in a third step an artificial PQ+Si₂H₄ molecule (see Fig. 4), using the atomic coordinates from the calculated adsorption geometry. The Si-O bonding leads to a charge redistribution in the molecule and to the formation of a new C=C double bond (V1 in Fig. 4) between the carbonyl group C atoms, which corresponds now to the highest occupied molecular orbital. By restricting the calculation to transitions between the three highest occupied π orbitals and the two lowest unoccupied π^* orbitals one obtains the third curve of Fig. 3. Obviously, the line shape and peak positions of the organic layer signal are well described by such a model for the constituents of the organic film.

Thus, the essential parts of the molecular contributions to the RAS can be traced back to a few π - π^* transitions within the PQ molecule. However, the bonding to the substrate must be taken into account: The feature M_1 arises solely from transitions involving the C=C double bond which forms as a result of the [4+2] Diels-Alder reaction with the Si=Si dimer. At the same time, the formerly pronounced M_4 and M_5 features are strongly reduced in amplitude and shifted in energy, due to the substrate-bonding related changes of the respective molecular orbitals. Fig. 4 shows the molecular states responsible for the RAS features related to the organic overlayer: M_1 , M_2 , and M_3 stem from $V_1 - C_2$, $V_2 - C_1$, and $V_3 - C_1$ transitions, respectively.

4 Conclusions

In conclusion, we calculated the optical response of clean, oxidized as well as organically modified Si(001) surfaces from *first principles*.

Comparison of the simulated optical spectra with oxidation experiments indicates that (i) the measured oscillations of the optical anisotropy are caused by the progression of the local strain pattern during the oxidation, (ii) the oxide layer directly above the interface is disordered and (iii) the oxidation proceeds layer-by-layer and there exists an one-to-one correspondence between the layer oxidation and the inversion of the interface optical anisotropy. The results thus suggest optical spectroscopy for monitoring and controlling the oxidation process with atomic resolution.

Strong modifications of the intramolecular transitions upon adsorption on Si(001) are found even for a molecule like 9,10-phenanthrenequinone, where bonding and functional groups are seemingly decoupled. This shows that a naive interpretation of the surface optical response in terms of molecular transitions fails. On the other hand, the optical anisotropy of the substrate is significantly altered. The total spectrum is dominated by contributions from

adsorption-modified Si bulk states. This indicates that optical spectroscopies may indeed be used to characterize organic-inorganic interfaces.

Our results show the wealth of information contained in the surface optical properties and the potential of state-of-the-art numerical simulations to unearth this information.

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Numerical Investigations of Nano-Systems in Reduced Geometry

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Summary. The structural and electronic properties of atomic wires and clusters have been analysed. Structural, energy-, flow-, and elastic- properties of model colloids have been studied with particular emphasis on the effect of external fields and of long ranged dipolar interactions. In the following sections an overview is given on the results of our recent computations on quantum effects, structures and phase transitions in such systems.

1 Introduction and general remarks

Nanostructures in reduced geometry and external fields have become interesting research fields in the last years. Despite the fact that by experimental techniques many structural-, elastic-, electronic-, and phase- properties of systems in the size of a few nanometers have been obtained, the theoretical investigations and analyses are still in an initial stage. This is partly due to the fact that systems which are far away from the thermodynamic limit (with infinitely many particles) due to their finite size are difficult to handle by analytical methods which are suitable for systems with either few particles (2-5) or in the limit of infinitely many particles. In this field computer simulations have become more and more important since nano-systems in reduced geometry contain about 10-10.000 particles, which is nearly ideal for the application of computer simulation methods. Many important results have been obtained by the support of HPC centres (HLRS, SSC, NIC) [1, 2, 3, 4].

In this paper we report on several new insights into electron transport in nano-wires, structural and electronic properties of Si clusters, ground state properties of two dimensional dipolar model colloids, and flow properties and phase transitions of model colloids in external potentials.

2 Electronic and structural properties of nano wires and clusters

Many experiments have shown that the conductance histograms of metallic atomic-sized contacts exhibit a peak structure, which is characteristic of the corresponding material. The origin of these peaks still remains as an open problem. In order to shed some light on this issue, we have computed conductance histograms of Au atomic contacts. In the HLRS/SSC project we have combined classical molecular dynamics simulations of the breaking of nanocontacts with conductance calculations based on a tight-binding model. This combination gives us access to crucial information such as contact geometries, forces, minimum cross-section, total conductance and transmission coefficients of the individual conduction channels. The ensemble of our results suggests that the low temperature Au conductance histograms are a consequence of a subtle interplay between mechanical and electrical properties of these nanocontacts. At variance with other suggestions in the literature, our results indicate that the Au conductance histograms are not a simple consequence of conductance quantization or of the existence of exceptionally stable radii. Moreover, we find that the main peak in the histogram close to one quantum of conductance is due to the formation of single-atom contacts and chains of gold atoms.

Atomic gold wires were studied recently by experimental methods [5, 6, 7], where wires have been stretched down to single atom contacts. In this context nano contacts under stress have been simulated [8, 9] using three different interactions: the “surface embedded atom”- interaction with a (up to 70 %) reduced electron density turned out to be not sufficiently stable, with Lennard-Jones interactions shifts of planes and single-atom contacts have been observed, however no atom chains. In case of the stretching of a nano contact with interactions according to the “effective medium theory” (EMT) single atom contacts as well as atom chains have been found. In order to prevent the heating of the wire due to the stretching work, a Nosé-Hoover thermostat has been implemented in the molecular dynamics simulation.

In cooperation with F. PAULY, J. HEURICH and C. CUEVAS, who developed [10]- by using a tight-binding-model and Greens function techniques- a program for the current through a nano contact (in different channels), conductivity curves have been determined. The qualitative agreement with the experiment is good, the conductivity fluctuations seem to be slightly higher compared to the experiment. The current through the contact depends on the atom type and the atomic configurations at the thinnest part of the chain. However it turns out that the atomic configuration in the surrounding of this position plays an important role as well.

This combination of numerical methods goes beyond previous computations of either structural or electronic properties of atomic-sized contacts since it permits the microscopic evolution of the conductance channels within

tight-binding approximation during the dynamical structural evolution of the stretched wire.

A typical computation of the structural and conductance evolution requires a computation with $1.1 \cdot 10^6$ MD steps where after the equilibration of the system every $4 \cdot 10^3$ MD steps a full conductance compilation is required. The resulting numerical effort is about 400 CPU-hours (single processor) for a single stretching process. The total CPU-time of our studies was about $20 \cdot 10^3$ CPU-hours.

In the experimental studies of a single stretching process a first plateau is found at a conductivity value slightly smaller than G_0 . Histograms show the result of averaging over many stretching processes at different temperatures. In order to compute such histograms and to be able to analyze the experimentally observed effects, in the HLRS project histograms have been computed by about 100 molecular dynamics simulations of single stretching processes.

In order to discuss in more detail the mechanical properties and stability of the contacts we have calculated histograms of the radius of the minimum cross-section for the three main crystallographic directions of the fcc-lattice. The results are summarized in Fig. 1. In this figure we have normalized the radius to the radius of an ideal linear chain $R_0 = 1.268 \text{ \AA}$ with nearest neighbor distance (lattice constant/ $\sqrt{2}$). The most prominent feature of the histograms is the presence of peaks, especially for the [100] direction. These peaks suggest the existence of exceptionally stable radii. This is relatively surprising at low temperatures (4.2K), where the gold atoms do not have enough kinetic energy to explore many configurations in order to minimize the surface energy.

It is important to remark that these peaks generally do not appear at the values $\sqrt{n} \cdot R_0$ ($n = 1, 2, 3, \dots$), and therefore we cannot infer that the cross-sections associated with these peaks correspond to multiple of the cross-section of a single-atom contact. Furthermore in the three cases the peak close to 1 is extremely pronounced. This is due to the fact that usually in the last stages a single-atom or a chain of atoms is formed. The next obvious question is whether this peak structure is an evidence of shell effects as observed for alkali metals [11] and suggested more recently for gold contacts [12, 13]. For shell effects the peaks are expected to be equidistant when plotted as a function of the radius R of the wire [11]. To test this idea in the inset of Fig. 1, we plot $k_F R$ as a function of the peak number for the histogram of the [100] direction. Here, k_F is the Fermi momentum, which is assumed to take the free-electron value of $1.21 \times 10^8 \text{ cm}^{-1}$. As one can see, the peak positions indeed follow a straight line with slope 0.60 ± 0.02 . This value of the slope lies in between the values observed in Ref. [13] for electronic shells (1.02) and for atomic shells (0.40). From our analysis we cannot draw any conclusion on the appearance of shell effects in our simulations for several reasons. First, the choice of the peak positions is not absolutely unambiguous, and second, a similar analysis for the histograms in the directions [110] and [111] does not show such a clear linear relation between the radius and the peak position. It is worth stressing that even though the peak structure of these histograms cannot be

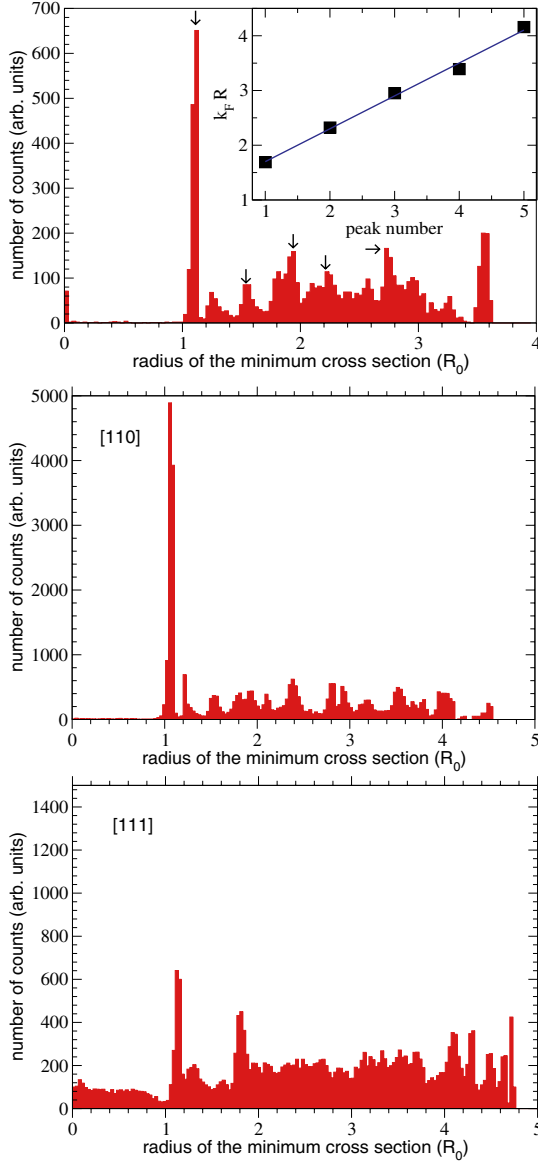


Fig. 1. Histograms of the radius of the minimum cross-section R , which is normalized in units of the radius of an ideal linear chain of gold atoms $R_0 = 1.268 \text{ \AA}$. The temperature is 4.2K. The different panels correspond to different crystallographic orientations. The number of simulations used to construct the histograms is 50 for each directions. The inset in the upper panel shows the peak positions in the [100] histogram, converted to $k_F R$, as a function of the peak index. The arrows in the upper panel indicate the peak positions used to construct this plot. The last peak of the [100] histogram is artificially generated by the starting configurations.

easily interpreted in terms of shell effects, it clearly shows that particularly stable configurations do exist, which most likely correspond to meta-stable geometries which are formed at low temperatures.

Next we want to address the origin of the peaks in the conductance histograms. Are these peaks simply due to the peaks in the minimum cross-section histograms as suggested in Ref. [14]? In order to answer this question, we have collected the conductance calculations for all our MD simulations in the [100] direction at 4.2K. The conductance histogram [9] has a pronounced peak close to $1 G_0$ and further maxima. The peak close to $1 G_0$ is highly correlated with the first peak in the corresponding minimum cross-section histogram, and it is therefore a consequence of formation of single-atom contacts (indeed, contacts with dimers) or chains of atoms. However, the other peaks are not reflected in the conductance histogram. As we found, the minimum cross-section is not the only ingredient that controls the conductance, and the geometry of the narrowest part and the disorder in the contact play also an important role. This means in practice that contacts with different radii can have similar values of the conductance. In particular, this is true for small contacts like the one we have analyzed in this work. Of course, the situation could be different for larger contacts, where semi-classical arguments are believed to provide a good description.

Based on these results a comparative study for different materials is planned. In parallel an improved treatment of the electronic components of the system at the single atom contact is planned by use of the Car-Parrinello-method and the results obtained at the SSC [15, 16, 17] with a program which is optimized for the IBM machine.

In addition Car-Parrinello- studies are performed for clusters at surfaces [18, 17], where in particular the cluster stability and their usefulness as building blocks as cluster material shall be analyzed.

Experimental results show that Si_4 and Si_7 clusters are possible candidates for a cluster material. For the simulations the implementation of DFT available at [19] was used. Calculations were performed using norm conserving pseudo potentials of the Trouiller-Martins type and PBE [20] Exchange Correlation functionals. As the interaction of the clusters with the (HOPG) surface is very weak, the surface was initiated by not allowing certain atoms to move out of the xy-plane. Following our studies of Si_4 clusters [15, 17], we focussed on the structural and electronic properties of Si_7 clusters.

In Fig. 2 (upper left) the energy of two Si_7 clusters approaching “head-to-head” is shown. In this and the next two figures the atoms of the pentagons are restricted to movements in the xy-plane. The red curve shows the results when the simulations are started from the “normal” ground state geometry. If the clusters are close to each other their geometry changes to a more “compact” structure. The green curve shows the results if the clusters are started from this structure. The peaks around $2.5 \text{ \AA}$ may be explained by the fact that the geometry optimizations are zero Kelvin simulations. In the “foot-to-head” configuration analyzed in Fig. 2 the two innermost atoms of the right cluster

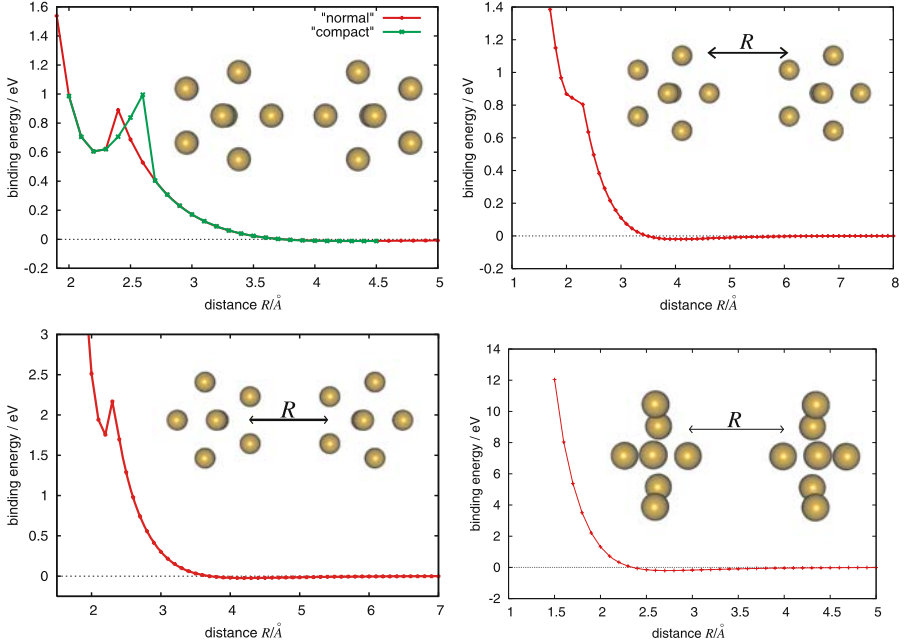


Fig. 2. Binding energy of two Si_7 clusters versus distance. Upper left: “head-head” geometry, upper right: “foot-head” geometry, lower left: “foot-foot” geometry, lower right: “top-top” geometry.

were allowed to move in the y-direction only, the nearest atom of the left cluster was fixed. The curve is not much different from the first and the step at 2 Å can be explained as before. There is a minimum close to 4 Å, but the structure does not change in this region. In Fig. 2 (lower left) the four innermost atoms of the whole configuration were allowed to move in y-direction only. The “foot-to-foot” configuration is the energetically worst of the structures investigated. In Fig. 2 (lower right) the clusters approach in a “top-top” configuration. The two nearest atoms of the clusters are fixed. This reaction channel probably does not show an in-plane configuration, but rather a cluster in the beam approaching another cluster already deposited on the substrate. This configuration seems to represent the experimental situation best.

Further studies will include a microscopic treatment of the graphite surface, consider additional reaction channels and the deposition process, investigate the role of oxygen in the experiments and other possible cluster material building blocks, for example C_{10} rings.

3 Confined dipolar fluids

In recent years, the physics of complex fluids such as colloidal dispersions, liquid crystals, polymers, biopolymers, and emulsions has attracted growing interest [21], stimulated in part by the important role of these materials in a variety of technological applications. Of particular interest is the class of complex fluids which consists of particles with electric or magnetic dipole moments [22]-[28]. The resulting dipole-dipole interactions are direction dependent and of long range. Recent theoretical and experimental research has demonstrated that fluids with dominant dipole-dipole interactions can display new, unexpected behavior such as self-assembly of the particles into dipolar chains [29], and crystallization into novel structures [30].

In order to investigate the properties of such systems in greater detail, in a first step we analyze the ground states of two-dimensional dipolar lattices. We consider systems composed of N particles which are spherically symmetric and carry a (three-dimensional) point dipole moment $\boldsymbol{\mu}_i$, $i = 1, \dots, N$ at their centers. The (potential part of the) Hamiltonian of the system is given as $H = H_{\text{sr}} + H_{\text{dip}}$, where H_{sr} contains contributions from some short-range potential depending only on the distance between particles, $r_{ij} = |\mathbf{r}_{ij}| = |\mathbf{r}_i - \mathbf{r}_j|$, and

$$H_{\text{dip}} = \frac{1}{2} \sum_{i=1}^N \sum_{j \neq i} \frac{\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j}{r_{ij}^3} - 3 \frac{(\boldsymbol{\mu}_i \cdot \mathbf{r}_{ij})(\boldsymbol{\mu}_j \cdot \mathbf{r}_{ij})}{r_{ij}^5}. \quad (1)$$

In this work we consider situations where the particles are fixed to the sites of a two-dimensional lattice located in the x - y -plane of the coordinate system. Thus, the particle positions are given as $\mathbf{r}_i = n_1(i) \mathbf{t}_1 + n_2(i) \mathbf{t}_2$, where n_1 and n_2 are integers and $\mathbf{t}_1$ and $\mathbf{t}_2$ are primitive vectors of the lattice. We consider both square and hexagonal lattices. For the first, $\mathbf{t}_1 = a\hat{\mathbf{x}}$, $\mathbf{t}_2 = a\hat{\mathbf{y}}$ (with a being the lattice constant), and n_1 and n_2 are arbitrary. The hexagonal lattice, on the other hand, can be described by the primitive vectors $\mathbf{t}_1 = a/2\hat{\mathbf{x}}$, $\mathbf{t}_2 = (a\sqrt{3}/2)\hat{\mathbf{y}}$, and the sum $n_1 + n_2$ has to be even.

In the following we are interested in the energies related to various configurations with *fixed* dipole moments. Specifically, we consider the following cases: 1) square lattice with in-plane ferromagnetic order ($\boldsymbol{\mu}_i = \mu\hat{\mathbf{y}}$); 2) square lattice with in-plane antiferromagnetic order; 3) square lattice with out-of-plane ferromagnetic order; ($\boldsymbol{\mu}_i = \mu\hat{\mathbf{z}}$); 4) square lattice with out-of-plane antiferromagnetic order; 5) hexagonal lattice with in-plane ferromagnetic order ($\boldsymbol{\mu}_i = \mu\hat{\mathbf{x}}$)

It is now well-established that the best way to calculate the energy of a system with long-range dipolar interactions is to replicate the “basis cell” containing the original N -particle system periodically in space and calculate the energy as the sum of interactions within the basis cell plus the interactions of the N dipoles with the periodically repeated images in the surrounding cell. In two spatial dimensions this sum is absolutely, but slowly convergent. It is therefore appropriate to employ Ewald summation techniques, by which the slowly convergent sum is transformed into two rapidly convergent sums, one in

real space, the other in reciprocal space, the rate of convergence is regulated by the parameter α . The resulting expression for a system with three-dimensional dipoles in two spatial dimensions is given by [23]

$$\begin{aligned}
 U_{\text{dip}} = & \frac{1}{2} \sum_{i \neq j}^N [(\boldsymbol{\mu}_i \cdot \boldsymbol{\mu}_j) B(r_{ij}, \alpha) - (\boldsymbol{\mu}_i \cdot \mathbf{r}_{ij}) (\boldsymbol{\mu}_j \cdot \mathbf{r}_{ij}) C(r_{ij}, \alpha)] \\
 & + \frac{\pi}{A} \sum_{\mathbf{k} \neq \mathbf{0}} \frac{\text{erfc}(k/2\alpha)}{k} \widetilde{M}_{\parallel}(\mathbf{k}) \widetilde{M}_{\parallel}^*(\mathbf{k}) \\
 & + \frac{\pi}{A} \sum_{\mathbf{k} \neq \mathbf{0}} \left(\frac{2\alpha}{\pi} \exp\left(-\frac{k^2}{4\alpha^2}\right) - k \text{erfc}\left(\frac{k}{2\alpha}\right) \right) \widetilde{M}_{\perp}(\mathbf{k}) \widetilde{M}_{\perp}^*(\mathbf{k}) \\
 & + \frac{2\sqrt{\pi}\alpha}{A} \left(\sum_{i=1}^N \mu_{i,z} \right)^2 - \frac{2\alpha^3}{3\sqrt{\pi}} N \mu^2
 \end{aligned} \tag{2}$$

In Eq. (2), the real space contribution has been formulated under the assumption that the convergence parameter α is large enough to consider only interactions within the central cell. This is satisfied with the present choice $\alpha/L = 7.0$. Furthermore, the functions B and C are defined by

$$\begin{aligned}
 B(r, \alpha) &\equiv \left[\frac{2\alpha r}{\sqrt{\pi}} \exp(-\alpha^2 r^2) + \text{erfc}(\alpha r) \right] / r^3, \\
 C(r, \alpha) &\equiv \left[\frac{2\alpha r}{\sqrt{\pi}} (3 + 2\alpha^2 r^2) \exp(-\alpha^2 r^2) + 3\text{erfc}(\alpha r) \right] / r^5,
 \end{aligned} \tag{3}$$

where erfc is the complementary error function. We evaluate the real-space part by employing periodic boundary conditions in the x - and y - directions and the minimum-image convention.

As to the Fourier-space part in Eq. (2), $A = L_x L_y$ is the area of the basic cell and $\widetilde{M}_{\parallel}^*$ and $\widetilde{M}_{\perp}^*$ are the complex conjugates of the quantities

$$\widetilde{M}_{\parallel}(\mathbf{k}) = \sum_{i=1}^N \boldsymbol{\mu}_{i,\parallel} \cdot \mathbf{k} \exp(i\mathbf{k} \cdot \mathbf{r}_i), \quad \widetilde{M}_{\perp}(\mathbf{k}) = \sum_{i=1}^N \mu_{i,z} \exp(i\mathbf{k} \cdot \mathbf{r}_i), \tag{4}$$

where $\boldsymbol{\mu}_{i,\parallel}$ is the in-plane part of the dipole vector of particle i , and $\mu_{i,z}$ is its out-of-plane component. Finally, the wave vectors $\mathbf{k}$ of the (rectangular) super-lattice are of the form $\mathbf{k} = (2\pi n_x/L_x, 2\pi n_y/L_y)$ where n_x and n_y are integers. Throughout the present study the reciprocal sums in Eq. (2) include $\mathbf{k}$ -vectors with length up to $n_x^2 + n_y^2 = 80$.

In Fig. 3 we show the ground state energy versus density and lattice constant. At a given density, the square lattice with antiferromagnetic order has the lowest energy. The ground state energies of the systems with only nearest neighbor interactions can be computed exactly and are shown in Fig. 3. The important effect of the long range nature of the dipolar interaction on the ground state energies versus lattice constant is shown in Fig. 3.

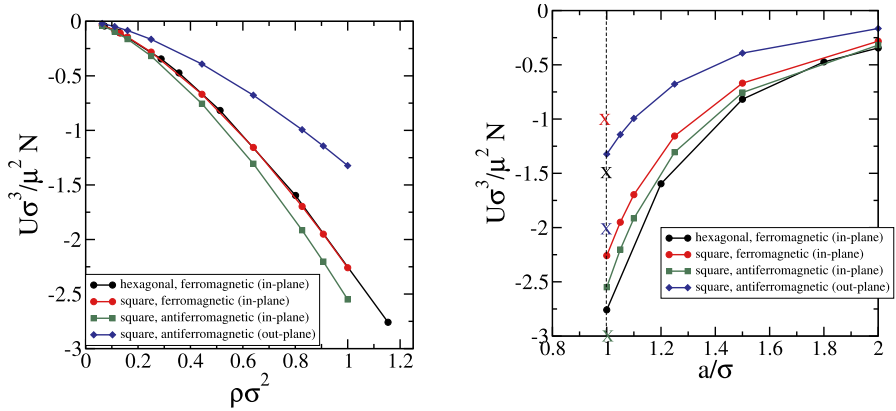


Fig. 3. Left: Ground state energies as function of density; right: ground state energies versus lattice constant, crosses indicate the values for the nearest-neighbor model.

4 Phase transitions and elastic properties of 2D model colloids

During the last decades, crystallization and melting of colloidal suspensions, both in two and three dimensions (2D and 3D), has been a continuous matter of interest. From the experimental point of view the research mostly focused on the analysis of structure and dynamics of the colloidal systems on different length and time scales through static or dynamic light scattering techniques. On the other hand, in theory the nature of the melting transition in 2D has been controversially discussed at least since the work of Kosterlitz and Thouless (KTHNY-theory). Obviously elastic constants play a crucial role in the solid to liquid phase transition: In 2D the KTHNY theory even claims that the melting process is entirely controlled by the elastic constants. However, both experimental and simulation studies of elastic constants are quite rare. Therefore, the development of tools for the determination of elastic constants in (colloidal) model systems is important.

The simulation approach makes use of a new coarse-graining procedure which has been successfully tested for a hard disk system. In this technique, elastic strains are calculated from the instantaneous configurations of the particles and averaged over subblocks of various linear dimensions $L_b \leq L$ of a system of total linear dimension L . From these data the correlation function of strain fluctuations in the thermodynamic limit can be extracted and the elastic constants then inferred from well known fluctuation formula.

This method has been applied to models of colloidal systems containing quenched point impurities and to colloidal mixtures [4, 31, 32, 33, 34, 35, 36, 37]. A substantial hardening of the material with impurities has been de-

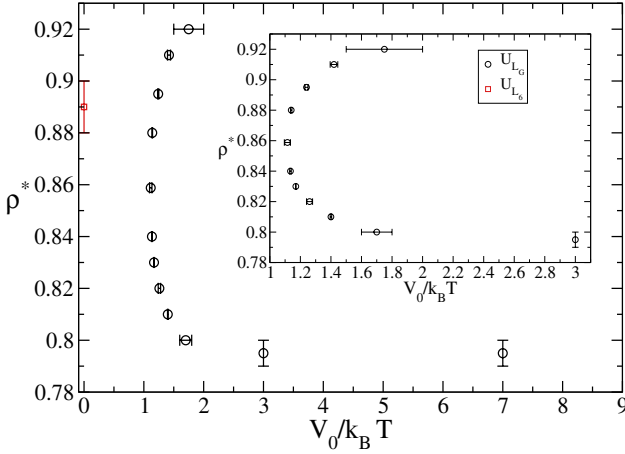


Fig. 4. Phase diagram of a hard disk system with $N=1024$ particles under the influence of an incommensurate potential with $\lambda/\sigma = 0.65579$.

tected, and interesting high pressure structures were found for binary colloidal mixtures of particles with different diameters in two and three dimensions. The liquid-solid transition in two dimensional systems of particles under the influence of external modulating potentials has recently attracted a fair amount of attention from experiments [38, 39, 40, 41, 42, 43, 44], density functional theory [45, 46], dislocation unbinding calculations [47, 48] and computer simulations [49, 50, 51, 52]. This is partly due to the fact that well controlled, clean experiments can be performed using colloidal particles confined between glass plates, producing essentially a two-dimensional system. These systems are subjected to a spatially periodic electromagnetic field generated by interfering two crossed laser beams. This field acts on the particles like a commensurate, one dimensional, modulating potential. One of the more surprising results of these studies is the fact that there exist regions in the phase diagram over which one observes reentrant [41, 42, 43] freezing/melting behavior. As a function of the laser field intensity the system first freezes from a modulated liquid to a two dimensional triangular solid. A further increase of the intensity confines the particles strongly within the troughs of the external potential, suppressing fluctuations perpendicular to the troughs, which leads to an uncoupling of neighboring troughs and to re-melting.

The interesting effect of “laser induced freezing” and “laser induced melting” has been studied by Monte Carlo simulations in two dimensions using commensurate [31, 36, 54, 55, 57, 58] and incommensurate [34] potentials. In the latter case incommensurate potentials have been applied to hard disk systems. As in the commensurate case the particles gather within the potential minima. Depending on the wavelength and potential strength different phases occur. In Fig. 4 the phase diagram for a system of hard disks of diameter σ in an

incummensurate potential, $V_{ext}(x, y) = V_0 \sin(2\pi x/\lambda)$ with $\lambda = 0.65579\sigma$, is shown. The phase diagram shows a laser induced freezing transition, but no reentrant melting, in contrast to the commensurate case.

Besides these classical simulation studies we explored the validity of our results on atomic length scales. In this context we were able to investigate the properties of quantum hard disks with a finite particle mass m and interaction diameter σ in an external periodic potential by path integral Monte Carlo [59]. Due to the quantum delocalization effect a larger effective particle diameter results, and in the external potential this delocalization is asymmetrical: in the direction perpendicular to the potential valleys we obtain a stronger particle localization than parallel to the valleys. As a result the reentrance region in the phase diagram is significantly modified in comparison to the classical case. Due to the larger quantum “diameter” the transition densities at small potential amplitudes are reduced in comparison to the classical values. At large amplitudes the classical and quantum transition densities merge. This effect is due to the approach of the effective quantum disk size to the classical value in the direction perpendicular to the potential valleys and leads to the surprising prediction, that the quantum crystal in a certain density region has a direct transition to the phase of the modulated liquid by an increase of the potential amplitude. This scenario is not known in the classical case.

5 Dynamics in micro channels

The dynamics of particles in micro-channels has been studied [33] by molecular dynamics simulations using particles with dipolar interaction,

$$V_{pp} = \frac{\mu_0 M^2}{4\pi r^3} \quad (5)$$

with the magnetization M , and thermalizing the system by a Nose-Hoover thermostat.

The particles are driven by the gravitational force due to the inclination of the micro channel, see Fig. 5. The channel walls are modeled as ideal hard walls, and open boundary conditions are applied in the flow direction, i.e. particles which drop out of the channel at the lower end will be inserted at

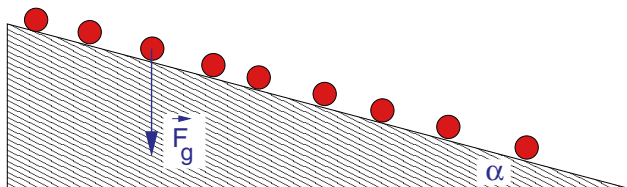


Fig. 5. Schematic picture of the micro channel geometry.

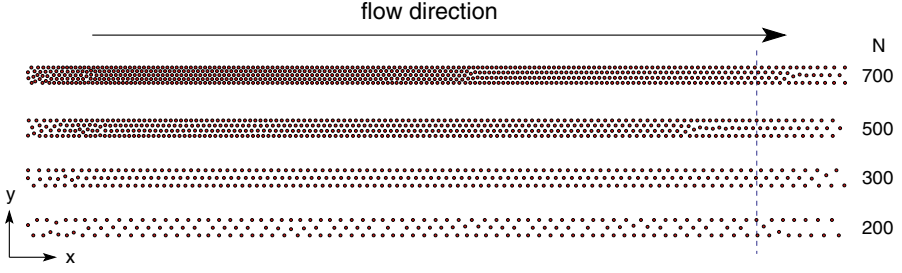


Fig. 6. Local density distribution of point particles with dipolar interaction ($M = 0.4912 \cdot 10^{-15} \text{ Am}^2$, $T = 1198 \text{ K}$) in the micro channel of length 1.25 mm and width $28 \mu\text{m}$.

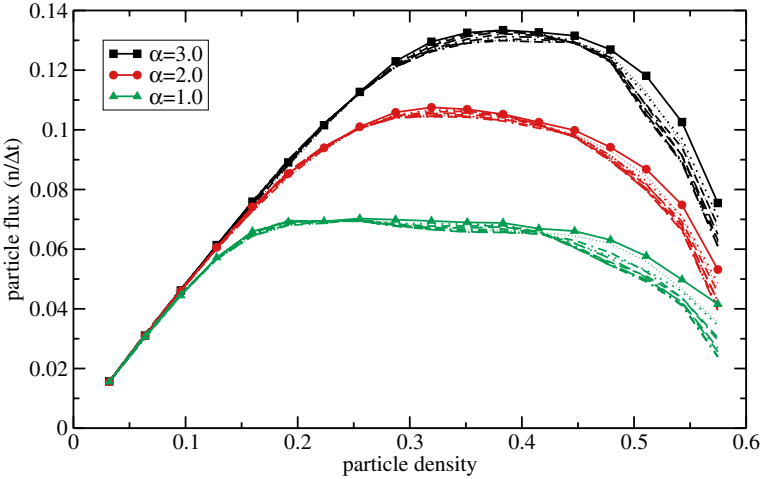


Fig. 7. Particle flow in dependence of the global particle density and the inclination α ($L_x = 600$, $L_y = 5.22$).

a random position at the beginning of the channel. Until now hydrodynamic interactions are neglected.

In all cases investigated the particles form ordered line structures in the lower part of the channel, see Fig. 6. During the simulation run we determined the particle flow at different positions in the channel. This was done for the three inclination angles $\alpha = 1.0, 2.0, \text{ and } 3.0$. The result is shown in Fig. 7. We conclude that the particle flow reaches a plateau value and decreases at high densities, and the plateau value increases with increasing inclination angle. This interesting new finding will be the subject of future investigations. In addition we plan to extend our studies to explore the flow behavior in dependence of the particle interaction range, the characteristics of the channel walls, and the channel geometry (bottlenecks, barriers).

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Computational Fluid Dynamics

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Numerical simulation has become a very attractive procedure to investigate complex fluid mechanical phenomena as soon as high performance computers and highly sophisticated numerical procedures became available. Since the flow processes in daily life are turbulent and may even include chemical reactions, phase changes, heat transfer and interference with structural movements the high performance computers are still by far too small in order to simulate for instance the turbulent flow around a complete aircraft. Despite this fact the following chapter on results in the field of computational fluid dynamics (CFD) obtained at HLR Stuttgart will demonstrate the usefulness of numerical simulation and the progress in gaining more insight into complex flow phenomena when the computer capacity is increased from NEC SX-5 to NEC SX-6 and further on to NEC SX-8 or to CRAY-Opteron Cluster.

The chapter starts with the direct numerical simulation (DNS) of non-linear transitional stages from laminar to turbulent flow in a laminar separation bubble. The DNS procedure is necessary since the flow is extremely complex and DNS is the proper way to study the flow structure in detail. This knowledge is necessary to prevent separation bubbles which increase the drag and can cause noise. Marxen and Rist offer in their contribution a detailed description of the flow field and the important parameters that control the instabilities. Investigations of this kind require a memory of 5.68 GB and 8.96 GB on the NEC SX-6 and NEC SX-8 (MPI), respectively. One simulation demands a computational time of 4619 hours on the NEC SX-6 and of 2517 hours (3175 hours) on the NEC SX-8 (MPI).

The second paper by Stemmer and Adams deals also with instabilities in boundary layers, however at hypersonic speeds. Therefore, the influence of high-temperature gas effects, e.g. dissociation, has to be included. As this kind of flow is very difficult to undertake in a wind tunnel on one hand but is very important on the other hand in the design of space-craft its simulation is not only attractive from an academic point of view. Stemmer and Adams show for instance that the vibrational temperature drops to about 2300 K inside the boundary layer compared to 4500 - 4800 K when performing equilibrium

calculations. For a $3001 \times 91 \times 181$ grid (49.4 million grid points) a main memory of 13.6 GB is necessary. On the NEC SX-6 series supercomputer a performance of 2825 MFLOPS on a single processor and 21.159 GFLOPS for a parallel calculation with 8 processors is reached. This is a speed-up of 7.5.

The third paper by Sander et al uses DNS to study multiphase flows, more specifically the break-up phenomena both in liquid jets and of colliding raindrops. They use DNS to bridge the gap between experimental and analytical descriptions of the complex phenomena. Three different disintegration mechanisms may appear, namely the Rayleigh type break-up, a wavy break-up and a disintegration phenomenon that leads to atomization of the jet into small droplets. The authors studied all three stages in good agreement with experiments. A typical grid size yields $3072 \times 96 \times 96$ grid points. Using 32 CPU's approximately 963 grid points per CPU are used on the HLRS-CRAY Opteron cluster. The computational time depends on the actual case and varies between 48 and 96 hours. The main problem in the simulation of collision-induced break-up of raindrops is to identify specific break-up modes and their relative appearance as well as to determine the corresponding specific fragment's size distribution functions. The first step of this investigation reveals interesting insights into the collision mechanisms and structures. A simulation with 8 CPU's and a grid resolution of $256 \times 256 \times 256$ requires approximately 20 hours of computation time.

DNS including all turbulent scales without any modeling is still restricted to low-Reynolds number flows and thus for industrial applications too expensive or even not possible. An alternative is the Large Eddy Simulation (LES) that resolves only the turbulent scales larger than the cell size of the grid. However, an adequate numerical resolution especially in the near wall region is required. On meshes that do not resolve viscous near-wall effects the simulation might fail, either with sub-grid simulation (SGS) or wall models. Magagnato et al investigate the flow around a turbine blade. They find that the upstream turbulence is underestimated in their simulation and transition is not modeled properly. In addition, the mesh down to the wall and along the wall is not fine enough which causes some deviation in comparison with experiments. However, the investigations will be continued to overcome the problems.

Zhang et al. present a hybrid LES/CAA (Computational Aeroacoustics) method for aero-acoustic investigations. They use LES to resolve the acoustic source region governed by nonlinear effects. In a second step they compute the acoustic field on a coarser grid by linear acoustic equations with the nonlinear effects lumped together in a source term that is obtained from LES. They use this hybrid LES/CAA method to simulate trailing-edge noise on a high-lift airfoil configuration and combustion noise in a turbulent non-premixed jet flame. For their first test case they use a total of 4,102,440 grid points and assure that the first grid point in wall normal direction is close enough ($y^+ \approx 2$). With this set-up the prediction of the aerodynamic characteristics of the airfoil with flaps is in good agreement with measurement. A memory of 3.5 GB is required. The authors reach a single processor performance of

about 2.4 GFLOPS on the NEC SX-5 and 4.3 GFLOPS on the NEC SX-6. Approximately 175 CPU hours on 10 SX-5 CPUs for a statistically converged solution are required for the airfoil-flap configuration. For the jet flame simulation a total of 106 cells is necessary. The ratio of the computation times between LES and CAA is approximately 4:1.

Q. Ye presents a numerical simulation of electrostatic spray-painting with movement of the atomizer using dynamic mesh models. The goal is to optimize the painting process that amounts to a high percentage of fixed and flexible costs. The numerical simulation of spray painting is performed with the commercial CFD code FLUENT using dynamic mesh models. The prediction of the film thickness distribution on the substrate needs some improvement with a new FLUENT code. The author expects to gain this improvement especially with a stable parallel solver. The presented investigation uses 5×10^5 cells and needs 144 hours of total CPU for one simulation on a Cray Opteron Cluster with single processor.

A. Schütte et al simulate complex manoeuvres of a combat aircraft. They couple the unstructured, time accurate flow solver TAU with a computational module that solves the flight-mechanic equations of motion and with a structural mechanics code that calculates the structural deformations. They use a loose coupling scheme between the aerodynamic and structural dynamic code that is conservative with regard to the forces, moments and the work performed on both. They apply a specific code for each discipline that was validated and optimized independently and that is executed on a platform for which it has been optimized. The CFD Code requires the largest computational effort and is run on an Opteron-based Linux-Cluster with 16/32 processors. A memory from 13 to 38 GB is necessary. The CPU time ranges from 14 to 156 hours for an X-31 steady calculation to a delta-wing unsteady calculation with 250 physical time steps and a coupled simulation.

Dietz, Kessler and Krämer present the numerical simulation of the aeroelastic behavior of the main rotor blades of a helicopter in forward flight. Strong coupling between the aerodynamics and the structural dynamics is mandatory. The correct trimming is also an essential part of the simulation. As in the paper before, the separate and optimized aerodynamic and dynamic code are coupled in a staggered procedure and run on separate platforms. The integration methods on both codes are second order accurate and are conservative. In order to get an accurate conservation of the tip vortices and thus to predict blade vortex interaction (BVI) the chimera technique is used to accurately capture the vortices. The grid consists of an eight-block cartesian background grid with 1.8 million cells, four blade grids with 150.000 cells each. This amounts to a total of 3.8 million cells. Even a high performance platform as the NEC SX-8 with 8 CPUs needs 64 hours CPU time per revolution (required memory: 5.7 GB). The authors use the code also to simulate individual blade control by trailing-edge flaps. In this case 2.540.000 cells were necessary for a single-blade simulation. The CPU time per rotor revolution was 15 hours on a NEC SX-6 (3.8 GB).

Walid Khier presents numerical simulations of the flow around a helicopter configuration with fuselage, main and tail rotor. To reduce computational costs he simulates the rotor flow by a quasi-steady actuator disk approach. He also uses a time accurate approach to simulate wind tunnel experiments. The chimera technique is applied. The grid consisted of approximately 11 million points distributed in 99 blocks in the first case and contained 13 million points in 480 structured blocks in the second case. A memory of 20 GB is required. Even on a high performance computer as the NEC SX-6 the simulation lasts 800 CPU hours.

In the contribution of Schnell et al. the numerical simulation of the flow and the water steam cycle in utility boilers is considered. The main processes are the transport of the heat released from the combustion reactions of the fossil fuel by radiation, convection and conduction in order to produce steam and finally electricity. By detailed numerical simulations it was shown that for an optimal operation of the unit, an effective, adequately dimensioned steam attemperator control system must be implemented to equalise the temperature distribution. The presented calculation for a geometry in 3D have been done on a single node consisting of 8 processors of the NEC SX-6. The maximal performance on the SX-6 system has been measured as 4.1 GFLOP/s which correspond to 46% of the maximum peak performance of the vector processor.

Direct Numerical Simulation of Non-Linear Transitional Stages in an Experimentally Investigated Laminar Separation Bubble

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Summary. This paper details a joint numerical and experimental effort to investigate a transition process in a laminar separation bubble, with the emphasis being put on the numerical contribution. A laminar separation bubble is formed if a laminar boundary layer separates in a region of adverse pressure gradient on a flat plate and undergoes transition, leading to a reattached turbulent boundary layer. Development of disturbances during the transition process in such a separation bubble is studied by means of direct numerical simulation with controlled disturbance input. Focus is put on the stage of non-linear development of these perturbations, for which a detailed comparison between numerical and experimental results is given. Beside physical phenomena like shear-layer roll-up and vortex shedding, computational aspects such as the performance of the numerical code on supercomputers are treated.

1 Introduction

Transition to turbulence in a two-dimensional separated boundary layer often leads to reattachment of the turbulent boundary layer and the formation of a laminar separation bubble (LSB). In environments with a low level of disturbances fluctuating in time, the transition process is governed by strong amplification of these disturbances. Such a scenario is typical for a pressure-induced LSB, e.g. found on a (glider) wing in free flight, or for an experiment where the region of pressure rise is preceded by a favorable pressure gradient that damps out unsteady perturbations (Watmuff, 1999). In the region of an adverse pressure gradient, disturbance waves are subject to strong amplification, and their saturation marks the location of transition to turbulence.

Laminar-turbulent transition in laminar separation bubbles has been the subject of numerous studies in the past. Only some of the most recent ones will be mentioned here. Watmuff (1999) carried out an experimental study of a LSB, while Spalart & Strelets (2000), Alam & Sandham (2000), Maucher *et al.* (2000), and Wissink & Rodi (2004) tackled the flow by means

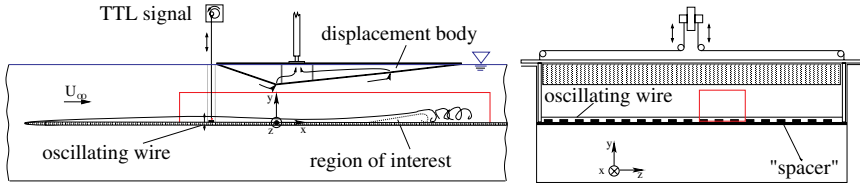


Fig. 1. Configuration for the experiment by Lang (2005) – sketch (provided by Matthias Lang) of the test section of the laminar water tunnel at the IAG

of direct numerical simulations (DNS). Most of the cited studies conclude that some type of linear instability (Tollmien-Schlichting or Kelvin-Helmholtz instability) is the cause for transition.

With the rise of computational fluid dynamics during the last decades, and especially with the availability of large (vector-)supercomputers, there also came up a cry to verify numerical simulations not only within themselves, e.g. by means of grid-refinement studies, but also by a comparison with the outcomes of available experiments. For flows with physical processes as complex as in a laminar separation bubble, a comparison of *only* time-averaged and root-mean-square quantities appears of little value and cannot be considered a true verification. Rather, a detailed quantitative time-accurate comparison of numerical results and experimental data obtained in a LSB is required. Both, experimental and numerical methods have certain, but different, weaknesses that make a meaningful comparison quite demanding.

This paper shall serve to demonstrate that the numerical method used within the project LAMTUR is capable to provide realistic space- and time-accurate simulations even of non-linear stages of the transition process in a laminar separation bubble. The method was adapted to represent a physical situation as given in Fig. 1, for which an experimental realization is available. The experiment was planned in a way as to minimize numerical difficulties as far as possible. A crucial point thereby is the explicit forcing of disturbances, so that the flow is not governed by the (hard to determine) background disturbances in the very tunnel that was used for the experiment.

The whole project LAMTUR aims at evaluating transition mechanisms in wall-bounded flows – in the present ‘subproject’ in a LSB – and is motivated by several considerations. Identifying the relevant disturbances and understanding their role in the transition process is a necessary condition for the prediction of transition in similar flows. In addition, it can be viewed as a first step towards control of the underlying flow field.

Here, the outcomes of a large-scale computation will be described. Physical insights gained within the subproject are discussed in more detail in Marxen *et al.* (2003, 2004, 2005); Marxen (2005). All calculations rely on a single case and mainly serve to illustrate transitional processes that *can* occur in a LSB.

2 Description of the Flow Field

The present case is defined by an experimental set-up specified in detail in Lang *et al.* (2004), Lang (2005). A sketch of the set-up was given in Fig. 1. Only a brief description is given here. The set-up was used during several measurement campaigns carried out by Matthias Lang at the Institut für Aerodynamik und Gasdynamik, Universität Stuttgart. Outcomes of these campaigns are taken for comparison with computational results throughout this paper. Specifically, results from measurements by means of Laser-Doppler Anemometry in 2000, denoted as *LDA (2000)* in the following, and 2001, *LDA (2001)*, as well as those obtained from Particle Image Velocimetry in 2001, *PIV (2001)*, are used.

2.1 General Parameters

A flat plate is mounted in the free stream ($\check{U}_\infty = 0.125 \text{ m/s}$) of the test section of a laminar water tunnel ($\check{\nu} = 10^{-6} \text{ m}^2/\text{s}$). A streamwise pressure gradient is imposed locally on the flat-plate boundary layer by a displacement body (length of the body $\check{L}_{DB}^{Exp} = 0.69 \text{ m}$), inducing a region of favorable pressure gradient followed by a pressure rise. The origin of the coordinate system corresponds to the narrowest cross section beneath the displacement body.

In the region of adverse pressure gradient (starting at $\check{x} \approx 0 \text{ m}$), a laminar separation bubble develops. The transition experiment is performed with controlled disturbance input. A 2-d time-harmonic perturbation is introduced upstream of the displacement body (at $\check{x} = -0.23 \text{ m}$) by an oscillating wire (fundamental frequency $\check{f}_0 = 1.1 \text{ s}^{-1}$). Additionally, 3-d disturbances are imposed by placing thin (height: 10^{-3} m) metal plates, so-called spacers, regularly underneath the wire (fundamental spanwise wavelength $\check{\lambda}_z = 0.058 \text{ m}$).

All quantities are non-dimensionalized. The global reference length is chosen to be $\check{L}_{ref} = 2/3 \text{ m} \approx \check{L}_{DB}^{Exp}$. The reference velocity is evaluated at a streamwise position where the flow field is still not strongly affected by the downstream presence of the separation bubble, yet already influenced by the displacement body. It was found that $x = -0.15$ is a convenient location for that purpose, since at that position only small wall-normal changes of the streamwise velocity are observable outside the boundary layer. Thus, the reference velocity amounts to $\check{U}_{ref} = 0.15 \text{ m/s} \approx 1.2 \cdot \check{U}_\infty$, resulting in a global Reynolds number $Re_{global} = 10^5$ in water. For DNS calculations, general physical parameters of the flow (see Table 1) are chosen to match the experimental set-up as closely as possible.

At the streamwise position of the inflow boundary $x_{ifl} = -0.6$, the measured boundary-layer profile can be approximated by a Falkner-Skan similarity solution with $Re_{\delta_{1,ifl}} = 900$ and $\beta_{H,ifl} = 0.13$. The outflow boundary is located at $x_{ofl} = 1.16$ with a preceeding damping region starting at $x_{st,oBZ} = 0.9911$. The useful region of the integration domain extends up to $x \approx 0.95$.

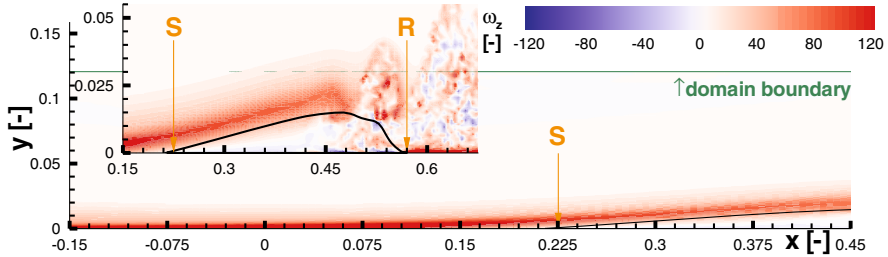


Fig. 2. Contours of the time- and spanwise-averaged spanwise vorticity $\bar{\omega}_z$ from DNS together with mean dividing streamline $\bar{\psi} = 0$. In the insert, the wall-normal direction is enlarged by a factor of 4 and an instantaneous view of ω_z is given

The pressure gradient is prescribed via streamwise and wall-normal velocity distributions $u_e(x), v_e(x)$ at a height $y_{max}=0.1207$. These distributions are chosen guided by potential(slip)-flow distributions u_{slip}, v_{slip} , but slightly adapted to compensate for errors introduced through the assumptions in deriving the potential-flow solution and to obtain the best possible overall matching of the DNS results with the experiment. The slip flow was estimated from experimental mean values $\bar{u}_{exp}, \bar{v}_{exp}$ at constant $y=0.06$. The procedure used to derive slip velocities from measured data is given in Marxen (2005). A rough estimate of the pressure-gradient parameter gives $P=\delta_2^*/\bar{\nu} \cdot \partial \bar{u}_{slip}/\partial \bar{x}|_{Separation} \approx -0.32$.

It was not possible to obtain a steady-state solution to the Navier-Stokes equations with the chosen distribution $u_e(x), v_e(x)$, i.e. the actual flow field observable downstream of transition is highly unsteady from $x=0.48$ onwards. For that reason, the subsequent discussion of the mean flow field is restricted to the laminar part of the LSB ($x \leq 0.45$).

2.2 Mean Flow and Boundary-Layer Properties

Contours of the spanwise vorticity ω_z are shown in Fig. 2, together with the mean dividing streamline $\bar{\psi}=0$. A fairly large but shallow separation region has developed. Its start is marked by the point of separation S ($x_S \approx 0.225$). To provide an impression of the size of the LSB, the whole bubble is included in the insert of Fig. 2, and the mean reattachment point is marked by R.

Table 1. Simulation parameters for DNS

$\check{U}_{ref}$	0.15 m/s	$\check{\nu}$	$10^{-6} \text{ m}^2/\text{s}$	Re_{global}	10^5	$Re_{\delta_{1,ifl}}$	900
y_{max}	0.1207	β_0	30.7	γ_0	72	$\beta_{H,ifl}$	0.13
x_{ifl}	-0.6	x_{ofl}	1.16	$x_{st,oBZ}$	0.9911	$x_{en,oBZ}$	1.1586
NMAX	2690	MMAX	241	KMAX	63	LPER	1200

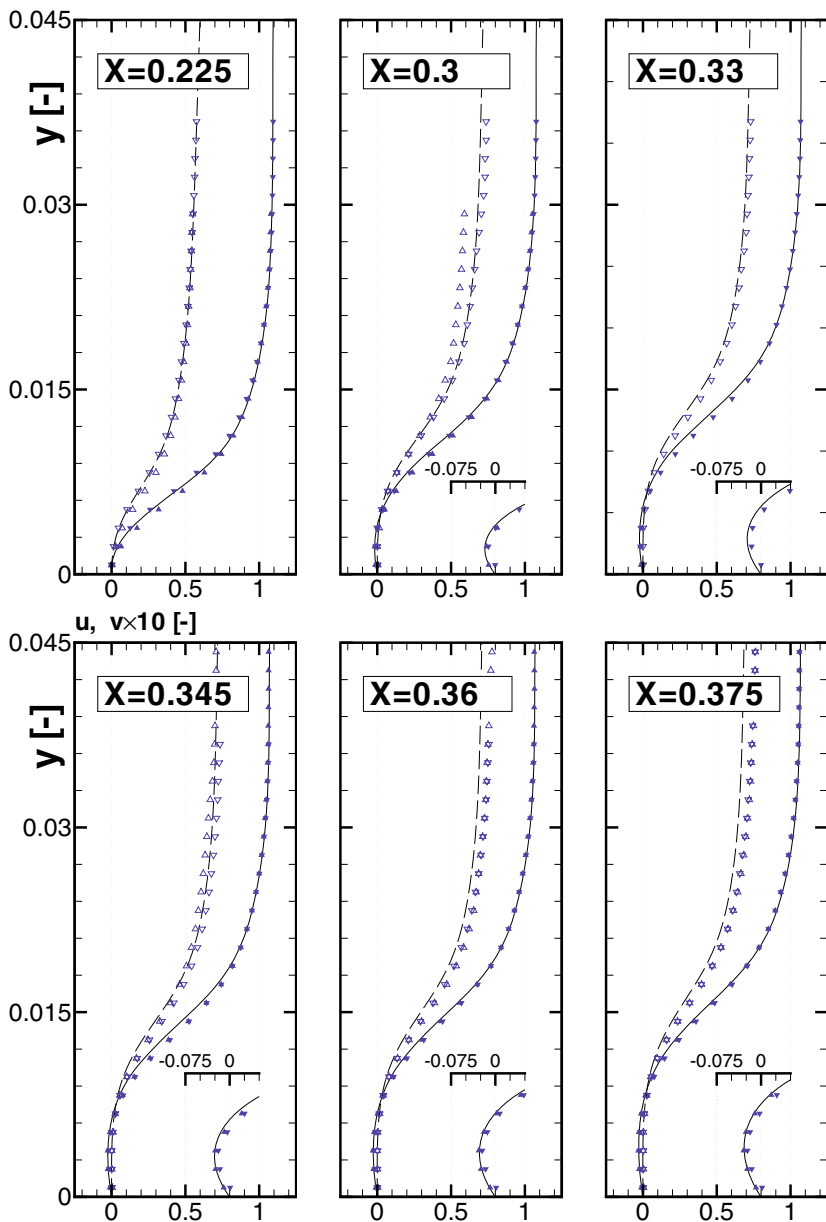


Fig. 3. Time- and spanwise-averaged streamwise (solid lines/filled symbols) and wall-normal (dashed lines/open symbols) velocity profiles at several streamwise positions in the laminar part of the LSB. Comparison of DNS (lines), LDA (2001) (deltas), and LDA (2000) (gradients). Inserts show u in the reverse-flow region enlarged by a factor of 4

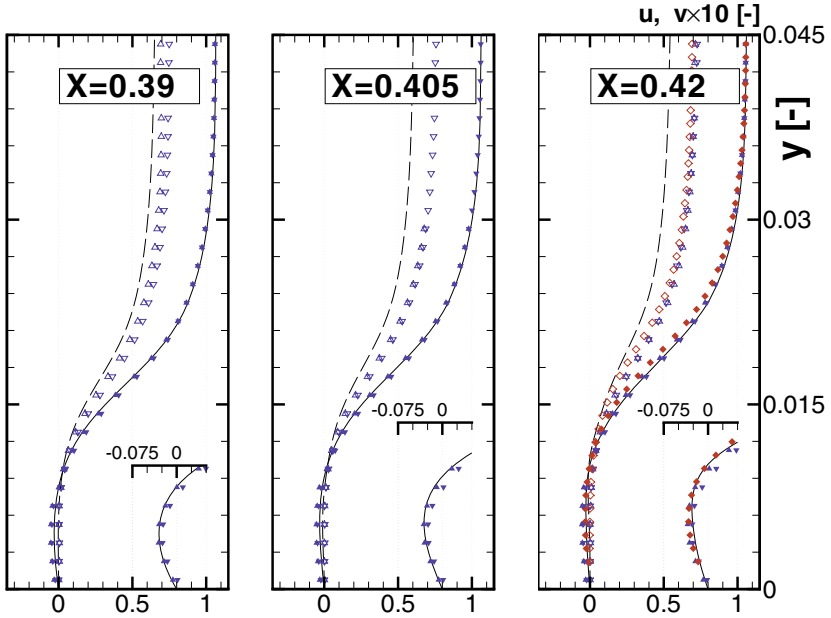


Fig. 4. Same as Fig. 3, except that streamwise positions $x=0.39$, 0.405 , and 0.42 are shown. Comparison of DNS (lines), LDA (2001) (deltas), LDA (2000) (gradients), and PIV (2001) (diamonds)

Figures 3 and 4 compare time- and spanwise-averaged velocity profiles at separation and in the reverse-flow region. Satisfactory agreement between DNS results and measurements for all streamwise positions even for the small wall-normal velocity component (note the different scaling for u and v in the figures) reveals that a separation bubble of approximately the same height is formed. The inserts showing the reverse-flow region of the LSB confirm that a comparable amount of reverse flow exists in the DNS and in the experiment. The last x -position shown is close to the transition location.

Boundary-layer quantities from DNS are computed using a pseudo velocity that is obtained by integrating the spanwise vorticity in wall-normal direction (Spalart & Strelets, 2000). Figs. 5 and 6 show the streamwise development of important boundary-layer parameters. A strong increase in the quantities related to the displacement of the boundary layer (such as the displacement thickness δ_1 or Re_{δ_1}) is visible in the separated region.

In Fig. 5, the pressure coefficient at the wall in case of slip flow $c_{p,slip}$ serves to illustrate the development of a pressure plateau due to the LSB. Comparing c_p obtained from potential-flow theory and from DNS, one can see that deviation of the pressure distribution is not restricted to the region around separation, but already visible far upstream from it. This can be attributed to the presence of the separation bubble (Marxen, 2005).

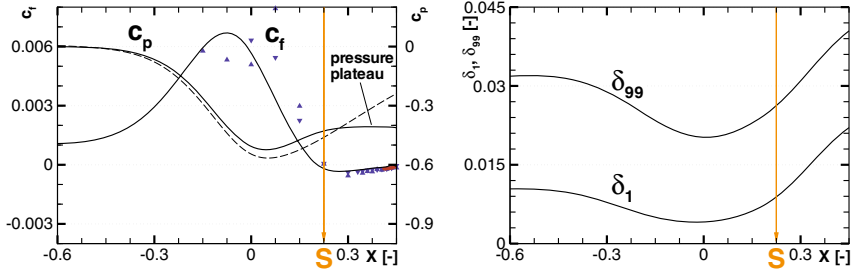


Fig. 5. Coefficients for surface pressure c_p , skin friction c_f (left), and boundary-layer thicknesses δ_1 , δ_{99} (right). Comparison of DNS (solid lines), slip-flow (potential-flow theory) results $c_{p,slip}$ (dashed line), LDA (2001) (deltas), LDA (2000) (gradients), and PIV (2001) (diamonds)

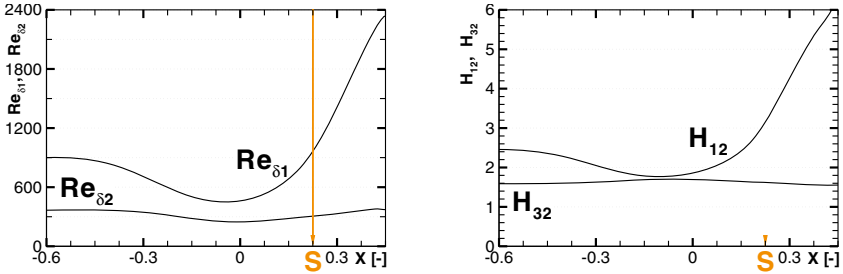


Fig. 6. Reynolds numbers Re_{δ_1} and Re_{δ_2} (left). Shape factors H_{12} and H_{32} (right)

2.3 Post-Processing of Time-Dependent Results

A double Fourier transform in time and spanwise direction of data sets from measurements or simulations yields disturbance amplitudes and phases. Below, the notation (h, k) will be used to specify the modes, with h and k denoting wave-number coefficients in time and spanwise direction, respectively.

In the simulations, the separation bubble showed low-frequency oscillations (so-called flapping) so that the Fourier analysis had to be carried out using a Hanning-window function to suppress aliasing effects. The amplitude of the subharmonic *after* using a Hanning-window was considerably lower than before and this was taken as proof that frequencies of the flapping and of the vortex shedding (see below) were indeed well separated. Four periods of the fundamental frequency were used in the analysis. The flow field is advanced in time until a quasi-periodic state is reached.

2.4 Linear Disturbance Evolution

Linear disturbance evolution in the considered flow shall only briefly be summarized – a detailed treatment can be found in Marxen *et al.* (2004, 2005);

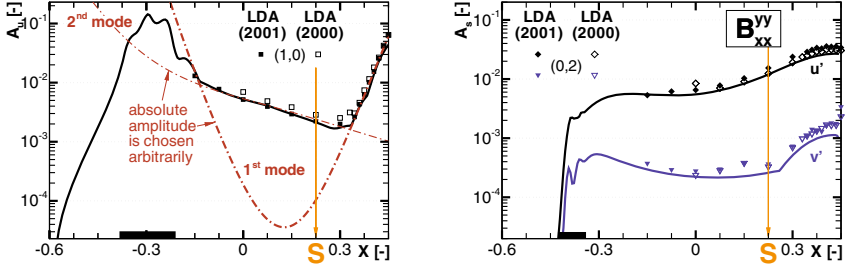


Fig. 7. Amplification curves for the maximum (in y) velocity fluctuations $|\hat{u}'_{max}{}^{(h,k)}|$, $|\hat{v}'_{max}{}^{(h,k)}|$. Left: 2-d mode (1,0) from DNS (solid line); LST (dash-dotted lines): first (thick), second (thin) mode; measurements LDA (2001) (filled symbols), LDA (2000) (open symbols). Right: steady 3-d mode (0,2) from DNS (lines) together with measurements LDA (2001) (filled symbols), LDA (2000) (open symbols)

Marxen (2005). All the results presented in this subsection have been obtained by means of a disturbance-flow computation (see Sect. 4), making use of the flow described in the last subsection as a base flow.

Linear stability theory (LST) based on the Orr-Sommerfeld equation (Schlichting, 1979) predicts that a discrete spectrum of eigensolutions exists for a certain velocity profile. For transition in low disturbance-level environments, out of these only the least damped, or most amplified, disturbance eigenmodes are relevant. An analysis of the stability characteristics for this flow field (Marxen, 2005) revealed that solely a single 2-d mode, here denoted as *first mode*, becomes amplified in the region of adverse pressure gradient, while at the same time precisely this mode is stronger damped in the acceleration region than another one, the *second mode*, existing in the flow.

In a numerical simulation or in the experiment, *all* eigenmodes with the respective frequency will inevitably be excited, though with different initial amplitude. For the present position of the oscillating wire in the experiment ($x = -0.345$), the second mode is initially visible, while further downstream the first one becomes dominant (Fig. 7, left). Therefore, it is sufficient to excite this first mode only in the DNS, e.g. with a disturbance strip placed in the location of pressure minimum ($x=0$) as it will be described below.

The evolution of a different class of linear disturbances – steady, three-dimensional ones – is shown in Fig. 7, right. A detailed discussion of this type of disturbance can be found in Marxen *et al.* (2004, 2005); Marxen (2005). The initial behavior of mode (0,2) in the region of favorable pressure gradient is associated with optimal transient growth, while further downstream a generic growth that is independent on initial condition can be observed. Again, good agreement of numerical and experimental results is visible. The two perturbations just discussed, the 2-d Tollmien-Schlichting wave and the 3-d steady streak, are the dominating disturbances up to the onset of non-linear stages of the transition process.

3 Non-linear Disturbance Evolution

Emphasis will be put now on the early non-linear stages for unsteady perturbations, i.e. stages where saturation and mutual interaction of disturbances occur for the first time. This restriction justifies to consider only spanwise symmetric perturbations.

Saturation of the disturbance waves leads to shear-layer roll-up and vortex shedding as it will be illustrated in the following. This vortex shedding is often essentially a two-dimensional phenomenon (i.e. strong spanwise coherence of the vortex structure), caused by either spanwise constant (2-d) small-amplitude waves, as it is the case here, or by spanwise-harmonic (3-d) waves with small obliqueness angles in an otherwise undisturbed flow.

Disturbances are forced via blowing and suction at the wall through a disturbance strip. The position and amplitude of the disturbance input for the simulation is given in Table 2. The fundamental frequency is $\beta_0=30.7$ and the fundamental spanwise wavenumber $\gamma_0=72.0$. Note that the disturbance strip is placed further downstream, i.e. not at the location of the oscillating wire in the experiment, due to the reasoning given in the last section.

Growth of a strongly oblique wave (mode (1, 2)) – despite its approximately neutral linear stability (Marxen *et al.*, 2004; Marxen, 2005) – is treated in Sect. 3.1. With the saturation of the fundamental, primarily amplified disturbances, non-linearly generated higher harmonics fill-up the disturbance spectrum in time (higher h) and span (higher k). This effect is discussed in Sect. 3.2 exemplarily for the two-dimensional perturbations.

3.1 Growth of Oblique Disturbances

Strong growth of mode (1, 2) inside the LSB is a result of non-linear generation, i.e. interaction of modes $(1, 0) \times (0, 2)$ and not due to a secondary instability, as proven by a variation in excitation amplitude of modes (0, 2) and (1, 2) in Marxen *et al.* (2004). Such a non-linear generation is seen to provide the experimentally observed growth rate (Fig. 8, left). Final growth and saturation of mode (1, 2) has to be attributed to an independent evolution of this mode. Equal behavior of the most relevant modes for the linear (thin lines) and non-linear (thick lines) computations verifies the applicability of the disturbance formulation discussed in Sect. 2.4.

Table 2. Forcing amplitudes A_v and location of the disturbance strip

	(1, 0)	(1, 1)
A_v	$1.15 \cdot 10^{-5}$	0.026
disturbance strip: $x \in [-0.0352, 0.0486]$	$[-0.4702, -0.3833]$	

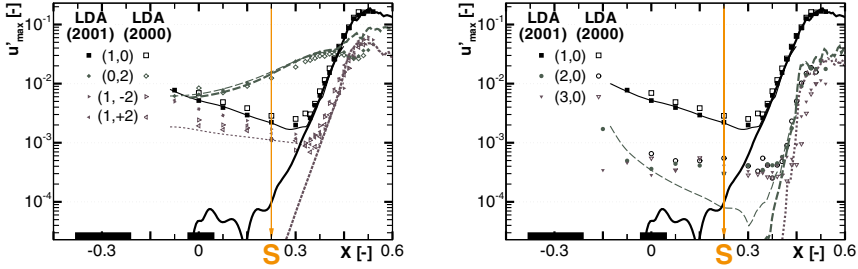


Fig. 8. Amplification curves for the maximum (in y) streamwise velocity fluctuation $|\hat{u}'_{max}|^{(h,k)}$. DNS results for linear (thin lines) and non-linear (thick lines) simulations; measurements LDA (2001) (filled symbols), LDA (2000) (open symbols)

3.2 Non-linear Generation, Shear-layer Roll-up, and Vortex-shedding

A comparison of the evolution of mode (1,0) in the linear and non-linear simulations (Fig. 8) reveals that instead of exciting both least-damped linear eigenmodes as discussed before, one can as well make sure that only the amplified first mode is visible by relocating the disturbance strip in the region around the pressure minimum ($x=0$). This does not alter the evolution of perturbation (1,0) deeper inside the LSB for $x>0.36$.

Comparing the DNS data with measurements (Fig. 8, right) it can be seen that in case of the experiment, mode (2,0) is not non-linearly generated by the fundamental disturbance in the interval $x \in [0, 0.375]$, but either possesses its own evolution or can be attributed to the accuracy-limit of the LDA. Outside this interval, and in particular deeper inside the LSB, mode (2,0) is indeed a true higher harmonic of the fundamental perturbation. The DNS is able to predict roughly the same location and amplitude level of disturbance saturation as observed experimentally for the unsteady disturbances (Fig. 8).

To illustrate the physical meaning of the saturation of the most relevant modes and the corresponding gain in amplitude of higher harmonics, we switch to the viewpoint in physical space, since the stage following disturbance saturation is associated with the development of coherent structures. In this stage, the phases and amplitudes of perturbations relative to each other are important, therefore it is convenient to look at them in physical space.

Reduction of information to a manageable level comes from looking at a single spanwise position only. Fig. 9 reveals that the non-linear processes given in Fourier space in Fig. 8 are associated with a roll-up of the separated shear-layer, i.e. the modes synchronize in a way as to form a spanwise vortex. The resulting vortex pumps outer, high-speed fluid towards the wall until it detaches from the shear layer and is shed downstream with fundamental frequency. This process is responsible for the reattachment of the flow in the mean.

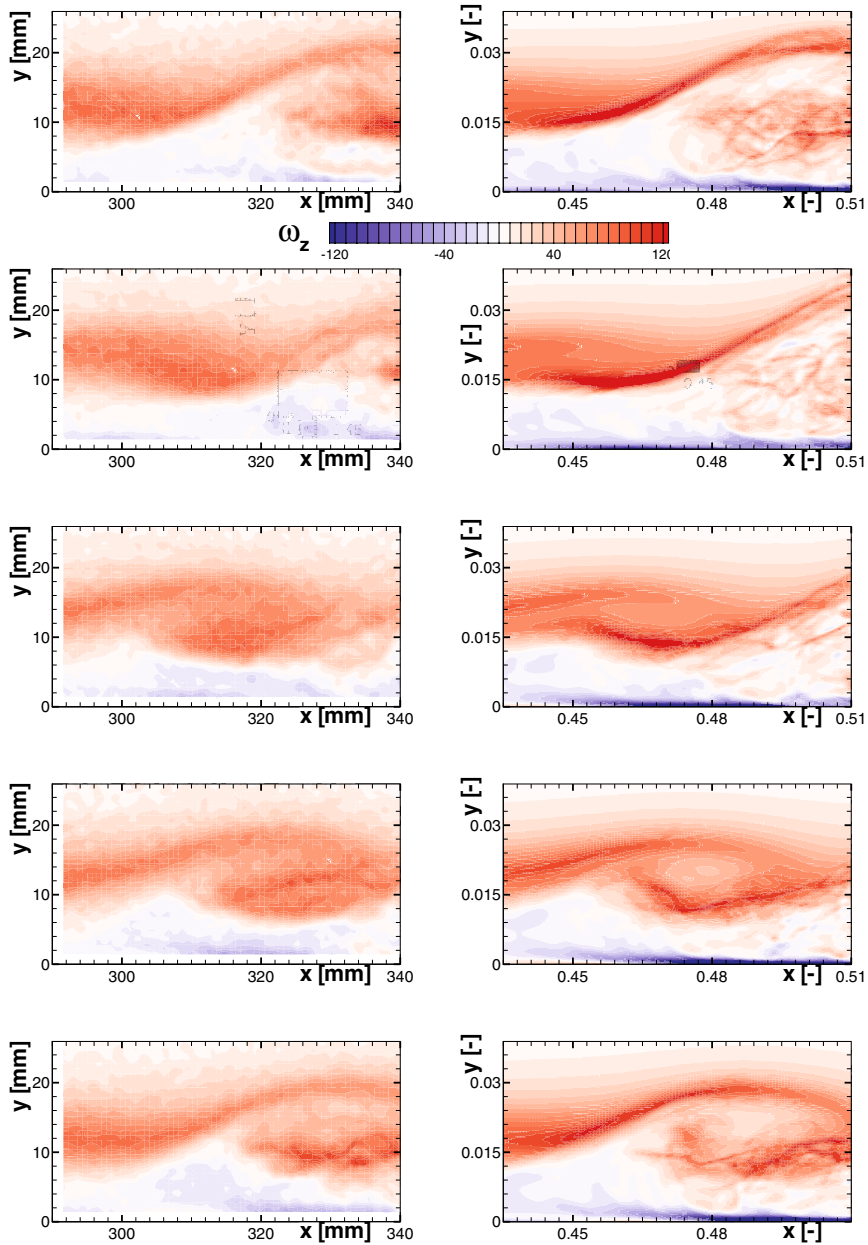


Fig. 9. Contours (levels: $\omega_z = -120 \dots 120$, $\Delta = 8$) of the spanwise vorticity at $z=0$ for single time instants (from top to bottom: $t/T_0 = 0, 0.2, 0.4, 0.6, 0.8$). Comparison of phase-averaged ($T_{aver} \geq 20$) results from PIV (2001) (left) and DNS (right)

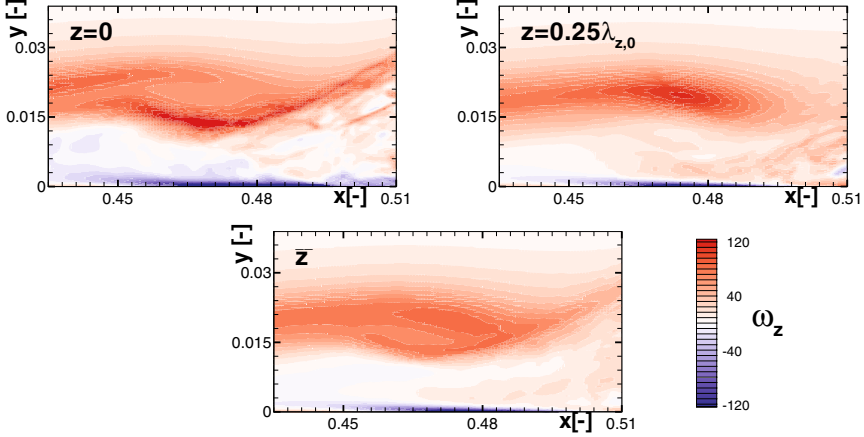


Fig. 10. Contours (levels: $\omega_z = -120 \dots 120$, $\Delta = 8$) of the phase-averaged ($T_{aver} = 20$) spanwise vorticity at $t/T_0 = 0.4$ from DNS. Comparison of peak $z=0$ (upper left), valley $z=0.25\lambda_{z,0}$ (upper right) position, and spanwise average (center)

However, the shear-layer roll-up is modulated in spanwise direction (Fig. 10). Even though we do not have an exact modulation of boundary-layer thickness caused by mode $(0, 2)$, still for $x < 0.45$ at some spanwise positions the top of the shear layer is closer to the wall ($z=0.25\lambda_{z,0}$), while at others it is further away ($z=0$). For that reason, Lang *et al.* (2001) denote this as a peak and valley structure similar to e.g. K -type breakdown. The fact that mode $(1, 0)$ is seen to possess the largest amplitude around and even after saturation (Fig. 8) – compared to 3-d modes – suggests that the 2-d structure mainly corresponding to this mode, i.e. the formation of the spanwise vortex, is dominant in the flow. This is confirmed by looking at Fig. 10, where it can be seen that the spanwise local evolution at peak and valley positions resembles each other as well as the spanwise average.

4 Computational Aspects

Simulation cases are set-up in a way as to economically apply available computational resources, relying on supercomputers only when it is essential. To maximize the physical outcomes with a minimum in computational effort, the following strategy was pursued: one large-scale computation was followed by several smaller ones and by theoretical investigations. The large-scale computation was carried out in total-flow formulation (the standard formulation typically used in CFD) to reproduce the experiment as closely as possible, and results of that computation have been presented in detail in Sect. 3 (denoted before as non-linear simulation). Based on the resulting flow field (after time averaging, i.e. the one described in Sect. 2.2), several smaller computations

Table 3. Performance of *n3d* in the present case for a typical run

Machine	CPU×Nodes	GFLOPS/CPU	Memory	CPU Time/Period
NEC SX-6	8×1	3.06	5.68 GB	30.79 <i>h</i>
NEC SX-8	8×1	5.38	6.19 GB	16.78 <i>h</i>
NEC SX-8, MPI	8×2	4.29	8.96 GB	21.17 <i>h</i>

could be run in disturbance formulation (before denoted as linear computations, see Sect. 2.4) with varying disturbance input. In addition, theoretical investigations were carried out.

For the present case, the total-flow formulation requires very long calculation times due to a slow convergence from the initially (arbitrarily chosen) attached boundary layer towards an almost time-periodic state of the flow field with a stable laminar separation bubble. Furthermore, such a simulation demands for a very high resolution due to the turbulent rear part of the separation bubble and requires a proper boundary-layer interaction model to capture the upstream influence of the entire LSB in the mean. Such a computation requires a supercomputer and will be discussed now.

4.1 Numerical Method for Direct Numerical Simulations

Spatial direct numerical simulation of the three-dimensional unsteady incompressible Navier-Stokes equations served to compute the flow field described above. The method uses finite differences of fourth/sixth-order accuracy on a Cartesian grid for downstream (NMAX) and wall-normal (MMAX) discretization (Kloker, 1998). Grid stretching in wall-normal direction allows to cluster grid points near the wall. In spanwise direction, a spectral ansatz is applied (KMAX + 1 modes). An explicit fourth-order Runge-Kutta scheme is used for time integration (LPER time steps per period of the fundamental disturbance). Upstream of the outflow boundary a buffer zone in the intervall $[x_{st,oBZ}, x_{en,oBZ}]$ smoothly returns the flow to a steady laminar state. Further details of the code *n3d*, i.e. the numerical method and the implementation, can be found in Meyer *et al.* (2003). Only a few adaptations compared to there have been made, namely the alteration of boundary conditions to allow for a total-flow formulation together with a boundary-layer interaction model.

4.2 Performance and Required Computational Resources

For the present resolution (see Table 1), the memory consumption and the performance observed is given in Table 3. A converged solution was achieved after 150 calculation periods, when mode (0.5, 0) – which can be viewed as a rough measure of low-frequency content in the flow – could be reduced to 10^{-3} in the first part of the LSB. This results in a computational time of 4619 *h* on the NEC SX-6 and of 2517 *h* (3175 *h*) on the NEC SX-8 (MPI). The actual degree of vectorization was $\approx 95\%$ for 15 periods.

5 Conclusions

The present DNS method has proven capable of providing quantitatively space- and time-accurate simulations of (early) non-linear stages of a transition process in a LSB. This has been shown by means of a comparison with experimentally determined data. The non-linear transitional stages featured the formation of coherent structures, namely shear-layer roll-up and vortex shedding as shown by a visualization based on the spanwise vorticity. Correctly capturing these stages of transition is believed to be an essential condition for a simulation of (very) late stages with their complex interactions of disturbances. However, concerning the very late stages, additional calculations are necessary in the future to improve CFD results.

The high computational cost associated with the usage of supercomputers required for a DNS does not justify to apply these computers to merely demonstrate the capabilities and accuracy of a numerical method. Instead, by a mutual comparison of results from numerical (DNS), experimental, and theoretical methods, more profound insights into the flow physics can be gained for a certain flow situation than it would be possible if only one of these methods were applied. This aspect is one of the main benefits of such an approach, reaching beyond a mere verification of either the numerical, experimental, or theoretical method: it exploits the fact that all these methods do not only have different weaknesses, but of course also have different advantages.

The performance of the code for the present case was found satisfactory, with a maximum performance of 5.38 GLFOPS/CPU on the NEC SX-8 for a typical run. For the computations in disturbance formulation a suitable production server is somewhat lacking. These runs cannot make use of a large number of processors, so that PC-Clusters are not favorably applicable. Rather, serial runs (or runs with less than 6 CPUs) on a fast machine would be preferable, yet in that case often the sum of queue and production time almost exceeds the wall-clock time for the large-scale computation.

Acknowledgments

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Instabilities in Hypersonic Boundary Layers Under the Influence of High-temperature Gas Effects

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Summary. Investigations on the spatial evolution of instabilities for hypersonic boundary-layer flows on a flat plate with dissociation are presented. A higher order compact numerical scheme allows for the detailed investigation of the linear and the non-linear evolution of the disturbance waves in the presence of chemical reactions. Compared to the ideal-gas case, lower temperatures in the boundary-layer are present. The three-dimensional disturbance behaviour is experiencing slight damping in the linear regime compared to equilibrium results. High-level disturbances can also lead to local shocklets that are treated with a hybrid ENO-scheme. Experiments for qualitative validation of the results at elevated Mach numbers are available by Mironov.

1 Introduction

The increased complexity of the reacting flows involving additional conservation equations for the chemical species involved require large and fast computers for the investigation of non-linear transitional boundary-layer flows. As the high Mach-number cases are very difficult to undertake in a wind tunnel and free-flight experiments are extremely rare and lack the resolution (in space and time) for transition research, direct numerical simulations provide a tool for the detailed investigation of such flows. As heat shields in (re-)entry problems are still overdimensioned as the exact flow properties are not well known, the development of better numerical tools to overcome this deficiency are necessary.

The 1950s and 1960s saw increased interest in high-velocity aircraft and spacecraft, but the numerical possibilities were limited. The Apollo and Space Shuttle programs brought increased research into the ongoing in dissociating boundary-layer flows, but mostly on the fields of material properties and

two-dimensional heat-transfer rates. The heat-shields of space missions in the 1990's were still designed with a safety factor of 3.

With the formulation of a compressible Linear Stability Theory by Mack [12], ideal gas stability calculation for supersonic Mach numbers became possible. Later, the incorporation of chemical reactions into the Linear Stability Theory has been achieved by Malik & Andersson [13] and Chang *et al.* [6]. With the increase in computational power, the direct solution to the Navier-Stokes equations (DNS) for compressible boundary-layer flows became feasible and overviews can be found in [7, 9, 8, 10]. Pruett & Chang [17] have presented a DNS of transition on a cone at Mach 8, but without the incorporation of high-temperature gas dynamics. The reason given are the lack of computer power at that time. They identify oblique second mode breakdown as “a viable path to transition for a high-speed boundary-layer flow on a cone”. But as Bertolotti [4] in stability calculations points out, the instability can be underestimated with the neglect of nonequilibrium effects.

An overview of early experimental work on high-speed flow experiments (wind tunnel and free flight) can be found in Schneider [18]. These experiments were very valuable for the identification of physical phenomena at the particular flow conditions. The resolution, nevertheless, of the measuring devices were not at all adequate to measure transitional non-linear development of instabilities which generally show frequencies in the upper kHz range. As wind-tunnel experiments in general cannot provide exact equivalence to the free-flight conditions (especially the Damköhler number), free-flight experiments would be needed which are terribly difficult to control and extremely expensive to undertake. Adequate numerical investigations (like DNS) can provide valuable insight into transitional high-speed boundary-layer flows that cannot be attained otherwise.

The late 80s and the early 90s were characterized by a boost in stability work and steady high-temperature simulations which are too numerous to mention here. As an example, the measurements of Stetson & Kimmel [22] on a sharp cone at $M=5-7$ and stability calculation of Stuckert & Reed [23] (for $M=25$ with chemical non-equilibrium) and Malik [13] (for $M=10$ and 15) provide many valuable results and numerous references that open the field of experimental and numerical work from that period. Recent experimental studies by Holden *et al.* are summarized in [24] and give a good insight in “hot” experiments on hollow cylinder/flare and double cone configurations which focus on steady heat transfer and separation as well as shock-interaction phenomena. A very detailed and recent experimental work on a very high Ma-number flow is conducted by Mironov & Maslov [14, 15] at $M=21$ which provides the possibility of a qualitative validation of the computational results.

2 Numerical procedure

The DNS code for both simulations is based on a compact finite-difference formulation for discrete points in all three spatial directions of high order (5th and 6th) developed by Adams [1, 2, 3]. A hybrid ENO method enables the local treatment of shocks whereas the other areas are continuously dealt with compact finite differences [11]. The code was adapted to account for the treatment of dissociation. Five species continuity equations and a conservation equation for the vibrational energy have been added [20]. The time advancement is realized through a three-step low-storage Runge-Kutta method. The boundary conditions are no slip at the wall and periodicity in spanwise direction. At the inflow, the laminar solution to the boundary layer equations is prescribed. The free-stream boundary is treated with a characteristic boundary condition. The outflow condition is characteristic for a flow without disturbances. For the disturbances, a well-tested outflow damping zone is applied.

2.1 Governing Equations

The complete, three-dimensional unsteady Navier-Stokes equations are treated in generalized coordinates which can be formulated as

$$\frac{\partial U}{\partial t} \frac{1}{J} + \frac{\partial F_E}{\partial \xi} \frac{1}{J} + \frac{\partial G_E}{\partial \eta} \frac{1}{J} + \frac{\partial H_E}{\partial \zeta} \frac{1}{J} = \frac{\partial F_S}{\partial \xi} \frac{1}{J} + \frac{\partial G_S}{\partial \eta} \frac{1}{J} + \frac{\partial H_S}{\partial \zeta} \frac{1}{J}. \quad (1)$$

The conservative variables are $U = \{\rho, \rho u, \rho v, \rho w, E\}$ with the energy being represented by $E = p/(\kappa - 1) + 1/2\rho(u^2 + v^2 + w^2)$ for the ideal-gas simulations without chemical reactions. The convective fluxes in the respective directions are denoted by the index E and the diffusive fluxes carry the index S . The variable J denotes the Jacobian of the mapping of the physical space (x, y, z) onto the computational space (ξ, η, ζ) .

For the hypersonic transition simulations an extra 6 equations for the 5 species continuity equations (the five species being the non-ionized species N, O, NO, N₂ and O₂) and the vibrational energy conservation equation are considered

$$\frac{\partial \rho_s}{\partial t} + \frac{\partial}{\partial \xi} \frac{\rho_s(u_1 + u_{Dx})}{J} + \frac{\partial}{\partial \eta} \frac{\rho_s(u_2 + u_{Dy})}{J} + \frac{\partial}{\partial \zeta} \frac{\rho_s(u_3 + u_{Dz})}{J} = mtr_s. \quad (2)$$

The index s denoting the five chemical species and u_{D_i} stand for the diffusion velocities. The mass transfer rates mtr are taken from Park [16]. The vibrational energy equation which is present only for the molecular species shows as

$$\frac{\partial e_v}{\partial t} + \frac{\partial}{\partial \xi} \frac{e_v u_1}{J} + \frac{\partial}{\partial \eta} \frac{e_v v}{J} + \frac{\partial}{\partial \zeta} \frac{e_v w}{J} = \frac{\partial}{\partial \xi} \frac{q_{v,x}}{J} + \frac{\partial}{\partial \eta} \frac{q_{v,y}}{J} + \frac{\partial}{\partial \zeta} \frac{q_{v,z}}{J} + w_v. \quad (3)$$

The heat transfer terms q_v are calculated from the vibrational temperature t_v and the term w_v describes the chemical heat transfer and the vibrational-translational heat transfer. The vibrational energy is built by

$$e_v = \sum_{ms=1}^3 \frac{\theta_{ms}}{e^{(\theta_{ms}/t_v)} - 1} R, \quad (4)$$

with the index ms denoting the molecular species and R is the real-gas constant.

All variables are non-dimensional according to the following relations: $\rho = \rho^*/\rho_\infty^*$, $u = u^*/U_\infty^*$, $E = E^*/(\rho_\infty^* U_\infty^{*2})$, $T = T^*/U_\infty^*$, $p = p^*/(\rho_\infty^* U_\infty^{*2})$ and $t = t^*/\delta_1^*/U_\infty^*$.

Details on the formulation and the calculation of the thermodynamic properties can be found in Candler[5] or in [19].

2.2 Grid

The grid is stretched in downstream (x -) and wall-normal (z -) direction and equidistant in spanwise (y -) direction. For the flat-plate flow, points are accumulated close to the wall and close to the boundary layer edge. The detailed procedure for the construction of the grid can be found in [1]. The maximum resolution for a full scale simulation was 3000x16x255. The results presented were obtained with a somewhat smaller grid.

3 Results

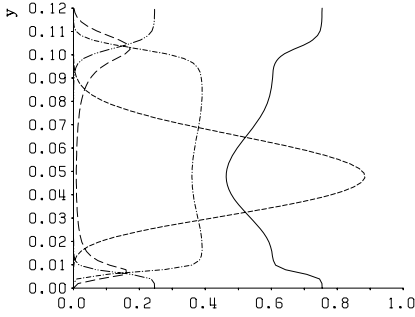
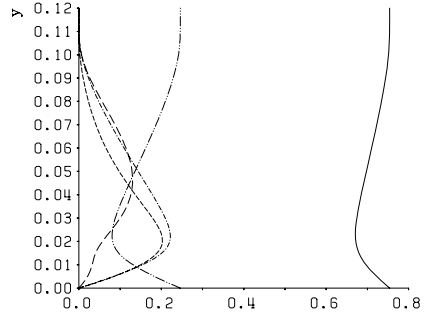
For the calculation of the hypersonic case, a flight case along the descent path of the Space Shuttle at a local Mach number of $M=20$ at an altitude of $H=50\text{Km}$ was chosen. The Knudsen number yields $Kn = 0.003$. The continuum approach still holds for this altitude. The parameters for this case are shown in Table 1.

For the ideal-gas case, the species concentrations are shown in Fig. 1, for the reacting case in Fig. 2. As can be expected, the species concentrations of the two-atomic molecule O_2 is almost zero inside the boundary layer as the temperature there reaches around 4800K in the ideal-gas case. The dissociation of O_2 starts (see [21]) relatively early at about 2500K, whereas the dissociation of N_2 doesn't start until $T > 4200\text{K}$. The drop in the N_2 -concentration is due to the presence of the NO molecule and the dissociation.

For the nonequilibrium case, the proportions are fundamentally different. The drop in the N_2 -concentration is rather gentle and the formation of NO is not as pronounced. This effect is due to the drop in vibrational temperature which lowers the reaction rates (see [21] for the dependencies of the reaction rates on the vibrational temperature). The O_2 -level is also larger in the nonequilibrium case. The NO -concentration is also higher inside the boundary

Table 1. Parameters for the hypersonic flat-plate simulation.

Parameter	Value	Comment
M_∞	20	
Re_{δ_1}	34 951	at inflow
δ_1^*	$8.787 \cdot 10^{-2}$	$[m]$, at inflow
T_∞^*	270.65	$[K]$
T_W	$3.0 T_\infty^*$	
U_∞^*	6596	$[m/s]$
p_∞^*	79.78	$[Pa]$
x_0	1.609	$[m]$
np _x	1501	number of points in x-direction
np _y	10	number of points in y-direction
np _z	255	number of points in z-direction


Fig. 1. Species concentrations c at $x=5.5m$ for the equilibrium ideal-gas case. ---- $N (\times 5)$; — N_2 ; - · - O ; · · · O_2 ; - - - $NO (\times 10)$

Fig. 2. Species concentrations c at $x=5.5m$ for the reactive non-equilibrium case. ---- $N (\times 10)$; — N_2 ; - · - O ; · · · O_2 ; - - - $NO (\times 10)$

layer, since the dissociation of NO leads to lower concentrations for temperatures above 3500K. In the nonequilibrium case, the mono-atomic species (N and O) are rather low in amplitude compared to the equilibrium case due to the presence of the inner degrees of freedom (vibrational energy) of the model.

The disturbance level development for the same disturbance input was checked for the ideal-gas simulation and the reacting case (Fig.3). The two-dimensional (second mode) disturbance shows the same amplitude level for the equilibrium and the nonequilibrium case, but the latter being more rugged. The most notable difference is the drop in the three-dimensional disturbance amplitude for the nonequilibrium case by a factor of 2~3.

The vibrational and the translational temperature for the reacting case are shown in Fig. 4. The translational temperature drops only slightly compared to the equilibrium case, but the vibrational temperature drops considerably to

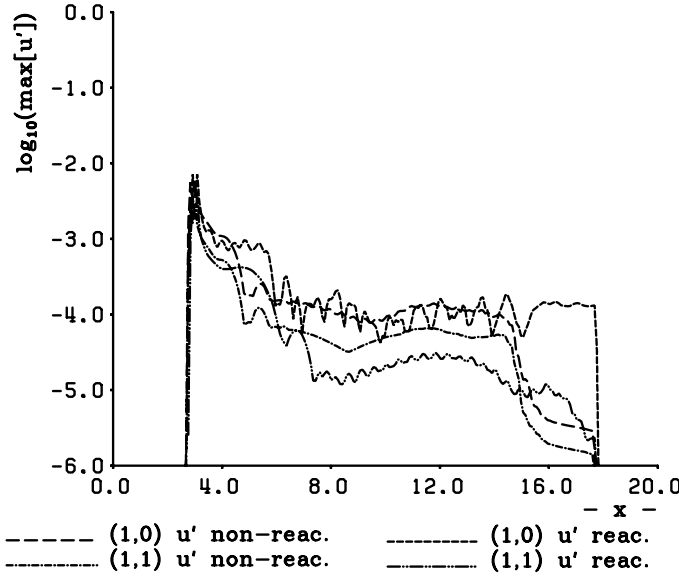


Fig. 3. Comparison of disturbance levels in ideal gas flow and reacting flow

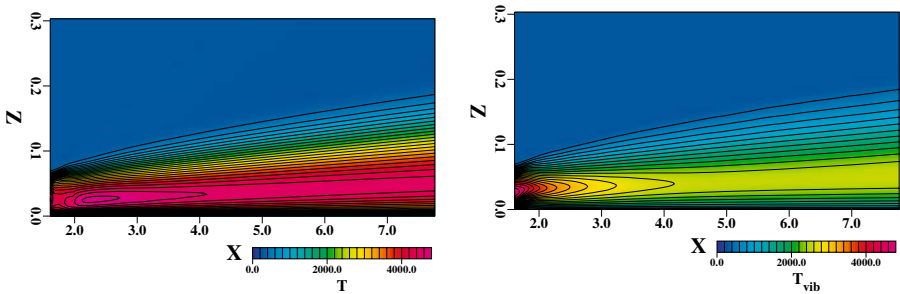


Fig. 4. Translational (left) and vibrational (right) temperature for the reacting gas case

about 2300K (compared to 4500-4800K for the equilibrium calculation) inside the boundary layer, where the highest temperatures are found. At the inflow, the equilibrium solution for the translational temperature is also given for the vibrational temperature, which explains the high level at the inflow boundary.

A closer examination of the introduction of the disturbances at the wall reveal that in the vicinity of the disturbance strip, an acoustic disturbance is introduced that is strongly attenuated (Fig. 5). The pressure disturbance that is associated with the propagating disturbance seems to vanish altogether, but is hidden in the scale since it has a smaller amplitude of ± 0.1 .

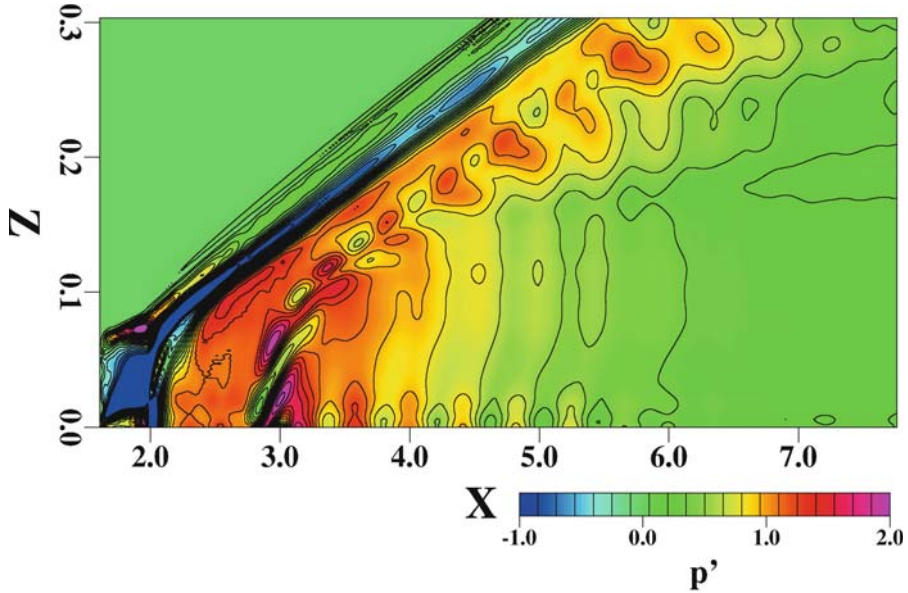


Fig. 5. disturbance pressure in the vicinity of the disturbance strip at the wall

4 Computational efficiency

The Fortran90 program runs with micro- and macro-tasking directives effectively on one node of the NEC SX6-series super-vector-computer. The vectorisation is optimized such that 99.4% of the program run in vector mode with an average vector length of 237.6 (out of 256). The exact performance depends on the size of the problem. For a 3001x91x181 grid 13.6 GB main memory was necessary. The average time per grid point and Runge-Kutta sub step of the 3-step scheme is $1.42\mu\text{s}$.

The MFLOPS-rate for a calculation on a single processor is 2825 and reaches 21,159 for a parallel calculation with 8 processors. The MOPS-rate for a parallel simulation with 8 processors accumulates 55 GOPS concurrent. This results in a speed-up of 7.5.

5 Conclusions and outlook

The three-dimensional disturbance development for the non-equilibrium case is not as pronounced as in the ideal gas case for linear disturbance amplitudes.

Ongoing work on the disturbance development in the nonequilibrium case (and comparative simulations for the equilibrium and frozen cases) will investigate for the nonlinear behaviour in the transitional regime. A possible

extension to a spanwise uniform three-dimensional base flow enable the consideration of cross-flow vortices and their non-linear interaction with the high-frequency disturbances.

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Direct Numerical Simulation of Breakup Phenomena in Liquid Jets and of Colliding Raindrops

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Summary. Since powerful computational resources are available, numerical simulation is one of the most attractive tools to bridge the gap between the experimental and analytical description of fluid flow phenomena. One of these tools is the *direct numerical simulation* (DNS) technique relying on a very high spatial and temporal resolution of fluid systems. Thus, all length scales of a fluid flow, only limited by the grid size, are captured by DNS. Since investigations of many fluid systems require a very fine resolution, considerable progress can only be made by both applying sophisticated numerical methods and using high performance computers. With the inhouse 3D DNS program FS3D (Free Surface 3D) based on the *Volume-of-Fluid* method it is possible to simulate two phase flows of fundamental interest in the automotive and aerospace industry, in meteorology and agriculture but also in the oil industry or medicine.

One part of this study focuses on the numerical simulation of the physical phenomena leading to disintegration of liquid jets. Although many researchers focused in the past on primary breakup phenomena and many experimental, analytical and also numerical results are available, these processes are not well understood. Therefore it was decided to simulate this breakup process by DNS. The results presented here demonstrate the capability of DNS on modern supercomputers. The first numerical simulation results on jet breakup agree qualitatively well with present experimental results. Differences are mainly due to the inflow condition which is a crucial problem for this phenomena.

The other part of this study is dedicated to a cloud microphysical process called 'collision-induced breakup' limiting the maximum size of raindrops. This process comprises a binary collision of raindrops and a subsequent disintegration of the coalesced body resulting in creation of a number of smaller fragment drops. The only very few experimental investigations of this process dating from the very past are reexamined by using the advanced fluid-mechanic program FS3D. The advantage of this numerical method is its high accuracy in simulating drop collisions. First results of fragment size distributions due to collisional breakup of raindrops are presented showing a good global agreement with those from laboratory experiments.

1 Introduction

In technical applications liquid jets usually are injected through a nozzle into a gaseous environment. Both the liquid and gaseous phase can have certain properties due to the pressure or the temperature typical for the process. This means that flow phenomena are influenced by the nozzle geometry, the fluid properties, and the ambient conditions, e.g. in a combustion chamber of an engine. Based on the given example the range of possible parameters influencing the flow is immense. At the same time the breakup and the spreading rate of the jet is crucial for the combustion efficiency and the resulting emissions.

With regard to rain evolution observations show that in natural rain the maximum size of raindrops is bounded from above: drops with diameters larger than 5 mm are very seldomly found. It is commonly assumed that the mechanism limiting the size of raindrops is collision-induced breakup [1]. Since the fragment droplets created by breakup are fed back into a pre-existing drop spectrum of a cloud breakup may change cloud and precipitation evolution as recently has been shown by [2] and [3].

Experiments related to collision-induced breakup are very rare. Only in the very past they have been performed by [4] and [5] considering only ten pairs of large raindrops as well as by [6] and [7] investigating only four drop combinations of small raindrops. Besides the very scarce number of drop pairs studied these experiments clearly suffer from specific uncertainties and limitations (reliable determination of sizes and fall speeds; problems in detecting very small fragment droplets). Consequently the outcome of these investigations as derived number and sizes of fragment drops rely, on one hand, on a very limited sample and, on the other hand, are fitted to noisy data. It should be noticed that the parameters derived from these experiments ([8],[9]) are the only ones applied in numerical simulation models of rain formation.

It is thus necessary (i) to assess the laboratory results and (ii) to extend the experiments to *all* relevant drop pair combinations.

2 Numerical method

The inhouse 3D CFD program FS3D [10] has been developed to compute the Navier-Stokes equations for incompressible flows with free surfaces. These equations are solved every time step without using a turbulence model according to the basic idea of *direct numerical simulation* (DNS).

The flow is governed by the conservation equations for mass and momen-

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u}) \otimes \mathbf{u} = -\nabla p + \nabla \cdot \mu \left[\left(\nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \right] + \rho \mathbf{k} + \mathbf{f}_v \quad (2)$$

tum where $\mathbf{u}$ denotes the velocity vector, t the time, ρ the density, μ the dynamic viscosity and p the pressure. Furthermore, the capillary stress tensor

$\mathbf{f}_v$ and an external body force denoted by $\mathbf{k}$ are added to the momentum equation. For the numerical solution of the equations a spatial discretization of the computational region is realized by a structured finite volume scheme on a staggered grid. In each phase, the discretization is second-order accurate. Due to the implemented projection method, a robust multigrid solver is used for solving the Poisson equation for the pressure.

Once the velocity field $\mathbf{u}$ of the flow is computed, the decoupled energy equation can be solved if required. The temperature field is governed by the energy equation

$$\frac{\partial}{\partial t}(\rho c_p T) + \nabla \cdot (\rho c_p \mathbf{u} T) = \nabla \cdot (k \nabla T) + \Phi, \quad (3)$$

where T denotes the temperature, c_p and k represent the specific heat capacity and the heat conductivity, respectively. The dissipation term Φ can be neglected for all mentioned flows due to the low Eckert number. The implementation and validation of the energy equation has been described in [11].

Based on the *Volume-of-Fluid* (VOF) method [12], the presence of liquid and gaseous phase has to be considered. Consequently an additional transport equation

$$\frac{\partial f}{\partial t} + \nabla \cdot (\mathbf{u} f) = 0 \quad (4)$$

is defined in order to describe the temporal and spatial evolution of the two phase flow. The variable f , called the VOF-variable, represents the volume of

$$f(\mathbf{x}, t) = \begin{cases} 0 & \text{in the continuous phase} \\ 0 < f < 1 & \text{at the interface} \\ 1 & \text{in the disperse phase} \end{cases} \quad (5)$$

(liquid phase) fluid fraction. Since fluid properties are required every time step in order to solve the Navier-Stokes and the energy equations the following relations for density ρ and viscosity μ are evaluated where the subscript c in-

$$\rho(\mathbf{x}, t) = \rho_d + (\rho_c - \rho_d) f(\mathbf{x}, t) \quad (6)$$

$$\mu(\mathbf{x}, t) = \mu_d + (\mu_c - \mu_d) f(\mathbf{x}, t) \quad (7)$$

indicates the continuous phase and d the disperse phase. Additional fluid properties like the specific heat, c_p , and the heat conductivity, k , are treated similarly.

To ensure a sharp interface and to suppress numerical dissipation of the disperse phase for each time step the interface is reconstructed by the PLIC (*piecewise linear interface calculation*) method proposed by [13]. After the reconstruction, the disperse phase is transported on the basis of the reconstructed distribution of the disperse phase. Due to the high gradients across the interface, a limiter is used to prevent the generation of oscillations and spurious solutions. The program, parallelized by the domain decomposition technique using the communication library *MPI*, can either be used on single-processor or on multi-processor systems.

3 Results

3.1 Breakup of Liquid Jets

It is known from literature [14] that breakup of liquid jets is a result of the aerodynamical interaction of the liquid jet and the surrounding gas. Analyzing the breakup phenomena, three different disintegration mechanisms, depending on the jet velocity, can be observed. Rayleigh type breakup given by the jet stability theory of Lord Rayleigh in 1878, which is mainly influenced by surface tension forces, is typical for low flow velocities. Higher jet velocities lead to a wavy breakup where unstable wave growth on the jet surface leads to a more complicated disintegration phenomena. High velocities lead to atomization of the jet into small droplets (spray) near the nozzle exit which is mainly caused by turbulence effects inside and outside the nozzle.

However, fluid properties e.g. surface tension, viscosity and density, ambient conditions such as velocity, pressure and temperature, nozzle geometry and unsteady effects lead to complicated conditions where friction between the liquid and surrounding gas, unstable wave growth and turbulence cause a disintegration of the jet. The specific behavior influenced by the various parameters cannot be exactly described in one approach. This is one of the main reasons for numerical simulation of this problem. Outside of experiments this is the only method to obtain precise results for a given problem. A clear advantage of direct numerical simulation results compared to experimental results is given by a high numerical accuracy combined with moderate efforts for various simulation setups once the implemented numerical schemes are validated and stable. Nevertheless, a crucial point in this context represents the requirement of computational resources, which can at the present time only be provided by multi-processor supercomputers such as HLRS-CRAY Opteron cluster in our case.

Computational domain and numerical setup

In order to simulate the current problem, the flow area must be discretized. This is performed on a rectangular geometry with an uniform mesh. The size of the computational domain depends mainly on the diameter, D , of the nozzle and the jet injection velocity, u_{inflow} , with respect to the specific spreading rate of the jet. For most simulations, the length of the domain was set to $L = 16H$ or $L = 32H$ while the height, H , and the width, W , of the channel usually was set to $H = W = 5D$ similar to the setup presented in Fig. 1. Figure 1 also shows how the domain is decomposed between the processors.

Once discretization of the domain is complete the boundary and the inflow conditions must be defined. In order to avoid influences of solid walls the boundary condition, except at the inflow side, is set continuous while the inflow side wall is set to a free slip condition. At the inflow, the nozzle diameter, D , and the inflow velocity of the jet are defined.

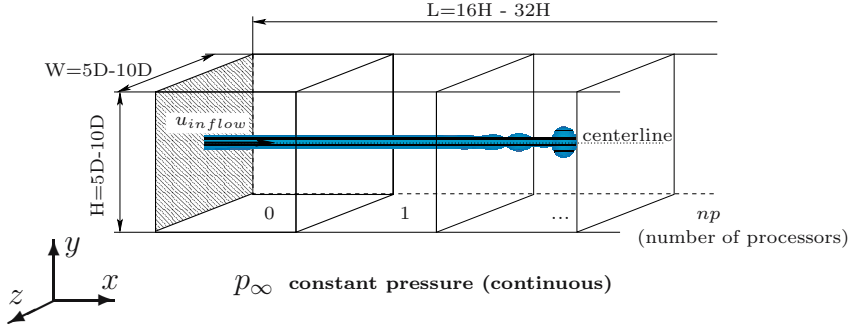


Fig. 1. Computational domain and grid

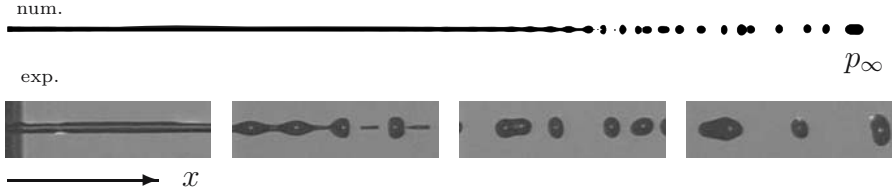
A crucial point in this context is the resolution of the computational domain. Of course it would be best to have an extremely fine spatial resolution according to the idea of DNS. Apart from this, it is also necessary to find a good compromise with respect to the computational resources. A typical grid size for the presented setup yields e.g. $3072 \times 96 \times 96$ grid points. Using 32 CPU's this yields 96^3 grid points per CPU in this case. Depending on the breakup length of each specific case, it is possible to set up the required computational domain by adapting the number of processors along the x -direction of the jet, as shown in Fig. 1.

Comparing results

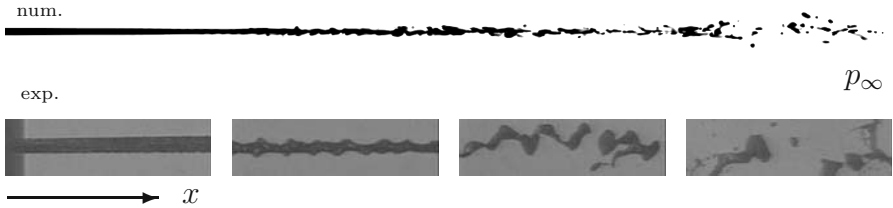
With the previously presented numerical setup, several numerical simulations were performed in order to control the capability of the numerical models implemented in FS3D for the given problem on the previously mentioned computational platform. The presented work represents a first step in order to demonstrate the capability and efficiency of DNS for breakup phenomena. It focuses basically on the accuracy and reliability of the numerical results which are compared to experimental data at different breakup types. The following results were obtained from similar numerical setups at various inflow velocities.

Firstly, the well known Rayleigh type breakup was simulated as presented in Fig. 2. For this, the numerical setup was selected as mentioned previously with an inflow velocity of the jet of 7 m/s and a jet diameter $D = 150 \mu\text{m}$.

The obtained results of the numerical simulation are represented by 2D contour plots from a 3D simulation of an n-pentane liquid jet ejected into air at atmospheric pressure. The comparison between the numerical and experimental results demonstrate the good qualitative agreement with several 'satellite' droplets rising from the continuous jet typical for Rayleigh breakup. While the diameter and the breakup length are not scaled, the breakup characteristics are qualitatively similar in this case.

**Fig. 2.** Rayleigh type breakup

With higher inflow velocities the breakup type changes from the Rayleigh type breakup to a wavy type breakup as presented in Fig. 3 where small instabilities lead to oscillations with respect to the jet axis and finally to a disintegration of the jet. The presented results were also obtained from a 3D simulation of an n-pentane liquid jet ejected into air at atmospheric pressure with an injection velocity of 100 m/s. From the comparison between the numerical and experimental results, once again a good qualitative agreement between the results can be found concerning the breakup phenomena.

**Fig. 3.** Wavy type breakup

Since 3D simulations at high grid resolutions require large computational resources, it is necessary to simplify the present problem in order to optimize the balance between the required simulation time and the computational effort. Due to the presented results and the unsteady character of the flow there is no possibility to create a simulation setup with symmetrical wall boundary conditions. Another simplification could be achieved by restricting the full 3D geometry into a 2D geometry. For this, the momentum transport in z -direction is disabled. The difference between the two models illustrated in Fig. 4 demonstrates the strong difference caused by this simplification. This leads to the conclusion that simulation of breakup phenomena cannot be simplified in this context either by 2D simulation or symmetry. Nevertheless it is important to mention that a 2D simulation leads to results obtained from disintegration of liquid sheets which have not been studied in this work so far.

Thus it is clear that breakup phenomena of circular liquid jets can only be simulated with a full 3D simulation model which leads to the need of higher computational resources depending on the spatial resolution. Besides this, the

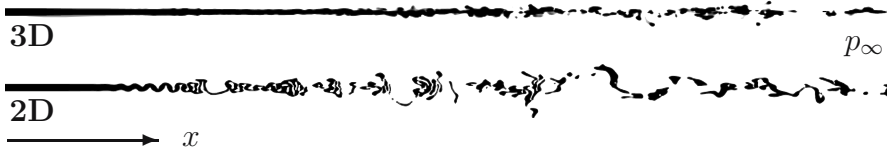


Fig. 4. 2D and 3D simulation results

temporal evolution of the breakup phenomena must also be captured. Direct numerical simulation provides a good possibility to achieve this requirement due to the very small time steps with respect to the grid size and the CFL (Courant-Friedrichs-Levy) criterion.

According to the presented results it finally makes sense to classify the breakup types depending on the injection velocity u_{inflow} of the jet. Since the liquid momentum is not large enough, a continuous jet cannot be formed and dripping from the nozzle tip can be observed. An increased injection velocity leads to a steady streaming jet. The ejected jet appears smooth and undisturbed near the nozzle tip, but after a certain distance downstream wavy disturbances appear at the liquid surface. These surface waves are propagated and amplified downstream. Once the amplitude corresponds with the jet diameter first liquid drops are pinched from the continuous jet. The length from the nozzle tip to the position where the first drop is formed is defined as breakup length L_b according to [14] (see Fig. 5). The breakup length increases linearly up to a maximum length inside the 'smooth jet region' where formed drops have almost a radius twice as high as the liquid jet. Higher velocities result in a decrease of the breakup length in a transient region. In the wavy region, droplets appear to be stripped off the jet where the average droplet radii are smaller. Finally the circular jet forms a core surrounded by small

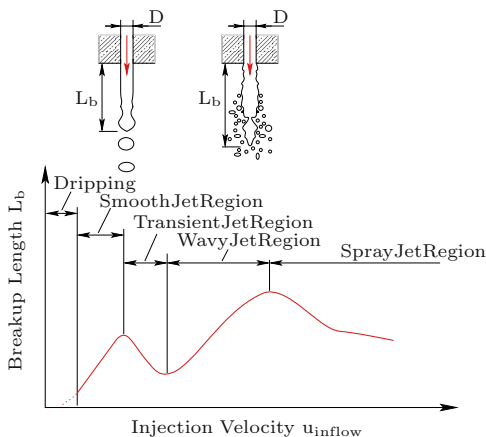


Fig. 5. Breakup length at different injection velocities (from [14] and [15])

droplets. The jet can be called atomized in this context. As the injection velocity increases further, the entire jet forms a small core near the nozzle tip surrounded by numerous droplets. The completely atomized jet can be called a spray.

According to [15] the breakup process and the breakup length, can be influenced by different inflow conditions such as specially designed injection nozzles. It can be assumed that different inlet conditions including cavitation and flow fluctuation caused by the nozzle design can greatly influence the breakup length. A similar behavior was also found by [16] for numerical results. Numerically generated inflow data for the inflow velocity of the jet was used to study the influence of prescribed turbulent length scales on the disintegration of the jet (see also [17]).

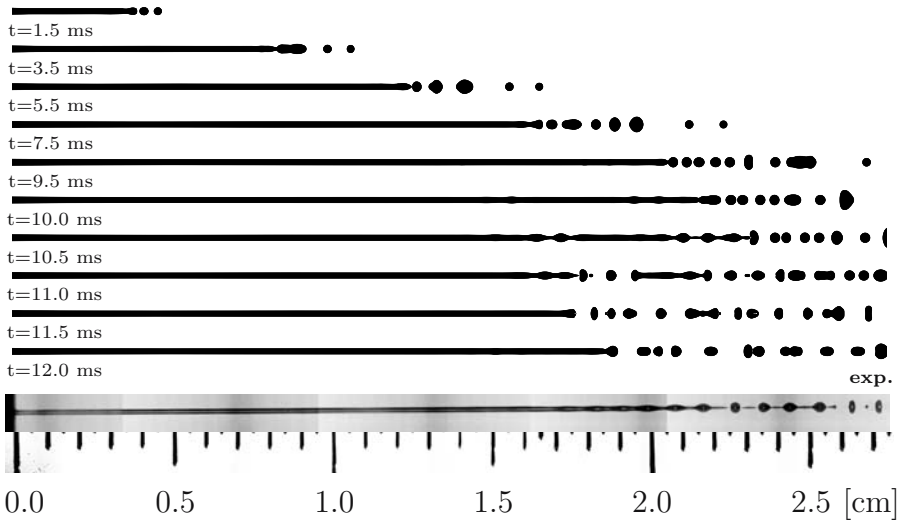


Fig. 6. Temporal evolution of a decane jet injected into nitrogen - 2D contour plot (experimental results by [18])

The highly transient breakup process of a decane liquid jet ($D=200\ \mu\text{m}$) ejected into nitrogen with an injection velocity of 5 m/s at an ambient pressure of 3 bar is presented in Fig. 6. The temporal evolution of this Rayleigh type breakup process can clearly be evaluated from the presented simulation results. In particular, the 'satellite' droplet formation, but also the breakup length, can be simulated. Since breakup mechanisms and the related breakup length is strongly dependent on the inflow condition it is not usual to reach a good quantitative accordance with experimental data. In particular the breakup length but also the spreading rate of the jet is influenced by this condition. Nevertheless, it is possible to realize a good overall agreement of the numerical results compared to the experimental data in this case.

3.2 Collision-induced Breakup of Raindrops

The time rate of change of a drop size distribution $f(m)$, m = drop mass, is commonly described by the stochastic collection equation [1]. That part of this equation concerning collisional breakup (CBU) reads (by neglecting for $f(m)$ its dependence on space and time for convenience)

$$\begin{aligned} \left. \frac{\partial f(m)}{\partial t} \right|_{CBU} = & \frac{1}{2} \int_0^\infty \int_0^x f(x)f(y)B(x,y)P(m;x,y)dydx \\ & - \int_0^\infty \frac{f(y)f(m)B(m,y)}{m+y} \int_0^{m+y} xP(x;m,y)dx dy \end{aligned}$$

with $B(x, y)$ = breakup function, $m = x + y$ and $P(m; x, y)$ = fragment density function. The first term on the r.h.s. represents breakup-induced production of drops with mass m by collisions of two drops with masses x and y whereas the second term describes the loss of drops with mass m taking part in a collision event with a drop of mass x or y , respectively. Besides the well-known breakup function $B(x, y)$ the fragment density function $P(m; x, y)$ contains the essential physics of the breakup mechanism. Physically $P(m; x, y)$ represents the conditional probability of obtaining a small drop in the mass interval $[m, m + dm]$ by collision and breakup of two drops with initial masses in the intervals $[x, x + dx]$ and $[y, y + dy]$ and can be expressed as product of a size distribution function of the fragments weighed with the relative occurrence of a specific breakup mode. In general, several modes of collisional breakup may have to be taken into account; in [5] the modes 'filament', 'sheet' and 'disk' are discriminated.

As mentioned in the Introduction it should be noted that up to now the only information on fragment density functions $P(m; x, y)$ stem from very few older laboratory experiments done by [4] and [5] as well as by [6] and [7].

Thus, ongoing and future simulations of raindrop breakup serve (i) to identify specific breakup modes and their relative appearance as well as (ii) to determine the corresponding specific fragment's size distribution functions. In a first step the results from the laboratory experiments cited above will be assessed by numerical experiments using FS3D. Thereafter the entire diameter ranges of colliding raindrops experiencing breakup is taken into account thus extending and completing the disparate data from the physical experiments. Finally $P(m; x, y)$ has to be expressed by mathematical formulae for use in models describing precipitation evolution.

Case studies according to the setup of [5]

Using FS3D first case studies on collisional breakup of raindrops have been performed with the diameter of the larger drops ranging between 0.18 and 0.46 cm and those of the smaller drops between 0.0395 and 0.18 cm, the same setup as investigated by [5] except that in the present study excentricity effects have additionally been considered: excentricity values ranged from 0.025

($\approx$ central impact) to 0.975 ($\approx$ grazing collision). For water standard material parameters are applied. The drops move in air at rest and have same temperature as the air.

An important feature of FS3D is that the fluid's circulation inside the drops interacting with the external flow field is simultaneously calculated the combination of which crucially influences the collision/breakup process [1]. As the equilibrium shape of large drops can deviate more or less strongly from sphericity this effect has been considered as initial condition by a relation of [19]. For the velocities of the drops the sophisticated formula [20] has been taken into account.

Due to the extremely fine temporal and spatial resolution of the numerical simulations the collision/breakup process could be followed in greatest detail. Computations are stopped after the collision/breakup event relaxed to a stable, i.e. stationary, configuration. The number and size of all fragments have been determined by a region growing method. Mass conservation was fulfilled in each case. To match the current results with those of [5] the data for different excentricities have been summed up by a weighed mean based on the relative mass difference for different excentricities.

Figure 7 exhibits the outcome of a collision event of two drops where the larger drop has a diameter of 0.36 cm (fall speed 8.64 m/s) and the smaller of 0.1 cm (fall speed 4.03 m/s) after an elapsed simulation time of 4.0 ms. The excentricity chosen is 0.7. It is clearly seen that due to the relatively large excentricity the smaller drop is at first only partly incorporated into the larger one followed by a continuous disruption where larger and smaller fragments are created: One may suspect that the size of the larger drop remains nearly equal as that of the smaller drop. This type of breakup is categorized as 'filament' mode.

However, compared to the initial configuration the size and mass differences, respectively, of the drops after collision/breakup account for the fragment drops showing a considerable size distribution quantified in Fig. 8. Note that some droplets of very small radii are produced. This is in contrast to the laboratory experiments of [5] and indicates the advantage of a precise numerical method or, vice versa, the limitation of physical experiments.

The blue line refers to a functional fit to the laboratory data based on [5] and the red stars show the data obtained from the numerical results. It is seen that in this case the initial large raindrop and to a lesser extent also the initial smaller one 'survive' whereas a considerable number of fragments in the diameter range < 0.1 cm appears. Note that the number of droplets with very small diameters increases with decreasing size. This feature is not represented by the formulae proposed by [5] who were not able to detect such tiny droplets in their experimental setup.

First results reveal that, compared to those of [5], the breakup modes identified in the laboratory experiments show up more or less pronounced also in the numerical simulations. Ongoing numerical experiments shall cover also size ranges not investigated by [5] with additionally considering excentricity.

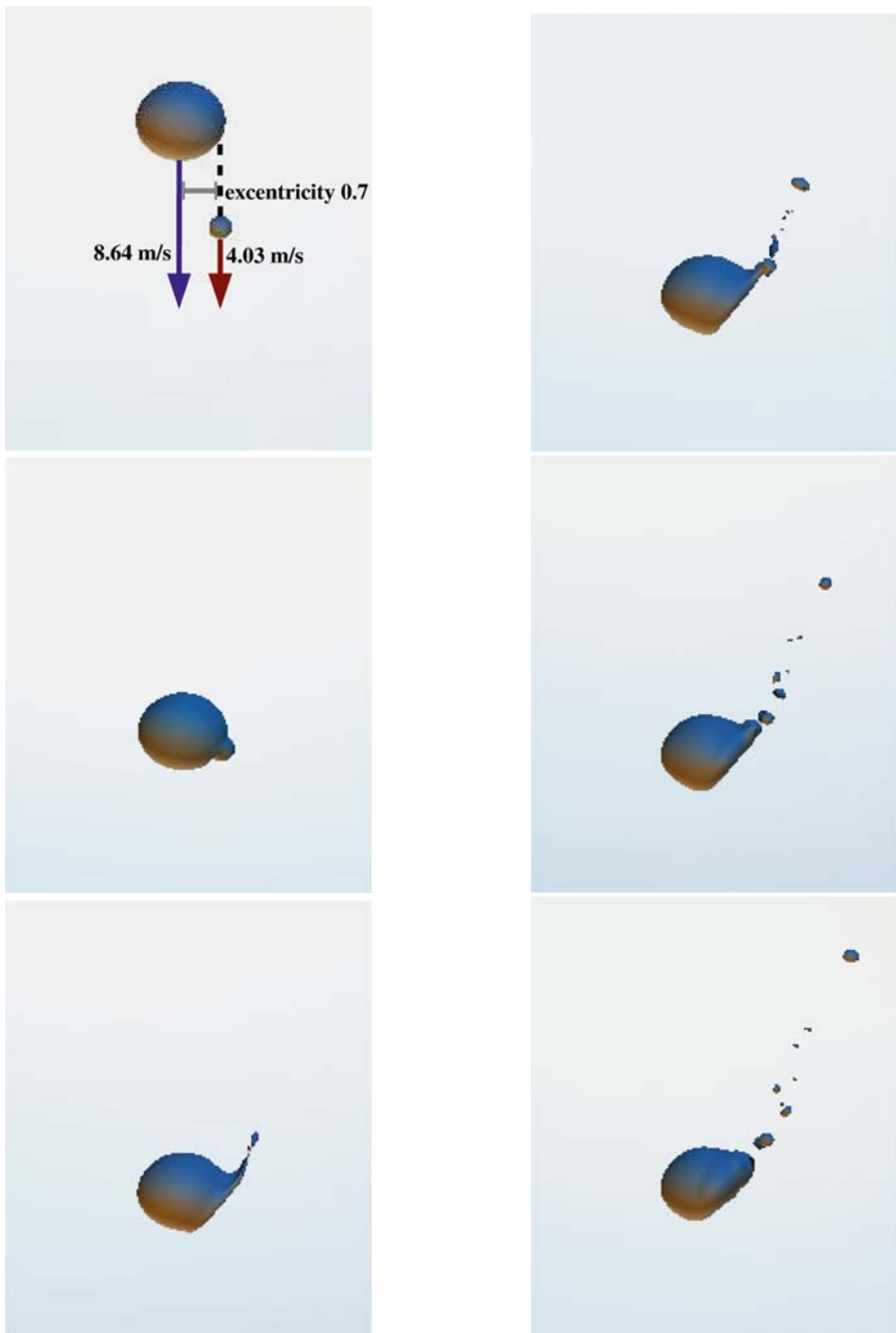


Fig. 7. Time series of a collision between two differently sized large raindrops showing breakup: Start at $t = 0$ s (left upper plate) and end after 4.0×10^{-3} s (lower right plate) in time intervals of 0.8×10^{-3} s. For details see text.

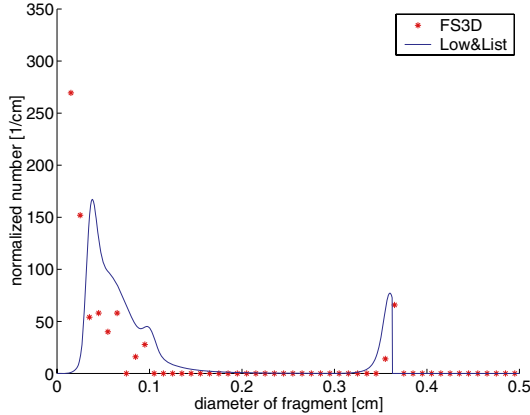


Fig. 8. Normalized number of fragment drops in cm^{-1} as function of diameters of these drops in cm for the case study of Fig. 7. For details see text.

After finishing the simulations presented so far a different setup will be chosen. As mentioned earlier further breakup experiments have been made by [6] and [7]. They considered pairs of drops where the diameter of the larger drop ranges between 0.055 cm and 0.085 cm and that of the smaller drop from 0.038 cm to 0.06 cm with varying excentricity. Comparing these diameter ranges to those investigated by [5] it is clear that they are disjoint. Thus the final goal of the present simulations is a close coverage of the entire range of raindrop diameters relevant to collisional breakup.

4 Computational Resources

All results presented in this paper have been computed on the CRAY-Opteron Cluster at the HLRS. Concerning the computational time for the presented breakup problem, time cycles vary due to the explicit time discretization with respect to the grid size and the CFL (Courant-Friedrichs-Levy) condition between approximately 10^{-6} s and 10^{-8} s at a velocity range between 5 m/s and 100 m/s. The grid resolution on each CPU was 96^3 (884,736 cells) while the number of required CPU's depends on the breakup length of the actual case. It can be assumed that the number of required CPU's usually varies between 16 and 32 depending on the mesh size of the grid and the size of the computational domain. The computational time also depends on the actual case and varies between 48 h up to 96 h or even more depending on the temporal evolution of the flow until a quasi stationary status is reached.

The raindrop breakup simulations have been done on the same system as for the jet calculations but with 8 CPU's and a grid resolution of $256 \times 256 \times 256$ cells. Also an explicit time discretization is applied so far which results -

owing to the fulfillment of the CFL criterion - in time steps of $\approx 10^{-5}$ s. The computational time is, depending on collision configuration, approximately 20 h made up by nearly 2100 time steps. The setup time was 46.8 s and the mean cycle duration 33.5 s.

5 Concluding Remarks

Two phase flow is of fundamental interest in various scientific disciplines. With experiments or analytical solutions many related questions have been answered in the past. Unfortunately it is not possible to resolve all problems with experiments or analytical solutions. The main reason for this situation usually is a very complex system of equations where analytical solutions cannot usually be found. Apart from this, experimental setups are restricted to a certain temporal and spatial resolution.

As presented in this study, direct numerical simulation is able to provide basic results concerning, e.g., the breakup process of liquid jets. Promising results have been presented and show a good qualitative agreement with experimental data. A very important aspect, especially for future research, must be consideration of inflow conditions caused by the nozzle flow. Since the breakup length and the breakup mechanisms are strongly coupled to the inflow condition it is necessary to focus in future setups on the influence of the inflow condition. Another important aspect here is linked to the question of how far disintegration of the liquid jet can be controlled by numerically generated inflow conditions according to the idea of digital filter based inflow data.

Regarding raindrop breakup the results obtained so far show convincingly the ability of numerical simulation to reliably describe the process under consideration: Mostly the findings of the laboratory investigations are recovered albeit some differences occur. Encouraged by this result the simulations will be continued by including different scenarios with the challenging chance to get a consistent data set for considering collision-induced breakup in cloud models – and, as an ultimate goal, for improving precipitation forecasts.

Acknowledgments

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Numerical Investigation of the VKI Turbine Blade by Large Eddy Simulation

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1 Introduction

The performance of turbine blades strongly depends on the turbulence occurrence. Appearance of heat transfer (with or without film cooling) makes this flow particular sensitive to turbulence. Thus, a key issue in CFD simulations of turbomachines is turbulence prediction. Some years ago, detailed experimental investigations of VKI turbine cascade were carried out by Ubaldi et al. [UZCG96]. The investigations were focused on the transitional boundary layer development at high Reynolds number (1.6×10^6). The ultimate goal of this project was to improve transition modeling in numerical simulations which is still not an entirely resolved problem. The database, produced by experiment, was adopted as official test case by ERCOFTAC Transition Modeling SIG10 and TRANSPRETURB [Pit02]. The test case was widely used in verification and validation of numerical codes as well as for development of turbulence models by many research groups.

In order to investigate the effect of Reynolds number on the blade boundary layer transition, Canepa et al. [CCPUZ03] have recently performed on the same geometry new experiments at lower Reynolds numbers (3.1×10^5 - 1.0×10^6). The measurements at Reynolds number 5.9×10^5 were made extensively. This, likewise the previous experimental investigations at Reynolds number 1.6×10^6 , gave a useful database for a comparison with numerical simulations.

The standard method to simulate flow fields is to solve the well-known Reynolds-averaged Navier-Stokes system of equations (RANS), that describe the evolution of the mean quantities. All turbulent fluctuations must be modeled to close the system. Turbulence models are usually developed and tested using simple geometries like 2D/3D channels, a flat plate and jets. They are also mainly based on empirical data. For more complex geometries those models are mostly adjusted for the particular case, therefore their usability is limited. Realistic flow comprises wide range of scales. The small scales depend

only on viscosity, where the large ones are mainly affected by the boundary conditions. This implies that the different scales should also be modeled diversely or, in other words, one model can hardly model the whole range of scales.

As mentioned above, it is hardly possible to model turbulence of different scales by means of only one turbulence model and DNS is numerically too expensive. To overcome those problems Large Eddy Simulation (LES) has been proposed. This approach is some kind of a compromise between RANS and DNS. The large scales, energy-carrying structures of turbulent flow are computed exactly, and only the smallest, subgrid scales (SGS) have to be modeled. The smallest, nearly isotropic eddies are less affected by the boundary conditions than the large ones. Thus, this suggests that SGS models should be simpler and more independent from complexity of geometries. LES, alike DNS, provides a three-dimensional, time dependent solution of the Navier-Stokes equations. It also requires fine meshes, but simulated flows can have a higher Reynolds number [PC96]. Michelassi et al. [MWR03] carried out investigations of the unsteady periodic flow in a low-pressure (LP) prismatic turbine vane at a Reynolds number of 5.18×10^4 . They performed calculations by means of DNS, LES and unsteady RANS (URANS), giving a great opportunity to look at differences.

The recent measurements carried out by Canepa et al. [CCPUZ03] at a lower Reynolds number (5.9×10^5) gave a great opportunity to apply Large Eddy Simulation on the well-known test case - the VKI turbine cascade. Hence numerical investigations of LES have been performed by means of our own code called SPARC. The comparison of the results with experimental data is presented in this paper. The investigations were focused on the prediction of the boundary layer on the suction side of the profile. The paper includes a discussion of problems appeared during investigation of the test case. The discussion involves boundary conditions and the mesh generation.

2 The code description

SPARC is parallelized by means of the Message Passing Interface (MPI). This code [Mag98] is compressible and solves 3D steady and unsteady Reynolds Averaged Navier-Stokes (RANS) equations as well as is able to perform LES and Direct Numerical Simulation (DNS). It is a block structured, Finite-Volume code using non-orthogonal grids and full multigrid methods. The code uses the cell-centered approach. For steady computations an explicit Runge-Kutta scheme is implemented, while for unsteady flows the explicit Runge-Kutta and the implicit dual time stepping schemes are used. Several turbulence and SGS models are implemented into the code. The box filter is implemented for filtering SGS. One can choose between different numerical schemes that are based on the artificial dissipation concept, proposed by Jameson et al. [JST81], Liou and Steffen [LS93] and Swanson and Turkel [ST96].

3 Description of test case

Geometrical characteristics and operating conditions

The blade profile is representative of a coolable hp gas turbine nozzle blade and is the same tested during the European project on time-varying wake flow characteristic on flat plates and turbine cascades [SCDMZ99]. A description of the considered cascade can be found in Table 1. The Reynolds number (Re_{2c}), given in the table, is based on chord length (c).

Table 1. Cascade characteristics

Chord length – c	$0.3m$
Pith-to-chord ratio – g/c	0.7
Aspect ratio – h/c	1.0
Stagger angle (with axial direction) – γ	49.83°
Inlet total pressure – p_{tl}	$400Pa$
Inlet total temperature – T_{tl}	$300K$
Inlet turbulence level – Tu	3%
Outlet isentropic Mach number – Ma_{2is}	0.086
Outlet Reynolds number – Re_{2c}	593200

Setup of computations

The geometry of the mesh used in the current investigations is shown in Fig. 1. The numerical mesh used for computations consists of about 8.8×10^6 nodes and is splitted into 168 blocks. The distance between the blade and the mesh boundary in the upstream direction is about one chord length and the downstream direction about two chord lengths. In the spanwise direction the mesh is extended to the length of 0.1 of the chord length with 33 cells. No wall-function is used, therefore the mesh is refined down to the wall to resolve the viscous sublayer of the flow. The first grid point at the blade is located at $y^+ \approx 1$. According to Piomelli and Chasnov [PC96] the grid spacing along the wall Δx^+ should be between 15 and 40. It was kept about $\Delta x^+ \approx 30$.

Only one blade has been calculated using periodic boundary conditions. Special care was taken to have an orthogonal mesh at the blade and within the boundary layer region. This was done at the expense of the mesh orthogonality near the periodic boundary condition - in the middle of the pitch. The mesh had to be “deformed” in order to satisfy block connection at the

periodic boundaries. The mesh was smoothed to improve orthogonality. This is presented in Fig. 2. Fig. 2 shows the 7th finest mesh for better visibility (about 17,000 cells) where in each direction every 8th line was left.

A total pressure condition with random fluctuations has been applied at the inlet boundary. The random fluctuations ought to emulate the incoming turbulence. The values were taken directly from the experimental data (see Tab. 1). At the outlet boundary the static pressure condition has been used, where the value of pressure was adjusted to obtain the isentropic Mach number $Ma_{2is} = 0.086$. In the third direction there is a periodic condition. Non-reflecting boundary conditions at the inlet/outlet boundary were also applied, but no remarkable differences were noticed. Hence they were not applied during the simulations.

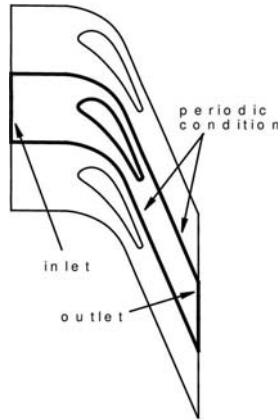


Fig. 1. The mesh geometry (thicker lines)

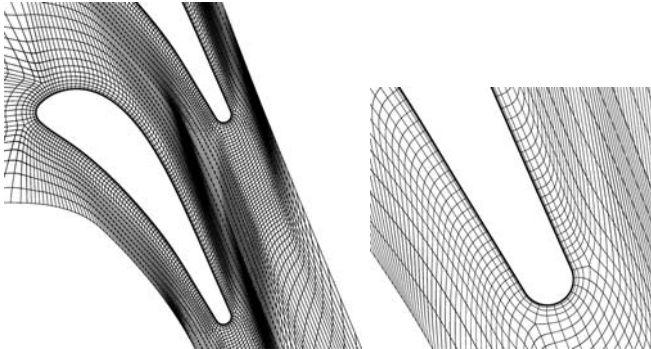


Fig. 2. Numerical mesh (every 8th node shown) and zoom of the trailing edge region

The numerical schemes used here are of second order accuracy both in space and time. The computations were performed using the Smagorinsky-Lilley model as well as the Monotonically Integrated Large Eddy Simulation (MILES) approach [FG99], where SGS structures modeling is based on an artificial dissipation approach.

Since the code uses an artificial dissipation method according to Jame-son et al. [JST81], an adequate dissipation factor has to be chosen by experience. Compared to URANS calculations this should be, according to our own experience, reduced to about 10% of the URANS dissipation factor otherwise the resolved fluctuations will be severely damped by the numerical scheme. Another way to provide low enough numerical dissipation is using the matrix dissipation scheme [ST96]. This is valid when a SGS model like the Smagorinsky-Lilley model is applied. Using the MILES approach the numerical dissipation must be greater. In this case the artificial dissipation does not only make the scheme stable but is also responsible for the SGS modeling. For MILES the dissipation factor was set to 20% of the URANS factor.

For marching in time the implicit dual time stepping scheme was employed. The first guess of the time step was made by means of the Strouhal number definition:

$$St = \frac{ls}{q},$$

where l is a characteristic length (here the thickness of the trailing edge $\approx 0.016m$), q - velocity (here velocity near the trailing edge $\approx 30\frac{m}{s}$), f - a vortex shedding frequency. The Strouhal number was set to 0.2. The period, calculated with the above assumptions and subdivided into 150 steps, gave an approximated time step of $1.8 \times 10^{-5}s$. A detailed investigation of the results enforces us to decrease the time step down to about $10^{-5}s$. In this case calculations with the implicit dual-time stepping scheme were chosen because of its efficiency.

Computational resources

The numerical simulations were carried out with the help of the *CRAY Opteron Cluster*. The typical number of used processors was 10 (5 nodes) at the beginning of computations, and 22 (11 nodes) later. The change was caused for better load balancing. The CPU time of the computation process (going through four mesh levels, flow developing phase and averaging) lasts ≈ 5.500 hours. The numerical simulations on the finest mesh needs about 12GB of memory, while during the averaging process about 18GB.

4 Results

In order to provide an insight into the three-dimensionality of the considered flow, the instantaneous profile of the spanwise component of the velocity w

is presented in Fig. 3. The noticeable three dimensionality appears in the boundary layer at $s/s_{max} \approx 0.5 \div 0.6$, approximately there, where - according to the experimental data at $s/s_{max} \approx 0.55$ - the laminar-turbulent transition ought to start. The strongest three-dimensionality is observed in the wake, close to the trailing edge, where the flow is highly turbulent. This high level of turbulence is caused by vortex shedding, where w can rise up to $\approx 50\%$ of the streamwise velocity.

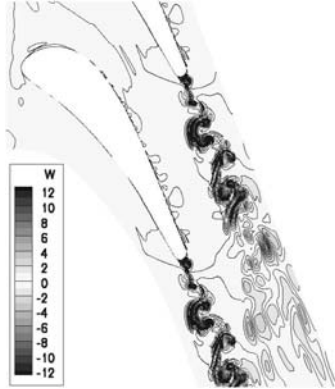


Fig. 3. Spanwise velocity component w (MILES approach)

Turbulence could be depicted by means of vorticity. It is also distinguishable in the Q -criterion pictures (see Fig. 4). The Q -criterion (positive values of Q) is a necessary condition for the existence of thin convex low-pressure tubes and therefore allows visualization of coherent vortices. The Q -criterion is defined as:

$$Q = \frac{1}{2} (\Omega_{ij} \Omega_{ij} - S_{ij} S_{ij}),$$

where

$$S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$$

and

$$\Omega_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right).$$

In Fig. 5 the comparison of the experimental data with the numerical results, obtained using Smagorinsky-Lilley model, of the boundary layer mean velocity profiles is shown. The chosen examples of the profiles show how the boundary layer develops along the suction side of the blade. The experimental data (points) shows at the beginning ($s/s_{max} = 0.32$) the typical laminar profile. The boundary layer at $s/s_{max} = 0.52$ indicates the tendency to separation. Next profile ($s/s_{max} = 0.56$) shows the boundary layer at the end of transition. The last plot represents the fully developed turbulent profile.

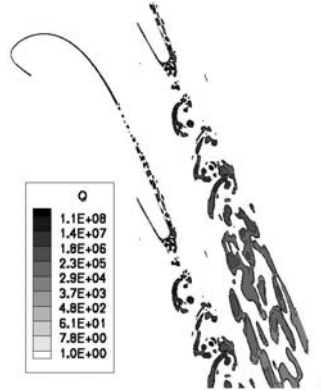


Fig. 4. Q-criterion (exponential scale)

Unfortunately only the first laminar profile of the simulations is in best agreement with the experiment. The boundary profile at $s/s_{max} = 0.52$ shows similar tendency to separation. The following profiles have turbulent shape, but reveal a turbulence deficiency in comparison to the experimental data.

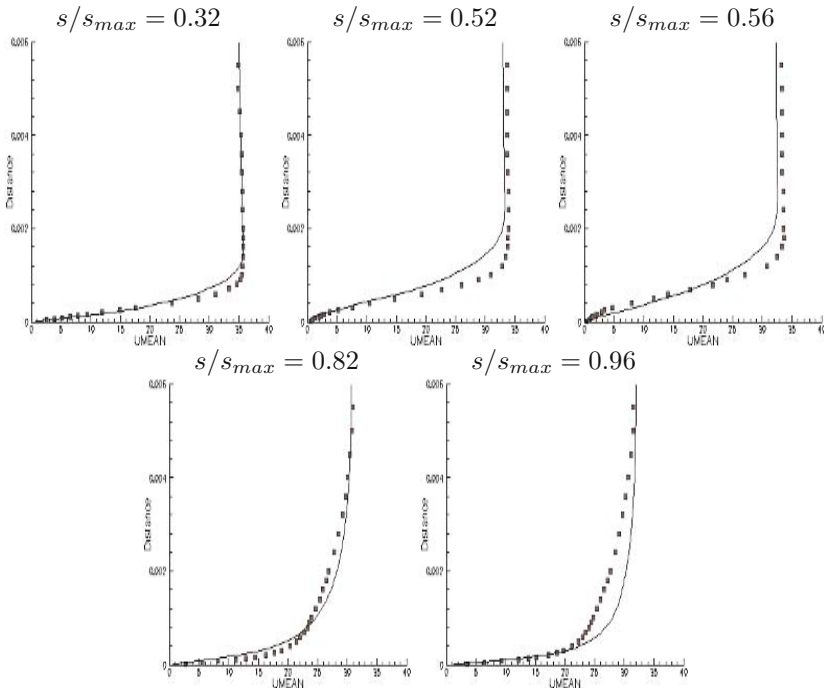


Fig. 5. Boundary layer mean velocity profiles at suction side – Smagorinsky-Lilley model (points – experimental data, lines – numerical results)

The discrepancy visible in the distribution of the streamwise velocity variance ($rms(u')$) along the suction side of the blade doesn't clarify the problem. In Fig. 6 one can see profiles of the $rms(u')$ variance within the laminar-turbulent transition region. The increase of the variance is mainly caused by the intermittent switches between laminar and turbulent states [CCPUZ03]. The peaks of $rms(u')$ indicate then the area of the laminar-turbulent transition. The experiment shows the transition between $s/s_{max} = 0.55$ and $s/s_{max} = 0.6$. In the numerical simulations the transition appears at the same position compared to the experiment.

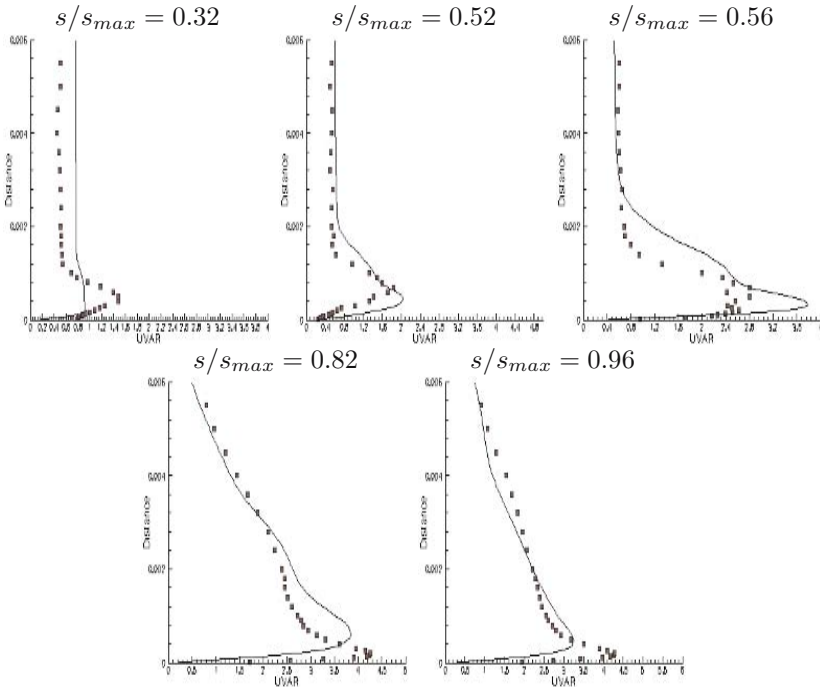


Fig. 6. The streamwise velocity component variance - Smagorinsky-Lilley model (points - experimental data, lines - numerical results)

Outside the boundary layer the calculated $rms(u')$ complies with the experiment. These streamwise fluctuations are enforced by the pulsating flow downstream. The maximal computed values of the $rms(u')$ in the laminar part of the flow ($s/s_{max} < 0.55$) are almost two times smaller than in the experiment. This seems to be caused by lack of upstream fluctuations. The turbulence development deficiency upstream of the transition region makes bypass transition impossible in the considered case. Therefore the transition in the simulations proceeds quietly and development of the turbulent boundary farther downstream is slower.

Figure 7 presents the profiles of the crosswise velocity component variance ($rms(v')$). The numerical calculations show lower fluctuations near the wall at $s/s_{max} = 0.82$ compared to the experimental data. This also indicates the deficiency of upstream turbulence.

The Reynolds shear stresses profiles are shown in Fig. 8. At the beginning they are almost equal to 0 and grow as the flow develops. The calculated Reynolds shear stresses are always lower in comparison to the experiment.

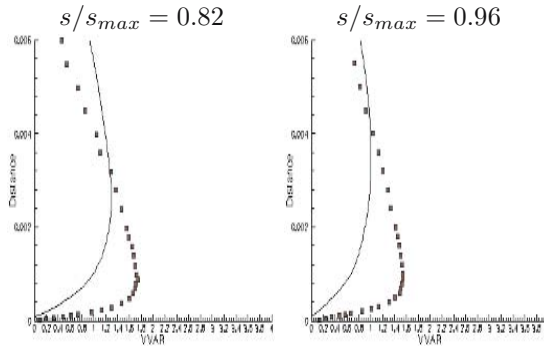


Fig. 7. Profiles of the crosswise velocity component variance - Smagorinsky-Lilley model

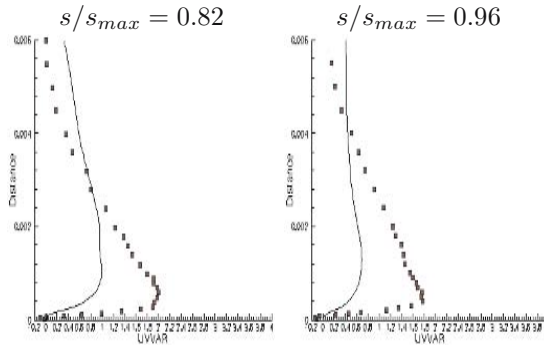


Fig. 8. Reynolds shear stresses - Smagorinsky-Lilley model

The incoming fluctuations inserted by means of the total inlet boundary condition with random fluctuations could not reach the cascade. This can be seen in Figs. 6÷8 - the values of the calculated rms and the Reynolds shear stresses values are low compared to the experimental data. The fluctuations were suppressed before they had arrived at the blade row. The random fluctuations are inserted at the inlet in such a way that the inflow has the correct

turbulent kinetic energy. Since these fluctuations are not coherent and have no correlations in space and time, they do not reflect real turbulent fluctuations. Turbulent coherent large-scale structures initiate the cascade of turbulent kinetic energy from large to small scales. The inflow fluctuations are inserted with the frequency of the time step hence they do not contain the whole energy spectrum of turbulence. As a result, the fluctuations have more energy in the high wave numbers and dissipate very fast without sustaining or initiating real turbulence. In order to overcome this problem one must apply a better inlet boundary condition.

We underestimated in the considered case the importance of correct upstream turbulence, therefore no suitable inlet boundary condition was applied to the simulations. This resulted in the deficiency of upstream turbulence and therefore the transition could not be enforced by the bypass mechanism. The transition in the simulation with Smagorinsky-Lilley model proceeded in the natural way.

The simulations carried out with employment of MILES approach suffer from the same reason. Within the laminar part of the boundary layer (see Fig. 9 at $s/s_{max} = 0.32$) computed boundary layer profiles stay in a good agreement with the experiment. In contrast to simulations where

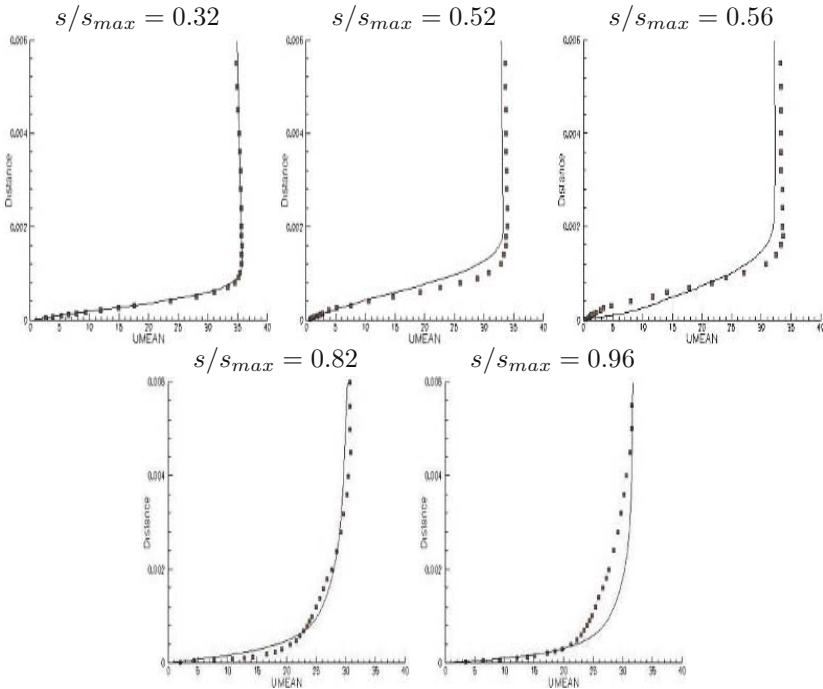


Fig. 9. Boundary layer mean velocity profiles at suction side – MILES approach (points – experimental data, lines – numerical results)

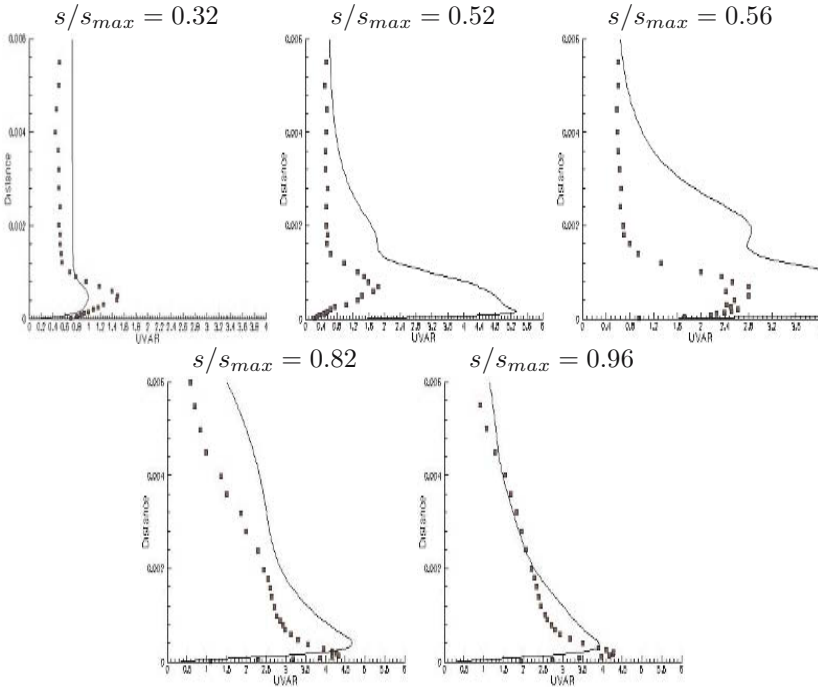


Fig. 10. The streamwise velocity component variance – MILES approach (points – experimental data, lines – numerical results)

Smagorinsky-Lilley model was applied, the upstream turbulence was not enough to prevent a small separation that appeared at $s/s_{max} = 0.52$.

In Fig. 10 one can recognize the separation through larger $rms(u')$ values. This separation enforced the start of the laminar-turbulent transition. Even the separation did not help to obtain enough turbulence behind the laminar-turbulent transition region (see the plot at $s/s_{max} = 0.96$ in Fig. 9).

5 Conclusions

In the frame of this work, the numerical investigations of the flow through the VKI turbine cascade were performed by means of Large Eddy Simulation.

The numerical simulation has delivered detailed aerodynamical information as well as showed problems and the importance of a proper mesh generation for LES. The mesh down to the wall and along the wall must be fine enough in order to resolve the expected structures.

The importance of upstream turbulence was underestimated. Therefore, no suitable inlet boundary condition was applied to the simulations. The lack of the upstream fluctuations caused deficiency of the turbulence development

in the boundary layer and therefore bypass transition was impossible. In the simulations the transitions proceeded in the natural way, hence the transitions were quieter and the development of the turbulent boundary farther downstream was slower.

At the present times computational resources necessary to perform a (U)RANS simulation of the considered case does not cause a problem. Computations of flows through complex geometries at higher Reynolds numbers with LES are still the challenge for CFD and super computers.

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A Hybrid LES/CAA Method for Aeroacoustic Applications

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1 Introduction

In aeroacoustics turbulence is often a source of sound. The direct approach of noise computation via a Direct Numerical Simulation (DNS) including all turbulent scales without any modelling is still restricted to low-Reynolds number flows and for real technical applications computationally too expensive. An attractive alternative is the Large Eddy Simulation (LES) which resolves only the turbulent scales larger than the cell size of the mesh. In order to take advantage of the disparity between fluid mechanical and acoustical length scales it is reasonable to separate the noise computation into two parts. In a first step, the LES resolves the acoustic source region governed by nonlinear effects. In a second step the acoustic field is computed on a coarser grid by linear acoustic equations with the nonlinear effects lumped together in a source term being calculated from the LES. The feasibility of such a hybrid LES/CAA method is demonstrated in the following by means of two different applications, airframe noise and combustion noise. The first part of the two-step method, the LES computation, is shown for airfoil flow. The present results will comprise a detailed analysis of the turbulent scales upstream of the trailing-edge, a thorough investigation of the surface pressure fluctuations and the trailing-edge eddies generated in the near-field wake based on LES findings. The simulation provides the data that allows the acoustic source functions of the acoustic wave equations to be evaluated. The second part, the application of the CAA method, is performed for combustion noise of unconfined turbulent flames. The acoustic analogy used for the acoustic field computation is the system of the Acoustic Perturbation Equations (APE) which have been extended to take into account noise generation by reacting flow effects.

2 LES for Trailing Edge Noise

Turbulent flow near the trailing edge of a lifting surface generates intense, broadband scattering noise as well as surface pressure fluctuations. The accuracy of the trailing-edge noise prediction depends on the prediction method of the noise-generating eddies over a wide range of length scales. Recent studies indicate that promising results can be obtained when the unsteady turbulent flow fields are computed via large eddy simulation (LES). The LES data can be used to determine acoustic source functions that occur in the acoustic wave propagation equations which have to be solved to predict the aero-acoustical field [5, 6, 7].

The turbulence embedded within a boundary layer is known to radiate quadrupole noise which in turn is scattered at the trailing edge [20]. The latter gives rise to an intense noise radiation which is called trailing-edge noise. Turbulence is an insufficient radiator of sound, particularly at low Mach number, $M_\infty \leq 0.3$, meaning that only a relatively small amount of energy is radiated away as sound from the region of the turbulent flow. However, if the turbulence interacts with a trailing edge in the flow, scattering occurs which changes the inefficient quadrupole radiation into a much more efficient dipole radiation [20].

The noise generated by an airfoil is attributed to the instability of the upper and lower surface boundary layers and their interactions with the trailing edge [9]. The edge is usually a source of high-frequency sound associated with smaller-scale components of the boundary layer turbulence. Low-frequency contributions from a trailing edge, that may in practice be related to large-scale vortical structures shed from an upstream perturbation, are small because the upwash velocity they produce in the neighborhood of the edge tends to be canceled by that produced by vorticity shed from the edge [9]. For this purpose, a large-eddy simulation is carried out to simulate the three-dimensional compressible turbulent boundary layer past an airfoil-flap configuration and airfoil trailing edge which can be used for an acoustic simulation.

3 Computational Setup for Airfoil Flow

One of the primary conclusions from the European LESFOIL project is that an adequate numerical resolution especially in the near wall region is required for a successful LES. On meshes which do not resolve the viscous near-wall effects, neither SGS models nor wall models were able to remedy these deficiencies [1]. According to the experience from LES of wall bounded flows, the resolution requirements of a wall resolved LES are in the range of $\Delta x^+ \approx 100$, $\Delta y^+ \approx 2$ and $\Delta z^+ \approx 20$, where x, y, z denote the streamwise, normal, and spanwise coordinates, respectively. During the mesh generation process, it became clear that it would lead to meshes with unmanageable total grid point numbers,

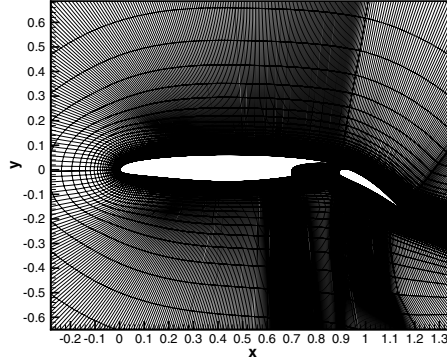


Fig. 1. Computational mesh in the x-y plane, which shows every second grid point.

if these requirements are to be followed strictly. For the preliminary study, the streamwise resolution is approximately $\Delta x^+ \approx 200 \sim 300$, whereas the resolution is set to $\Delta y_{min}^+ \approx 2$ and $\Delta z^+ \approx 20 \sim 25$ in the wall normal and in the spanwise direction, respectively. The mesh of the preliminary study is shown in Fig. 1.

The extent of the computational domain is listed in Table 1. The spanwise extent of the airfoil is 0.32 percent of the chord length. A periodic boundary condition is used for this direction. The relatively small spanwise extent is chosen because of the following two reasons. On the one hand, it was shown for flat plate flows that due to the high Reynolds number of $Re = 1.0 \times 10^6$, two-point correlations decay to zero already in about 250 wall units [3] and on the other hand, since a highly resolved mesh was used in the wall normal and tangential direction the computational domain must be limited to a reasonable size to reduce the overall computational effort. Towards the separation regions in the flap cove and at the flap trailing edge, the boundary layer thicknesses and the characteristic sizes of turbulent structures will increase. Therefore, especially for these areas, the spanwise extent of the computational domain needs to be increased in further computations. A no-slip boundary condition is applied at the airfoil surface, and a non-reflecting boundary condition according to Poinso & Lele [14] is used for the far field.

Another possibility to enlarge the spanwise extent without increasing the total number of grid points and as such the overall computational effort, is to focus the analysis on the zone of the flow field that is of major interest for the sound propagation. For the airfoil flow problem this means that a local

Table 1. Computational domain and grid point distribution, SWING+ Airfoil ($Re = 10^6$) .

L_X	L_Y	L_Z	$N_x \times N_y$	N_z	Total Grid Points
-4.0 ... 5.0	-4.0 ... 4.0	0 ... 0.0032	241.320	17	4.102.440

analysis of the flow in the vicinity of the trailing edge has to be pursued. To do so, we apply the rescaling method by El-Askary [3] which is valid not only in compressible flows but also in flows with weak pressure gradients. This procedure is a consistent continuation of the approach that was already successfully applied in the analysis of the trailing edge flow of a sharp flat plate [7, 5, 16, 4, 15].

4 Airfoil Flow Results

In the following, we discuss first the LES of the airfoil-flap configuration and then turn to the zonal analysis of the airfoil trailing edge flow. In both problems numerical and experimental data are juxtaposed.

In the flow over the SWING+ airfoil with deflected flap, separations exist in the flap cove and at the flap trailing edge. In the current numerical simulation, both separation regions are well resolved. They are visible in the time and spanwise averaged streamlines of the numerical simulation (Fig. 2).

The turbulent flow is considered to be fully developed such that the numerical flow data can be time averaged over a time period of $\Delta T = 3.0 c/u_\infty$, and then spanwise averaged to obtain mean values. The distribution of the mean pressure coefficient c_p over the airfoil surface is plotted in Fig. 4. A good agreement with the experimental data [22] is achieved. It is worth mentioning, that the onset of the turbulent flow separation and the size of the separation bubble in the vicinity of the flap trailing edge are captured quite exactly by the numerical simulation. This can be seen by the plateau in the c_p -distribution near the trailing edge of the flap.

In the experiments carried out by the Institute of Aerodynamics and Gasdynamics of the University Stuttgart, profiles of the wall tangential velocity were measured at five locations two of which were on the airfoil and three on the flap [22] (Fig. 3). The mean velocity profiles from the experiments and

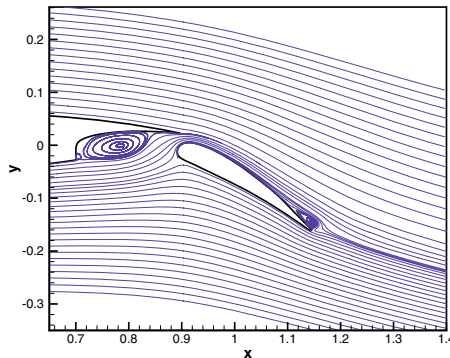


Fig. 2. Time and spanwise averaged streamlines.

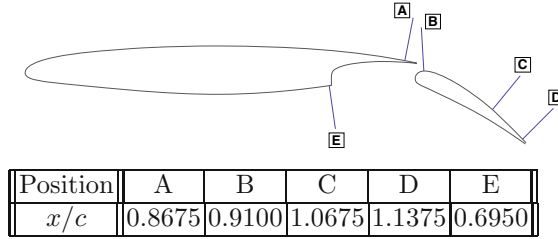


Fig. 3. Locations of the velocity measurements on the airfoil and flap.

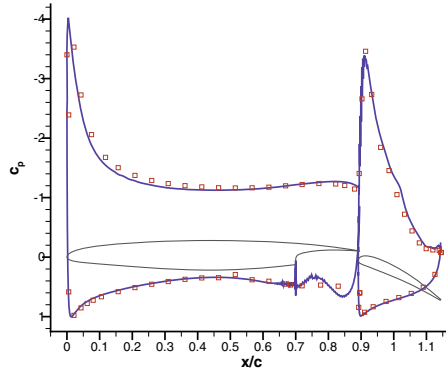


Fig. 4. Time and spanwise averaged pressure coefficients. Solid line: numerical data, Symbols: experimental data [22].

the numerical simulation are compared in Fig. 5. The qualitative trends of the velocity profiles agree with each other. Note that in the near wall region of position D, the measuring location lies in the separation area, where the hot wire probe cannot obtain the correct velocity information. This is the reason for the different signs of the velocity profiles in the near wall region.

As can be expected from the good agreement of the c_p distribution over the airfoil, the lift coefficient agrees very well with the experimental value [22]. The drag coefficient, however, is over-predicted by the numerical simulation, which is not surprising due to the discrepancies in the velocity profiles.

We now turn to the discussion of the zonal large eddy simulation of an airfoil trailing-edge flow at an angle of attack of $\alpha = 3.3$ deg. The trailing-edge length constitutes 30% of the chord length c . The computational domain is shown in Fig. 6. All flow parameters are given in Tab. 2, in which Re_c is the Reynolds number based on the chord length. In the present simulation the inflow section is located at a position of an equilibrium turbulent boundary layer with a weak adverse pressure gradient. Therefore, all inflow data for the upper side boundary layer of the airfoil δ_u ($\delta_u = 0.01972c$) and for the lower side boundary layer δ_l ($\delta_l = 0.0094745c$) are extracted from two separate LES of flat plate boundary layers with an equilibrium pressure gradient, which

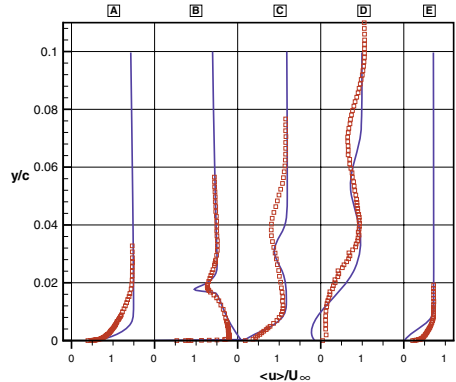


Fig. 5. Time and spanwise averaged profiles of the wall tangential velocity components. Solid line: numerical data, Symbols: experimental data [22].

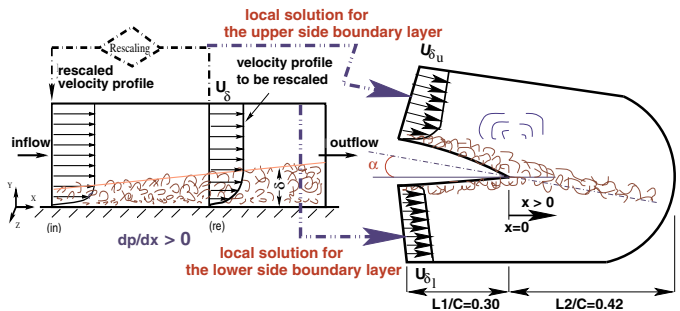


Fig. 6. Computational domain for the airfoil trailing edge flow (right) and inflow distribution from a flat plate boundary layer with an equilibrium adverse pressure gradient via the slicing technique.

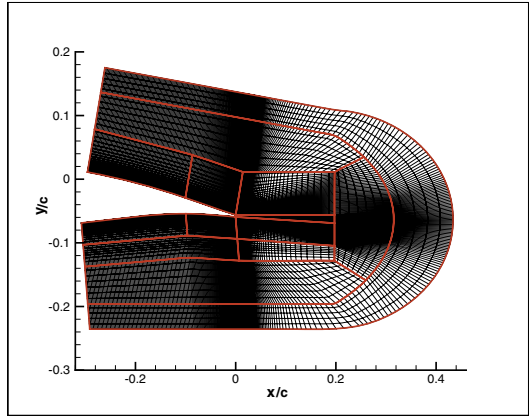


Fig. 7. LES grid of a turbulent flow past an airfoil trailing edge.

Table 2. Parameters and domain of integration for the profile trailing-edge flow simulation. See also Fig. 6

Re_c	Re_{δ_o}	δ_o/c	M_∞
$8.1 \cdot 10^5$	15989	0.01972	0.15
L_1	L_2	L_z	grid points
$0.3 \, c$	$0.42 \, c$	$0.0256 \, c$	$8.9 \cdot 10^6$
$\Delta x_{\min}^+$	$\Delta x_{\max}^+$	$\Delta y_{\min}^+$	Δz^+
5	87	2	32

use the new rescaling formulation for a variable pressure pressure gradient. A total of 8.9×10^6 computational cells are employed with mesh refinements near the surface and the trailing edge (Fig. 7). The resolution used for the present results is $\Delta y_{\min}^+ \approx 2$, $\Delta z^+ \approx 32$, and $\Delta x^+ \approx 87$ at the inlet and $\Delta x^+ \approx 5$ near the trailing edge, see Tab. 2.

The vortex structures in the boundary layer near the trailing edge and in the near wake are presented by the λ_2 contours in Fig. 8. A complex structure can be observed immediately downstream of the trailing edge. This is due to the interaction of two shear layers shedding from the upper and lower airfoil surface. An instantaneous streamwise velocity field in the mid-span is plotted in Fig. 9. Note that in the velocity distribution a small recirculation region occurs right downstream of the trailing edge.

Comparisons of the mean streamwise velocity profiles with experimental data of [22] are presented in Figs. 10(a) and 10(b) for the upper and lower side, respectively, at several streamwise locations: $x/c = -0.1, -0.05, -0.02, 0.0$ measured from the trailing edge. Whereas in the near wall region a good agreement is observed between the computed and measured mean-velocity profiles. Pronounced deviations occur in the log- and outer region of the boundary layer, which could be caused by the coarsening of the mesh.

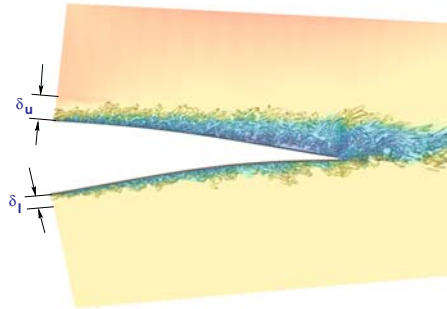


Fig. 8. Vortex structures in the boundary layer near the trailing edge and in the near wake (λ_2 contours).

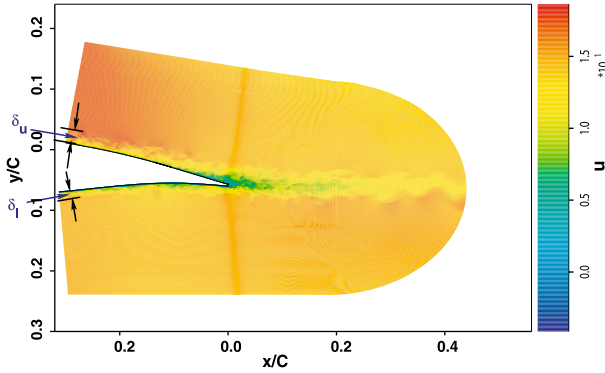
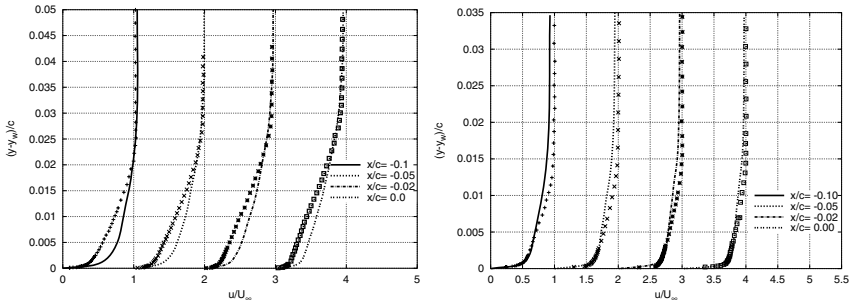
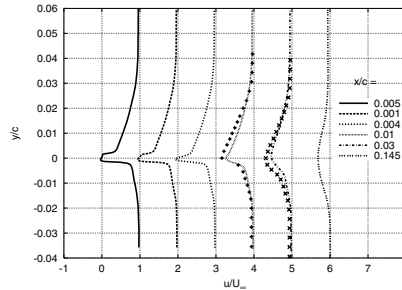


Fig. 9. Instantaneous velocity contours in the boundary layer near the trailing edge and in the near wake.



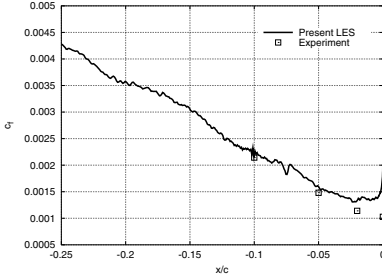
(a) Mean streamwise velocity profiles near the trailing edge (upper side).

(b) Mean streamwise velocity profiles near the trailing edge (lower side).

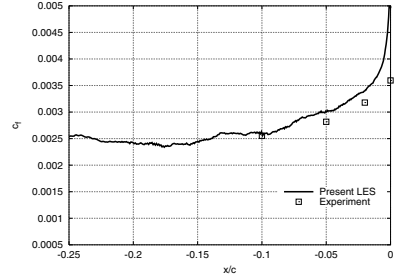


(c) Mean streamwise velocity profiles in the wake.

Fig. 10. Mean streamwise velocity profiles compared with experimental data (symbols) [22].



(a) Skin-friction coefficient on the upper side of the trailing edge.



(b) Skin-friction coefficient on the lower side of the trailing edge.

Fig. 11. Skin-friction coefficients compared with experimental data (symbols) [22].

Further downstream of the trailing edge, asymmetric wake profiles are observed as shown in Fig. 10(c) in comparison with the experimental data. This asymmetry is generated by varying shear layers on the upper and lower surface shed from the trailing edge. Even at $x/c = 0.145$ no fully symmetric velocity distribution is regained. Note the good qualitative and quantitative experimental and numerical agreement for the velocity distributions.

For the analysis of airfoil flow the skin-friction coefficient is one of the most critical parameters. Its distribution evidences whether or not the flow undergoes separation. Comparisons of the present computations with the experimental values are shown in Figs. 11(a) and 11(b) on the upper and lower surface, respectively. The simulation results are in good agreement with the data of [22] except right at the end of the trailing edge. This could be due to an insufficient numerical resolution near the trailing edge or could be caused by some inaccuracies in the experimental data in this extremely susceptible flow region.

The simulations were carried out on the NEC SX-5 and NEC SX-6 of the High Performance Computing Center Stuttgart (HLRS). The vectorization rate of the flow solver is 99%, and a single processor performance of about 2.4 GFlops on a SX-5 and 4.3 GFlops on a SX-6 processor is achieved. The memory requirement for the current simulation is around 3.5 GB. Approximately 175 CPU hours on 10 SX-5 CPUs for statistically converged solution data are required for the airfoil-flap configuration and roughly 75 CPU hours on 10 SX-5 processors for the zonal approach.

5 Conclusions and Outlook for Airfoil Flow

The flow over an airfoil with deflected flap at a Reynolds number of $Re = 10^6$ has been studied based on an LES method. The main characteristics of

the flow field are well resolved by the LES. The comparison of the numerical results with the experimental data show a very good match of the pressure coefficient distribution and a qualitative agreement of the velocity profiles. The results achieved to date are preliminary but encouraging for further studies. The main reason for the deficiency in the numerical results is the fact, that the resolution requirement for an LES cannot be met everywhere in the computational domain at this high Reynolds number.

The zonal approach results in a pronounced improvement of the local accuracy of the solution. The skin-friction coefficient distribution and the near wall as well as the wake velocity profiles show a convincing agreement with the experimental data.

The experience with the present global LES method evidences, that good results can be achieved if the resolution requirements are met [3]. For this reason, the next step will be to concentrate on the improvement of the computational setup. Since the outer part of the flow field over an airfoil is predominantly two-dimensional and laminar, only a quasi-2d calculation will be performed in this area in the next step. For this purpose, a 2D/3D coupling technique has been developed for the structured solver. With this technique, it is possible to increase the near wall resolution while keeping the overall computational cost at a relatively low level. Next, hybrid RANS/LES coupling techniques are contemplated for the improvement of the overall numerical method. Furthermore, with respect to the simulation of the sound field the LES data from the zonal approach will be postprocessed to determine the source terms of the acoustic perturbation equations, which were already successfully used in [7].

6 CAA for Combustion Noise

This research project is part of the Research Unit FOR 486 “Combustion Noise”, which is supported by the German Research Council (DFG). The objective of the Institute of Aerodynamics of the RWTH Aachen University is to investigate the origin of combustion noise and its mechanisms. The LES for the two-step approach is performed by the Insitute for Energy and Powerplant Technology from Darmstadt University of Technology, followed by the CAA simulation to compute the acoustical field. This hybrid LES/CAA approach is similar to that in [7]. However, in this study the Acoustic Perturbation Equations (APE) [6] are extended to reacting flows. In flows, where chemical reactions have to be considered, the application of such an approach is essential as the disparity of the characteristic fluid mechanical and acoustical length scales is even more pronounced than in the non-reacting case.

It is well known from the literature, e.g. [17, 2], that noise generated by combustion in low Mach number flows is dominated by heat release effects, whereas in jet or airframe noise problems the major noise contribution originates from the Lamb vector ($\mathbf{L}' = (\boldsymbol{\omega} \times \mathbf{u})'$), which can be interpreted as a

vortex force [6, 18]. In principle it is possible to treat this task by extending Lighthill's Acoustic Analogy to reacting flows as was done in the past [17, 2]. This, however, leads to an inhomogeneous wave equation with an ordinary wave operator e.g. [2, 10], which is valid for homogeneous mean flow only. Therefore, this approach is restricted to the acoustic far field. The APE approach remedies this drawback. It is valid in non-uniform mean flow and takes into account convection and refraction effects, unlike the linearized Euler equations [6].

7 Acoustic Perturbation Equations for Reactive Flows

To derive the extended APE system the governing equations of mass, momentum, and energy for reacting flows are rearranged such that the left-hand side describes the APE-1 system [6], whereas the right-hand side (RHS) consists of all non-linear flow effects including the sources related to chemical reactions.

$$\frac{\partial \rho'}{\partial t} + \nabla \cdot (\rho' \bar{\mathbf{u}} + \bar{\rho} \mathbf{u}') = q_c \quad (1)$$

$$\frac{\partial \mathbf{u}'}{\partial t} + \nabla (\bar{\mathbf{u}} \cdot \mathbf{u}') + \nabla \left(\frac{p'}{\bar{\rho}} \right) = \mathbf{q}_m \quad (2)$$

$$\frac{\partial p'}{\partial t} - \bar{c}^2 \frac{\partial \rho'}{\partial t} = q_e \quad (3)$$

As was mentioned before, the heat release effect dominates the generation of combustion noise. Therefore the investigations have been performed using q_e only, i.e. assuming $q_c = 0$ and $\mathbf{q}_m = 0$.

7.1 Thermoacoustic Source Terms

In the proposed APE system the source term containing heat release effects appears on the RHS of the pressure-density relation, i.e. q_e . This term vanishes when only isentropic flow is considered. However, due to the unsteady heat release in a flame the isentropic pressure-density relation is no longer valid in the combustion area. Nevertheless, it is this effect, which defines the major source term in comparison to the sources (q_c , $\mathbf{q}_m$) in the mass and momentum equations within the APE system. Concerning the other source mechanisms, which lead to an acoustic multipole behavior though it can be conjectured that they are of minor importance in the far field. Using the energy equation for reacting flows the pressure-density relation becomes:

$$\begin{aligned} \frac{\partial p'}{\partial t} - \bar{c}^2 \frac{\partial \rho'}{\partial t} &= -\bar{c}^2 \cdot \frac{\partial \rho_e}{\partial t} \\ &= \bar{c}^2 \left[\frac{\bar{\rho}}{\rho} \cdot \frac{\alpha}{c_p} \cdot \left(\sum_{n=1}^N \frac{\partial h}{\partial Y_n} \right)_{\rho, p, Y_m} \rho \frac{DY_n}{Dt} + \nabla \cdot \mathbf{q} - \frac{\partial u_i}{\partial x_j} \tau_{ij} \right] \end{aligned}$$

$$\begin{aligned}
& -\nabla(\mathbf{u}\rho_e) - \frac{1}{\bar{c}^2} \left[\left(1 - \frac{\bar{\rho}\bar{c}^2}{\rho c^2} \right) \cdot \frac{Dp}{Dt} - \frac{p - \bar{p}}{\rho} \cdot \frac{D\rho}{Dt} \right] \\
& + \left[-\frac{\gamma - 1}{\gamma} \mathbf{u} \cdot \nabla \bar{\rho} - \frac{p}{\bar{c}^2} \cdot \mathbf{u} \left(\frac{\nabla \bar{p}}{\bar{p}} - \frac{\nabla \bar{\rho}}{\bar{\rho}} \right) \right] \quad (4)
\end{aligned}$$

where ρ_e is defined as

$$\rho_e = (\rho - \bar{\rho}) - \frac{p - \bar{p}}{\bar{c}^2} \quad (5)$$

Perturbation and time averaged quantities are denoted by a prime and a bar, respectively. The volumetric expansion coefficient is given by α and c_p is the specific heat capacity at constant pressure. For an ideal gas the equation $\alpha/c_p = (\gamma - 1)/c^2$ holds. The quantity Y_n is the mass fraction of the n th species, h the enthalpy and $\mathbf{q}$ the heat flux.

7.2 Evaluation of the Thermoacoustic Source Terms

The investigations have been performed by considering q_e only. Reformulating the energy equation for a gas with N species [2] leads to

$$\frac{D\rho}{Dt} = \left[\frac{1}{c^2} \frac{Dp}{Dt} + \frac{\alpha}{c_p} \cdot \left(\sum_{n=1}^N \frac{\partial h}{\partial Y_n} \bigg|_{\rho, p, Y_m} \rho \frac{DY_n}{Dt} + \nabla \cdot \mathbf{q} - \frac{\partial u_i}{\partial x_j} \tau_{ij} \right) \right] \quad (6)$$

Since the combustion takes place at ambient pressure and the pressure variations due to hydrodynamic flow effects are of low order, the whole combustion process can be assumed to be at constant pressure. From our analysis [18] and from literature [2] it is known that combustion noise is dominated by heat release effects and that all other source mechanisms are of minor importance. Assuming combustion at constant pressure and neglecting all mean flow effects q_e reduces to sources, which are related to heat release effects, non-isomolar combustion, heat flux and viscous effects. Adding up all these sources under the aforementioned restrictions the RHS of the pressure-density relation can be substituted by the total time derivative of the density multiplied by the square of the mean speed of sound and the ratio of the mean density and the density

$$q_e = \bar{c}^2 \left[\frac{\bar{\rho}}{\rho} \cdot \frac{\alpha}{c_p} \cdot \left(\sum_{n=1}^N \frac{\partial h}{\partial Y_n} \bigg|_{\rho, p, Y_m} \rho \frac{DY_n}{Dt} + \nabla \cdot \mathbf{q} - \frac{\partial u_i}{\partial x_j} \tau_{ij} \right) \right] \quad (7)$$

$$= \bar{c}^2 \frac{\bar{\rho}}{\rho} \frac{D\rho}{Dt}. \quad (8)$$

8 Numerical Method for Combustion Noise

8.1 LES of the Turbulent Non-premixed Jet Flame

In the case of non-premixed combustion, the chemical reactions are limited by the physical process of the mixing between fuel and oxidizer. Therefore, the flame is described by the classical mixture fraction approach by means of the conserved scalar f . The filtered transport equations for LES are solved on a staggered cylindrical grid of approximately 10^6 cells by *FLOWSI*, an incompressible finite-volume solver. A steady flamelet model in combination with a presumed β -Pdf approach is used to model the turbulence chemistry interaction. The subgrid stresses are closed by a Smagorinsky model with a dynamic procedure by Germano [12]. For the spatial discretization, a combination of second-order central differencing and total-variation diminishing schemes is applied [21]. The time integration is performed by an explicit third-order, low storage Runge-Kutta scheme. At the nozzle exit, time averaged turbulent pipe flow profiles are superimposed with artificially generated turbulent fluctuations [13], while the coflow is laminar.

8.2 Source Term Evaluation

The total time derivative of the density, which defines the major source term of the APE system, has been computed by the unsteady flow field in a flame region where the main heat release occurs (Fig. 12).

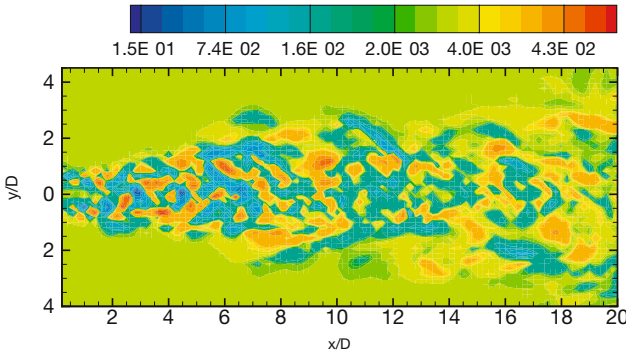


Fig. 12. Contours of the total time derivative of the density ($D\rho/Dt$) at $t = 100$ in the streamwise center plane

8.3 Grid Interpolation

Since the source terms have been calculated on the LES grid they need to be interpolated on the CAA grid. Outside the source area the APE system

becomes homogeneous. This means, the RHS is defined in the source region only. Therefore, the CAA domain has been decomposed into a multiblock domain such that one block contains the entire source area. This procedure possesses the advantages that the interpolation from the LES grid to the CAA source block is much faster than onto the whole CAA domain and that the resulting data size for the CAA computation can be reduced dramatically. The data interpolation is done with a trilinear algorithm.

8.4 CAA Computation for Combustion Noise

For the CAA computation this proposed APE-System has been implemented into the PIANO (Perturbation Investigation of Aeroacoustic Noise) Code from the DLR (Deutsches Zentrum für Luft- und Raumfahrt e.V.).

The source terms on the right-hand side of the APE system has to be interpolated in time during the CAA computation. Using a quadratic interpolation method at least 25 points per period are required to achieve a sufficiently accurate distribution. Hence, the maximal resolvable frequency is $f_{max} = 1/(25\Delta t) = 800\text{Hz}$ since the LES solution comes with a time increment of $\Delta t = 5 \cdot 10^{-5}\text{s}$ [11]. This frequency is much smaller than the Nyquist frequency. The CAA code is based on the fourth-order DRP scheme of Tam and Webb [19] for the spatial discretization and the alternating LDDRK-5/6 Runge-Kutta scheme for the temporal integration [8]. At the far field boundaries a sponge-layer technique is used to avoid unphysical reflections into the computational domain.

Solving the APE system means to solve five equations (3D) for the perturbation quantities ρ', u', v', w' and p' per grid point and time level. No extra equations for viscous terms and chemical reaction need to be considered since these terms can be found on the RHS of the APE system and are provided by the LES within the source region. On the other hand the time step within the CAA computation can be chosen much higher than in the LES. This means, using a rough estimation, that the ratio of the computation times between LES and CAA is approximately $t_{LES}/t_{CAA} \approx 4/1$.

9 Combustion Noise Results

Figure 13 shows a snapshot of the acoustic pressure field in the streamwise center plane at the dimensionless time $t = 100$. The source region is evidenced by the dashed box. This computation was done on a 27-block domain using approximately 4×10^6 grid points, where the arrangement of the blocks is arbitrary provided that one block contains all acoustical sources.

The acoustic directivity patterns (Fig. 14) are computed for different frequencies on a circle in the $z = 0$ plane with a radius $R/D = 17$ whose center point is at $\mathbf{x} = (10, 0, 0)$. The jet exit diameter is denoted by D . From 150° to 210° the directivity data is not available since this part of the circle is outside

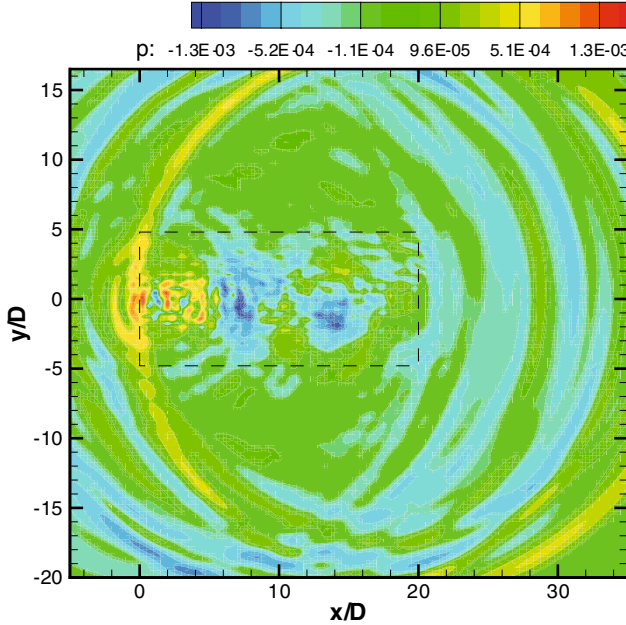


Fig. 13. Pressure contours of the APE solution at $t = 100$ in the streamwise center plane

of the computational domain. In general an acoustic monopole behaviour with a small directivity can be observed since this circle is placed in the acoustic near field.

10 Conclusion for Combustion Noise

The APE system has been extended to compute noise generated by reacting flow effects. The heat release per unit volume, which is expressed in the total time derivative of the density, represents the major source term in the APE system when combustion noise is analyzed. The main combustion noise characteristic, i.e., the monopole nature caused by the unsteady heat release, could be verified. In the present work we have demonstrated that the extended APE System in conjunction with a hybrid LES/CAA approach and with the assumptions made, is capable of simulating an acoustic field of a reacting flow, i.e., of a non-premixed turbulent flame.

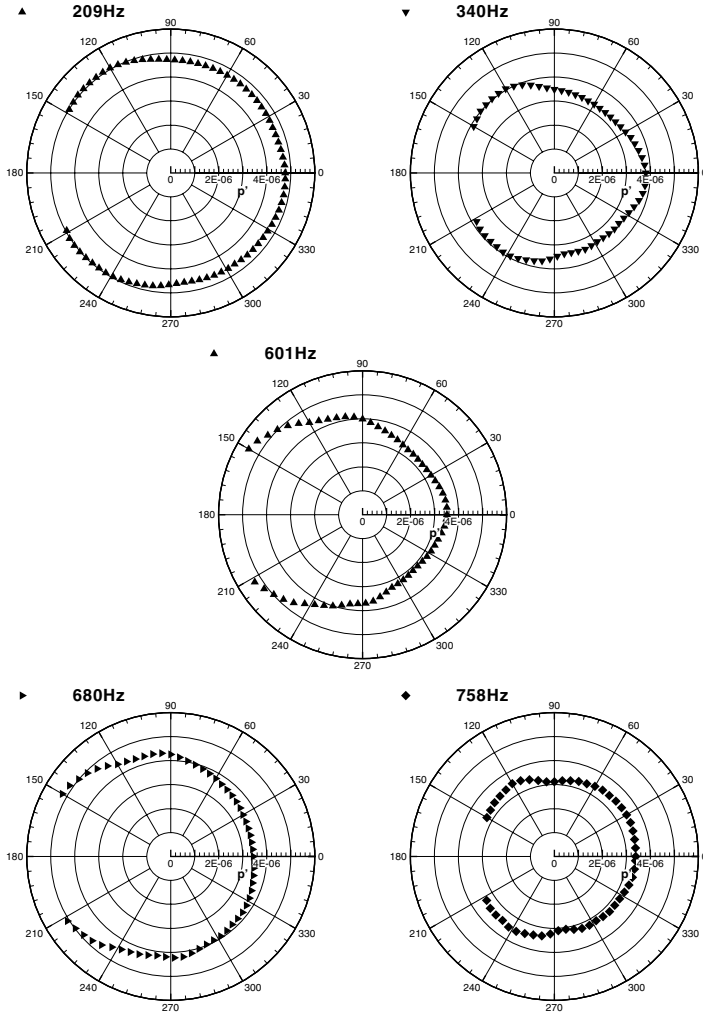


Fig. 14. Directivity patterns for different frequencies

Acknowledgments

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Using Dynamic Mesh Models to Simulate Electrostatic Spray-Painting

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Summary. In this paper a numerical simulation of electrostatic spray-painting with movement of the atomizer has been performed using dynamic mesh models. As atomizer the high-speed rotary bell with external charge was used. Simple movement of the atomizer and simple geometry of the substrate were considered. Numerical results with two different dynamic mesh models, i.e., dynamic layering and local remeshing are discussed. The simulated film thickness distribution was compared with the experimental result.

1 Introduction

In order to optimise the painting process, which amounts to a high percentage of fixed and flexible cost in automotive production, numerical simulation of spray painting for the automotive industry, especially using high-speed rotary bell and electrostatically supported methods, has been performed [1, 2] in the Fraunhofer-Institut für Produktionstechnik und Automatisierung (IPA) by means of the CFD (Computational Fluid Dynamics) code FLUENT.

The previous numerical studies were concerned with the prediction of film thickness distribution and transfer efficiency based on the quasi-steady airflow field with a static atomizer. Three-dimensional turbulent airflow and the electrostatic field including space charge were calculated. Based on the Lagrangian approach, the trajectories of the paint droplets were modelled considering electric and aerodynamic forces. The FLUENT code was extended to account for the relevant electrical effects in the spray-painting process. From the simulation the so-called static film thickness distribution or the static spray pattern could be obtained on the surface of arbitrary 3D-objekts. Figure 1 shows, for instance, a typical static film thickness pattern on the car door. In industrial application, however, only the dynamic film thickness distribution is useful. The static spray pattern has to be used to derive the dynamic film thickness by artificially moving the spray pattern along a given path and integrating the mass, given that the physical conditions of the work piece are essentially the

same as those in the simulation with a static atomizer during the integration. A typical dynamic film thickness distribution is shown in Fig. 2, which was created based on the static film pattern in Fig. 1 and by moving the spray pattern from the left door to the right using DLS (Dynamic Lacquer Simulation), a code developed by IPA. A cross section profile in the middle of the car door in Fig. 2 was compared with the experiment. A quite good agreement was obtained [2].

It is difficult, however, to obtain the dynamic film distribution using such an integration method for an irregular object shape, such as the frame of the car door in Fig. 2, where the geometry changes continuously, corresponding to unsteady physical boundary conditions with respect to the moving direction.

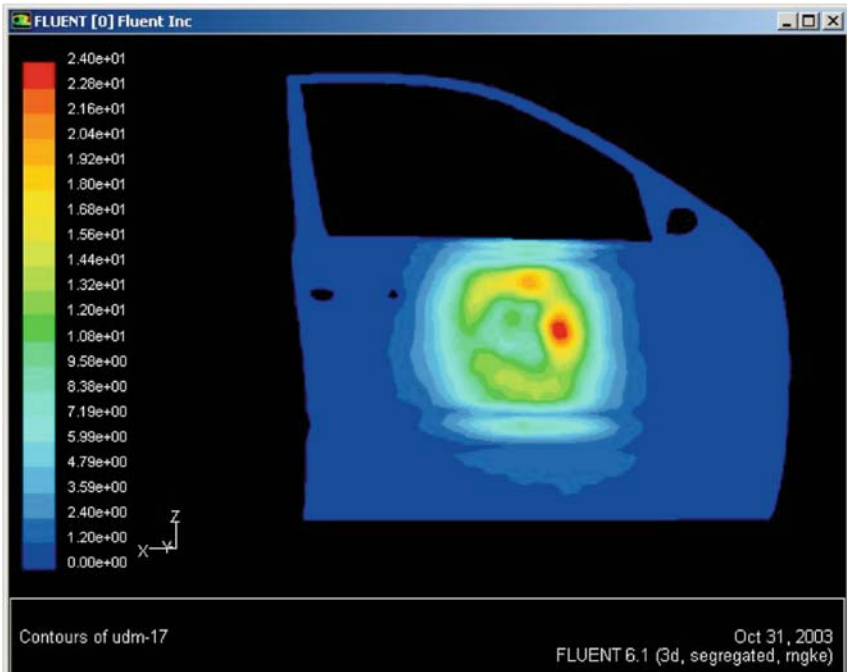


Fig. 1. Static film thickness distribution (μm)

In the practical spray-painting process in automotive industry, neither the atomizer is static, nor is the object shape regular. The spray-painting process itself actually involves the phenomena of a time-dependent turbulent flow field. Numerical simulation of the real dynamic painting process should be carried out, which involves the unsteady flow calculation with dynamic mesh model. The spray simulation has to be coupled with the highly complex motion of robot arms. This new feature requires to read the robot motion files, convert the motion to FLUENT commands and apply all this to the atomizer

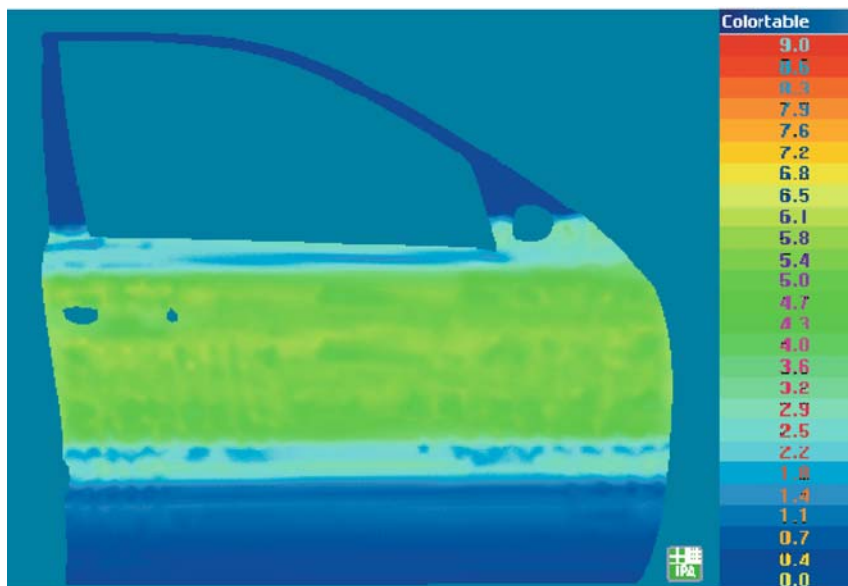


Fig. 2. Dynamic film thickness distribution (μm)

(motion and bell rotation axis) and the injected paint droplets (position and initial direction). Additionally, grid adaption and coarsening are used to refine only the focussed region in order to limit the total computational resources needed. Clearly, such numerical simulations are more complicated and time consuming compared to the simulations done previously.

In the current paper, the numerical simulation of spray-painting with dynamic mesh models will be presented for a simple movement with a simple target geometry, e.g., a flat plate, where high-quality measurements are available, in order to verify the algorithm for transient, dynamic calculations in general.

2 Numerical Methods

2.1 Grid generation and dynamic mesh models

A high-speed rotary bell with external charge system is applied in the current numerical simulation using the CFD code FLUENT 6.1 [4]. A simple geometry of the grounded work piece, i.e., a flat plate, was used. The rotary bell was moved horizontally above the plate with a single direction and a constant moving velocity of 50 mm/s.

Three mesh motion methods are available in FLUENT, i.e., spring-based smoothing and dynamic layering, as well as local remeshing. For the purely

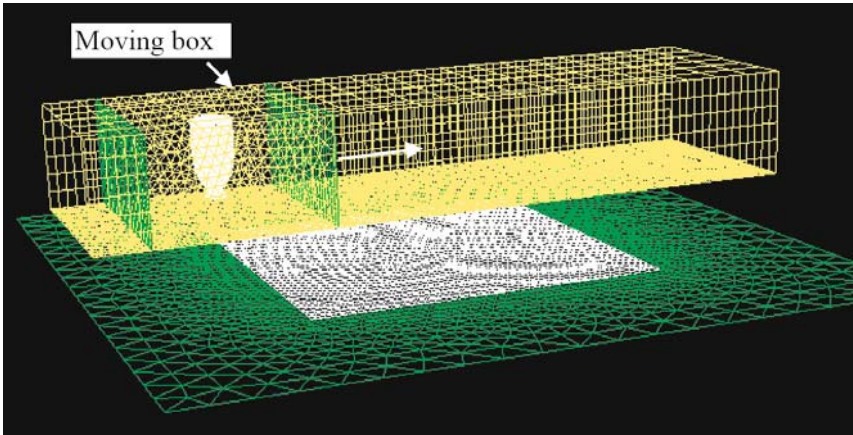


Fig. 3. 3D view of part of the mesh for the layering model

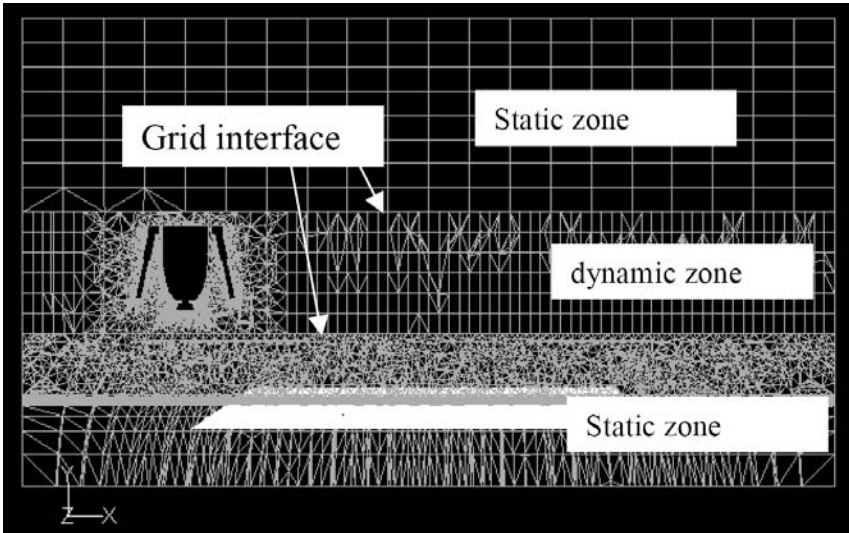


Fig. 4. Grid cross-section details for the layering model

linear motion, as mentioned above for the simple case, dynamic layering can be used. A grid that is suitable for the layering model was first created, namely, hexahedral elements are required in the dynamic zone. Figures 3 and 4 show the mesh details for the layering model. The atomizer is included in a moving box bounded with a quad surface mesh (Fig. 3), in which tetrahedral elements are fulfilled. The box moves in the dynamic zone, a channel bounded with quad elements (yellow coloured in Fig. 3). Cells in the dynamic zone are added or deleted adjacent to the box as the box moves. In order to limit the total mesh size, the grid in the static zone above the dynamic zone is quite coarse.

Another kind of the dynamic model consists in a local remeshing that is suitable for the relative boundary motions that involve both translation and rotation. Using local remeshing will give more practical sense, since the movement of the atomizer with respect to the car body is highly complicated. Therefore, a numerical simulation with local remeshing model will be presented more detailed in the following.

Local remeshing in FLUENT is only available for tri/tet meshes. Figure 5 shows the grid for the local remeshing model. The mesh on the rotary bell and the electrodes is quite fine. In order to avoid difficulties and to keep the grid quality during the mesh movement, it is necessary to create a cylinder region with interior boundary around the atomizer. Both the cylinder region and the atomizer are defined as moving zone. Since the local grid adaption with dynamic meshing is not available in FLUENT version 6.1, the cylinder zone with fine mesh cells in downstream region is created quite close to the plate in the current case, to ensure the grid resolution. The initial position of the atomizer is located 300 mm away from the edge of the plate. During the movement the grid within the moving zone and the boundary layer mesh above the plate are not modified. An update of the grid topology in the dynamic zone is, however, performed after every time step, if user-specified skewness and size are exceeded. Using size function and smoothing parameter, local remeshing with regular change of the cell size, i.e. fine mesh around the

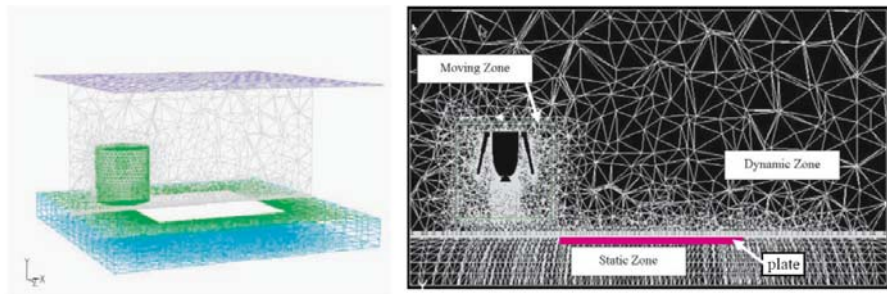


Fig. 5. Grid 3D view and cross-section for local remeshing

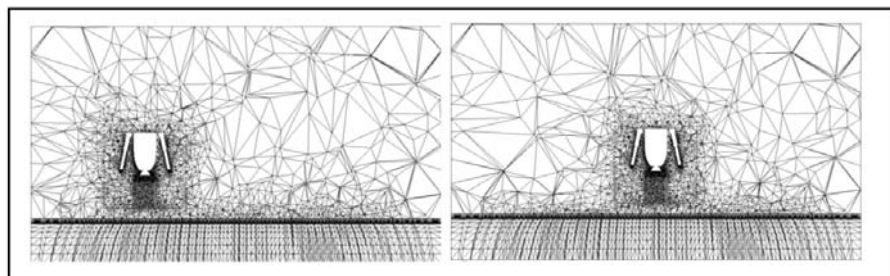


Fig. 6. Grid cross-section in different positions of the atomizer

moving zone and coarse cell far away from this zone can be guaranteed (Fig. 6). Detailed parameters concerned with local remeshing can be found in [5].

2.2 Computational details

The numerical simulations presented in this work were carried out with the FLUENT code based on finite-volume approach. The time-dependent, three-dimensional, incompressible Reynolds-averaged Navier-Stokes equations with a k-RNG turbulence model were solved for the turbulent airflow. The computational domain is $2 \times 2 \times 1.7 \text{ m}^3$ with ca. 500 000 cells. The droplet phase created by the high-speed rotary bell was calculated using Lagrangian approach with a stochastic tracking model. In the simulation, two-phase coupling was taken into account. Numerical models concerned with electrical field, electrical force on the particles and particle charge etc. which have been reported in pervious studies [1, 3] will not be stated here. Standard application parameters in the spray painting process, i.e., shaping air 150 l/min, bell speed 45 000 rpm, liquid flow rate 150 ml/min and high voltage -60 kV, were applied in the simulation. By solving the electrical field the steady governing equation for the ion flow was still assumed. After getting convergent solutions of the airflow and the electrical field at the initial position of the atomizer, mesh movement and the coupling calculation between continuous phase and discrete phase started with a time step size of 0.02s. The maximum number of outer iterations required per time step was about 30. 1300 computational particles with a measured size distribution from $1\mu\text{m}$ to $80\mu\text{m}$ were released initially from the bell edge at each time step. During the calculation there were more than 40 000 computational particles in the domain, as the particle resident time is about 0.1-1 s. Increasing the initial number of the computational particles will increase the CPU time. Table 1 shows the computing effort with different dynamic mesh models and grid sizes.

Table 1. CPU Time Information

Dynamic Case	Grid size (cell elements)	CPU time per time step (min/ts)	Total Time step	Total CPU time (hour)
Layering	445727	7.2	1200	144
Remesh1	368695	5.2	1200	104
Remesh2	505021	7.2	1200	144

Although the dynamic mesh models are compatible with all physical models in FLUENT 6 and are fully parallelized, a serial FLUENT code has to be used in the current simulation, as the parallel calculation with particle injection during the mesh movement in FLUENT 6.1 is not yet stable. A CPU time of 144 hours is required for the whole simulation with a moving distance of 1.5 m.

3 Results

3.1 Results using dynamic layering model

Simulations for the airflow and the electrical field by using the layering model (Fig. 3 and 4 were performed. The isolines of the velocity and the electrical potential for the position, where the atomizer is located above the middle of the plate, are depicted in Fig. 7 and 8, respectively. It can be seen that the isolines are broken in some positions that correspond to the grid interfaces (see Fig. 4). The break-up of the isolines in the position above the atomizer might not create a significant effect for the final results, namely the deposition of the droplets on the work piece. However, disconnections of the contours under the atomizer will certainly influence the particle trajectories. In order to improve the distributions of the velocity and electrical fields in the interfaces, more effort should be made in the future, for instance, keeping the similar cell-size on both sides of the interface. In the current study, the calculation of droplet trajectories was performed only with the local remeshing model, shown as follows.

3.2 Results using local remeshing model

In this section, the results of the numerical simulation based on the local remeshing model are presented. Contours of the electrical potential at different time steps, corresponding to different positions of the atomizer, are depicted in Fig. 9. Figure 10 shows the corresponding velocity fields. At the positions, where the atomizer is located outside of the flat plate, the velocity contour is characterised by a narrow spray jet. As soon as the atomizer moves above the plate, the boundary conditions for flow and electrostatic field are changed, resulting in the flow field with a broad spray. For the atomizer position above the middle of the plate, both the isolines of the electrical potential and the velocity field in Fig. 9, 10 are the same as those obtained in a previous study based on the static atomizer [1].

The final film thickness distribution on the plate is plotted in Fig. 11. It can be seen that close to the left and right edges of the plate the film thickness is lower, due to the unsteady boundary conditions with respect to the moving direction. The film thickness distribution in the middle region of the plate is relatively stable, where a higher film thickness can be observed. A cross-section film thickness profile in the middle of the plate ($x = 0$) was obtained and converted to the dry film thickness distribution that was compared with the measured result, as shown in Fig. 12. The shape of the simulated film thickness profile is quite similar to that from the experiment. However, the simulation underestimates the film thickness about 20%, corresponding to a lower transfer efficiency of the liquid paint. By using a static atomizer in the previous numerical simulation [1], a good agreement between simulated and measured film thickness profiles was obtained however. Therefore, further

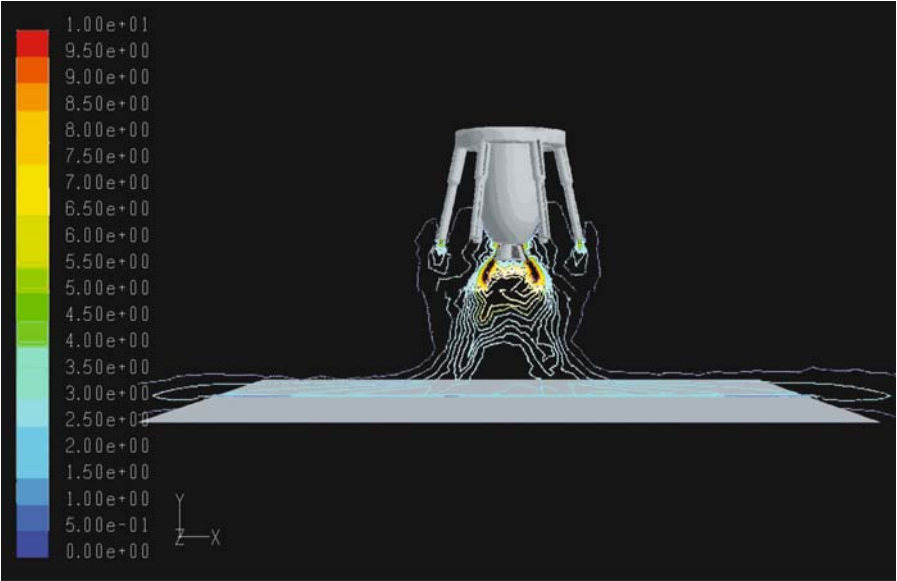


Fig. 7. Velocity contours (layering model)

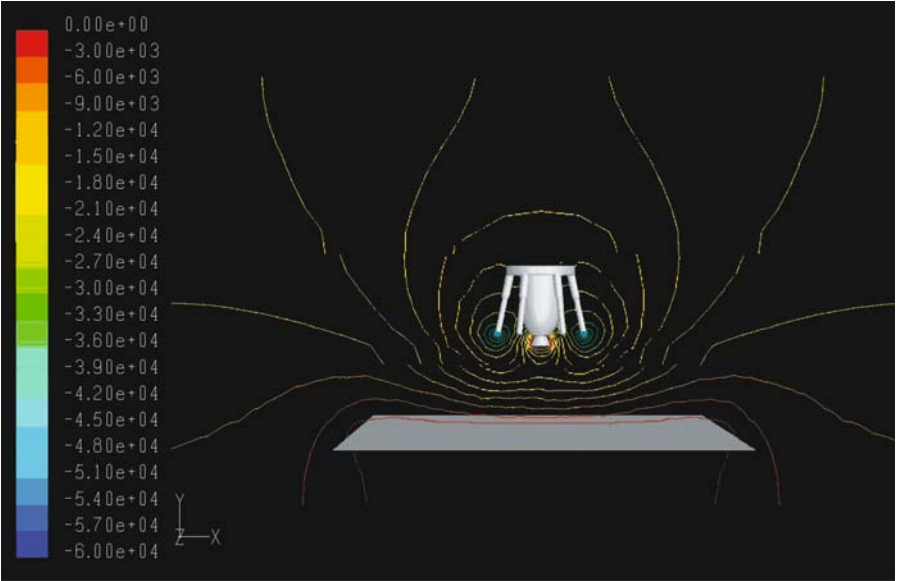


Fig. 8. Electrical potential (V) (layering model)

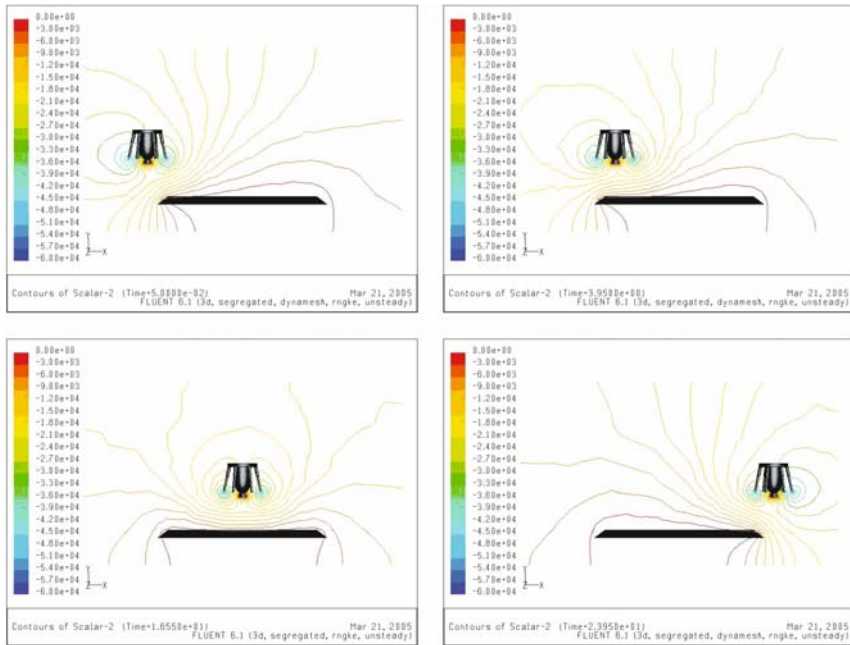


Fig. 9. Visualization of the electrical potential (V) (remeshing model)

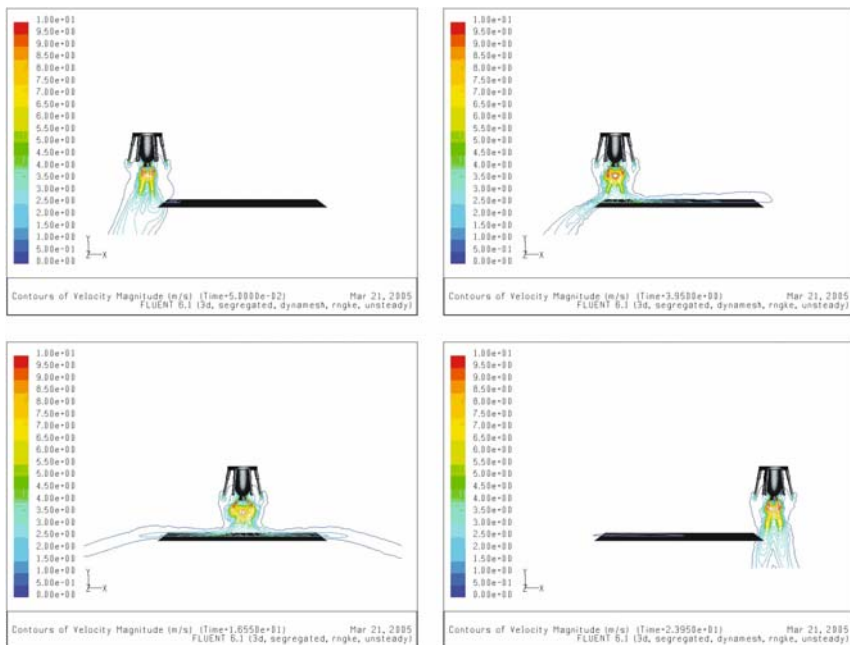


Fig. 10. Visualization of the flow field (m/s) (remeshing model)

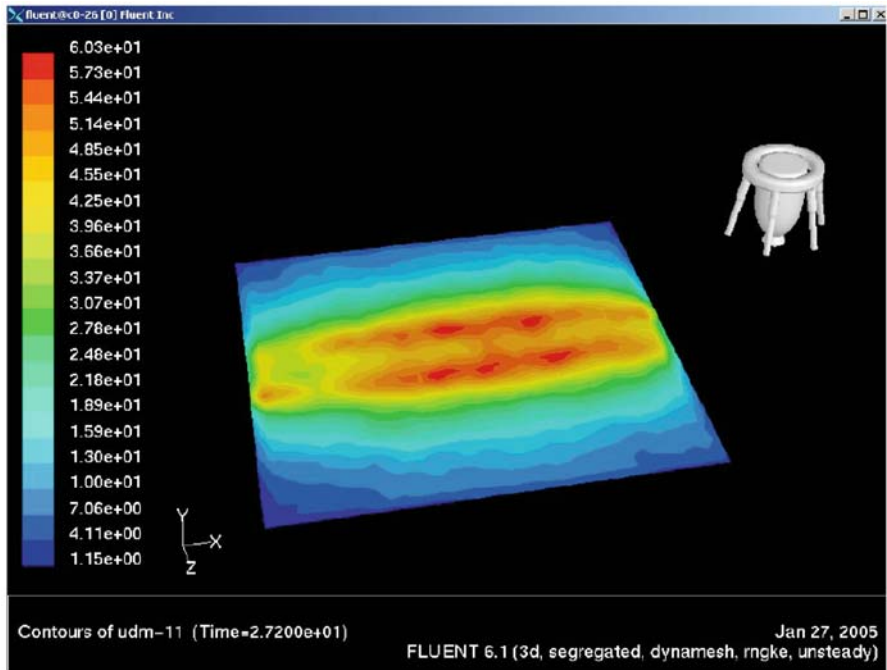


Fig. 11. Wet film thickness (μm) distribution on the flat plate (remeshing model)

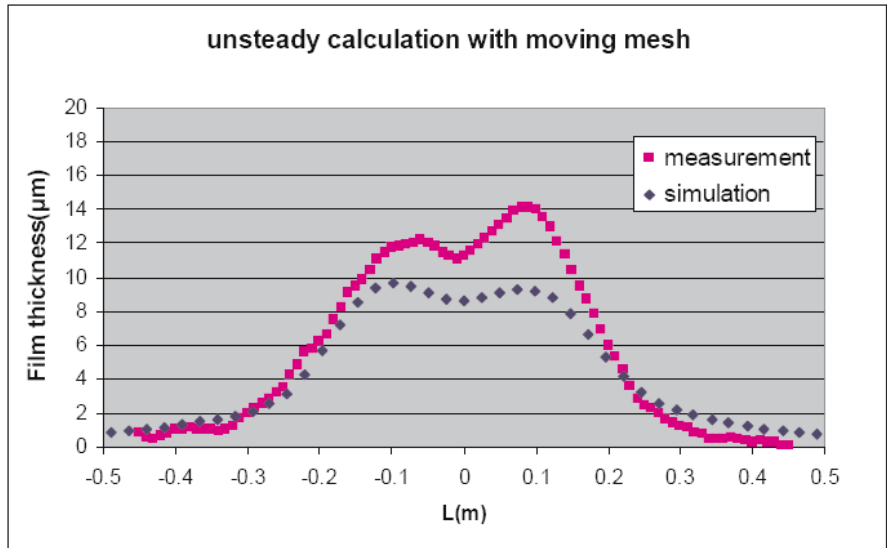


Fig. 12. Comparison of the simulated and the measured dynamic film thickness distribution (μm)

investigation concerning dynamic mesh models together with particle phase model should be carried out.

4 Conclusion

For the first time, a dynamic spray painting simulation with moving atomizer was carried out using dynamic mesh models. An electrostatically supported high-speed rotary bell was applied. Linear translation of the atomizer and a flat plate as substrate were used. It was found that the calculated airflow field and electrical field using a local remeshing model are much better than using dynamic layering. The predicted film thickness distribution on the substrate was still beyond the acceptable accuracy, comparing with the experiment. Detailed investigation concerned with the local remeshing model, e.g., local grid adaption in the new FLUENT code, and the unsteady discrete phase simulation should be carried out.

For the present computation, mesh size and computational particles are limited, in order to reduce the total computational resources needed. With the improvement of the CFD code, e.g., stable parallel solver for the discrete phase model and local grid adaption during mesh movement, simulations with increased mesh size and number of computational particles should be performed in the future.

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Numerical Simulation of Maneuvering Combat Aircraft

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Summary. An overview about recent results of the DLR-Project SikMa-“Simulation of Complex Maneuvers” is presented. The objective of the SikMa-Project is to develop a numerical tool to simulate the unsteady aerodynamics of a free flying aeroelastic combat aircraft, by use of coupled aerodynamic, flight-mechanic and aeroelastic computations. To achieve this objective, the unstructured, time accurate flow-solver TAU is coupled with a computational module solving the flight-mechanic equations of motion and a structural mechanics code determining the structural deformations. By use of an overlapping grid technique (chimera), simulations of a complex configuration with movable control-surfaces is possible.

Nomenclature

Θ	Incidence angle, pitch angle at $\Phi = 0$	l_i	Chord length of the model
α	Angle of attack	Ma	Mach number
Φ	Roll angle	$\text{Re} = \frac{V_\infty \cdot l_i}{\nu}$	Reynolds number
Φ_0	Initial roll angle	$q_\infty = \frac{\rho_\infty}{2} V_\infty^2$	Dynamic pressure
$\Delta\alpha$	Angle-of-attack amplitude	$\omega^* = 2\pi f \cdot l_i / V_\infty$	Reduced Frequency
η	Flap deflection angle	$c_M = \frac{M}{q_\infty F l_i}$	Pitching moment coefficient
t	Time	$c_L = \frac{L}{q_\infty F}$	Lift coefficient
F	Reference area	$c_p = \frac{p - p_\infty}{q_\infty}$	Pressure coefficient
		$c_l = \frac{l}{q_\infty F l_i}$	Rolling moment coefficient

1 Introduction

The improvement of maneuverability and agility is a substantial requirement of modern fighter aircraft. Currently, roll-rates of 200°/s and more can be achieved, especially if the design of the aircraft is inherently unstable. Most

of today's and probably future manned or unmanned fighter aircraft will be delta wing configurations. Already at medium angles of attack the flow field of such configurations is dominated by vortices developed by flow separation at the wings and the fuselage. The delay in time of vortex position and condition to the on-flow conditions of the maneuvering aircraft can lead to significant phase shifts in the distribution of loads. In such a case, reliable results for the analysis of the flight properties can only be achieved by a combined non-linear integration of the unsteady aerodynamics, the actual flight motion, and the elastic deformation of the aircraft structure.

Today, these types of data can only be obtained by flight tests, and not during the design period. Flight tests, as well as modifications after the design phase, lead normally to an increase in costs. In order to decrease the costs incurred by extensive flight-tests and the post-design phase modifications, it would be helpful to have a tool which enables aircraft designers to analyze and evaluate the dynamic behavior during the design phase.

The main objective of this paper is to focus on the necessity for developing an interactive, multidisciplinary engineering tool for predicting the unsteady critical states of complex maneuvering aircraft. Such a simulation environment has to bring together aerodynamics, aeroelasticity and flight mechanics in a time accurate simulation tool. In order to deliver such a tool in the near future, the DLR Project SikMa- "Simulation of Complex Maneuvers" has been initiated to combine these three disciplines into one simulation environment.

For validating the numerical simulations several wind tunnel experiments in both the low speed and transonic regime will be done within the SikMa project.

2 Numerical Approach

2.1 CFD Solver TAU

The behavior of the fluid-flow affecting the object of interest is simulated with the TAU-Code, a CFD tool developed by the DLR Institute of Aerodynamics and Flow Technology [Galle97][Gerhold97]. The TAU-Code solves the compressible, three-dimensional, time-accurate Reynolds-Averaged Navier-Stokes equations using a finite volume formulation. The TAU-Code is based on an hybrid unstructured-grid approach, which makes use of the advantages that prismatic grids offer in the resolution of viscous shear layers near walls, and the flexibility in grid generation offered by unstructured grids. The grids used for simulations in this paper were created with the hybrid grid generator Centaur, developed by CentaurSoft [cent]. A dual-grid approach is used in order to make the flow solver independent from the cell types used in the initial grid. The unstructured grid approach is chosen due to its flexibility in creating grids for complex configurations, e.g. a full-configured fighter aircraft with control surfaces and armament, the capability of grid

adaptation and straightforward parallelization of all the main TAU modules.

The TAU-Code consists of several different modules, among which are:

- The Preprocessor module, which uses the information from the initial grid to create a dual-grid and the coarser grids for multigrid.
- The Solver module, which performs the flow calculations on the dual-grid.
- The Adaptation module, which refines and derefines the grid in order to capture flow phenomena like vortex structures and shear layers near viscous boundaries, among others.
- The Deformation module, which propagates the deformation of surface coordinates to the surrounding grid.
- The Post-processing module, which is used to convert TAU-Code result files to formats usable by popular visualization tools.

In the Solver module, several upwind schemes, as well as a central scheme with artificial dissipation, are available for the spatial discretization. Both Spalart-Allmaras and $k\text{-}\omega$ turbulence models are implemented. For steady calculations an implicit LU-SSOR multistage Runge-Kutta time stepping scheme is used [Dwight04]. For time accurate computations, an implicit dual-time stepping approach is used. The TAU-Code is parallelized using grid partitioning, and a multigrid approach is used in order to increase the performance.

The TAU-Code can handle simulations containing multiple bodies in relative motion with one another, e.g motion of control surfaces with respect to the aircraft, by use of a hierarchical motion-node structure. The motion of each body can either be calculated internally by the TAU-Code, or supplied by an external program through a Python implemented external interface.

2.2 TAU-Code Extension: Chimera Technique

The chimera technique provides the capability to perform calculations with systems of overset grids. By allowing large relative body movement without the need for local remeshing or grid deformation, the technique is invaluable for the simulation of maneuvering combat aircraft, where large-amplitude control surface deflections and/or store release are a standard part of the simulation. The current implementation can handle multi-body simulations where the overset-grid boundaries have been predefined; a version that allows 'automatic-hole-cutting' is currently under development. The chimera search algorithm, which is based on a state-of-the-art alternating digital tree (ADT), is available for both sequential and massively parallel architectures (Linux Clusters). A more detailed description of the chimera approach is given in [Raichle04].

2.3 Flight Mechanics

For the numerical simulation of the flight mechanics, the simulation environment SIMULA developed at the DLR Institute of Flight Systems is used

[Moen91]. SIMULA provides the three basic functionalities necessary for flight simulation and flight control purposes: trimming, i.e. the determination of the initial state and control values, linearization and stability analysis, and simulation, i.e. the numerical integration of the equations of motion.

Single and multi-body flight-mechanic models, ranging from 1 to 6 degrees of freedom, are made available to the simulation by SIMULA. The amount of data that is exchanged between SIMULA and TAU is of a scale that can be easily transported directly through a TCP/IP socket connection, which is offered by the TENT simulation environment.

2.4 CSM-Code

For the coupling of the aerodynamic and structural dynamic simulations in the time domain, a loose coupling scheme has been implemented. The coupling scheme is conservative with regards to the forces, moments and the work performed on both the aerodynamic and structure dynamic side. Furthermore, it is verified that no dissipation or accumulation of net energy occurs.

The main characteristics of the aeroelastic fluid structure interaction in the time domain are as follows:

- loose coupling of computational fluid dynamics (CFD) and computational structure dynamics (CSD) through file input/output,
- use of an implicit or explicit Newmark algorithm for the time integration of the CSD equations of motion,
- use of different scattered data interpolation methods with and without compact support radius for coupling in space domain,
- data exchange based on adjusted conventional serial staggered (CSS) algorithm modified with a predictor-corrector scheme,
- structural behavior is described by the complete FE-Model of the delta-wing and the support.

2.5 Integration Framework

The integration framework TENT [Schr02] provides a graphical user interface for controlling and monitoring coupled simulation workflows. The various codes used in the SikMa simulations will be made available in the TENT system, where a simulation workflow can be built by connecting icons representing each code using a graphical workflow editor. Java wrappers containing the basic control functionality for the TAU and SIMULA applications are already integrated in the TENT environment. The wrapper for the CSM-Code as well as the extension of the functionality to handle the coupling between all three disciplines is under development.

While TENT is providing the data transfer and the communication between the applications, the communication logic for the simulation workflow is contained within a coupling manager script. The coupling manager is a user-extensible script based on a Python and Java interface, where functionality to control the flow of the simulation has been implemented.

3 Computer Resources and Performance

Two common simulation environment strategies for the numerical simulation of multi-disciplinary problems are the single, monolithic computational code approach, and the discipline-distributed code approach. In the monolithic approach the discipline specific solvers are all contained within a single code, which is executed on a single computational platform. The advantages of this approach are low communication latencies between the discipline-specific codes, and a unified simulation environment interface. Some of the disadvantages of the monolithic approach are code complexity and non-optimal computational platforms for parts of the code, e.g. scalar-type code parts on vector computers.

In SikMa the discipline-distributed approach is used. Each discipline-specific code, which has been validated independently from the multi-disciplinary simulation, is executed on a platform for which it has been optimized, and the communications between the codes are accomplished using standard network protocols. A unified simulation environment for the different codes is accomplished using the TENT simulation framework, which is also responsible for the data-transfer between the codes. For the simulations of the SikMa specific scenarios, the CFD-Code requires the largest amount of computational resources, and since the TAU-Code has been optimized for high-performance Cluster environments, the platform chosen for the CFD calculations is an Opteron-based Linux-Cluster (www.hlrs.de/hw-access/platforms/strider). In the following table the amount of processors used, calculation time and storage requirements are listed.

Case	Memory [GB]	Proc's [-]	CPU-Time [h]	Cycles [-]
Delta-wing steady calc. One operational point	13	16/32	22	40000
Delta-wing unsteady calc. 72 physical timesteps	13	16/32	51	57600
Delta-wing unsteady calc. 250 physical timesteps coupled simulation	13	16/32	156	200000
X-31 steady calc. One operational point	38	16/32	14	40000

4 Experimental Data

For the validation of the numerical simulation software, various wind-tunnel experiments, designed specifically for the SikMa project, are performed. Experimental data, both steady and unsteady, are available for a 65°-swept delta-wing-fuselage-model-configuration which has been tested in the DNW

Transonic-Wind-Tunnel Göttingen (DNW-TWG). The model has movable trailing-edge flaps and can be used for both guided and free-to-roll maneuver simulations around its longitudinal axis. The model has a chord length of 482mm and a span of 382mm. For the verification of the aerodynamic-structure coupling a steady and dynamic system identification of the delta-wing and the support within the wind tunnel is done. The system parameters are used to setup the FE-model for the coupled simulation.

The main experiments are done in the DNW Low-Speed-Wind-Tunnel Braunschweig (DNW-NWB). In order to perform these experiments, a wind-tunnel model has been designed and built for the SikMa project. The model, shown in Fig. 1, is based on the X-31 experimental high angle-of-attack aircraft configuration. The X-31 model is a 1:7 scaled model with a span of 1000mm and an overall length of 1800mm. The model is equipped with remotely controlled moveable control devices driven by internal servo-engines. Measurement equipment is installed to determine the aerodynamic forces and moments on the model, as well as span-wise pressure distributions at locations of 60% and 70% chord length. The experiments include steady-state measurements using PSP- “Pressure Sensitive Paint”, which provide detailed information on the surface pressure distribution for the whole wing. The experiments will culminate with maneuver simulations, where the movement of the aircraft and the control devices will be synchronized. For the maneuver experiments the model will be mounted on the MPM- “Model Positioning Mechanism” of the DNW-NWB.



Fig. 1. X-31 Remote control model in the DNW-NWB Braunschweig.

5 Results

For the verification and validation of the simulation environment the results of the numerical simulations are compared against data collected from various experimental simulations. To show the capability of the TAU-Code to predict the unsteady aerodynamic behavior of configurations with vortex dominated

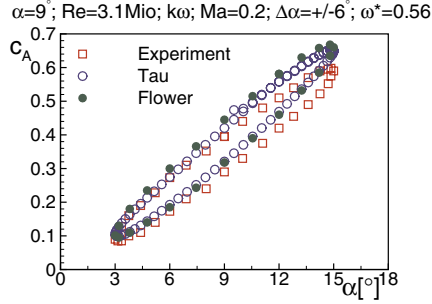


Fig. 2. Lifting coefficient vs. angle of attack in pitching motion of a 65°-swept delta-wing.

flow fields the delta-wing-configuration described in section 3 is used. Fig. 2 shows a result of a delta-wing in rigid body pitching motion. In this calculation the $k\omega$ turbulence model is used. For all simulations presented a central spatial discretization scheme is used. Depicted is the hysteresis loop of the lift coefficient over the angle-of-attack α . The wing is pitching around $\alpha = 9^\circ$ with an amplitude of $\Delta\alpha = \pm 6^\circ$. The wing is oscillating with a reduced frequency of $\omega^* = 0.56$. It is seen that the calculation compares well with the experimental data. For higher angles-of-attack the calculation tends to predict higher lift, because with the common turbulence models a different load distribution over the wing is predicted compared to the experiment. At higher angles of attack the vortex structure and the location of vortex breakdown will not be correctly predicted. The same behavior has been found to occur in simulations using the structured DLR FLOWer-Code.

Figure 3 the result of a coupled simulation between CFD and flight-mechanics is shown using the delta-wing with trailing-edge flaps. To simulate the motion of the control surfaces (trailing-edge flaps) the chimera approach has been used. The maneuver shown in Fig. 3 is a 1 DoF rotation around the

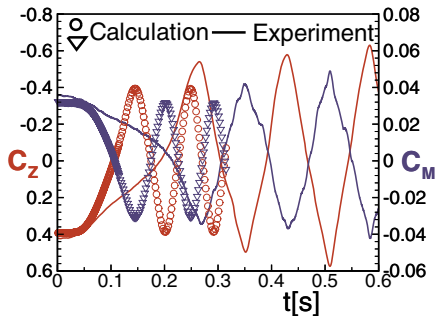


Fig. 3. 1 DoF Free-to-Roll maneuver of delta-wing-flap conf. through trailing-edge flap deflection of $\eta = \pm 3^\circ$.

longitudinal axis of the delta-wing induced by an asymmetric deflection of the flaps by $\eta = \pm 3^\circ$. The initial aircraft attitude is at $\alpha = 9^\circ$ and $\Phi_0 = 0^\circ$. It is seen that the wing enters a periodic roll motion in both the numerical and experimental simulations. One of the sources for the difference seen between the numerical and experimental results is the mechanical friction in the experimental setup, which is not taken into account in the numerical simulation, thus leading to a higher frequency of rotation. Currently only a one equation turbulence model is used in the coupled simulations. It is known that for sharp leading-edge delta-wings the $k\omega$ turbulence model delivers better results and will be used in further simulations.

The capability to predict the elastic deformations of the delta-wing configuration during a guided roll maneuver is shown in Fig. 4. In the coupled simulation between the TAU-Code and the structural mechanics tool developed within SikMa the delta-wing and the rear-sting support are considered to be elastically deformable. For the coupled simulation the finite element model [Neum03] takes into account both the delta wing configuration as well as the flexible support. The FE-Modell is validated based on results of both ground vibration and static deformation tests.

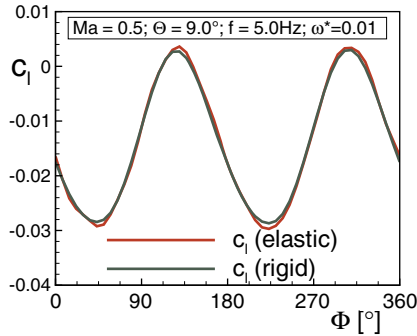


Fig. 4. Comparison of rolling moment between rigid- and elastic-body motion of delta-wing during constant rotation. Time accurate coupled CFD(Euler)-CSM simulation.

In Fig. 5 the corresponding history of the model deflection due to the elasticity is seen. Depicted is the displacement of the delta-wing nose-tip and sting relative to the rigid-body motion case. It is seen that the wing tip is describing an elliptic motion during the rotation. The green loop in Fig. 5 shows the tip movement from the system identification in the experiment due to the integration of the acceleration. Because of the integration the shift in z-direction can not be captured. However, it is shown that the numerics predict the characteristic movement of the wing tip accurately. Due to this deformation the effective angle-of-attack at the same roll angle is higher in

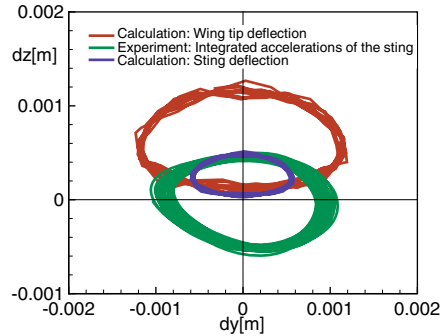


Fig. 5. History of the delta-wing nose and sting deflection during elastic-body motion comparison with experiment. Time accurate coupled CFD(Euler)-CSM simulation.

the elastic case. This leads to a higher amplitude of the rolling moment, as is seen in Fig. 4.

For the X-31 configuration, results from steady-state numerical simulations have been obtained. These simulations show the capability of the TAU-Code to simulate complex delta-wing configurations with rounded leading-edges. Figure 6 shows the numerically simulated 3D flow field over the X-31 configuration, which is a good indication of the complexity of the vortex flow topology over the wing and fuselage. Comparisons with experimental data show good agreement regarding the vortex topology.

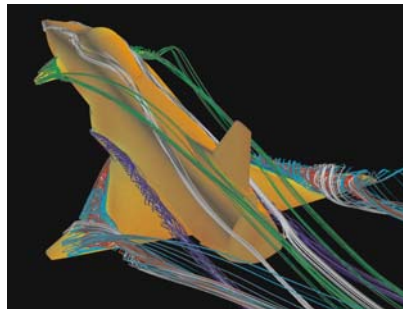


Fig. 6. 3D flow field over the X-31-Configuration at 18° angle-of-attack.

In Fig. 7 an oil flow picture of the X-31 clean-wing from low speed experiments is shown. The angle-of-attack is $\alpha = 18^\circ$ at a Reynolds number of 1.0Mio. The separation line of the strake vortex and the main wing vortex as well as the attachment line of the main wing vortex near the leading-edge is emphasized. In Fig. 8 the corresponding CFD calculation is depicted. It is seen that the flow topology from the calculation fits quite well with the

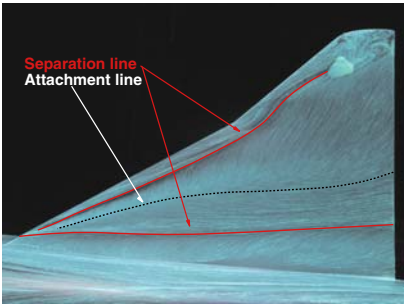


Fig. 7. Oil flow visualization of the X-31 clean wing at $\alpha = 18^\circ$, $Re=1.0Mio$.

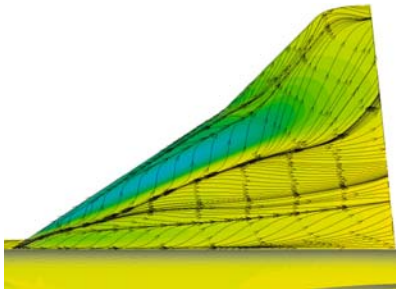


Fig. 8. TAU calculation: Visualization of surface streamlines at $\alpha = 18^\circ$, $Re=1.0Mio$.

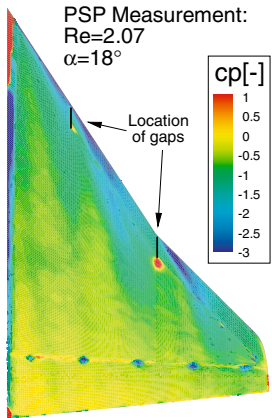


Fig. 9. Steady PSP measurement of the pressure distribution over the X-31 wing.

experiment. Further experimental results delivering steady pressure distributions upon the wing were done within another X-31 test campaign. The PSP result at $\alpha = 18^\circ$ at a Reynolds number of 2.07Mio is shown in Fig. 9. Comparing the pressure distribution in Fig. 9 with the CFD calculation in Fig. 10

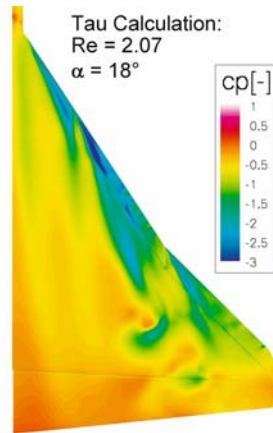


Fig. 10. Steady TAU RANS calculation of the pressure distribution over the X-31 wing (clean wing).

shows that the main footprints of the vortices are captured by the numerics, but the suction-strength and the vortex location are not. However, in this case the experiment is done with mounted leading-edge flaps. The gaps between the leading-edge flaps probably influence the vortex formation considerably. Additional calculations will follow taking all geometric features into account.

6 Conclusions

In this paper the activities and recent results of the DLR-Project SikMa were presented. In SikMa a simulation tool will be developed that is capable of simulating a maneuvering elastic aircraft with all its moveable control devices. The simulation tool combines time-accurate aerodynamic, aeroelastic and flight-mechanic calculations to achieve this objective. Preliminary verification of the functionality of the simulation tool has been shown by simulating a sharp leading-edge delta-wing during a guided motion pitching maneuver and free-roll maneuvers due to flap deflections. Furthermore, first perspectives were presented regarding the time accurate coupling between the TAU-Code and the numerical Structure-Mechanical Tool. Initial results of the steady flow field around the X-31 configuration were presented.

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Advanced Rotary Wing Aeromechanics

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Abstract. This paper presents recent developments and results in the aerodynamic and aeroelastic simulation of helicopter main rotors. Our current work focusses on two aspects which are of high relevance for the further improvement of helicopter rotors: The aeroelastic simulation of active rotor concepts and the correct reproduction and prediction of Blade Vortex Interaction.

1 Introduction

Helicopter aerodynamics and aeroelasticity has been an extensive field of research at the Institut für Aerodynamik und Gasdynamik (IAG) within the past years and it has become evident that a helicopter rotor is a highly complex and strongly coupled system which needs to be investigated in an interdisciplinary manner [10, 11]. Even the plain aerodynamic simulation of a helicopter rotor in forward flight is still one of the most ambitious tasks in Computational Fluid Dynamics, as the flow field is characterized by highly three-dimensional, unsteady transonic effects.

At the IAG advanced numerical analysis tools are used for the coupled aerodynamic/dynamic analysis of rotary wings [1, 3, 6, 8]. The flow field is calculated by the CFD code **FLOWer** which is provided by DLR. Interfaces for strong (time accurate) and weak fluid structure coupling have been implemented into **FLOWer** at IAG. Furthermore, the code has been extended with a simulation tool for active rotor trailing-edge flaps and an additional feature which allows highly accurate blade tip vortex conservation by applying Chimera subgrids adapted to the vortex path. The calculation of the blade dynamics in combination with the strong coupling approach is carried out by the finite element solver **DYNROT** [3], whereas the flight mechanics code **HOST** provided by Eurocopter is going to be used for weak coupling.

2 Mathematical Formulation and Numerical Scheme

2.1 Governing Flow and Structure Models

Aerodynamics. FLOWer solves the three-dimensional, unsteady Reynolds-averaged Navier-Stokes equations (RANS) in integral form in the subsonic, transonic and supersonic flow regime. The equations are derived for a moving frame of reference and are given by

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{E}}{\partial \xi} + \frac{\partial \mathbf{F}}{\partial \eta} + \frac{\partial \mathbf{G}}{\partial \zeta} - \frac{1}{Re_0} \left(\frac{\partial \mathbf{E}_v}{\partial \xi} + \frac{\partial \mathbf{F}_v}{\partial \eta} + \frac{\partial \mathbf{G}_v}{\partial \zeta} \right) = \mathbf{R} . \quad (1)$$

$\mathbf{Q}$ represents the solution vector containing the conservative variables. Centrifugal and coriolis accelerations are included in the source term $\mathbf{R}$ and Re_0 is the reference Reynolds number evolving from non-dimensionalization.

The parabolic-hyperbolic system of partial differential equations can be closed by assuming a thermally and calorically perfect gas as well as Newtonian fluid properties. Turbulence can be modelled either by algebraic or by transport equation models. For the present RANS calculations the algebraic model according to Baldwin&Lomax has been applied.

The numerical procedure is based on structured meshes. The spatial discretization uses a central cell-vertex, cell-centered or an AUSM (Advection Upstream Splitting Method) finite volume formulation. Dissipative terms are explicitly added in order to damp high frequency oscillations and to allow sufficiently sharp resolutions of shock waves in the flow field. On smooth meshes, the scheme is formally of second order in space. The time integration is carried out by an explicit Runge-Kutta scheme featuring convergence acceleration by local time stepping and implicit residual smoothing. The solution procedure is embedded into a sophisticated multigrid algorithm, which allows standard single grid computations as well as successive grid refinement. Unsteady calculations are carried out using the the implicit Dual Time Stepping Scheme which reduces the solution of a physical time step to a steady-state solution in pseudo time. This approach is very effective as all convergence acceleration methods mentioned above can be used.

The code is written in a flexible block structured form enabling treatment of complex aerodynamic configurations with any mesh topology. It is fully portable for either scalar or vector architectures on sequential and parallel computers.

FLOWer is capable of calculating flows on moving grids (arbitrary translatory and rotatory motion). For this purpose the RANS equations are transformed into a body fixed rotating and translating frame of reference. Furthermore the Arbitrary-Lagrangian-Eulerian (ALE) method allows the usage of flexible meshes which is essential in the context of fluid structure coupling. Arbitrary relative motion of grid blocks is made possible by the Chimera technique of overlapping grids.

Structure Dynamics. In combination with the time accurate strong coupling approach the IAG in-house code DYNROT is used, which represents the rotor blade as quasi one-dimensional Timoshenko beam. In contrast to Euler's beam theory, where cross sections remain plane and keep a tangential orientation along the beam axis, Timoshenko's theory allows a deviation from this orientation due to shear forces. The physical representation of the quasi one-dimensional beam consists of infinitesimally thin cross-sectional layers. For a given cross-section the center of gravity, the torsion center and the bending center must not necessarily coincide which leads to a structural coupling of torsion and bending. Furthermore the aerodynamic center may have an offset to the other axes, thus allowing an aerodynamic coupling of the torsional and bending degrees of freedom.

The deflection of each rigid slice is described by three rotational and three translational degrees of freedom, subsumed in the vectors ϕ and $\mathbf{u}$. The kinetic and potential energy of the cross-section can be formulated as length-related energy density functions in coordinates of the rotating reference system $[R]$, yielding

$$\begin{aligned} l = \frac{1}{2} & (\rho A \dot{\mathbf{u}} \dot{\mathbf{u}} + \omega \mathbf{\Theta} \omega \\ & + E A \dot{u}_{2T}^2 + \gamma^T \mathbf{G} \gamma + \check{\phi}^T \mathbf{T} \check{\phi} \\ & + N^0 (\phi_1^2 + \phi_3^2)) + \rho A \mathbf{g}_{(R)} . \end{aligned} \quad (2)$$

After the integration over the beam length has been performed, an inhomogeneous system of differential equations can be obtained by applying Hamilton's principle. The resulting system of differential equations is solved using a finite element formulation which is introduced into the Lagrange density function. Finally a linear ODE-system is obtained which is given by

$$\mathbf{M} \ddot{\mathbf{Q}} + \mathbf{D} \dot{\mathbf{Q}} + \mathbf{K} \mathbf{Q} = \mathbf{F}^{RHS} . \quad (3)$$

The time integration is performed by a generalized- α method, which is unconditionally stable and of second-order accuracy.

The flight mechanics code HOST is used for weak fluid structure coupling. It represents the rotor blade as a chain of rigid, one-dimensional elements, connected to each other by fictive articulations. The dynamic response of the blade in flap, lag and torsion is obtained by solving the Lagrange equation, which is given by

$$\frac{d}{dt} \left(\frac{\partial T}{\partial \dot{q}_i} \right) - \frac{\partial T}{\partial q_i} + \frac{\partial U}{\partial q_i} = Q_i \quad (4)$$

where T is the kinetic energy, U the elastic energy, Q_i the generalized loads and q_i the generalized coordinates. In order to reduce the calculation time HOST expresses the solution as a superposition of the blade's mode shapes. As the solution is periodic in case of a steady forward flight, the contribution

of each eigenmode to the total dynamic response, its generalized coordinate, is given as a distinct function of the blade's azimuth angle. Thus, any degree of freedom $h(r, \psi)$ can be expressed by

$$h(r, \psi) = \sum_{i=1}^{modes} q_i(\psi) \cdot \bar{h}_i(r) \quad (5)$$

where q_i are the generalized coordinates and $\bar{h}_i$ are the modal shapes, depending on the blade radial position r .

2.2 Fluid Structure Coupling

Strong Coupling. The coupling of fluid code and structure code in a time accurate manner is called *Strong Fluid Structure Coupling*. This means the data exchange between FLOWer and the structure code DYNROT is performed on a time step basis. Both codes are coupled using a modular approach which maintains the full autonomy of the individual methods. Fluid code and structure code can be run on different platforms and the data exchange on the common interface, the deformed blade surface, is performed via TCP/IP. FLOWer calculates the loads on the blade surface, which are used by DYNROT for an update of the blade deformation. This deformation is introduced into the flow solver by applying a deformation of the blade grid. In order to ensure the required accuracy of the overall method and to obtain a true representation of the underlying physics, a sophisticated coupling scheme must be introduced. The coupling scheme used for the calculations presented in this paper was developed by Hierholz [7]. The integration methods on both sides are of second order accuracy. Considering that the structure integration algorithm can be transformed into the midpoint rule by an appropriate choice of parameters and under retention of the order of accuracy, a non-iterative coupling scheme is obtained, illustrated in Fig. 1. The overall accuracy of the aeroelastic analysis is of second order. A characteristic feature of this scheme is an offset of half a timestep between the structure and fluid modules.

Weak Coupling. The weak coupling scheme is started by the HOST code. HOST computes the blade dynamic response and deformation by trimming the rotor with its simplified 2D aerodynamics provided by airfoil tables. The HOST output, given as the significant harmonics of the generalized coordinates and all related mode shapes, is provided to FLOWer. FLOWer then re-assembles this information to the deformed blade surface. In the following step the CFD computation determines the force and moment distribution versus the blade radius and azimuth angle for an entire revolution, taking into account the respective deformation of the blade grids. Based on the harmonics of the CFD loads HOST applies a correction to its aerodynamic loads and re-trims the rotor. This cycle is repeated until convergence has been

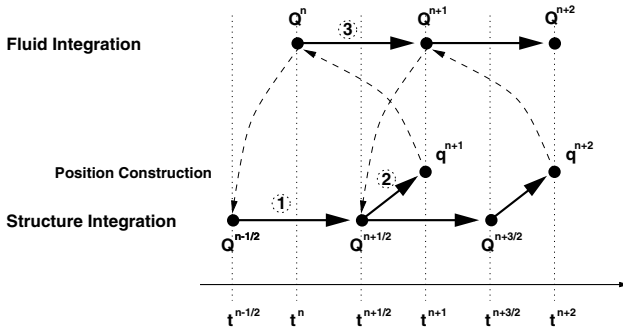


Fig. 1. Implicit/Implicit Scheme of 2nd Order

reached. In case of convergence the simplified HOST aerodynamic model has been completely replaced by the CFD aerodynamics. The advantage of the weak coupling method in comparison to the strong coupling approach is the faster trim of the rotor, which makes the method better suited for rotor design calculations.

2.3 Grid Deformation Tool

For aeroelastic computations, a robust algebraic grid deformation tool utilizing Hermite polynomials is applied prior to each time step in order to update the structured aerodynamic mesh according to the surface deformation provided by the structure solver. The deformed surface is determined by bending and twisting the blade quarter-chord line.

In order to minimize the amount of grid deformation and thus maintain a high level of grid quality, the entire virgin grid is rotated into the root-tip secant of the deformed quarter-chord line prior to updating the 3D grid according to the current deformed blade surface. While automatically satisfied on rigid grids, the Geometric Conservation Law (GCL), relating the time rate of volume change of a given grid cell and the relative normal velocities of the individual cell faces, must be taken into account when dynamic grids are used in order to avoid non-conservative inconsistencies in the numerical analysis.

3 Blade Tip Vortex Conservation

The correct reproduction and prediction of Blade Vortex Interaction (BVI) on a helicopter rotor is a major challenge in Computational Fluid Dynamics. The effects of BVI on rotor performance, rotor noise and vibration can only be insufficiently modelled up to now, as the dissipation of the blade tip vortex is too high compared to reality. One possibility to improve the vortex conservation is to refine the CFD grid. This approach is currently investigated at IAG.

A helicopter rotor in forward flight is commonly modelled using the Chimera approach of overlapping grids. This means rotating blade grids are embedded into a so called background grid. Forward flight of the rotor is realized by setting the appropriate far field flow values at the background grid boundaries. The communication between the different grids, i.e. the exchange of flow values, is established by interpolation. The flow field in the background grid is interpolated onto the blade grid block boundaries, whereas the flow field in the blade grids is transferred into the background grid by applying hole cutting in the background grid. Basically the conservation of the tip vortex shed from a given blade and thus the prediction of its influence on the following blades can be improved by providing a finer background grid and finer blade grids. But this approach is inefficient as a finer grid resolution is only needed in the region of the blade tip vortex and otherwise unnecessary. The method which is currently applied at IAG circumvents this drawback by adding special vortex adapted Chimera subgrids. The position of these tube-shaped vortex adapted grids varies with time to fit the current position of the blade tip vortex. The position of the grid centerline is currently prescribed using the analytical blade tip path and taking into account the rotor downwash. In the nonrotating rotor hub system the blade tip vortex path is given as follows:

$$\begin{aligned}
 \text{longitudinal coordinate:} \quad & \frac{z}{R} = -\cos(\psi_w - \psi) - \mu \cdot \psi_w \\
 \text{lateral coordinate:} \quad & \frac{y}{R} = -\sin(\psi_w - \psi) \\
 \text{axial coordinate:} \quad & \frac{x}{R} = -\lambda \cdot \psi_w
 \end{aligned} \tag{6}$$

ψ is the blade's azimuth angle, ψ_w is denoted as the wake age, μ is the rotor advance ratio in the tip path plane and λ is denoted as the rotor inflow angle which is calculated from

$$\lambda = \frac{V \cdot \sin \alpha_{TPP} + v_i}{\Omega \cdot R} . \tag{7}$$

v_i is the induced rotor velocity which is calculated from the rotor thrust coefficient. Note that the current approach does not take into account a variation of the induced velocity over the rotor disc. An example Chimera grid setup for a BVI flight case is shown in Fig. 2. The grid features an eight-block cartesian background grid (1.8 mio cells), four blade grids (150.000 cells each) and four vortex adapted grids (360.000 cells each), i.e. an overall number of 3.8 mio. grid cells.

The flow exchange between the vortex adapted grids and the other grids is established by Chimera interpolation and appropriate hole cutting. The vortex which is shed from the blade is immediately interpolated onto the front face of the associated vortex adapted grid. All remaining block faces of the vortex grid obtain their flow condition from the background grid. The flow transfer from the vortex adapted grid into the following blade grids and

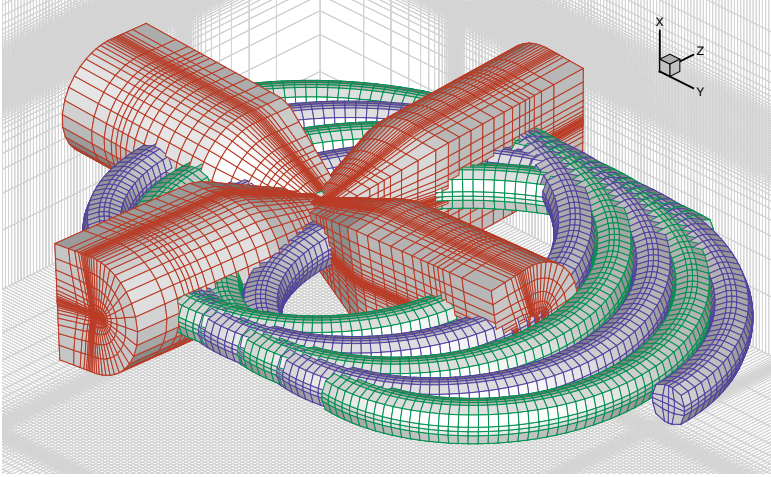


Fig. 2. Chimera grid setup

the background grid is accomplished by additional holes which are shown in Fig. 3. Two additional types of hole definitions have been added compared to a standard Chimera setup:

- Hole Cutting in the blade grid ensuring an accurate flow transfer from the vortex grid into the blade grid (marked red)
- Hole Cutting in the background grid ensuring the flow transfer from the vortex grid into the background grid (marked blue)

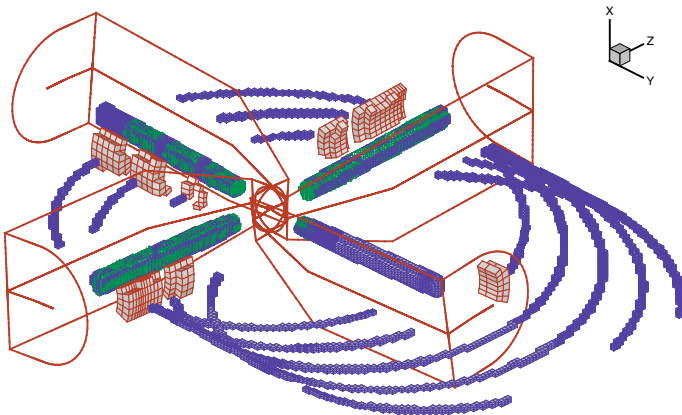


Fig. 3. Chimera hole setup

Fig. 4 shows a vortex visualization using the well-known λ_2 -vortex criterion. An iso-surface of $\lambda_2 = -0.0001$ is shown. In addition, the y -vorticity is plotted on the iso-surface as contour variable showing the sense of rotation with respect to the flight direction. It can be clearly seen that the vortex conservation has significantly improved compared to previous calculations featuring about the same number of cells. In Fig. 5 λ_2 is plotted as contour variable for equidistant axial sections of a vortex adapted grid, showing that the vortex is well captured by the grid even for wake ages greater than one rotor revolution.

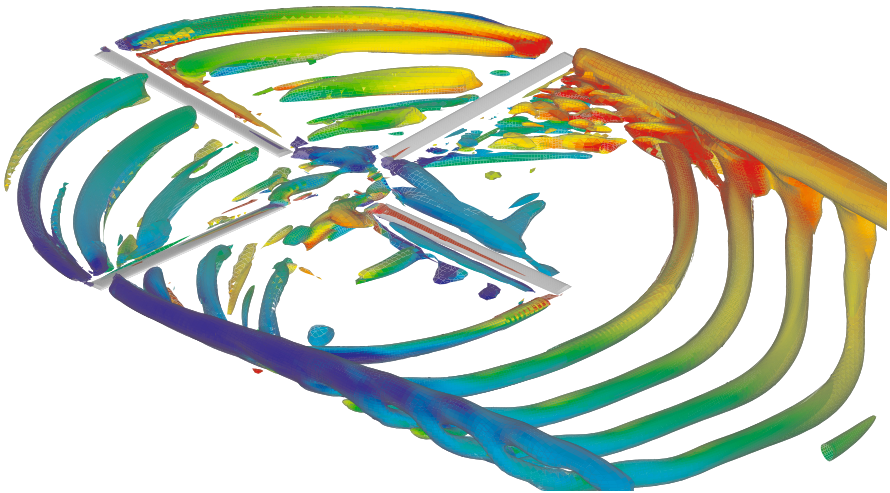


Fig. 4. λ_2 -vortex visualization ($\lambda_2 = -0.0001$)

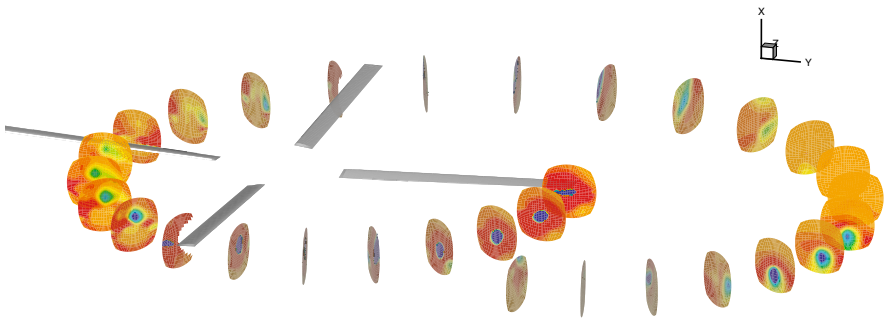


Fig. 5. λ_2 -contour levels in sections of the vortex adapted grid ($\lambda_2 = -0.0001$)

Table 1. Code performance on NEC–SX8 platform

Platform	SX8
Number of cells	3,800,000
Number of CPUs	8
GFLOPS	20.58
Vector operation ratio	97.7%
CPU-time per rotor revolution	64h
Required memory	approx. 1.5 kB/cell

This calculation was carried out on the NEC–SX8 supercomputer using eight CPUs. Table 1 contains significant performance data of this Navier-Stokes computation.

4 Active Rotor Simulation

The performance of a helicopter rotor with respect to power consumption, noise and vibration can be improved by introducing higher harmonic control. One possibility to achieve this is to use a rotor which is equipped with active trailing-edge flaps. In order to correctly capture the effect of the flap control it is absolutely mandatory to perform an aeroelastic analysis. As a rotor blade is a torsionally flexible structure, the flap acts as a servo flap. This means a positive flap angle (downward deflection) will cause a negative (nose down) twist of the blade due to the negative pitching moment in the flap region. This leads to a reduction of the overall blade lift. Therefore qualitatively wrong results will be obtained if aeroelastic coupling effects are neglected.

The servo flap is modelled by a local deformation of the blade grid in the flap region. At the inner and outer flap segment boundary the deflection angle is reduced to zero within a certain smoothing area, neglecting a possible side gap. The deformed blade surface is generated in two steps as illustrated in Fig. 6. In the first step the blade surface is locally deformed according to the flap deflection. In the second step the blade deformation due to the coupling process is applied to this pre-deformed surface. If the structure model is left unchanged the pure aerodynamic effect of the flap control can be simulated. If the flap is supposed to be taken into account on the structure side as well, the structure description (in terms of bending and torsional stiffness etc.) has to be adapted to the current flap deflection.

In the following results of a strongly coupled single blade calculation are presented. The computation was performed for a generic untwisted NACA0012 rotor blade. The blade features a free flap hinge at $r/R = 0.036$. The radial position of the flap segment runs from $r/R = 0.74$ to $r/R = 0.9$ with a chord size of $0.2c$. A cyclic $1/rev$ flap deflection with 9° amplitude has been prescribed. Fig. 7 shows the rotor thrust coefficient versus the blade azimuth

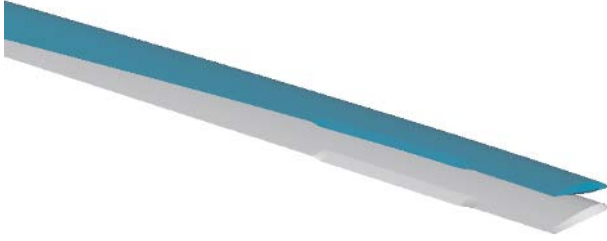


Fig. 6. Deformation of a blade surface due to servo flap and blade dynamics

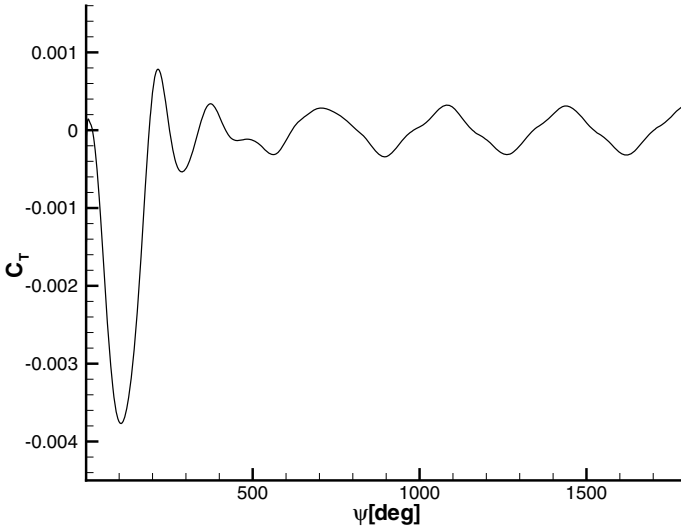


Fig. 7. Rotor thrust coefficient versus azimuth

angle. It can be seen that a fully periodic solution is obtained after about five rotor revolutions.

The quantitative relation between servo flap angle, blade tip torsion and blade tip deflection is plotted versus the azimuth angle in Fig. 8. A positive deflection of the servo flap is linked to a negative (nose down) tip torsion which causes a maximum negative tip deflection amplitude with a phase angle of approx. 90° . The phase angle is actually slightly smaller as the hub distance of the flap hinge of $r/R = 0.036$ is not exactly zero. The performance data of this single CPU Navier-Stokes calculation on NEC-SX6 is given in Table 2.

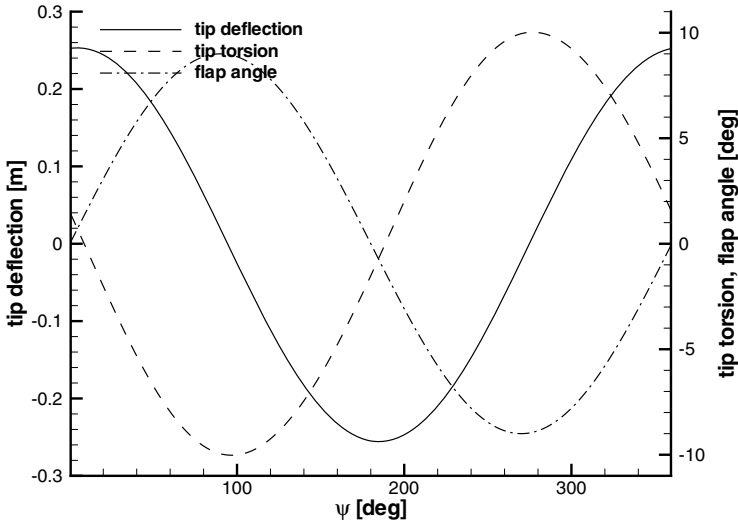


Fig. 8. Servo flap angle, blade tip torsion and blade tip deflection versus azimuth

Table 2. Code performance on NEC-SX6 platform

Platform	SX6
Number of cells	2,540,000
Number of CPUs	1
GFLOPS	1.3
Vector operation ratio	98.0%
CPU-time per rotor revolution	15h
Required memory	approx. 1.5 kB/cell

5 Conclusions and Outlook

We presented advanced methods for the aerodynamic and aeroelastic analysis of helicopter rotors. Currently strongly coupled calculations applying the technique of vortex adapted Chimera child grids are underway. We expect to significantly improve the prediction of BVI with respect to the influence on the blade loading as well as on the impulsive noise. Considering the simulation of active rotors we started to perform rotor performance calculations which will be trimmed using the weak coupling technique in combination with HOST. Furthermore we plan to extend our activities from stand-alone main rotor simulations towards complete helicopter configurations.

Acknowledgement

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Time-Accurate versus Actuator Disk Simulations of Complete Helicopters

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Summary. This report describes numerical simulation of the flow around helicopter fuselage-main rotor-tail rotor configurations using the quasi-steady actuator disk approach and the time-accurate simulation that resolves the relative motion of the main and tail rotors with respect to the fuselage. The computations predict both the instantaneous and quasi-steady flow fields by solving the Reynolds-averaged Navier-Stokes (RANS) equations in three dimensions using a finite volume method and block structured grids. Turbulence effects are taken into account via a two-equation $k - \omega$ model. The motion of the rotors was accomplished by an overlapping grid technique (Chimera). The DLR CFD code FLOWer was applied in parallel mode to obtain the solution at each time step. The computations were performed on 8 processors of the NEC-SX6 at Höchstleistungsrechenzentrum Stuttgart¹ (HLRS)

1 Introduction

Air flow past helicopters ranks among the most complicated types of flow in the aeronautic field. The flow around helicopters exhibits strong vortices generated at blade tips and in the wake of the fuselage. Highly unsteady, interaction between these different flow regimes takes place and varies continuously with time due to the motion of the rotors. Numerical prediction of this class of flows must be capable therefore to capture three dimensional flow phenomena, and to account properly for turbulent effects.

There are two main approaches to simulate rotors numerically. The first resolves the motion of the blades in time, where grids generated around the blades are allowed to rotate intersecting a background grid by means of an overlapping grid technique (Chimera). Several rotor revolutions are usually required for complete evolution of the flow field. The choice of the time intervals, and consequently the number of time steps, is governed by the desired time accuracy and other numerical considerations concerning the overlapping

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grid method. Alternatively, the momentum jump and mass flow across the rotor are introduced to the flow as a special boundary condition (actuator disc approach). These discontinuities are calculated by blade element or momentum theories allowing variations in the radial and azimuth directions on the disc. The actuator disc model is particularly attractive as it removes the need for unsteady simulation of the rotor and represents its effects by a simple, computationally inexpensive boundary condition. Therefore most of the literature dealing with rotor-fuselage configurations is based on the quasi-steady actuator disk approach (see [1, 2, 3]. Only very few publications compute the unsteady flow around such configurations using the chimera technique (e.g. [4, 6, 7, 8]) because of the enormous computational effort especially in terms of CPU time.

Proper resolution of the motion and the geometry requires high performance computing to obtain results in a practical turnaround time. Although the SX6 is a computer with a remarkable performance, 6 to 8 weeks (48-64 CPU weeks) were necessary to obtain periodic behavior of the flow. The computational costs were mainly covered by the DLR (around 90%), as opposed to the original plans where the reported computation should have been carried out as a part of the current (TAAD) project.

2 Numerical tools

In the present project the DLR's CFD simulation code FLOWer [9, 10] was applied to predict the flow fields. FLOWer solves the integral form of either the time-dependent or the steady compressible Navier-Stokes equations on structured, multi-block grids based on finite volume discretization.

Mass, momentum and energy fluxes are discretised in space using either cell-vertex (making use of the supercell concept) or cell-centred, whereby flow unknowns are located either at grid nodes or at cell centres respectively. Spatial discretisations of convection fluxes result from the application of either the Jameson scheme (central fluxes plus second and fourth order dissipation) or the upwind AUSM/Van Leer scheme [11], while viscous fluxes are centrally discretised, and time integration is carried out by means of a 5-stage Runge-Kutta cycle. Acceleration techniques like local time-stepping, implicit residual smoothing and multigrid cycling are then used to enhance the convergence properties. FLOWer can also handle low velocities by means of preconditioning [12], possesses a full implementation of Chimera features [13] (no hierarchical mesh dependencies) and has further unsteady developments [14]: an implicit time integration using the dual-time stepping method by Jameson, an extension of the equation formulation to moving and deforming meshes and a geometry conservation law. The Reynolds-stress tensor is modeled using Boussinesq's assumption and the resulting eddy viscosity in turn can be calculated by the algebraic Baldwin-Lomax model or in integrating the 1-transport equation Spalart-Allmaras model or a series of 2-transport equation models,

the most famous of which is the Wilcox $k - \omega$ model. Convection fluxes of the turbulence equations are discretised by a first order accurate Roe scheme and turbulence variables are integrated in time by means of a single grid implicit DDADI (diagonal dominant alternating direction implicit) scheme [15]. Boundary conditions for the conservative and turbulence variables follow the one-dimensional characteristics theory on far-field boundaries, mirror the variables on symmetry planes and set a no-slip condition on solid bodies. Finally, the code has been parallelised [16] making use of the MPI framework.

The relative rotary and pitching motions of the blades with respect to the fuselage are accomplished by moving a Chimera overlapping grid method. Theoretically an unlimited number (up to the code dimension limits) of hierarchies of relative motions can be specified in time, and applied to the different elements of the geometry. Each level of the hierarchy defines a separate reference frame in which motions can be specified indepently of the inertial frame of reference, thus allowing any combination of translatory and rotary motions to be realized by a series of simple co-ordinate transformations.

3 Computational model and grid

Actuator Disk approach

The first test case is the BO105 helicopter. The grid has been generated at DLR and contains approximately 11 million points distributed in 99 blocks. An O-block topology has been used around the fuselage, while an H-topology was retained around the disc and its hub, which has been neglected. General flight conditions are given by the upstream Mach number M_∞ , the angle of incidence α and the Reynolds number per meter Re_∞ . Specific rotor parameters are the tip Mach number M_{tip} , the thrust coefficient C_T and advance ratio μ . Their numerical values are: $\alpha=-0.66^\circ$, $M_\infty=0.125$, $Re_\infty=2.91 \times 10^6$, $M_{tip}=0.638$, $C_T=0.006315$, $\mu=0.2$. The rotor has been modeled by a uniform pressure jump.

The Dauphin 365N configuration was chosen as the second test case. This configuration has been experimentally tested, meshed and computed at ONERA, see [5] and references therein. In this context, experimental data, a structured multi-block mesh and a ready-to-use actuator disc map have been made available to DLR by ONERA. The mesh of the Dauphin is made of around 7 million points gathered in 94 blocks. The fuselage as well as the disc are embedded within O-topologies and the stabilisers and the fin within C-topologies. This grid was particularly designed to allow efficient vorticity convection, especially marginal vortices of the disc, and in respect thereof has proven to be of high quality. Flight and rotor conditions are: $\alpha=-3.0^\circ$, $M_\infty=0.044$, $Re_\infty=1.07 \times 10^6$, $M_{tip}=0.294$, $C_T=0.006196$, $\mu=0.15$. where the relatively small value of M_{tip} is due to the smaller tip radius of the wind tunnel model. The upstream flow makes with the disc an angle of $\alpha_{shaft}=-7^\circ$.

Time accurate approach

Time accurate approach was applied to simulate wind tunnel experiment carried out in the HELINOVI research project. The model used in the experiment (Fig. 1) is 1:2.5th scale of the original BO-105 helicopter. The model has a total length of 3.5 m. The main and tail rotors diameters are 4 and 0.773 meter, respectively.

Mach number at the tips of both rotors (M_{tip}) is equal to 0.64. The flight conditions are set to Mach number $M_\infty = 0.1766$ and an angle of incidence $\alpha = -5.2^\circ$. The corresponding free stream Reynolds number (Re_∞) is equal to 13.5×10^6 based on the total length of the model.

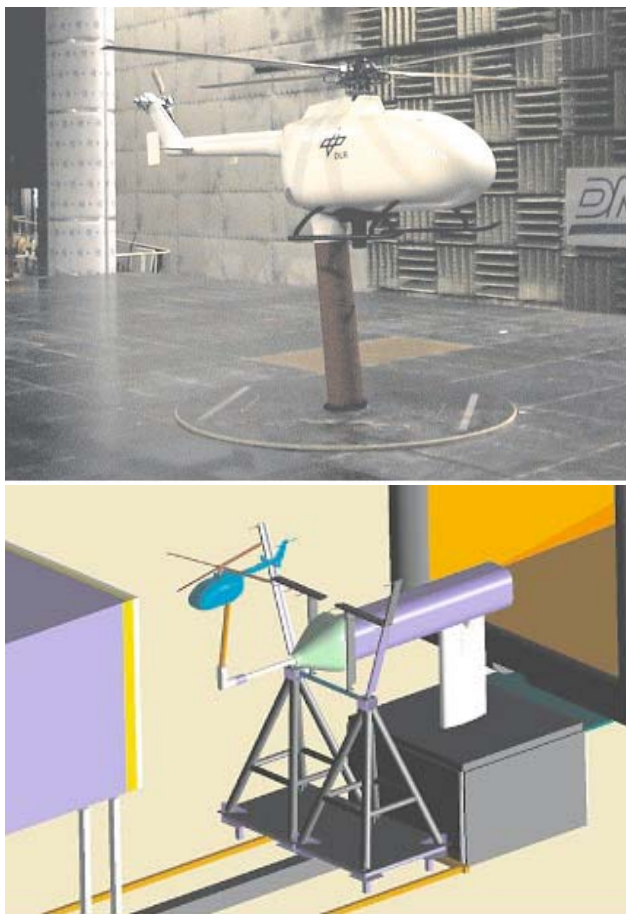


Fig. 1. Helinovi wind tunnel measurements. a) Wind tunnel model, b) 3D sketch of the experimental setup

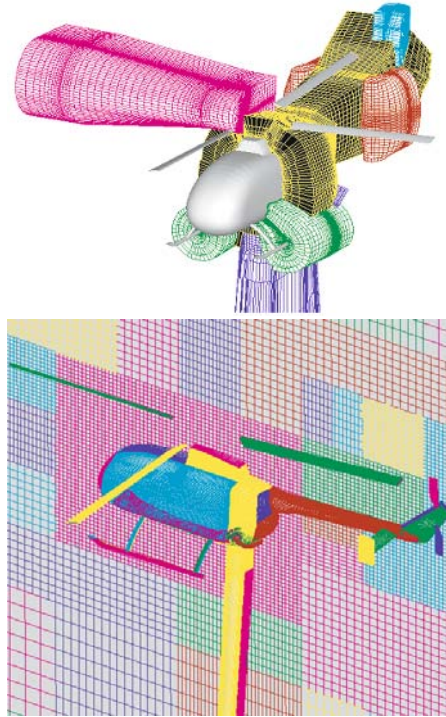


Fig. 2. CFD geometry and numerical grid a) Cross section view showing the background grid at symmetry. b) View of components grids

The simulated configuration consisted of 13 different elements grouped in 7 main groups. Fig. 2 shows the computational CFD configuration and the numerical grid.

Each element of the configuration had its own component (child) grids. Child grids are embedded in a large background grid and may have partial overlap, thus ensuring continuity of the flow via the overlap regions. The grid consists of 480 structured blocks and a total number of 13 million points.

4 Results

Actuator disc approach

Figure 3 displays the distribution of normalised total pressure along with streamlines in the symmetry plane, whereby it appears clearly that the fin and the stabilisers experience a totally different flow in comparison to an isolated fuselage simulation.

The insert in the same picture shows the pressure distribution along the top centerline, where experimental points (hollow squares) are relatively well

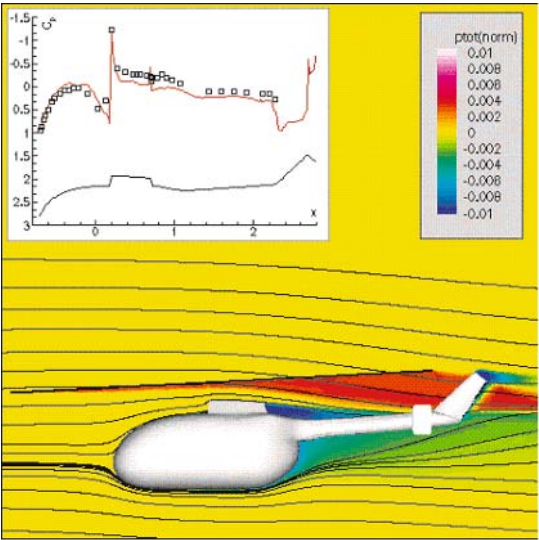


Fig. 3. BO105 - Normalised total pressure distribution

reproduced by the computation (solid line). However, modeling the hub and specifying a more realistic force distribution on the disc could further improve the agreement. Pressure coefficient distribution on the fuselage and normal velocity component on the disc are displayed in Fig. 4 .

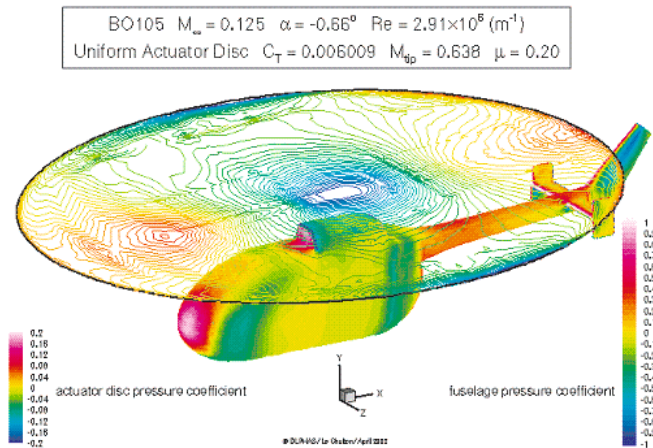


Fig. 4. BO105 - Pressure coefficient distribution

The blocking influence of the fuselage is to be seen on the front part of the disc where the inflow is reduced in comparison to the sides. Also to be noted are the thin zones on both sides where the fluid flows from bottom to top. More insight in the BO-105 test-cases can be found in [8].

For the Dauphin 365N configuration, validation runs have been carried out with and without actuator disc map and have been compared to computational results presented in [5]. Figure 5 depicts pressure distributions along sections normal to the fuselage axis. Experimental points are identified with squares and the computation with the solid line: good agreement has been reached notably thanks to the use of preconditioning.

The presence of the rotor head, in both cases during the wind tunnel experiment, inevitably modifies the flow-field downstream of it, which is not reproduced here in the present simulations. Further comparisons have been done and show good global agreement with results given in the aforementioned

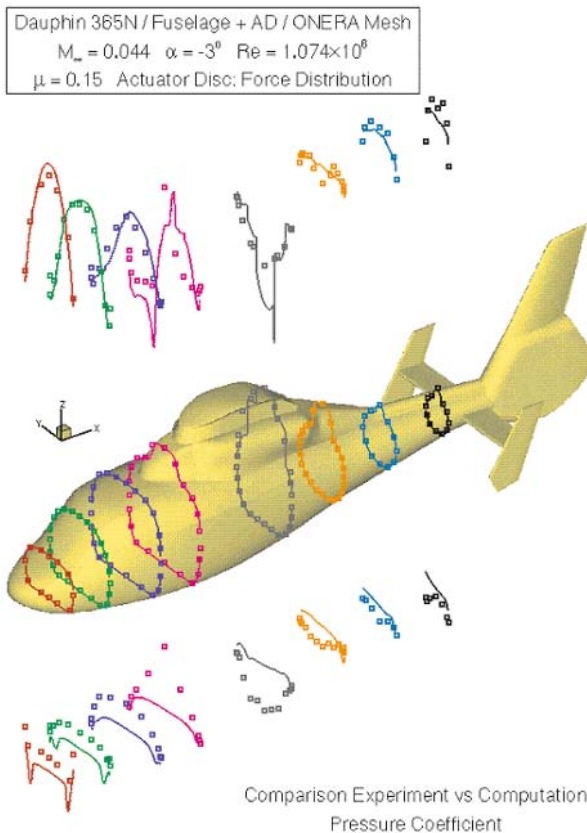


Fig. 5. Dauphin 365N - Pressure coefficient distributions

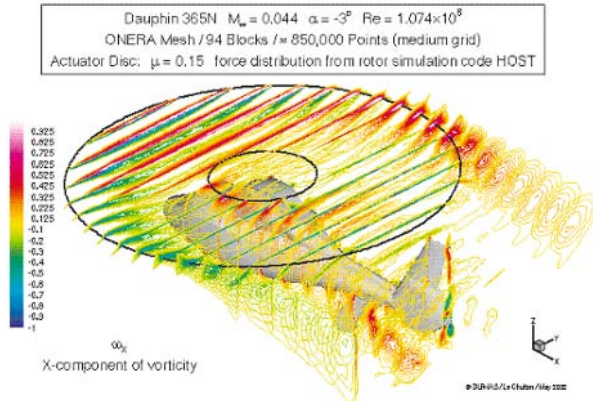


Fig. 6. Dauphin 365N - Distribution of the X-Component of Vorticity

reference, which the interested reader is referred to. In Fig. 6 the distribution of the x-component of the vorticity vector in a series of planes parallel to each other and all perpendicular to the main dimension of the configuration is presented. Since the actuator disc map sets source terms in all three space directions, a relatively strong shearing takes place between the upper and lower sides, which causes the coloured vorticity stripes all over the disc surface.

Time accurate approach

The computed vortex structure is shown in Fig. 7 by constant λ_2 surfaces. Evident blade-vortex interaction can be observed. Also clearly seen is unsteady vortex shedding from the helicopter skids and the model support. The computations could reproduce the interaction of the main rotor wake with the tail rotor, which is typical for this advance ratio.

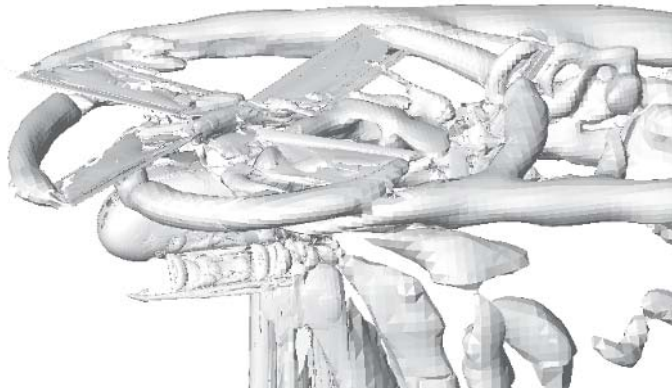


Fig. 7. Iso-surfaces of computed λ_2

A large stagnation region on the front of the motor fairing is evident. The high pressure zone at the fuselage front end is affected by the main rotor's downwash where an asymmetrical pressure pattern is found instead of the symmetric distribution usually found on isolated fuselages.

Surface pressure contours are shown in Fig. 8 at 365° main rotor azimuth position. Examination of the figure reveals significant differences in pressure on the different blades of the main rotor. Large suction areas can be seen on the advancing blade (the rotors rotates counter clockwise seen from above) near the tip with large pressure gradients indicating most probably formation of shocks. A completely different pressure pattern is observed on the retreating blade. Similar observation can be found on the tail rotor (note the opposite sense of rotation).

Figure 9 illustrates the phenomenon further. The figure shows computed pressure distributions on the main rotor blade at 98.5% of the radius for 90° , 180° , 270° and 360° azimuth positions. Clearly seen is a suction peak on the upper side of the advancing blade (90° position) followed by a steep pressure increase possibly due to a shock. The pressure behaves completely different on the retreating blade (270° position) showing significantly weaker suction and pressure peaks.

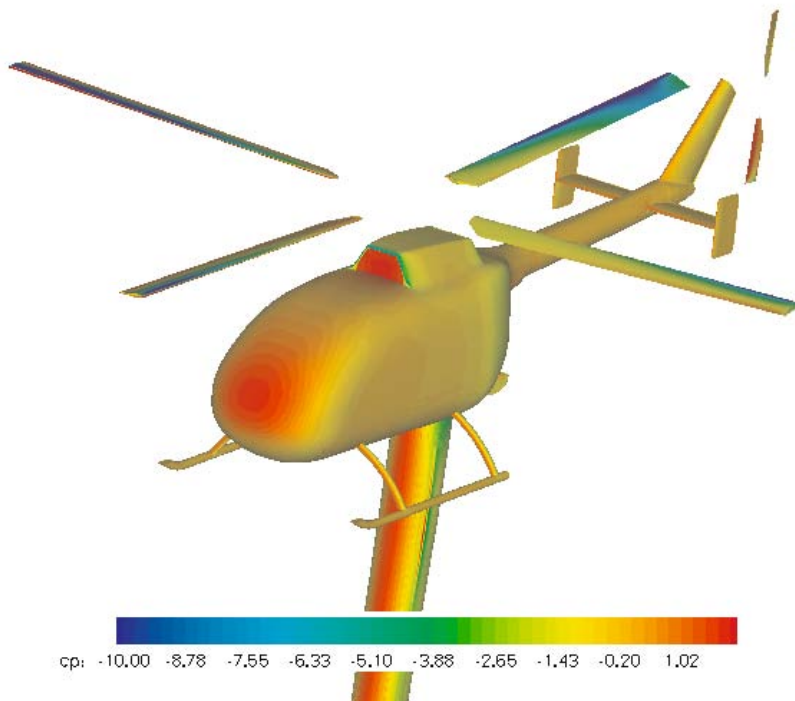


Fig. 8. Instantaneous pressure coefficient on the surface of the model

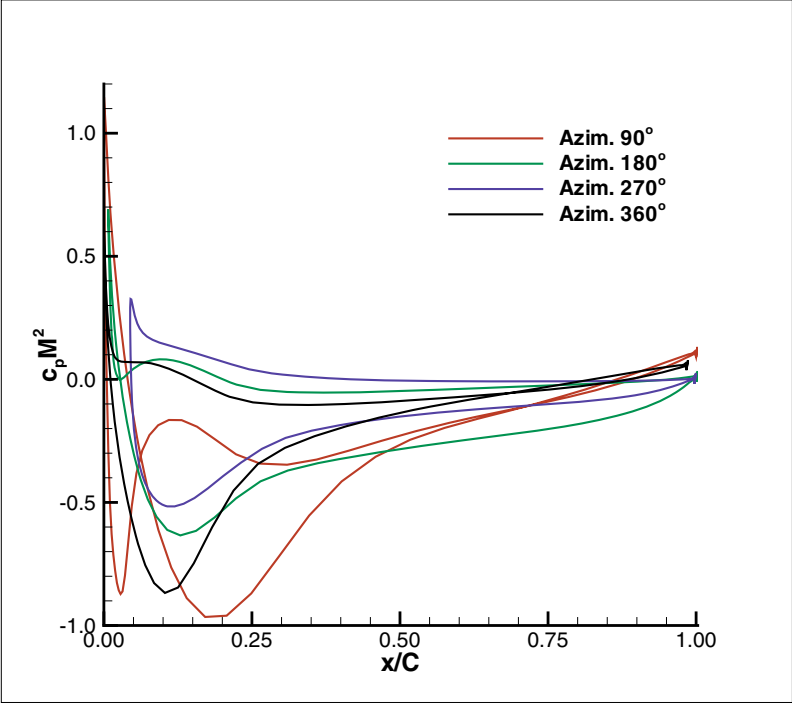


Fig. 9. Instantaneous pressure coefficient on the surface of the model

Performance

Several modifications have been introduced to FLOWer during the project to improve its performance on the NEC-SX6. The outcome of FLOWer development is summarized in Table 1. As can be seen from the table, Chimera search algorithm was the bottle neck on vector computers. Enhancement of Chimera performance could reduce the CPU time to 44%.

Table 1. Performance improvement of Chimera search algorithm

	Chimera	Flow solver	CPU sec. /time step /proc.
Original status	750	465	1215
New compiler	460	465	925
Loop unrolling	370	465	835
Hole cutting			
vectorization	80	465	545
Current state	69	465	534

5 Conclusions

Quasi-steady and time accurate simulation of the flow around a BO-105 fuselage-main rotor-tail rotor wind tunnel model and a Dauphine 365N helicopter have been carried out by the solution of Reynolds Averaged Navier-Stokes equations. Despite the relative simplicity of the wind tunnel model geometry compared to the real aircraft, 7 to 13 million grid points were necessary to properly resolve the surface geometry and the thin viscous layer near the body. The flow field was computed at time intervals corresponding to 0.4 degree angular displacement of the main rotor. CPU memory and time required were in the order of 20 GB and 800 hours respectively. CFD computations at such a scale can be performed nowadays only using a high performance computer like NEC-SX6 at HLRS. The original plans were to finance the computations by the research project TAAD. However, the budget of the project was dramatically reduced and DLR had to provide the financial resources for about 90% of the total computational cost.

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LES of Shock Wave/Turbulent Boundary Layer Interaction

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Summary. Well-resolved Large-Eddy Simulations (LES) are performed in order to investigate flow phenomena and the turbulence structure of the boundary layer along a supersonic compression ramp. The numerical simulations directly reproduce an available experiment. The compression ramp has a deflection angle of $\beta = 25^\circ$. The mean free-stream Mach number is $M_\infty = 2.95$. The Reynolds number based on the incoming boundary-layer thickness is $Re_{\delta_0} = 63560$ in accordance with the reference experiment. About 18.5×10^6 grid points are used for discretizing the computational domain. For obtaining mean flow and turbulence structure the flow is sampled 1272 times over 703 characteristic time scales. Statistical data are computed from these samples. An analysis of the data shows a good agreement with the experiment in terms of mean quantities and turbulence structure. The computational data confirm theoretical and experimental results on fluctuation-amplification across the interaction region. In the wake of the main shock a shedding of shocklets is observed. The temporal behavior of the coupled shock-separation system agrees well with experimental data. Unlike previous DNS the present simulation data provide indications for a large-scale shock motion. Also evidence for the existence of three-dimensional large-scale stream-wise structures, commonly referred to as Görtler-like vortices, is found.

1 Introduction

Shock-wave/turbulent-boundary-layer interaction on compression-ramp flow is a canonical test configuration for statistical turbulence modeling. Extensive experimental data are available, whereas computational data focus mainly on Reynolds-averaged computations employing a wide range of turbulence models. In Fig. 1 basic flow features are sketched [14]. The undisturbed incoming turbulent boundary layer interacts with the shock wave, for sufficiently large deflection angles resulting in a separation region near the compression corner, and a λ -shock system containing the separation region. Subsequently the disturbed boundary layer passes through the Prandtl–Meyer expansion near the decompression corner and finally relaxes towards a developed zero-pressure-

gradient boundary layer. The most prominent features are highlighted in the insets of Fig. 1, where separation and reattachment points are indicated by S and R respectively: 1,2: unsteady shock system and the turbulence amplification due to shock-turbulence interaction within the boundary layer and in the external flow; 3: damping of turbulent fluctuation by interaction with the expansion; 4: re-initialization of the boundary layer after reattachment; 5: three-dimensional large-scale structures (Görtler-type vortices); 6: possible flow relaminarization in the reversed-flow region.

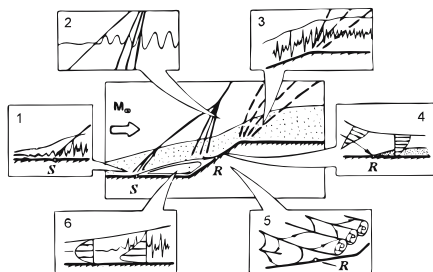


Fig. 1. Essential flow physics in compression ramp flows (for explanations see text on page 221)

Although numerous computations based on the Reynolds-averaged Navier-Stokes equations (RANS) were performed, most of them failed to predict some essential characteristics (e.g. skin-friction and heat transfer)[15],[9]. Main conclusion on RANS computations is that they fail since some essential physical flow features are precluded. LES is the most appropriate numerical tool for an analysis of unsteady transitional and turbulent flows. Although a wide range of different sub-grid-scale (SGS) models exists, to our knowledge no successful LES computations have been performed for the configuration investigated in this paper matching exactly the experimental flow parameters [10].

The current numerical investigation is aimed at a direct comparison with an available experiment. For this purpose all flow parameters and the flow geometry are matched to this experiment [16], [17]. The free-stream Mach number is $M_\infty = 2.95$, the Reynolds number based on the incoming boundary-layer thickness is $Re_{\delta_0} = 63560$, the ramp deflection angle is $\beta = 25^\circ$. By matching directly the experimental parameters the prediction quality of the employed sub-grid-scale model can be assessed without further assumptions. Given a successful validation, the computational results will provide an important source to analyze the flow physics in detail. Presently results of the compression corner simulation is considered mainly. The subsequent downstream interaction of the reattached boundary layer with the expansion near and along the decompression ramp is currently in progress. The short outline of the latter investigation will be given.

2 Simulation method

In the following the subscripts ‘₁’, ‘₂’ and ‘₃’ correspond to the streamwise, spanwise, and wall-normal coordinate, respectively. We write the fundamental equations in the Cartesian (x_1, x_2, x_3) physical space, using a transformation to computational space (ξ_1, ξ_2, ξ_3) which is detailed in [1]. Figure 2 shows a side-view of the computational domain, where only each 10th mesh line is displayed. The selected stations are indicated by arrows, there streamwise positions together with brief explanations can be found in Table 1.

Table 1. Selected station positions

letter	x_1 position	comment
<i>E1</i>	-14.8	experimental section 1
<i>I</i>	-6.1	just before interaction
<i>S</i>	-4.5	separation position
<i>P</i>	-1.5	pressure plateau in the separation zone
<i>R</i>	2.5	reattachment position
<i>E2</i>	4.2	experimental section 2

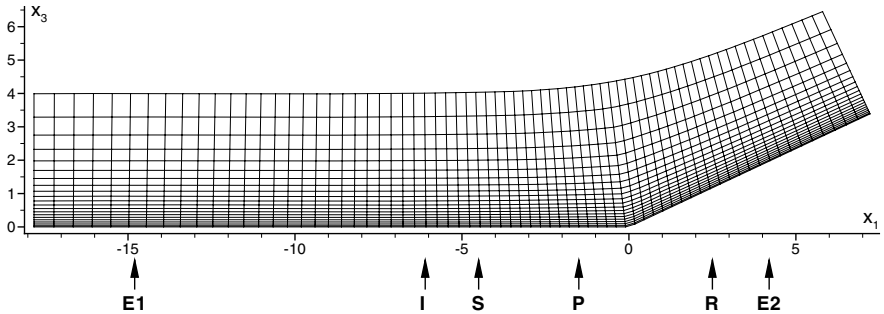


Fig. 2. Computational mesh (each 10th line is shown); selected stations are indicated by arrows (see Table 1 for details).

In this section, dimensional quantities are marked by an asterisk. As a reference length we use the mean boundary layer thickness δ_0^* at section 1 (Fig. 2). The integration domain has the extents $L_1^* = 25.8\delta_0^*$, $L_2^* = 4\delta_0^*$, $L_3^* \approx 4\delta_0^*$ the mesh consist of $701 \times 132 \times 201$ points in the streamwise, spanwise and wall-normal directions, respectively. We assume the solution to be L_2 -periodic in x_2 .

A perfect gas with a specific-heat ratio of $\gamma = 1.4$ is assumed and the viscosity is calculated according to Sutherland’s law.

Given a Reynolds number $Re = U_\infty^* \rho_\infty^* \delta_0^* / \mu_\infty^*$ and a Mach number $M = U_\infty^* / a_\infty^*$ we can write the compressible Navier-Stokes equations in curvi-linear coordinates as

$$\frac{\partial U}{\partial t} \frac{1}{J} + \frac{\partial F_E}{\partial \xi_1} \frac{1}{J} + \frac{\partial G_E}{\partial \xi_2} \frac{1}{J} + \frac{\partial H_E}{\partial \xi_3} \frac{1}{J} = \frac{\partial F_S}{\partial \xi_1} \frac{1}{J} + \frac{\partial G_S}{\partial \xi_2} \frac{1}{J} + \frac{\partial H_S}{\partial \xi_3} \frac{1}{J} \quad , \quad (1)$$

where the conservative variables are $U = \{\rho, \rho u_1, \rho u_2, \rho u_3, E\}$, and J is the Jacobian of the mapping $(x_1, x_2, x_3) \leftrightarrow (\xi_1, \xi_2, \xi_3)$. F_E, G_E, H_E are the convective fluxes and F_S, G_S, H_S are the diffusive fluxes in the respective coordinate directions. For the detailed flux definitions we refer to [1].

For LES equations 1 are filtered at the expense of the appearance of unclosed subgrid-scale terms. For closure the approximate deconvolution model (ADM) [13] is used. Boundary conditions are as follows. At the inflow we prescribe all variables in time, using data from a separate zero pressure gradient flat plate boundary layer computation (see in [12]). At the outflow a sponge-layer technique is used, which is detailed in [1]. At the upper truncation plane non-reflecting conditions combined with sponge layer are imposed. The wall is assumed to be isothermal, and no-slip conditions are imposed on the velocity. The wall temperature distribution along the streamwise direction is taken from the experiment.

The conservation equations for the filtered density, momentum and total energy are solved in curvilinear coordinates. A 6-th order compact finite-difference scheme [11] is used for spatial discretization and an explicit low-storage 3-rd order Runge-Kutta scheme is applied for time advancement.

3 Numerical results

A flat plate boundary layer simulation used for generating inflow boundary conditions was discussed in a previous report [12]. Here we mainly concentrate on the compression corner simulation results. The initial data for the simulation were artificially composed out of inviscid data and laminar similarity boundary layer data. After an initial transient the compression corner simulation was continued for 703.45 characteristic time scales of the incoming boundary layer δ_0 / U_∞ . Such a long period was chosen in order to capture at least one period of low frequency shock motion (see subsection 3.1) and to get smoother statistical correlations as suggested earlier [2]. During this time range the flow field was sampled 1272 times for statistical analysis. Various statistical quantities and time-history data have been saved. Now the simulation of the compression corner is complete and we can analyze obtained data with more confidence.

Flow features described in section 1 can be found in calculations. They are illustrated by Fig. 3a where Schlieren-type photo visualization is approximated by mean density gradient averaged in spanwise direction. Averaging

time corresponds to ≈ 2.6 ms exposure if recalculated accordingly to conditions of the reference experiment. The numbers indicated in the figure refer to the following flow features: 1: incoming turbulent boundary layer; 2: unsteady shock wave; 3: separation region as result of interaction; 4: shear layer; 5: traveling compression waves (will be discussed later).

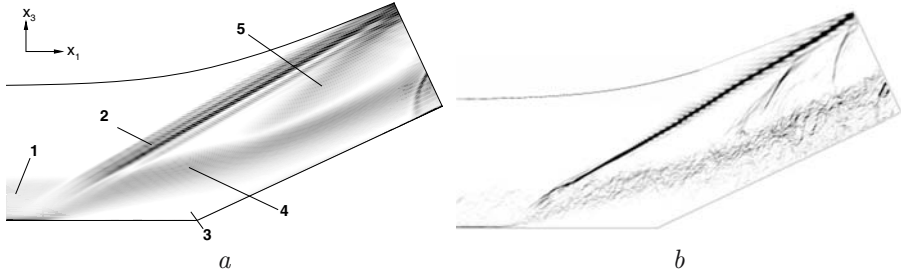


Fig. 3. Density gradient $\|\nabla\rho\|$ averaged in spanwise direction of the mean-flow (a) and instantaneous field ((b)); numbers are detailed in section 3.

Accordingly to the Reynolds number the separation shock (1) wave penetrates deeply inside the boundary layer and transformed into compression waves near the wall. For given conditions pressure gradient is high enough to separate the turbulent boundary layer. The separated shear layer (4) contained region of the reverse flow (3). The snapshot captured several positions of an unsteady shock. An example of such random shock motion is clearly demonstrated by [6]. This feature will be discussed in section 3.1. Highly unsteady second stem of the λ -shock configuration, clearly visible at instantaneous snapshots (see Fig. 3b), is transformed into compression waves fan (5) when averaged in time.

Despite of the fact that a two-dimensional configuration is considered computed mean flow is three-dimensional. This has been suggested before based on experimental findings [16] and it is clearly demonstrated by Fig. 4. Here the computational domain boundary is shown by thin black lines, slices are coloured with mean temperature, semitransparent isosurface visualise the shock using mean pressure $\langle p \rangle = 0.1$. A rake of 10 coloured mean streamlines starting from inflow clearly show non-planar motion in the separation zone and rotational motion after reattachment. Vorticity isosurface of equal magnitude with clockwise (“magenta” color) and anticlockwise (“cyan”) rotation identify vortices. Rotational motion is quite weak in that region, we used only streamwise component of vorticity vector aligned with gridlines to visualise it. For smoother visualization the vorticity field was passed through a box filter several times. There are 4 streamwise counter-rotated vortices existing after the reattachment line.

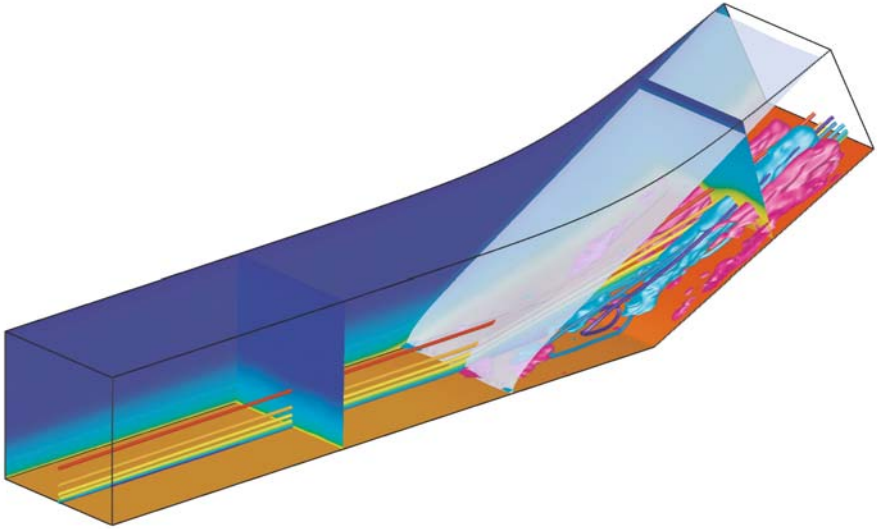


Fig. 4. Three-dimensional meanflow.

These streamwise vortices affect turbulence structures and the mean properties significantly [8]. For example, the mean wall skin-friction distribution is shown in the picture 5. The dashed vertical line shows the compression corner position. The x_1 -location of separation and reattachment can be read off the thin solid lines ($C_f = 0$) for each x_2 position. Evidently these locations vary considerably in spanwise direction. Further downstream in the reattachment region two streamwise oriented convergence at $x_2 \approx 1$ and $3\delta_0$ as well as divergence lines at $x_2 \approx 2$ and $4\delta_0$ can be identified from the skin-friction distribution. A vortex core is located between divergence and convergence lines. One of them rotates clockwise and together its adjacent contra rotating counterpart forming downwash (above divergence line) and upwash (convergence) regions in the flow. The width of the vortex pair about $2\delta_0$ is consistent with reports in the literature (see [8] for example). Similar patterns are also found in the experimental oil-flow visualisation at a higher value of the Reynolds number $Re_{\delta_0} = 144000$ (Fig. 6), as well as at our reference of value $Re_{\delta_0} = 63560$ [16]. Again the vertical dashed line denotes the corner position, oil accumulation bit downstream associated with reattachment region. Several convergence and divergence lines can be clearly identified.

Such patterns can be associated with the footprints of Görtler-type streamwise vortices. Görtler vortices arise from an instability of laminar flow with sufficient concave streamwise curvature. The acting mechanism for the origin of these vortices in turbulent flow is yet unknown.

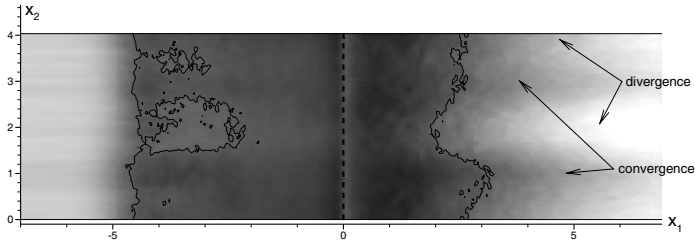


Fig. 5. Distribution of the mean skin-friction coefficient at the wall.

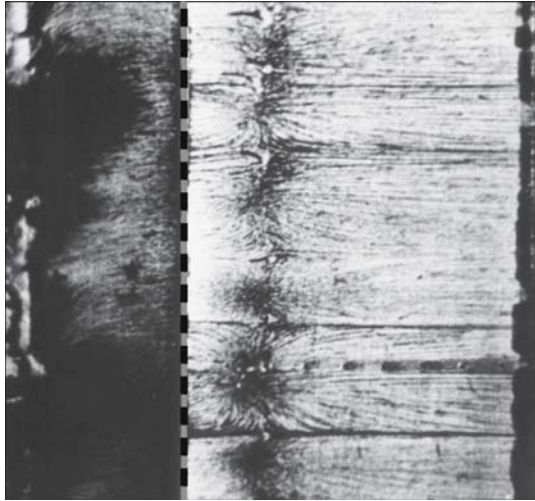


Fig. 6. Oil-flow visualization pattern from [16], $Re_{\delta_0} = 144000$

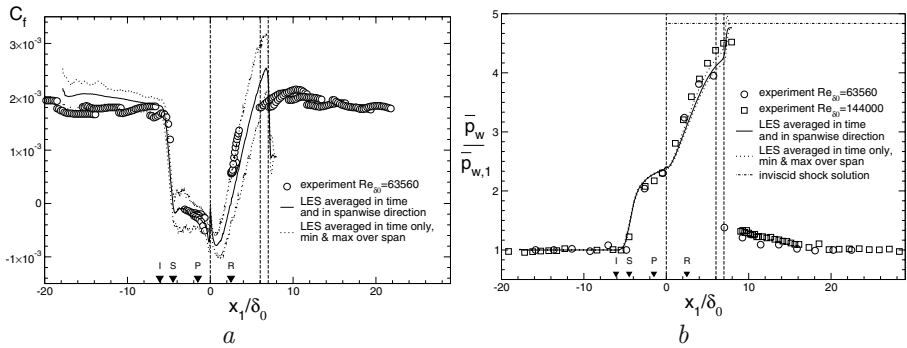


Fig. 7. Averaged skin-friction coefficient (a) and wall pressure (b) distributions along the streamwise direction.

The spanwise mean flow properties variation should be taken into account when compare computational data with experiment since in the experiment data usually collected only in one section $x_2 = \text{const}$. But apparently it does matter at which spanwise position with respect to the large-scale streamwise vortexes measurements are taken. Comparison of computed skin-friction with experiment is presented in the Fig. 7(a) Along with the spanwise and time-averaged quantities (thick line) also the minimum and maximum of the time-averaged distribution (dotted lines) over spanwise is indicated. Open symbols denote experimental values, the left-most vertical dashed line indicates the compression corner position, the middle line indicates the decompression corner (not considered in the present simulation), the right-most line indicates the outflow sponge-layer position (boundary condition). The solution within the sponge-layer at the outflow is physically not meaningful. Separation and reattachment positions are determined by zero spanwise averaged skin-friction are displayed with S and R respectively. Apparently, the spanwise variation after reattachment region is on the order of the value within the incoming-boundary-layer. The mean surface skin-friction measurements have been performed using the Global Interferometry Skin Friction technique (GISF) [4]. The data in Fig. 7 corresponds to some section between the longitudinal convergence and divergence lines. They are in good agreement with the computations averaged in time and in spanwise. Separation line is located at $x_{1S} = -4.5 \pm 0.25\delta_0$ and reattachment occurs at $x_{1R} = 2.5 \pm 0.7\delta_0$ The separation zone length L_{sep} can be estimated as $7\delta_0$, but significant variation of L_{sep} is observed in spanwise (see also Fig. 5).

Less sensitive to the existence of these vortexes is the wall pressure which is shown normalised by the mean pressure in the undisturbed boundary layer value at position $E1$, refer to Fig. 2 and Table 1. There is no expressive pressure plateau with constant pressure observed in the separation region, we define it as curve inflection point P . The agreement of the computational results with the experiment is very good. Significant differences between computational and experimental values can be seen only in the region of sponge layer at the outflow boundary and just before the decompression corner position.

3.1 Shock wave structure

We start the shock wave structure description from computed Schlieren-type visualisation taken at time instant (Fig. 3b). This corresponds roughly to a spark shadowgraph of the flow. Time-series of instantaneous pictures clearly showed unsteady motion of the shock system and compression waves. The separation shock undergo small scale motion and large scale excursion. The second stem of λ -configuration is highly unsteady and seems to disappear from time to time.

In order to identify shock foot location and shock motion [7] measured instantaneous wall pressure signal. We apply a similar analysis here to our numerical simulation data. Time-histories of the wall pressure at four point

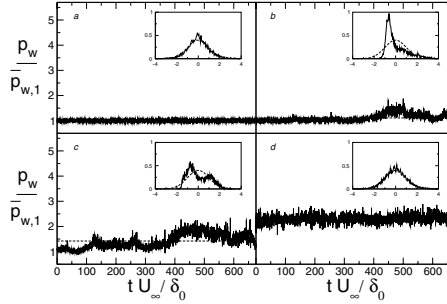


Fig. 8. Wall pressure history and probability distribution

tracers positions are shown at Fig. 8. Tracers were placed in the mid-span of the domain, streamwise positions correspond to: (a) undisturbed boundary layer, station I ; (b) beginning of interaction, i.e. where initial mean pressure rise above undisturbed value $\langle p \rangle = 1.1\langle p \rangle_I$ (see Fig. 7b); (c) maximum pressure fluctuation position (see peak on Fig. 9); (d) inside separation region, station P (Fig. 7). The dashed line shows time-averaged value. The data is normalized to the mean value of the pressure at station I . There are normalised probability-density-function (PDF) of the signal is shown at insets, Gaussian PDF is depicted by dashed curve for reference purpose. Evidently PDF distribution is essentially Gaussian in the incoming boundary layer and in the separation region. Off-centre peak in PDF at beginning of interaction (Fig. 8b) indicate that shock wave is not simply oscillate near the mean position, but the greater excursions have high probability. The streamwise length of this excursion can be estimated as $1.3\delta_0$. Another evidence of large scale low frequency shock motion is shown by next tracer, Fig. 8c. At the beginning the pressure is below average (shock wave is downstream of its mean position), then shock moves forward and pressure became higher and again return to initial position. One cycle of shock excursion can be roughly estimated as $675\delta_0/U_\infty$ or 2.5 ms for the reference experiment. It is higher then value of ≈ 1 ms reported in [7] at $Re_{\delta_0} = 1400000$. It should be noted that there is no true periodicity in shock motion observed: shock wave suddenly can jump downstream during its upstream motion (see peaks at $t \approx 125$ and $275\delta_0/U_\infty$). Also it can spend some time near some (not necessarily mean) position. This observation as well as PDF distribution of the pressure signal is in agreement with conclusions of [6], [7]. While it is widely acceptable that small scale shock wave fluctuation are driven by incoming boundary layer bursting events, there is no conclusive conception concerning to the large scale low frequency motion ([2], [5]). In our simulation such low frequency motion definitely cannot be imposed by periodically repeated inflow conditions, because inflow data was turned over more then 12 times during one large-scale cycle.

The wall loads maybe further qualified by intensity of wall pressure fluctuations. This is measured by the standard deviation of the and shown in

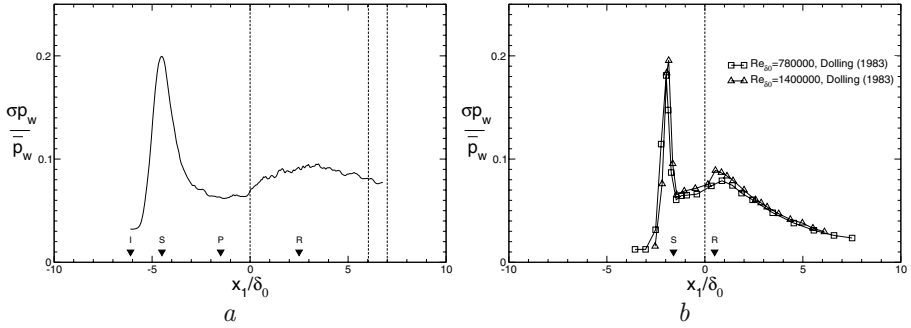


Fig. 9. Standard deviation of wall pressure fluctuation (*a*) computation and (*b*) experiment of [6] at $Re_{\delta_0} = 780000$ and $Re_{\delta_0} = 1400000$, vertical lines have the same meaning as in Fig. 7.

Fig. 9*a*. The values are normalised by the local mean wall pressure. A global maximum is observed in the separation region at $x_1 \approx -4.5\delta_0$ this corresponds to the mean separation S position. Its magnitude is more than 20% of the mean wall pressure which agrees well with experimental data of [6] at larger Reynolds number, shown in Fig. 9*b*.

Compression waves are travel downstream with convective speed $\approx 0.1 - 0.4U_\infty$. Higher values correspond to the shocklets, they are in order of magnitude of speed of largest eddies in the disturbed shear layer (4). Rankine-Hugoniot condition was checked in order to prove that these waves are true shocklets. This estimation is done taking into account the speed and angle of the wave relatively to the flow behind the separation shock. The pressure raise in shocklets is satisfied shock relations. Shocklet strength is determined by Mach number varies in range of 1.23 – 2.2. Latter corresponds to second stem of the λ -shock which is more stable and has lower velocity.

These travelling compression waves discovered by LES is an important phenomenon which explains the nature of turbulence increasing in the external flow between the separation shock and shear layer revealed by the hot-wire measurements in [17]. As was shown in this paper the acoustic mode is typical for this region. Such conclusion is in agreement with the calculated flow-field structure.

3.2 Turbulence evolution

One of the most significant outcome of turbulent boundary layer interaction with shock is turbulence amplification inside boundary layer and in the outer flow ([17], [3]). The amplification of turbulent fluctuations is illustrated in Fig. 10. Profiles of root-mean-square (RMS) values of the mass-flux (*a*), density (*b*) and velocity (*c*) fluctuations are shown at positions E1 and E2, again refer to Fig. 2 and Table 1. Due to technical limitations of the experiment only relative changes with respect to undisturbed boundary layer values of

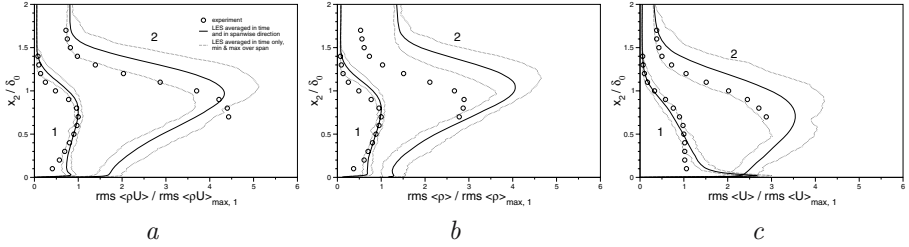


Fig. 10. Amplification of RMS of momentum (a), density (b) and velocity (c) fluctuations between position E1 and position E2.

the RMS values can be assessed. So profiles are normalised to maximum value in the first section. The computation gives larger values for the fluctuation amplifications near the local RMS maxima for all quantities, $0.7\delta_0 < x_3 < 1\delta_0$ at position E2, and in the external flow for density fluctuations, $x_3/\delta_0 > 1.5$. Taking into account, however, the accuracy of the experimental data which is at least between 15% and 20% the agreement can be considered as satisfactory. Near-wall maxima of the RMS distributions are not captured by the experiment due to the lack of near-wall resolution.

4 Decompression corner

The simulation of subsequent interaction of the disturbed boundary layer with Prandtl-Meyer rarefaction waves is considered as a separate stage. In order to accomplish this task, another computation was set up. The side-view of the computational domain is shown on Fig. 11. The mesh consist of $401 \times 132 \times 201$ points in the streamwise, spanwise and wall-normal directions respectively. The spanwise length is chosen to be equal to compression corner domain. Further more the first section of the decompression corner domain exactly corresponds to a cross-section from compression corner domain (thick line in Fig. 11). During the compression corner simulation all conservative variable are saved from this cross-section. This provides data for inflow boundary conditions for decompression corner simulation. The inflow boundary conditions are implemented in the same way as for compression corner simulation. The sponge layer technique at inflow ensures better stability and shorter transient distance, caused by temporal interpolation of inflow data.

The simulation currently in progress. So far the collected statistics is too small to give even preliminary analysis. We intend to investigate shocklets behavior after passing Prandtl-Mayer expansion. Our expectation that they will not fully decay in expansion waves sustaining high turbulence level in the external flow as it was observed in the experiment [17]. This higher level of external turbulence might be important for heat transfer and cannot be predicted by conventional RANS simulations.

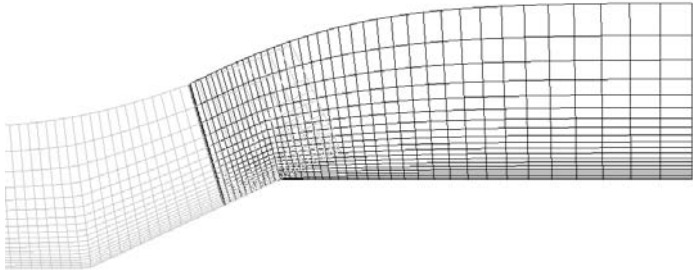


Fig. 11. Computational mesh for decompression corner (each 10th line is shown). Part of compression corner mesh is displayed by grey lines, junction section denoted by thick line.

5 Computational details

For the current computation a FORTRAN code designed and optimized for shared memory vector-parallel computers is used. Computations are performed on the NEC SX-5 system available at HLRS. Parallelization and vectorization of the code relies on the compiler automatic parallelization and manual tuning in critical sections with compiler directives (the NEC FORTRAN90/SX compiler is used). Typical values for production runs on NEC SX-5 machine are given in the Table 2. The performance ratio is in accordance with previously obtained data at another SX-5 computer with 8 GFLOPS peak performance (CSCS, Switzerland). It varies slightly when running on different number of processors. Approximately 10000 CPU hours are used on this platform. Significant performance ratio decreasing was observed when calculation was running on NEC SX-6 platform (see Table 3). A dependence on the number of CPUs is significant in this case. We spent more then 8000 CPUh on SX-6 platform. The simulation is requires a vast amount of disk space to save results since a lot of instantaneous data have to be saved for time-history analysis. More than 500 GigaBytes of data have been saved for post-processing.

Table 2. Details of the production runs on SX-5 platform

parameter	value	comment
Memory, GB	6.7	7.7 with concurrent postprocessing
Performance, MFLOPS	1748	$\approx 44\%$ of peak performance
Number of CPU	5	tried 4 – 12 CPUs
Vector optimization ratio, %	99.3	
Wall clock time, hours	185.3	for 694.8 CPUh user time

Table 3. Details of the production runs on SX-6 platform

parameter	value	comment
Memory, GB	6.9	
Performance , MFLOPS	2763 $\approx$ 30% of peak, varies 25–34%	
Number of CPU	6	
Vector optimization ratio, %	99.3	
Wall clock time, hours	38.9	for 163.3 CPUh user time

6 Conclusions

Large-Eddy Simulations at flow parameters matching reference experiments are feasible if recent LES modeling techniques and high-resolution numerical discretizations are used. In particular unprecedented results are achieved for the very challenging problem of shock-wave/turbulent-boundary-layer interaction at compression ramps. Analysis of the computational data compared with reference experiment not only confirms the experimental data and suspected but so-far unconfirmed large-scale flow structures and large scale low frequency shock motion. A mechanism for turbulence amplification in the external flow by traveling compression waves is proposed. Evidence for the existence of three-dimensional large-scale structures (Görtler-type vortices) is provided. The investigation of the subsequent boundary-layer acceleration in a Prandtl-Meyer rarefaction at the decompression ramp is currently in progress.

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Detailed Combustion and Steamside Simulation of Fossil-fuel Fired Utility Boilers

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Summary. In the “DAMPFSIM” project, a detailed simulation methodology of a fossil-fuel fired utility boiler using a Computational Fluid Dynamics code for the coal combustion process coupled with a water/steam simulation code was employed. The results are useful to analyse the influence of non-uniform heating resulting from combustion properties or operational conditions on the steam generation process in order to reduce critical conditions, and to enhance the operational performance and reliability of the boiler. For both parts, combustion and steamside simulation, in-house developed codes which have been extensively validated with experimental data in many previous projects have been used.

1 Introduction

Utility boilers are commonly used worldwide for electricity production in fossil-fuel fired power plants and for thermal waste treatment. The steam generation process and the plant efficiency depend on the interaction of the heating from the combustion side and the design of the heat exchangers. As the heat exchanger tubes in the boiler of a power plant are under high pressure, the tube material has a certain maximum allowable load which limits the maximum allowable temperature. Mass flow and heat flux distributions in the parallel tubes of heat exchangers may lead to different steam and material temperatures. Higher safety margins have to be kept in boiler design to account for non-uniform distributions, and the tube material cannot be utilised equally in all tubes up to its maximum allowable load. For the optimization of the design of the heat exchanger system and to identify deviations from the optimum operational conditions, the application of detailed mathematical simulation programs is very beneficial [17], [18], [19], [15].

On the flue gas side of the boiler, the heat transfer is mainly dependent on the gas temperature and its velocity. On the steam side, the tube material is cooled by the water/steam flow which mainly depends on the steam temperature and its mass flow density. In parallel tubes of a heat exchanger, the latter

is primarily defined by the arrangement of the tubes between inlet and outlet header. For the calculation of the steam generation process, the water/steam-cycle simulation program DYNAMIC [3], [7] is used. In order to obtain the temperature and velocity distribution of the flue gas, and the local heat fluxes along the tubes of the heat exchangers the Computational Fluid Dynamics code AIOLOS [13] is applied. AIOLOS was previously validated with extensive in-furnace measurements under different operational conditions [4], and a comprehensive evaluation of the models using the experimental data was performed. Furthermore, the predictive quality of the Computational Fluid Dynamics code AIOLOS coupled with the water-/steam cycle simulation program DYNAMIC has been approved in previous projects in detail [2], [1], [10].

In terms of computational aspects, AIOLOS was successfully used on the following platforms, using different methods of parallelisation: Intel Paragon XP/S-5/72, Intel Paragon XP/S-35/512, Cray C94, Cray J916, Cray T3D/32, Cray T3E/512, NEC SX-4/32 and NEC SX-5Be/32M2, achieving high parallel efficiencies [10], [9], [5], [6], [11], [12], [8].

The calculations presented here were done on a single node (8 processors) of a NEC SX-6. The degree of vectorisation of AIOLOS, defined as the ratio between the time spent in the vector unit and the total user time, reached 99.7 %. A single processor speed of 1.7 GFLOP/s was measured using the hardware performance monitor on the NEC SX-6. This is approximately 38 % of the maximum sustained performance of 4.5 GFLOP/s obtained by benchmark calculations. Thus the concurrent node performance reaches 13.6 GFLOP/s. Depending on the problem size and applied models, AIOLOS maximum sustained performance on the SX-6 system has been measured as 4.1 GFLOP/s which corresponds to 46 % of the maximum peak performance of the vector processor.

2 Theory

In utility boilers the heat released from the combustion reactions of the fossil fuel is transferred by radiation, convection and conduction in order to produce steam and, finally electricity. Radiation is the predominant mechanism of heat transfer in the lower part of coal-fired boilers whereas convection prevails in the tube bundle heat exchangers in the upper part of the boiler. The flue gas side convective heat transfer in tube bundle heat exchangers is a function of geometry, temperature and velocity. Thus, different heat transfer coefficients for different heat exchanger tubes result from flue gas streaks with temperature and/or velocity profiles significantly differing from the respective mean values along the heat exchanger bundles. Ash deposition and its removal by soot blowers can lead to an additional non-uniform heat resistance due to conduction in the deposit layer.

In order to meet the goal of maximum possible efficiency, the heat exchanger layout in modern utility boilers is characterized by very sophisticated designs. But some operational issues cannot be answered without understanding and questioning the design and its consequences. For this purpose, detailed simulation models for the reheater/superheater section have been introduced into the DYNAMIC code, e.g., a parallel tubes model, an inlet and outlet headers model and a parallel steam lines model. The parallel tube model allows to account for different heating conditions in different parallel tubes. The pressure distribution in the headers and thus the steam mass flow in the parallel tubes are derived from the header-model [14]. In the reheater and superheater section of utility boilers, parallel steam lines are commonly used in order to reduce the influence of non-uniform combustion side heating conditions. From the interaction of these three models the temperature, mass flow and pressure along each single tube of a heat exchanger is obtained. As a result of the simulations, the performance of the steam line arrangement can be analysed, and the amount of injected cooling water into the individual steam lines can be obtained. For example, a good header design leads to outlet steam temperatures and mass flow densities in parallel tubes which do not differ significantly from each other.

3 Application

For the numerical simulation with AIOLOS, the boiler under consideration was discretized using a three-dimensional grid including the convective section (see Fig. 1, left). 12 pulverized coal burners on three burner levels are located on each wall. The furnace walls, consisting of inclined tubes, are the evaporator section. Tube bundle heat exchangers, acting as reheaters and superheaters, are arranged in the upper part of the boiler.

In Fig. 1 (right), the computational grid of the tubes with a piping scheme of the reheater section including the inlet and outlet headers is shown [16]. The superheaters and reheaters, consisting of two sections, are arranged alternating along the flue gas flow, i.e. along the height of the boiler. This explains the spare distance between reheater I and reheater II. The lower a heat exchanger is located in the furnace the higher flue gas temperatures and the higher velocities it is exposed. For the analysed reheaters being located downstream of two superheater tube bundles in the flue gas flow it is assumed that convective heat transfer is predominant with a strong dependency on flue gas velocity and flue gas temperature, and consequently, radiative heat transfer is assumed to be negligible.

Figure 2 (left) shows a rotating flame vortex induced by the tangential firing system along the vertical centre axis of the furnace. The simulation results reveal that overfire air which is injected between the upper burner level and the beginning of the convective section does not reach the centre of the cross section, i.e., the core of the flame vortex. Consequently, there

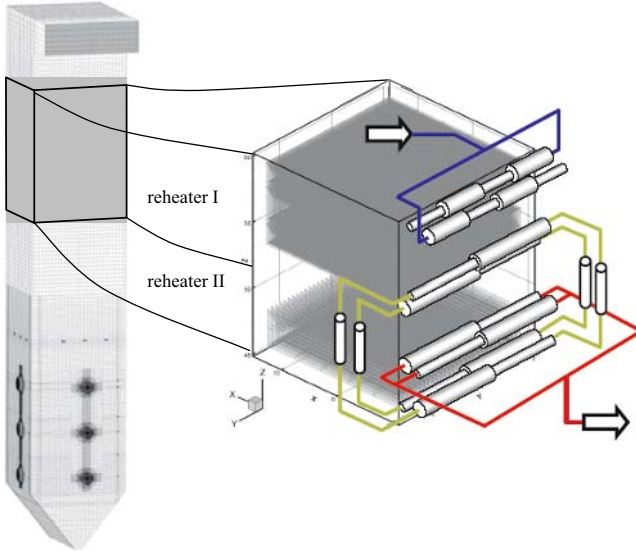


Fig. 1. Numerical grid for AIOLOS (left) with grid and piping scheme of the reheater I and reheater II section (right)

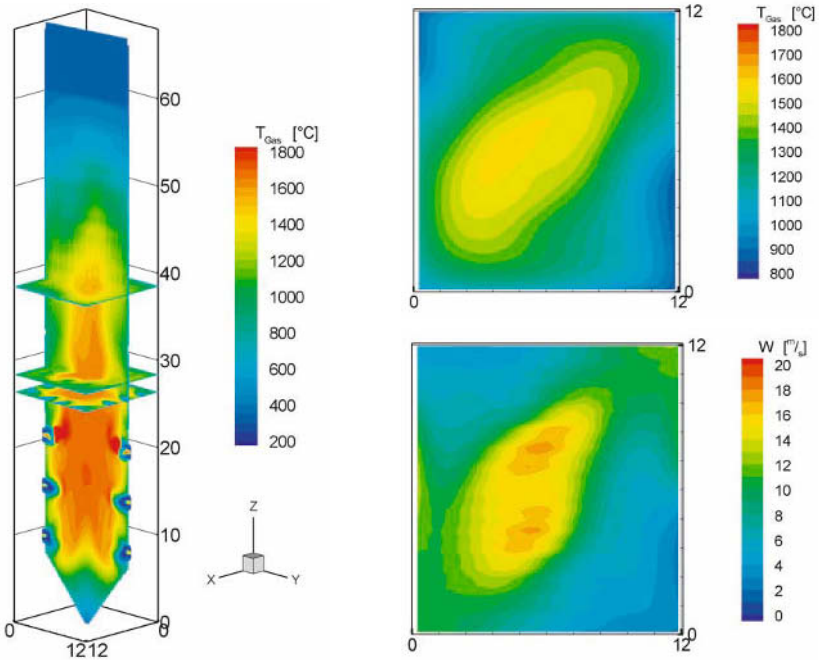


Fig. 2. Flue gas temperature distribution along the boiler height (left) and cross-sectional flue gas temperature and velocity distribution at the beginning of the tube bundles (right)

is an area at the beginning of the convective section where the flue gas is still very hot and has a high velocity whereas the gas temperature and the gas velocity are lower in the peripheral area. This non-uniform distribution implies unbalanced heating conditions of the convective tube bundle heat exchangers and unequally distributed production of steam.

Results obtained from the simulation with DYNAMIC using the models mentioned in the “theory” section and assuming equal water injection in the steam attemperators of the different steam lines are shown in Fig. 3 [16]. The abscissa is divided in four sections representing the four parallel steam lines of reheater I (red) and reheater II (blue) over the parallel tubes of the heat exchangers, i.e. the furnace cross section (from left to right). Between the two reheaters a steam line intersection is implemented such that steam line 1 is located in the most left (peripheral) section of the boiler in reheater I and in the inner right section in reheater II. From the steam side models some constraints are imposed. This means that in the dead ends of the headers where two steam lines meet from different side no pressure differences must occur. Also the pressure drop in all steam lines must be the same over the

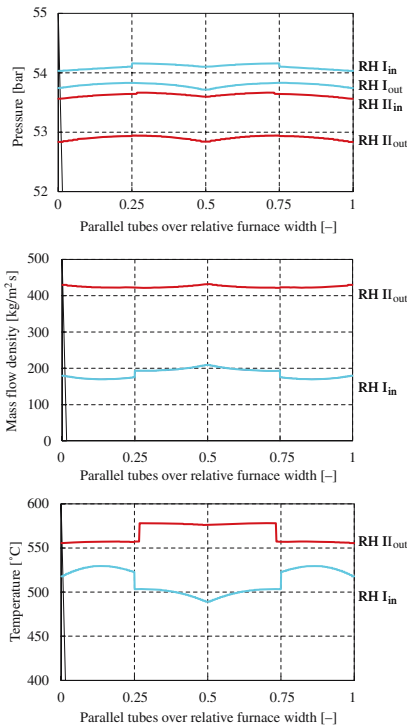


Fig. 3. Pressure, mass flow density, and temperature distribution along the inlet and outlet headers

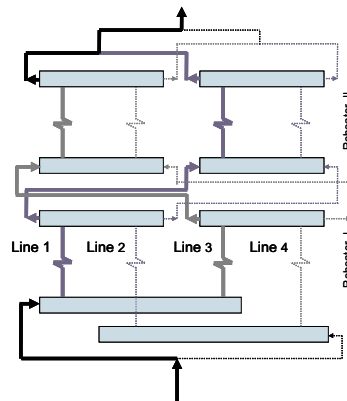


Fig. 4. Path of the four reheater steam lines

whole reheater system. This leads to a complex iterative nested calculation to find the mass flow, temperature and pressure along each single tube. In the present case some tubes from the outer steam line of reheater I do not meet steam line 1 or 4 but steam line 2 or 3 in reheater II in order to rise the mass flow in these lines and to meet the mentioned pressure drop (see Fig. 4). Comparing Fig. 4 with Fig. 1 it is obvious that the reheaters consist of four parallel steam lines with a U-header arrangement in each.

The design of the boiler under consideration with only two inlet headers in reheater I results in higher mass flow and lower temperatures in the tubes of the steam lines 2 and 3 (inner sections in reheater I). For the same reason the outlet temperatures of the tubes in the steam lines 1 and 4 are higher. The non-uniform outlet temperatures in reheater II can be equalised by injecting different mass flows of water in the steam attemperators. These results have been verified by comparison with power plant data [14].

4 Conclusions

In utility boilers, the steam generation process in the parallel tubes of the heat exchangers is influenced by the heat transfer distribution from the combustion side as well as by the design of the heat exchangers and the piping system. Therefore, the numerical simulation using a Computational Fluid Dynamics code coupled with a detailed water/steam-cycle simulation program enables to take into account the effects of the design of the boiler and furnace and to predict the influences of operational conditions on the thermal performance and the utilisation of the boiler material. As one exemplary result from the coupled simulation, it was shown that for optimum operation of the unit, an effective, adequately dimensioned steam attemperator control system must be implemented to equalise the temperature distribution.

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Chemistry

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Over the last years, computational chemistry has developed substantially. At the heart of quantum chemistry is still the elucidation of the molecular and electronic structure of small to medium-sized molecules and the rationalization of the bonding situation encountered therein. This is an important topic, and several examples of such applications are described in the contribution of Gernot Frenking and Ralf Tonner. A large part of this work is devoted to the *qualitative* understanding of the bonding situation. Although accurate numbers are important, they alone provide no understanding. In many cases, such numbers could, at least in principle, also be obtained by spectroscopic instruments. But in contrast to a real spectroscopic device, one can ask our *in silico spectrometer* (i.e., the computer) why the results are as they are. For example, the classification of chemical bonds being more covalent or electrostatic in character is a highly successful means of rationalizing trends in chemical behaviour. Although there is some arbitrariness because a quantitative assessment in this context is not a quantum mechanical observable, such results can be highly useful. Of course, one must be sure that the “hard facts”, e.g. bond lengths, binding energies, vibrational frequencies etc. are calculated accurately before one tries a decomposition of the binding energy. One of the most accurate quantum chemical methods available today for routine applications is the coupled cluster method in the variant CCSD(T). Such methods have been formulated such that most of the computation is done in matrix multiplications, and therefore supercomputers with vector facilities have found good use.

Parallel to the increase in hardware performance, new algorithms have been designed that make quantum chemical codes more suitable for applications to large systems containing many (up to thousands of) atoms. This development also enabled quantum chemistry to make contributions to new fields such as materials science. The contribution of Péter Deák et al. provides a typical example. Using the SIESTA code on a parallel computing platform (the Cray T3E), they asked themselves what boron atoms dispersed in silicon actually do. Being left alone with this question, even powerful quantum

chemical methods could not contribute much, but together with experimental information (mostly Raman data), results from quantum chemical calculations are a key ingredient in the assignment of Raman data to different types of interstitial boron clusters.

The applications described above are all static in nature. Both in the calculations on individual molecules (gaseous state) and in the solid-state calculations, local minima of the total energy with respect to a variation of nuclear coordinates have been searched, and the vibrational problem is solved in the vicinity of such a local minimum. The liquid state is completely different, as molecules can no longer be treated individually (as in the gaseous state) but also no longer hold fixed positions as in the solid state. To simulate the liquid state, one has to be aware that contacts (bonds) are established and broken again and again, a scenario which calls for long molecular dynamics runs to extract the relevant information. In the case of liquid aluminum chloride, covalent bonds are reorganised over time such that Barbara Kirchner and coworkers used Car-Parinello simulations which is one of the ways to interface quantum chemistry with molecular dynamics. After simulating the system for some time, one can extract quantities such as radial distribution functions which are directly related to experimental (measured) results. But again, the reproduction of data that could also be obtained experimentally is not the whole story. Based on the calculation, details in the radial distribution function can be related to certain structural features like the presence of AlCl_4 tetrahedra which share a Cl-Cl edge.

Looking at the reports in the present volume, one sees that supercomputer applications in chemistry move from vector to parallel computers built from more or less standard CPUs. The reason for this is clear: for many quantum chemical programs, it is difficult to parallelize the code while keeping optimum vector performance, and the power of a *single* vector CPU is not sufficient for many key applications. Most likely, this trend of migrating from vector to parallel supercomputers for chemistry applications will continue in the near future.

Computational Chemistry

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Theoretical Investigations of Main Group Compounds and Transition Metal Complexes

1 Introduction

Transition metal complexes show a wide variety of chemical reactions. To gain insight into the bonding situation of these complexes and the transition states involved in these reactions is not only crucial for understanding the underlying principles, but even more for finding new reaction pathways or optimizing reaction conditions in chemical industry. Where experiments fail to obtain the needed results, modern quantum chemical approaches can be utilized to investigate chemical systems and predict their properties. This is a challenging task for computational chemists and demanding in computational resources. Such calculations have been carried out in order to predict geometries, bond energies and chemical properties of various compounds. A number of projects are still in progress which include CCSD(T) and MP2 calculations with large basis sets that have been carried out at the HLR. The following chapters give an overview about the research of our group using computational resources of the HLR Stuttgart in the year 2004.

2 The Nature of the Chemical Bond Revisited: An Energy-Partitioning Analysis of Nonpolar bonds

2.1 Introduction

According to the classical view of chemical bonding, nonpolar bonds between identical fragments R in a molecule R-R are established through covalent interactions. The model of a covalent bond consisting of a pair of electrons

shared between two atoms was introduced into chemistry by Lewis.[1–3] This type of chemical bonding, which leads in most cases to an accumulation of the interatomic electronic charge,[4] is conceptually different from ionic bonding which can be rationalized in terms of classical Coulomb attraction that arises when two charges of opposite sign attract each other. In modern terminology, covalent bonding comes from shared electron interactions while ionic bonding arises from closed shell interactions between separated fragments which carry opposite charges, i.e. charged species whose electron densities do not overlap. The latter bonding can be described by the laws of classical electrostatic interactions.

The nature of the chemical bond in nonpolar molecules has been investigated with the help of the energy decomposition analysis (EPA) of the ADF program using DFT calculations. The EPA divides the bonding interactions into three major components, i.e. the repulsive Pauli term, quasi-classical electrostatic interactions and orbital interactions. It is shown that atomic partial charges may be misleading for analyzing the nature of the interatomic interactions, because they do not reveal the topography of the electronic charge distribution. A true understanding of the strength and trends of the chemical bonding can only be achieved when the Pauli repulsion is considered. The repulsive ΔE_{Pauli} term is in most cases the largest term in the EPA in an absolute sense.

2.2 Method

The geometries of the molecules have been optimized at the non-local DFT level of theory using the exchange functional of Becke[5] in conjunction with the correlation functional of Perdew[6] (BP86). Uncontracted Slater-type orbitals (STOs) were employed as basis functions for the SCF calculations.[7] The basis sets have triple- ζ quality augmented by two sets of polarization functions, i.e. p and d functions on hydrogen and d and f functions on the other atoms. This level of theory is denoted BP86/TZ2P. An auxiliary set of s, p, d, f and g STOs was used to fit the molecular densities and to represent the Coulomb and exchange potentials accurately in each SCF cycle.[8] Scalar relativistic effects have been considered using the zero-order regular approximation (ZORA).[9–11] All structures have been verified as minima on the potential energy surface by calculating the Hessian matrices.[12, 13]

The atomic partial charges have been calculated with the Hirshfeld partitioning scheme.[14] The calculations were carried out with the program package ADF(2.3).[15–17] The binding interactions were analyzed by means of the energy partitioning scheme of ADF [18–20] which was originally developed by Morokuma[21, 22] and later modified by Ziegler and Rauk[23]. The focus of the bonding analysis is the instantaneous interaction energy, ΔE_{int} , of the bond, which is the energy difference between the molecule and the fragments in the

frozen geometry of the compound. The interaction energy can be divided into three main components:

$$\Delta E_{int} = \Delta E_{elstat} + \Delta E_{Pauli} + \Delta E_{orb} \quad (1)$$

ΔE_{elstat} gives the electrostatic interaction energy between the fragments, which are calculated using the frozen electron density distribution of the fragments in the geometry of the molecules. The second term in equation 1, ΔE_{Pauli} , refers to the repulsive interactions between the fragments, which are caused by the fact that two electrons with the same spin cannot occupy the same region in space. ΔE_{Pauli} is calculated by enforcing the Kohn-Sham determinant of the orbitals of the superimposed fragments to obey the Pauli principle by antisymmetrization and renormalization. The stabilizing orbital interaction term, ΔE_{orb} , which includes the Heitler-London resonance phenomenon[24] but has additional contributions from polarization and relaxation is calculated in the final step of the energy partitioning analysis when the Kohn-Sham orbitals relax to their optimal form.

This term can be further partitioned into contributions by the orbitals belonging to different irreducible representations of the point group of the interacting system. The interaction energy, ΔE_{int} , can be used to calculate the bond dissociation energy, D_e , by adding ΔE_{prep} , which is the energy necessary to promote the fragments from their equilibrium geometry to the geometry in the compounds (see eq. 2).[25] Further details of the energy partitioning analysis can be found in the literature.[26, 27]

$$-D_e = \Delta E_{prep} + \Delta E_{int} \quad (2)$$

It is important to recognize the physical meaning and the relevance of the energy terms given by the EPA, ΔE_{elstat} , ΔE_{Pauli} and ΔE_{orb} , in order to avoid misinterpretations of the calculated numbers. In particular, we want to point out that the calculation of ΔE_{elstat} uses the electron density distribution of the fragments without considering the polarization of the charge distribution that comes from the chemical interactions. The polarization is only considered in the final step of the EPA, which means that the stabilization due to polarization and relaxation is completely included in the ΔE_{orb} term. Thus, the calculated electrostatic interaction energy ΔE_{elstat} of the unpolarized fragments is not the same as the total potential energy change in the bond formation, because the final electron density differs from the superposition of the two fragment densities. While the ΔE_{elstat} term contains only quasi-classical electrostatic interactions which come from the frozen electron densities of the fragments, the ΔE_{orb} term contains electrostatic attraction coming from quantum interference, potential energy changes due to polarization and relaxation and kinetic energy contributions. The ΔE_{Pauli} term contains also potential energy contributions because electronic charge is removed from the overlap area of the fragments closer to the nuclei which is actually lowering the energy. The increase of the total energy due to the ΔE_{Pauli} term

comes from the kinetic energy of the electrons which is much higher when they come closer to the nuclei. This is the reason that the ΔE_{Pauli} term is sometimes called kinetic repulsion.[26, 27] The EPA has been used in the past mainly for analyzing the interactions between closed-shell species. To the best of our knowledge, the extension of the method to electron-pair bonding was done for the first time by Bickelhaupt et al.[28]

2.3 Results

The interaction energy of a chemical bond can be meaningfully interpreted in terms of quasi-classical electrostatic interaction, Pauli repulsion and orbital interactions. The contributions of all of the three terms must be considered when chemical bonds shall be compared with each other. Chemical bonding is caused by classical electrostatic terms and by the specific quantum mechanical kinematics of the electrons, resulting in Pauli repulsion of occupied overlapping orbitals and resonance and deformation of partially occupied orbitals.

Table 1. EPA^[a] of the N≡N bond in N₂ at the BP86/TZ2P level of theory.

	N ₂
ΔE_{int}	−240.5
ΔE_{Pauli}	802.4
$\Delta E_{elstat}^{[b]}$	−312.9 (30.0 %)
$\Delta E_{orb}^{[b]}$	−730.0 (70.0 %)
$\Delta E_{\sigma}^{[c]}$	−479.8 (65.7 %)
$\Delta E_{\pi}^{[c]}$	−250.3 (34.3 %)
E–E bond length [$\text{\AA}$] ^[d]	1.102 (1.09768) ^[e]
$D_e^{[d]}$	240.5 (228.5) ^[e]
$D_0^{[d]}$	237.1 (225.0) ^[e]

[a]Energy values are given in kcal/mol. [b]The percentage values in parentheses give the contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb}$. [c]The percentage values in parentheses give the contribution to the orbital interaction ΔE_{orb} . [d]The experimental values are given in parentheses. [e]Ref.[29]

The results of the EPA show that nonpolar covalent bonds between main group elements of the first and higher octal rows of the periodic system have large contributions by quasi-classical electrostatic attraction between the bonded fragments that may be even stronger than orbital interactions. The bonding interactions in H_nE-EH_n (E = Li to F; n = 0 - 3) possess between 20.7% (E = F) and 58.4% (E = Be) electrostatic character (see Table 2). The nature of the bonding interactions in H₂, which comes exclusively from orbital interactions is atypical for chemical bonds. The electrostatic bonding arises from the attraction between areas of electronic charge concentration

Table 2. EPA^[a] of the H_nE-EH_n single bond (E = Li to F) at the BP86/TZ2P level of theory. Calculated atomic partial charges q_E and the E-E bond lengths are also given.

	Li ₂	Be ₂ H ₂	B ₂ H ₄	C ₂ H ₆	N ₂ H ₄	O ₂ H ₂	F ₂
Symm.	<i>D_{∞h}</i>	<i>D_{∞h}</i>	<i>D_{2d}</i>	<i>D_{3d}</i>	<i>C₂</i>	<i>C₂</i>	<i>D_{∞h}</i>
Δ <i>E</i> _{int}	−20.6	−70.3	−114.5	−114.8	−76.8	−62.6	−52.8
Δ <i>E</i> _{P_{multi}}	1.9	41.1	161.7	201.6	407.9	384.6	145.8
Δ <i>E</i> _{elstat} ^[b]	−8.4 (37.3 %)	−65.1 (58.4 %)	−140.5 (50.9 %)	−130.9 (41.4 %)	−178.3 (36.8 %)	−145.8 (32.6 %)	−41.1 (20.7 %)
Δ <i>E</i> _{orb} ^[b]	−14.1 (62.7 %)	−46.3 (41.6 %)	−135.7 (49.1 %)	−185.5 (58.6 %)	−306.4 (63.2 %)	−301.4 (67.4 %)	−157.5 (79.3 %)
Δ <i>E</i> _o ^[b]	−14.1 (100 %)	−46.3 (100 %)	−119.7 (88.2 %)	−175.5 (94.6 %)			−151.3 (96.1 %)
Δ <i>E</i> _π ^[c]			−16.0 (11.8 %)	−10.0 (5.4 %)			−6.2 (3.9 %)
Δ <i>E</i> _{prep}	0	1.6	6.1	21.7	4.2	3.2	0
<i>D_e</i>	20.6	68.7	108.4	93.1	72.6	59.4	52.8
<i>D₀</i> ^[d]	20.1 (26.4 ± 1.0)	64.9 (71.7) ^[e]	103.0 (104.0) ^[e]	83.4 (89.9 ± 0.5)	62.8 (65.8)	53.6 (50.9 ± 1.0)	51.5 (37.9)
q _E [e]	0.0	0.196	0.081	−0.105	−0.214	−0.153	0.0
E-E [Å] ^[h]	2.737 (2.673)	2.101 (2.101) ^[h]	1.623 (1.656) ^[g]	1.532 (1.535)	1.443 (1.449)	1.473 (1.464) ^[h]	1.421 (1.412)

[a]Energy values are given in kcal/mol. [b]The percentage values in parentheses give the contribution to the total attractive interactions Δ*E*_{elstat} + Δ*E*_{orb}. [c]The percentage values in parentheses give the contribution to the orbital interaction Δ*E*_{orb}. [d]The experimental values are given in parentheses. Unless otherwise noted they have been taken from ref. [30]. [e]The theoretical value was taken from high-level (CBS-Q) ab initio calculations, see ref. [31]. [f]The theoretical value was taken from ref. [32]. [g]The theoretical value was taken from ref. [33]. [h]Ref. [34]

in the valence shell distribution of one atom with the nucleus of the other atom. The electronic charge distribution of the valence shell of E in the fragment H_nE is highly anisotropic except for Li. However, even fragments with a spherically symmetrical electronic charge distribution may strongly attract each other through quasi-classical electrostatic forces. This becomes obvious by the calculated value $\Delta E_{elstat} = -312.9$ kcal/mol for N_2 (see Table 1). A true understanding of the nature of the chemical bonding can only be achieved when the Pauli repulsion is considered. The binding interactions in H_2N-NH_2 and $HO-OH$ are weakened by strong Pauli repulsion.

The double bonds in the molecules $HB=BH$, $H_2C=CH_2$, $HN=NH$ have a higher degree of orbital interactions than the respective single bonds in H_nE-EH_n (see Table 3). An even higher degree of covalent bonding coming from orbital interactions is found in the $HC\equiv CH$ triple bond. The relative contribution of the ΔE_{elstat} term increases, and the relative contribution of the

Table 3. EPA^[a] of the $HB=BH$, $H_2C=CH_2$, *trans*- $HN=NH$ and $HC\equiv CH$ multiple bonds at the BP86/TZ2P level of theory. Calculated atomic partial charges q_E and the E-E bond lengths are also given.

	B_2H_2	C_2H_4	<i>trans</i> - N_2H_2	C_2H_2
Symm.	$D_{\infty h}$	D_{2h}	C_{2h}	$D_{\infty h}$
ΔE_{int}	-159.8	-191.1	-137.4	-280.0
ΔE_{Pauli}	116.3	281.9	599.4	255.4
$\Delta E_{elstat}^{[b]}$	-110.6 (40.1 %)	-181.6 (38.4 %)	-254.6 (34.6 %)	-147.5 (27.6 %)
$\Delta E_{orb}^{[b]}$	-165.5 (59.9 %)	-291.4 (61.6 %)	-482.2 (65.4 %)	-387.9 (72.4 %)
$\Delta E_o^{[c]}$	-111.1 (67.1 %)	-212.2 (72.8 %)	-392.6 (81.4 %)	-215.5 (55.6 %)
$\Delta E_{\pi}^{[c]}$	-54.4 (32.9 %)	-79.2 (27.2 %)	-89.6 (18.6 %)	-172.4 (44.4 %)
ΔE_{prcp}	4.4	12.9	5.6	32.8
D_c	155.4	178.2	131.8	247.2
$D_0^{[d]}$	149.8	168.3 (175.4 ± 2)	123.7 (123.8 ± 1) ^[e]	238.7 (230.9 ± 2)
q_E [e]	0.031	-0.086	-0.106	-0.093
E-E	1.526	1.333	1.249	1.206
[Å] ^[d]	(1.498) ^[f]	(1.339)	(1.252) ^[g]	(1.203)

[a]Energy values are given in kcal/mol. [b]The percentage values in parentheses give the contribution to the total attractive interactions $\Delta E_{elstat} + \Delta E_{orb}$. [c]The percentage values in parentheses give the contribution to the orbital interaction ΔE_{orb} . [d]The experimental values are given in parentheses. Unless otherwise noted they have been taken from ref. [30]. [e]Ref. [35]. [f]The theoretical values were taken from ref. [36]. [g]Ref. [37]

π bonding decreases, when E becomes more electronegative. The π bonding interactions in $\text{HC}\equiv\text{CH}$ amount to 44.4% of the total orbital interactions. The interaction energy in $\text{H}_3\text{E}-\text{EH}_3$ ($\text{E} = \text{C}$ to Pb) decreases monotonically as the element E becomes heavier. The electrostatic character of the E-E bond increases from $\text{E} = \text{C}$ (41.4%) to $\text{E} = \text{Sn}$ (55.1%), but then becomes less when $\text{E} = \text{Pb}$ (51.7%).

3 Benchmark Results for Carbodiphosphoranes and Adducts

3.1 Introduction

The chemical bonding calculated for carbodiphosphoranes (see Fig. 1) has been investigated in our group.[38] Starting with the hexaphenyl carbodiphosphorane and its properties the research led to the Lewis acid adducts of the compounds. Inspired by the experimental work of Prof. Petz in Marburg, the structures and dissociation energies of the adducts were examined. Although the CS_2 and CO_2 adducts are well known since the 1960s[39, 40] the bonding in the double ylidic compounds has not yet been analyzed. A critical issue in the recently published paper were the differences between the dissociation energies calculated with MP2 and DFT methods (BP86 and B3LYP) where a basis set of triple zeta quality has been applied throughout the calculations. This lead us to extensive benchmark calculations on the dissociation energies for the lewis acid adducts of carbodiphosphoranes.

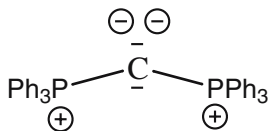


Fig. 1. Hexaphenyl-Carbodiphosphorane

3.2 Method

The geometries have been optimized at the BP86/TZVP and MP2/TZVP levels of theory applying the resolution-of-identity-technique [41–47] Characterisation of the stationary points has been carried out at BP86/SVP[48, 47, 49, 5]. For the phenyl groups Ahlrich's benzene-basis set has been applied at the SVP level which uses heavily contracted SZ-basis sets for aromatic rings. Single point calculations have been carried out with the TZVPP basis set which contains the polarization functions of the cc-pVTZ basis set[50]. The CCSD(T) method has been used together with correlation consistent basis sets [51, 52] without freezing any virtual orbitals.

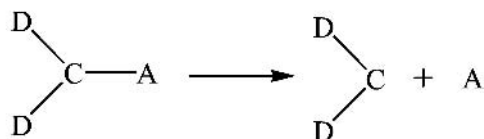
3.3 Results

In Table 4 the dissociation energies for several Lewis acids and three phosphine groups at the central carbon atom are given at the BP86, MP2 and CCSD(T) level of theory.

The lack of experimental heats of formation led us directly to a highly correlated method as reference for the oftenly diverging results of the DFT and MP2 calculations. Additionally as BSSE effects seem to be important in these calculations, counterpoise corrections of the CCSD(T) values have been evaluated.

A second point that makes carbodiphosporanes interesting is their obvious ability to act as a σ - and π -electron donor towards Lewis acids or transition metals[53]. This is a result of the two lone pairs at the central carbon atom which can be “seen” in orbital plots and also in NBO calculations together with a highly negative charge (> 1.5 e, depending on the phosphine substituents[38]). To get more detailed informations we calculated the dissociation energies for a second Lewis acid bound at the carbodiphosphorane (see Table 5). The same levels of theory as mentioned above have been applied. Again, a discrepancy between DFT and MP2 values gives rise to benchmark calculations at the coupled cluster level. The previous results show that the answer to the question if BP86 or MP2 give the better description of the carbodiphosphorane adducts can only be given if highly correlated benchmarks are applied. Especially - as this is one aim of our work - if suggestions to the experimentalist shall be given which molecules are worth to search for by synthesis. With up to 450 contracted basis functions and nearly 40 million configurations the need for supercomputers with large memory availability is obvious.

Table 4. Dissociation energies of carbodiphosphorane-Lewis-acid-adducts.

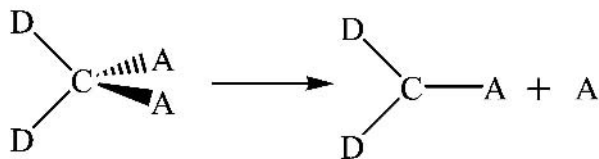


D	Method	A											
		H ⁺		BH ₃		BCl ₃		AlCl ₃		CO ₂		CS ₂	
		D _e	D _e +BSSE	D _e	D _e +BSSE	D _e	D _e +BSSE	D _e	D _e +BSSE	D _e	D _e +BSSE	D _e	D _e +BSSE
PH ₃	BP86/TZVP	263.8	(262.7)	42.2	(40.6)	40.2	(37.1)	51.6	(49.1)	14.6	(12.1)	34.0	(30.9)
	BP86/TZVPP*	261.2	(261.1)	41.3	(40.8)	37.5	(36.6)	48.2	(47.4)	13.7	(12.8)	32.1	(31.2)
	MP2/TZVP	270.7	(266.4)	45.2	(36.9)	53.3	(38.3)	62.6	(53.0)	14.7	(1.5)	32.9	(16.6)
	MP2/TZVPP**	263.9	(262.2)	43.3	(40.5)	49.8	(44.6)	59.6	(56.1)	16.2	(10.4)	34.1	(28.1)
	CCSD(T)/cc-pvDZ**	272.1	(268.5)	42.8	(35.8)	45.6	(33.4)	58.9	(48.8)	10.0	(-4.5)	31.2	(17.3)
	CCSD(T)/cc-pvTZ**	267.3	(265.2)	42.4	(39.2)	46.8	(41.2)	59.0	(54.7)	16.9	(10.5)	35.3	(29.4)
PMe ₃	BP86/TZVP	287.7	(287.1)	46.3	(45.3)	42.1	(39.6)	58.6	(56.3)	18.0	(16.4)	25.1	(22.5)
	BP86/TZVPP*	286.9		46.0		39.5		55.4		16.2		22.6	
	MP2/TZVP	290.4	(286.7)	49.9	(42.2)	59.3	(41.7)	72.6	(60.0)	18.2	(7.3)	32.0	(13.1)
	MP2/TZVPP**	286.0		49.5		56.0		69.8		18.9		29.4	
	CCSD(T)/cc-pvDZ**	295.4		49.8		53.3		71.0		19.7		27.8	
PPh ₃	BP86/TZVP	289.0	(288.6)	34.6	(33.8)	26.6	(23.9)	43.5	(40.9)	3.9	(2.1)	12.7	(10.2)
	BP86/TZVPP*	288.2		34.1		23.7		40.0		2.6		10.4	
	MP2/TZVP	288.8	(285.9)	42.1	(34.0)	60.4	(37.2)	72.5	(54.1)	8.8	(-5.7)	32.6	(9.7)
	MP2/TZVPP**	285.9		41.0		53.3		66.5		8.0		27.3	

All values in kcal/mol.

* at BP86/TZVP geometries

** at MP2/TZVP geometries

Table 5. Dissociation energies of a second Lewis acid bound at a carbodiphosphorane.

D	Method	A											
		H ⁺		BH ₃		BCl ₃		AlCl ₃		CO ₂		CS ₂	
		D _e	D _e + BSSE	D _e	D _e + BSSE	D _e	D _e + BSSE	D _e	D _e + BSSE	BSSE	D _e + BSSE	BSSE	D _e + BSSE
PH ₃	BP86/TZVP	125.4	(124.0)	38.8	(37.2)	17.5	(13.7)	29.3	(26.2)	-2.3	(-11.7)	-3.0	(-15.2)
	BP86/TZVPP*	121.7	(121.5)	37.4	(37.0)	14.6	(13.4)	26.7	(25.7)	-0.8	(-11.3)	-0.9	(-15.1)
	MP2/TZVP	129.8	(125.7)	43.2	(35.2)	35.8	(16.4)	43.0	(30.3)	-11.9	(-21.4)	-19.8	(-19.7)
	MP2/TZVPP**	122.1	(120.5)	41.8	(39.0)	33.0	(26.3)	40.9	(36.4)	-5.4	(-13.4)	-6.5	(-10.7)
	CCSD(T)/cc-pvDZ**	131.3	(128.4)	41.4	(34.5)	27.5	(12.5)	39.6	(27.6)	-14.3	(-24.0)	-15.1	(-24.9)
	CCSD(T)/cc-pvTZ**	124.9	(123.5)	40.7	(37.6)	27.8	-	38.4	-	-	-	-	-
PMe ₃	BP86/TZVP	168.0	(167.2)	40.6	(39.5)	8.3	(5.0)	28.9	(26.2)	-2.1	(-10.8)	-3.1	(-17.8)
	BP86/TZVPP*	166.7		39.3		5.0		26.1					
	MP2/TZVP	167.7	(164.0)	47.6	(39.5)	33.7	(10.7)	47.1	(31.7)	-12.5	(-15.0)	-21.4	(-14.8)
	MP2/TZVPP**	163.8		46.4		28.4		45.6					
	CCSD(T)/cc-pvDZ**	171.6		46.2		22.7		43.8					
PPh ₃	BP86/TZVP	196.6	(196.0)	25.6	(24.7)	-31.2	(-34.5)	-4.1	(-6.9)	-2.0	(-18.9)	-3.0	(-33.9)
	BP86/TZVPP*	195.7		24.2		-35.8		-7.5					
	MP2/TZVP	197.1	(193.7)	36.6	(27.4)	-21.4	(-47.5)	5.4	(-15.1)	-14.4	(-36.3)	-26.4	(-48.1)
	MP2/TZVPP**	193.8		35.5		-24.3		n.c.***					

All values in kcal/mol.

* at BP86/TZVP geometries

** at MP2/TZVP geometries

*** not converged

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Quantum Mechanical Studies of Boron Clustering in Silicon

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1 Introduction

Boron-interstitial clusters (BICs) are known to be a key problem to controlling diffusion and activation of ultra-shallow boron implants in ULSI silicon device technology. During post-implantation annealing the self-interstitials, which had been created by the radiation damage, mediate fast transient diffusion of boron, during which stable and metastable BICs are formed. The BICs are either electrically inactive or the number of holes they can provide per number of boron atoms is significantly less than one. This causes a significant decrease in the activation rate. Therefore, sophisticated annealing strategies have to be developed to regain isolated boron substitutionals from BICs.

In recent years attempts have been made to determine the energetics of BIC formation from first principles theoretical calculations but, apparently, energy calculations alone are not sufficient to establish the key players in the clustering process. Therefore, we have chosen, as an alternative strategy, to identify the most important BICs based on their spectroscopic properties. In the first years we have established a database of calculated vibration frequencies for a wide variety of BICs (see Fig. 1) [1], then we have determined the electronic structure of those clusters [2]. The usual nomenclature of BICs, B_nI_m is based on the number n of boron atoms and the number m of interstitials involved in the cluster, irrespective of the fact that the interstitial is a boron or a silicon atom. In this notation, BI may as well mean an interstitial boron or a silicon self-interstitial next to a substitutional boron. Such systems are configurational isomers with the same number of atoms. In order to be able to differentiate among the possible isomers the present study uses the notations Si_i , B_i , and B_s for interstitial silicon and boron, and for substitutional boron, respectively.

One of the most important fingerprint of these clusters are the local vibrational modes which might be detected by infrared (IR) absorption or

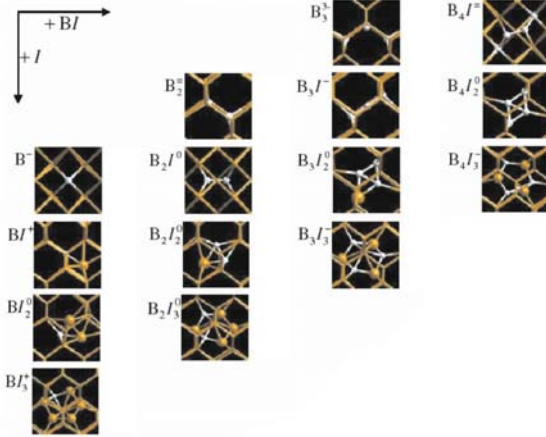


Fig. 1. Structure and energetics of the BICs considered by Windl et al. [3]. The small white balls are B atoms, the large balls are Si atoms involved in the cluster. All other Si atom are shown as a stick-only network.

by Raman-measurements. To establish the equilibrium geometry and local vibrational modes of the clusters in the charge state relevant in this study (when the Fermi-level is pinned to the midgap) we have used the so-called GGA approximation within the Density Functional Theory (DFT). Most of these cluster are electrically active, i.e., they produce defect levels in the band gap. These defect levels can be occupied/emtpied either optical or thermal excitation resulting in lines in the IR or photoluminescence spectrum, or those can be detected by deep level transient spectroscopy (DLTS). These defect levels are also charachteristic to the clusters and they could help in their identification by comparing the calculated and experimental values. However, it is well known that the DFT-GGA leads to band gaps which are by 30-50% lower than the experimental values. This makes the position of the calculated defect levels uncertain. Due to the problems of “pure” DFT, the use of empirically determined hybrid potentials was suggested in quantum chemistry. We have adopted the approach is based on the empirical mixing of the exact exchange and GGA exchange while using the GGA correlation potential, to fit the experimental band gap. Both the elastic constants and the parameters characterizing the quality of the electronic structure have optimum values in the 10-15% range of mixing. The best agreement with experiment can be obtained at 12% mixing of exact exchange (ME). Table 1 shows the calculated values compared to experimental data [4] and to traditional LDA calculations [5, 6]. As can be seen, the structural and elastic data fit the experimental values about the same way as the traditional plane wave LDA results (which are better converged in terms of the basis set). At the same time the electronic structure obtained with the mixed exchange gives an excellent agreement. It

Table 1. The properties of bulk silicon calculated with 12% mixing of exact exchange into GGA, as compared with the experimental data, and with “traditional” plane-wave LDA calculations. (a: lattice constant; E_b : binding energy; B_0 : elastic constant; VB_{width} : width of valence band; E_{Ig} : indirect gap; E_{dg} : direct gap)

	a [Å]	E_b [eV]	B_0 [Mbar]	VB_{width} [eV]	E_{Ig} [eV]	E_{dg} [eV]
12 % ME	5.466	4.95	0.99	12.65	1.16	4.21
Exptl.[4]	5.431	4.75	0.99	12.5	1.17	4.19
Plane wave	5.433	4.84	0.92	12.2	0.5	2.5
LDA	[5]			[6]		

should be emphasized that not only the indirect (minimum) gap is reproduced well, but also the relative energies in the conduction band are correct. We used the CRYSTAL code [7] to accomplish this task. This code is not yet massively parallelized, therefore the GGA calculations were carried out on HLRS. The geometries obtained by GGA calculations were used in the ME calculations, and post relaxations by using ME were carried out only if it was necessary. Nevertheless, we report the results obtained by both methods.

2 Methodology and Usage of High Performance Supercomputer Center in Stuttgart

We use the SIESTA code [8] to carry out the GGA calculations. SIESTA implements DFT combined with the pseudopotential approximation, and uses numerical atomic orbitals (NAO) as a basis set. It is aimed at large-scale calculations with linear-scaling simulations but is also capable of employing conventional diagonalization methods. In this work, only the latter capability was used. Norm-conserving pseudopotentials have been generated according to the Troullier-Martins [9] scheme, in the Kleinman-Bylander [10] separable form. Core radii of 1.78 and 1.89 bohr were used for B and Si, respectively. The program requires the use of a grid to compute some of the contributions to the matrix elements and total energy and also for performing the Fourier transforms needed to evaluate the Hartree potential and energy by solving Poisson’s equation in reciprocal space. A grid - fine enough to represent plane waves with kinetic energy up to 90 Ry - have been used. Calculations have been carried out using the same GGA functional [11] as with CRYSTAL. The NAO basis set consisted also of double- ζ plus polarization functions. The maximum extent of these functions was 5.965 Å. Structural relaxations have been performed by means of the conjugated gradient algorithm until the forces were smaller than 0.04 eV/Å. In order to keep the usage of resources within the available framework without compromising the predictive power of the results, careful convergence tests had been carried out [1]. Based on those results, all calculations were done in a 64-atom supercell, using a 2^3 Monkhorst-Pack (MP) k-point set [12] in the Brillouin zone (BZ) summation.

The calculation of local vibrational modes is extremely time demanding process. In addition, we have investigated more than 10 complexes in their different charge states and configurations. The usage of supercomputers is necessary to accomplish this task. We have used the CRAY-T3E machine with MPI library in the High Performance Supercomputer Center of Stuttgart to execute the program SIESTA parallel.

First, the geometry was optimized in 64 and 216 atom supercells with different K-point sets (single Γ -point (1^3 MP) and four K-points (2^3 MP)). The execution time scales linearly with the number of K-points. Typically, 64 processors have been used for 64 atom - 1^3 MP calculations for geometry optimization by requiring 10 SUs per processors, which means about **640 SUs** as total usage. After obtaining the optimized geometry in 64 atom supercell, we have used this as an input in 216 atom supercell. For 216 atom - 1^3 MP calculations 128 processors needed with typically 7.5 SUs per processors, which means about **960 SUs** as total for a single geometry optimization run.

The calculation time of second derivatives scales linearly with the number of vibrating atoms. For $(B_s)_2$ defect, the number of the atoms up to the second neighborhood (2NN) is 17. The calculation of the (2NN) second derivatives within 1^3 MP K-point in a 64 atom supercell required about **224 SUs** (using 64 processors). This means that a typical run with 2^3 MP K-points is in the order of **1000 SUs**.

It is apparent that the supercomputer resources of HLRS indeed helps to carry out the necessary calculations needed to investigate the behavior of BICs.

3 Results

First, we report the calculated local vibrational modes. In Table 2 the calculated vibration frequencies of the BIC-related LVMs are given assuming the presence of either only ^{11}B or only ^{10}B (the latter values in parentheses). From the two possible isomers of BI, B_i does not give rise to LVMs above the phonon continuum. Even though B_2 , alias $(B_s)_2$, appears to be metastable with respect to two isolated B_s atoms, it might be created in the dissolution process of larger BICs. It has a double acceptor level above that of the single boron acceptor, therefore, both the neutral and the double negative charge state has been calculated, for the former should occur in p -type (where the level of boron activation is high) and the latter in compensated samples (or where the activation level of boron is low). Among the possible isomers of B2I the following were considered: the boron pair splitting a substitutional site in a [001] dumbbell configuration and two B_s on neighbor sites with a Si_i between them (D_{3d} in the neutral, and a puckered C_{1h} symmetry in the doubly negative charge state) Further $2B_s + \text{Si}_i$ complexes are possible in other charge states. $(B_2)_s^0$ is more stable than $(B_s - \text{Si}_i - B_s)^0$ by 0.64 eV, but the activation energy for rearrangement appears to be significant. Among the higher BICs

Table 2. LVMs of BICs calculated in the 64 atom supercell with the 2^3 MP set, 2NN shells around the BIC vibrating. The numbers in italics- and bold-type correspond to IR and Raman active modes, respectively, while bolded-italics numbers denote LVMs which are both IR and Raman active. Values above the phonon continuum are given for isotopically pure complexes of ^{11}B (^{10}B) in (cm^{-1}).

BIC		LVM	Frequency	LVM	Frequency
B_s^-	$\text{B}^- \text{ T}_d$	T_2 (IR/R)	<i>607(632)</i>		
B_i^+	$\text{BI}^+ \text{ T}_d$		<520		
$(\text{B}_s+\text{Si}_i)^+$	$\text{BI}^+ \text{ C}_{1h}$	A' (IR/R)	<i>693(723)</i>		
$[(\text{B}+\text{Si})_s+\text{Si}_i]^-$	$\text{BI}_2^- \text{ C}_{1h}$	A' (IR/R)	<i>671(698)</i>	A'' (IR/R)	<i>658(684)</i>
$(\text{B}_s)_2^0$	$\text{B}_2^0 \text{ D}_{3d}$	A_{1g} (R)	<i>644(674)</i>	E_u (IR)	<i>527(547)</i>
$(\text{B}_s)_2^{2-}$	$\text{B}_2^{2-} \text{ D}_{3d}$	A_{1g} (R)	<i>627(657)</i>	E_u (IR)	<i>577(602)</i>
$(\text{B}_2)_s^0$	$\text{B}_2 \text{I}^0 \text{ D}_{2d}$	A_1 (R)	<i>1099(1152)</i>	E (IR/R)	<i>577(602)</i>
$(\text{B}_s-\text{Si}_i-\text{B}_s)^0$	$\text{B}_2 \text{I}^0 \text{ D}_{3d}$	A_{1g} (R) E_g (R)	<i>672(706)</i> <i>586(608)</i>	A_{2u} (IR) E_u (IR)	<i>882(908)</i> <i>604(628)</i>
$(\text{B}_s-\text{Si}_i-\text{B}_s)^{2-}$	$\text{B}_2 \text{I}^{2-} \text{ C}_{1h}$	A' (IR/R)	<i>821(852)</i> <i>666(692)</i> <i>573(594)</i>	A'' (IR/R)	<i>719(748)</i> <i>582(604)</i> <i>569(589)</i>
$[(\text{B}_2)_s+\text{Si}_i]^0$	$\text{B}_2 \text{I}_2^0 \text{ C}_{1h}$	A' (IR/R)	<i>926(969)</i> <i>565(585)</i>	A'' (IR/R)	<i>684(710)</i> <i>539(560)</i>
$(\text{B}_s+\text{B}_i+\text{B}_s)^-$	$\text{B}_3 \text{I}^- \text{ D}_{3d}$	A_{1g} (R) E_g (R)	<i>842(882)</i> <i>612(635)</i>	A_{2u} (IR) E_u (IR)	<i>1264(1326)</i> <i>652(679)</i>
$[(\text{B}_s(\text{B}_2)_s\text{B}_s)]^0$	$\text{B}_4 \text{I}^{2-} \text{ C}_2$	A' (IR/R)	<i>1095(1148)</i> <i>729(763)</i> <i>639(665)</i> <i>566(589)</i> <i>564(587)</i>	A'' (IR/R)	<i>814(853)</i> <i>637(663)</i>
$[(\text{B}_s(\text{B}_2)_s\text{B}_s)]^0$	$\text{B}_4 \text{I}^{2-} \text{ C}_{2v}$	A_2 (R)	<i>641(667)</i>	A_1 (IR/R) B_1 (IR/R) B_2 (IR/R) B_2 A_1 (IR/R)	<i>1019(1068)</i> <i>744(780)</i> <i>730(759)</i> <i>652(679)</i> <i>609(637)</i>

isomerism has only been considered for B_4I , for the arrangement of the two B_s atoms around the central $(\text{B}_2)_s$ dumbbell in a C_{2v} and in a C_2 geometry differs only by 0.35 eV in energy (in favor of the latter). The LVMs of complexes have also been calculated (see Table 3).

The expected accuracy of the calculated vibration frequencies are about $\pm 30 \text{ cm}^{-1}$. Therefore, identification of experimentally observed vibrational centers with the models, based on the calculated values, can only be trusted if more than one mode of the center is known and possibly the effect of isotope substitution has also been measured. Unfortunately, the available experimental information about the vibrations of BICs is scarce. The LVM of the isolated boron acceptor has been measured by both infrared (IR) and Raman [13, 14] spectroscopy but further boron related vibrations are only known from IR spectra of electron irradiated compensated samples [15, 16, 17]. (Compensa-

Table 3. LVMs of BICs calculated in the 64 atom supercell with the 2³ MP set, 2NN shells around the BIC vibrating. The numbers in *italics*- and **bold-type** correspond to IR and Raman active modes, respectively, while **bolded-italics** numbers denote LVMs which are both IR and Raman active. Values above the phonon continuum are given for isotopically mixed complexes in (cm⁻¹).

BIC	LVM	Frequency	LVM	Frequency
(B _s) ₂ ⁰	B ₂ ⁰ C _{3v}	A ₁ (IR/R)	E(IR/R)	<i>540</i>
(B _s) ₂ ²⁻	B ₂ ²⁻ C _{3v}	A ₁ (IR/R)	E(IR/R)	<i>592</i>
(B ₂) _s ⁰	B ₂ I ⁰ C _{2v}	A ₁ (IR/R)	B ₁ (IR/R)	<i>738</i>
			B ₁ (IR/R)	<i>738</i>
(B _s -Si _i -B _s) ⁰	B ₂ I ⁰ C _{3v}	A ₁ (IR/R)	A ₁ (IR/R)	<i>897</i>
		E (IR/R)	E (IR/R)	<i>622</i>
(B _s -Si _i -B _s) ⁻	B ₂ I ⁻ C _{1h}	A' (IR/R)	A'' (IR/R)	<i>721</i>
				<i>593</i>
				<i>582</i>

tion is necessary to get rid of the free carrier absorption which would mask the LVMs. In case of neutron irradiation the created damage provides for compensation [18].) Matters are complicated by the presence of oxygen in Cz-Si samples which gives rise to a huge band between 1000 and 1100 cm⁻¹ in the IR spectrum making the observation of other features in this region extremely difficult. Based on circumstantial evidence (number of modes, splitting on isotope substitution, stability range) the boron related centers in the IR spectrum (called P-, Q-, R- and S-lines) have been tentatively assigned to various models [15]. In Table 4 we have compared the calculated LVMs of these models (in a charge state appropriate for compensated samples) with the observed data. The calculated frequency of the single acceptor, 607 cm⁻¹ with an isotope shift of 25 cm⁻¹, against the observed 623 cm⁻¹ with an isotope shift of 23 cm⁻¹ marks the accuracy of the calculations. The R line was assumed to originate from a complex of substitutional boron with one or more self-interstitials. At present we only have the LVMs of the (B_s+Si_i)⁺, alias BI⁺, and the [(B+Si)_s+Si_i]⁻, alias BI₂⁻ complex, at 693(723) cm⁻¹ and 671(698) cm⁻¹ for the isotope ¹¹B (¹⁰B), respectively. The deviation from the observed 730(757) cm⁻¹ is not small enough in either case, to make the identification convincing based on just a single mode. The Q-line was assigned to interstitial boron [15] but Yamauchi et al. suggested the (B₂)_s complex (alias B₂I) instead, based on their calculations. Our result for the IR mode, 738(767) cm⁻¹ is even closer to the experimental 733(760) cm⁻¹ but Raman measurements on FZ-Si would be needed to confirm the assignment by finding the high-frequency Raman-active mode.

In case of the S-lines, with two known IR modes, the situation is more favorable. The suggestion of ref. [15] was a complex of two boron atoms with trigonal symmetry. Since B₂ (i.e., (B_s)₂) has no high frequency modes the B₂I isomer with trigonal symmetry, B_s+Si_i+B_s can be considered. The calculated

Table 4. Comparison of early experiments on e -irradiated compensated or n -irradiated material with calculated frequencies of those BICs which have been suggested as the origin of the observed vibrational centers. Only pure ^{11}B BICs are considered here. The numbers in italics- and bold-type correspond to IR and Raman active modes, respectively, while bolded-italics numbers denote LVMs which are both IR and Raman active. The I2 center has been observed in photoluminescence.

Center	acceptor	R-lines	S-lines	Q-lines	P-lines	I2-center
Stability range ($^{\circ}\text{C}$)		< -40	$-40 - -10$	$-10 - 200$	> 300	> 200
Expt. LVM	<i>623</i>	<i>730</i>	<i>903</i> <i>599</i>	<i>733</i>	<i>553</i>	843 242
Assignment	B_s^-	$\text{B}_s + n\text{Si}_i$	2B trig. sym.	B_i	$(\text{B}_s)_2$	$2\text{B}_s + \text{Si}_i$ low. sym.
Model	B_s^-	$(\text{B}_s + \text{Si}_i)^+$ $(\text{B}_s + 2\text{Si}_i)^-$	$\text{B}_s + \text{Si}_i + \text{B}_s$	$(\text{B}_2)_s$	$(\text{B}_s)_2$ or $(\text{B}_s)_2^{2-}$	$(\text{B}_s + \text{Si}_i + \text{B}_s)^{2-}$
Yamauchi et al. (theory) [19]	T_2 <i>612</i>			A_1 1026 E 760	A_{1g} 585 E_g 603 E_u <i>530</i>	
PRESENT (theory)	T_2 607	A_1 693 A_1 671	A_{2u} <i>882</i> A_{1g} 672 E_u <i>604</i> E_g 586	A_1 1099 E 738	(0) / (2-) A_{1g} 644 / 627 E_u <i>527</i> / <i>577</i>	A 821 719 666 582 573 569

IR modes, at 882(908) and 604(628) cm^{-1} are reasonably close to the observed values 903(928) and 599(-) cm^{-1} for the isotopically pure complexes. Also the calculated modes for the mixed complexes, 897 and 622 cm^{-1} fit the observed 917 and 603 cm^{-1} agreeably. It should be noted, though, that the mixed complex has lower symmetry (no inversion) and the other two modes which are Raman-active in the isotopically pure complex should become visible in IR around 688 and 592 cm^{-1} . From the boron related centers in the IR spectrum (called P-, Q-, R- and S-lines), only the Q-line is stable at room temperature and only the P-line survives annealing up to 300 $^{\circ}\text{C}$. The P-lines have been assigned to a pair of substitutional boron atoms [15]. Despite of finding the $(\text{B}_s)_2$ complex metastable, Yamauchi et al. [19] confirmed that the calculated IR-active mode of $(\text{B}_s)_2^0$, 530 cm^{-1} , is reasonably close to the experimentally observed 553 cm^{-1} . Our result for the IR mode, 527 cm^{-1} , is close to that of ref. [19] (even though we only get one Raman active mode, E_g , above the continuum with a frequency much higher than that of Yamauchi et al.) We note, however, that in compensated samples the stable charge state should be $(\text{B}_s)_2^{2-}$, for which we obtain 577(602) cm^{-1} for the isotopically pure complexes and 592 cm^{-1} for the mixed one. (Note that in the mixed complex an additional mode at around 642 cm^{-1} should become IR-visible.)

The observed values, $553(570) \text{ cm}^{-1}$ for the pure and 560 cm^{-1} for the mixed complex are still within the accuracy of the calculation. Additional support for the assignment stems from the report of a feature at 615 cm^{-1} correlating with the P-lines. This could be the mode which is only IR-active in the mixed complex. Still, a definite identification required the knowledge of the corresponding Raman spectra. In addition to IR centers, LVM assisted sidebands of the boron related photoluminescence (PL) center, called I2, has also been observed [20, 21]. Originally, this center has been attributed to two boron and a self-interstitial atom with trigonal symmetry [20] but later a reduced symmetry was reported [21]. The calculated frequencies of the neutral B_2I (D_{3d}) isomer ($\text{B}_s\text{-Si}_i\text{-B}_s$)⁰ obviously do not fit the modes of the I2 center. The highest frequency of the doubly negative (C_{1h}) isomer is, however, quite close to the observed I2 mode. Since we cannot, at present, calculate intensities, it is not clear why the other modes were not observed, if this complex is the origin of the I2 center.

Within the framework of the FRENDECH-EAST project, the MTA-MFA started the IR/Raman investigation of silicon samples, heat treated after high dose boron implantation (^{11}B doses of 10^{16} and $2 \cdot 10^{15} \text{ cm}^{-2}$). The first Raman spectra taken after a 900°C annealing showed several boron related features. The features at 618 and 683 cm^{-1} are present in both Raman spectra, the first increasing, the latter decreasing with the dose. Since the increasing implantation dose creates more damage and with that a stronger level of compensation, it is tempting to assign these two features to the Raman-active modes of $(\text{B}_s)_2^{2-}$ and $(\text{B}_s)_2^0$, with calculated frequencies at 627 and 647 cm^{-1} , respectively, assuming that increasing the level of compensation - and thereby raising the Fermi level - makes the former more and the latter less abundant. Electrical measurements on these samples as well as IR spectra are needed for the confirmation of this suggestion.

Beside the local vibrational modes we have also calculated the electronic structure of BICs. We started on the simplest BIC, the BI complex, for which many experimental results are known: it is has been linked with the so-called G28 electron paramagnetic resonance (EPR) center [22] and with occupation levels found by deep-level transient spectroscopy (DLTS) [23]. DLTS measures the adiabatic internal ionization energy of a defect, i.e., the position of the Fermi level, at which two charge states of the defect have the same total energy. The measured values correlating with the G28 EPR center are $E_C - 0.13 \text{ eV}$ for the $(+/0)$ charge states, and $E_C - 0.37 \text{ eV}$ for the $(0/-)$ charge states. In other words: $E_F(+/0) = E_V + 0.99 \text{ eV}$ and $E_F(0/-) = E_V + 0.75 \text{ eV}$, using the room temperature gap of silicon. The G28 center is a negative-U bistable defect, which can only be detected in non-equilibrium EPR experiments (e.g. under illumination), for EPR measures the paramagnetic neutral charge state. The observed $\hbar f$ interactions imply a defect with C_{1h} symmetry. Previous (pure DFT) theoretical studies have found [24, 25, 26], indeed, that the BI defect is bistable. In the $(+)$ charge state it consists of a Si_i at the tetrahedral site next neighbor to a B_{Si} . This defect has C_{3v} symmetry. In the $(-)$ charge state,

the boron shares a lattice site with a Si in a dumbbell configuration in the (110) plane, with C_{1h} symmetry. In the (0) charge state both configurations constitute local minima of the total energy surface. So far, all calculations have predicted the C_{3v} configuration to be more stable (by 0.21 eV in LDA and by 0.07 eV in GGA) than the C_{1h} one - in contrast to the experimental observation. This has always been suspected [26] to be the consequence of the band gap error. We have calculated the geometry of the BI defect in both the (+), and the (-) charge state using the 12% ME. The details of the geometries did not deviate significantly from those obtained by pure GGA. However, in the neutral charge state, our calculation resulted in the C_{1h} configuration being more stable by 0.14 eV than the C_{3v} - in agreement with experiment! The occupation levels, determined by DLTS depend also on the position of

Table 5. Comparison of the occupation levels calculated by different methods for the BI defect with the DLTS results for the G28 center. Values are given in (eV) with respect to the valence band edge.

Method	LDA [26]	LDA [24]	GGA [27]	Present GGA	Expt. [23]
Correction	No correction	Empirical correction using test cases	Scissor correction (+ charge correction)	12% ME	
(+ / 0)	0.66	1.07	1.1	0.94	0.99
(0 / -)	0.55	0.79	0.7	0.66	0.75

the one-electron levels, since the total energy of any charge state contains the sum of the energies of occupied one-electron states. Shifts of the gap states in the order of the band gap error (≈ 0.5 eV in silicon) may easily reverse the energetic sequence of different configurations. In addition, the error related to this is different in various charge states, influencing the position of occupation levels. Our calculated values are compared to those of (a posteriori corrected) pure LDA and GGA calculations, as well as to experimental data in Table 5.

It can be stated that our procedure is at least as effective as other a posteriori correction schemes in predicting DLTS results. (N.B.: unlike ref. [27], our results do not yet contain a correction for the charged supercell.) It should be emphasized, however, that the one-electron levels of the 12% ME calculations are correct in themselves, and the same calculation also provides the correct total energy sequence among various configurations in the neutral state.

We have then studied the electronic structure of all the BICs depicted in Fig. 1. The electronic structure of the BICs fall into two categories. In the first one, the boron atoms (which are always negatively charged but may be compensated by the interstitial) introduce delocalized, occupied effective mass states very near the VB edge (the distance falling within the error bar of the calculation). The BIC series B_n^{n-} and BI^+ , B_2I^0 , B_3I^- , B_4I^{2-} fall into this category. Loss of activation occurs only due to the compensating effect of the

self-interstitial in the latter series. It should be noted that the clusters $(B_s)_2^{2-}$, and $(B_s)_3^{3-}$ have positive formation energies with respect to the isolated B_s^- , obviously because of the repulsion of two negatively charged B atoms. With the hybrid functional we find, however, that a $(B_s)_2^0$ complex, in which the boron atoms relax back into the plane of their respective three Si neighbors into an sp^2 configuration and are not bonded to each other, is energetically favored over isolated B_s^0 atoms. This fact may be used to explain why $(B_s)_2^{2-}$ complexes can after all be observed by infrared spectroscopy (see Refs. [3, 28] and references therein).

The second category of BICs introduces localized states in the band gap. The estimated position of the isolated defect levels are given in Table 6. As can be seen, these states are not too deep for the B_nI_3 series and likely to be filled even after annealing. In contrast, the B_nI_2 series introduces states near midgap, and are likely to become empty when annealing of the intrinsic defects causes the lowering of the Fermi level. Therefore, this is the class of BICs which impair the activation rate the most. The results given in Table 6 indicate that,

Table 6. Estimated level position of isolated B_nI_m clusters with respect to the VB edge in (eV). Always the highest occupied localized acceptor state is given for the charge state relevant to a Fermi level pinned to midgap.

	n = 1	n = 2	n = 3	n = 4
m = 1	< 0.1	< 0.1	< 0.1	< 0.1
m = 2	0.53	0.47	0.40	~0
m = 3	~0	0.07	0.22	0.14

based on the electronic structure, it will be difficult to distinguish between BICs containing the same number of interstitials and different number of boron atoms. On the other hand, if recent suggestions about the average value of $m/n \approx 1.2$ get confirmed, the diagonal of Table 6 show clear differences among the possible compositions.

From the experimental point of view, the $m=1$ series will only be observable by methods which measure the activation energy of conductance (e.g. photoconductivity). The $m=2,3$ series may bind an exciton or can give rise to defect-to-band luminescence, measurable by photoluminescence. The $m=2,3$ series have levels deep enough to be measurable by electrical (CV, DLTS) measurements, as well. It should be pointed out, though, that these methods measure the occupation levels, and not the one-electron levels reported here. Still, the values given in Table 6 can be used to correct the occupation level obtained, from earlier pure DFT calculations, for the gap error.

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Ionic Liquids from AlCl_3

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1 Introduction

Recently, new solvents and solutions are discussed in chemical research because many of the solvents and solutions commonly used in laboratories and in the chemical industry are considered as unsafe for reasons of environmental protection. [9] On the list of damaging chemicals, solvents rank highly, because they are often used in huge amounts and because they are volatile liquids difficult to contain. The introduction of cleaner technologies has become a major concern throughout both academia and industry. The development of environmentally benign so called neoteric solvents, constituting a class of novel solvents with desirable, less hazardous, new properties is one of the major topics in green chemistry.

The new solvents called ionic liquids are salts/salt mixtures with melting points below ambient temperature. In contrast to classical molten salts, which are usually high melting, viscous and very corrosive substances, ionic liquids are fluid at low temperatures ($> 350\text{K}$) and have a relatively low viscosity. [9] Ionic liquids are known since 1929. Since then, their application as solvents in chemical reactions has increasingly gained attention. [9]. Applications of ionic liquids are found for a variety of reactions, for example the Friedel–Crafts alkylation, the Friedel–Crafts acylation, some hydrogenations and hydroformylations, the Heck reaction as well as some oligomerisations and polymerizations.

This report is dedicated to liquid AlCl_3 and ionic liquids formed by the salts of AlCl_3 . These salts exhibit attractive properties such as low-temperature eutectics of possible relevance to energy storage. The thermodynamic and physical properties of these low-melting acidic mixtures, i.e. more than 50% AlCl_3 , show a strong compositional dependences that are not completely understood. Complex ions as AlCl_4^- , Al_2Cl_7^- and $\text{Al}_3\text{Cl}_{10}^-$ are found in these acidic mixtures and with increasing AlCl_3 concentration the proportion

of Al_2Cl_7^- is increasing. All complex ion species are essentially polymeric build up by the same fundamental unit of AlCl_4^- tetrahedra being connected with each other. However, the precise structures are not well established and there is some disagreement concerning the structure of the Al-Cl-Al bridge in the Al_2Cl_7^- species. Although quantum chemical calculations ([1] and references therein) indicate a bent bridge in the AlCl_3 -Dimer the important structural features could be different in condensed phase. The established model of the molten AlCl_3 is that of fluid Al_2Cl_6 dimers formed by edge sharing of two distorted AlCl_4^- tetrahedra units, which is in accordance to quantum chemical studies. Inspired by the similarities between ZnCl_2 and AlCl_3 – both have a low melting point and a very low conductivity – the structure has been re-investigated and a ‘sparse network liquid’ has been suggested. [1] The liquid seems to consist of Al_2Cl_6 dimers, but it also might be a liquid with reduced connectivity and strong covalent bonding. [1]

In this report we study the systems by means of Car-Parrinello simulations. [3] With the Car-Parrinello simulation technique one is able to treat polarization and molecular many-body effects as in each simulation step the electronic structure is calculated on the fly. Due to the large computational costs, the calculations are restricted to gradient corrected density functional theory.

2 Methodology

The Car-Parrinello calculations are performed with the CPMD code [4]. Gradient corrected local density functionals for exchange and correlation, i.e., BLYP [2, 6] and PBE [7] are chosen throughout and the Kohn–Sham orbitals are expanded in a plane wave basis with a kinetic energy cutoff of 50 Rydbergs for the BLYP functional calculation and 25 Rydbergs for the PBE calculations making use of ultrasoft pseudopotentials. Norm conserving pseudopotentials of the Troullier–Martins type [8] are taken with pseudization radii in Bohr units) of $s=1.25$, $p=1.55$, $d=1.40$, and $s=2.0$, $p=1.6$, $d=1.82$ for aluminum and for chlorine atoms, respectively. The pseudopotentials are applied in the Kleinman–Bylander representation [5] with s and p angular momentum in non-local form and d angular momentum as local potential. Employing periodic boundary conditions the Brillouin zone sampling is restricted to the Γ point. All Car-Parrinello simulations are performed in an NVE ensemble.

Single molecule calculations are performed in a cubic box of $12\text{\AA}$ length with the PBE functional. The fictitious electron mass was set to 1000 a.u. while the time step was 0.148 fs. The temperature was fixed to 470 K with Nose-Hoover thermostats coupled to the ionic degrees of freedom. A special Poisson solver was used in order to avoid spurious box effects for the isolated molecule calculations.

The PBE simulation of the liquid encounters 64 aluminum chloride units. The molecules are placed randomly as monomers in a cubic box of $22.7\text{\AA}$

length. After an equilibration of several ps data was collected from a 10 ps trajectory. The fictitious electron mass was set to 1000 a.u. and the time step was 0.148 fs. In the case of the BLYP simulation at each third time step the maximally localized Wannier-functions were calculated. Data collected from a trajectory of 1.4 ps length.

3 Results

3.1 Basics to the AlCl_3 systems

Figure 1 depicts the two dimer conformers with different distances and angles. As can be seen in Fig. 1 there are three characteristic parameters to distinguish the two conformers. The Al–Al distance is much longer in the case of the corner conformer. There is one very large Al–Cl bond length in the corner dimer, it is a distance to the bridge atom, which we mark in Fig. 1 with a capital B. Another good criteria to distinguish the two conformers is the Al–B–Al angle. It is smaller in the case of the edge dimer which will assist to distinguish the connectivity of the AlCl_3 unities in the simulations. Although these criteria do not reveal which n-mer is dominant in the simulation they are helpful in deciding which connectivity of the monomers is present.

To analyze the simulations we will also use information from molecular dipole moments. Monomer dipole moments for the edge dimer are 2.64 Debye. The corresponding values for the corner dimer are 1.18 Debye and 0.68 Debye. Whereas the dipoles in the edge sharing dimer point in opposite direction and therefore cancel, the ones in the corner dimer must amplify each other. This information can be used to determine the connections of the monomer units in the liquid phase simulations.

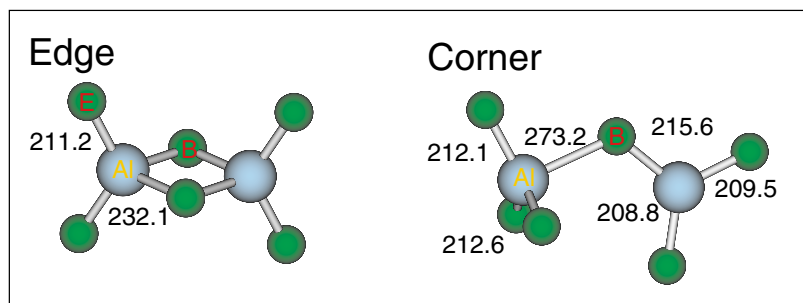


Fig. 1. The two dimer conformers. Left: Edge conformer. Right: Corner conformer. Distances and angles are given in pm respectively degrees and are obtained from BLYP calculations.

3.2 Isolated neutral dimers

In Fig. 2 we depict the dipole distributions from the simulations of the isolated cluster, i.e. the monomer, the edge-sharing dimer and the corner dimer. Whereas the monomer (0-2 D) and the edge dimer (0 D) have a sharp distribution, see blue and red curve in Fig. 2, the corner dimer provides values in the range of 0-8 Debye. This will help to distinguish both of the dimer

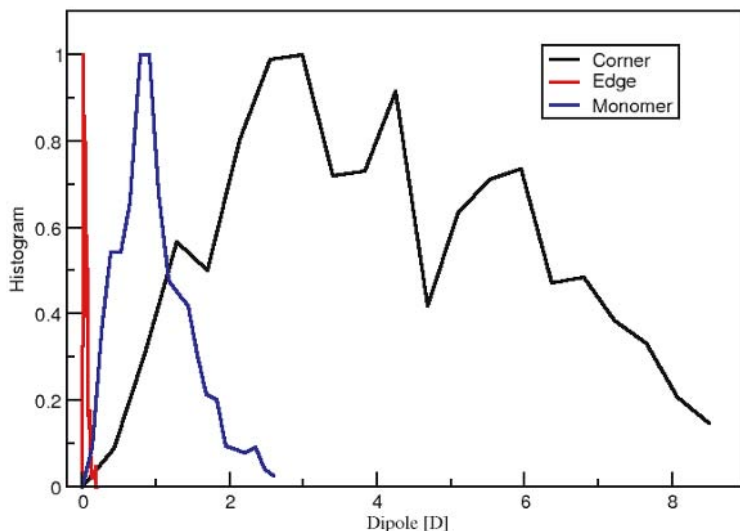


Fig. 2. Dipole distribution of different monomers.

configurations in the liquid. Although the edge is more stable by 60 kJ/mol, no transformation from or to the edge- or corner-dimer could be investigated. This points to a substantial barrier for the interconversion of the two forms.

For the liquid this might be different, since the negative charged dimer $Al_2Cl_7^-$ is only stable in the edge configuration. Thus assuming the liquid polarize each of the dimers, the barrier for the transformation reaction might be lowered. We tried to calculate the reaction barrier for the transformation but failed due to the difficulties of finding a good reaction coordinate.

3.3 The structure of liquid $AlCl_3$

In Fig. 3 we depicted six snapshots from the simulation. As can be recognized from these pictures there are more than one configurations apparent.

Furthermore it can not be decided on the grounds of these pictures to what extend, monomers, dimers and in what configuration they are present. Detailed structural features of a liquid can only be captured from further analysis of the trajectory, such as the radial pair distribution function.

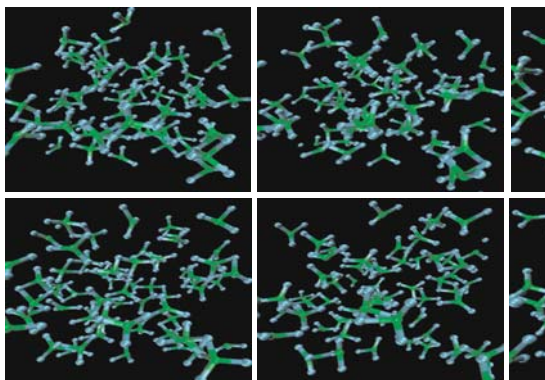


Fig. 3. Snapshots from the simulation

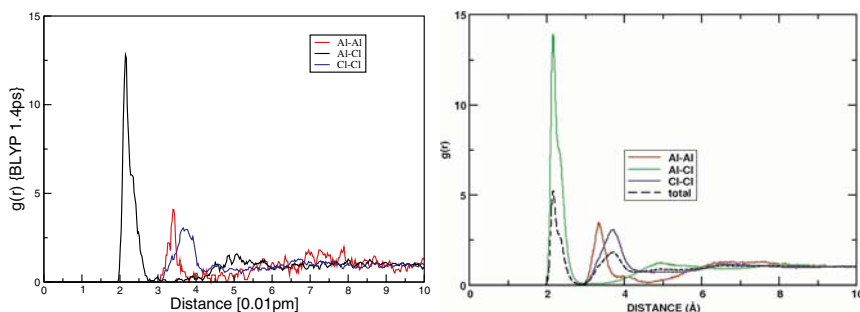


Fig. 4. Radial pair distribution function from 1.4 ps of the BLYP simulation left and from the PBE simulation right.

In Fig. 4 the radial pair distribution function for the BLYP and the PBE run is depicted. Both simulations show similar curves for the pair functions. The functions for the BLYP run are less smooth due to shorter simulation time. Due to the similarities of both simulations we will in the following always discuss the data from the PBE simulation. There is a large peak indicating the intramolecular Al-Cl bond at approximately 214 pm in the Al-Cl function (see green curve Fig. 4).

A noticeable shoulder is also apparent at about 235 pm. This distance corresponds to the dimer in the edge-sharing conformation. Furthermore the Al-Al partial function (red line Fig. 4) shows the first peak at around 328 pm, which is another attribute of the edge-sharing conformer. There might also be a very small amount of corner-sharing conformers present, since the functions shows a not vanishing probability at 414 pm. However, this peak is not enough pronounced to decide its importance for the liquid structure.

It should be kept in mind, that the liquid needs not to consist only of monomers and dimers. To further gain insight into the structural behavior

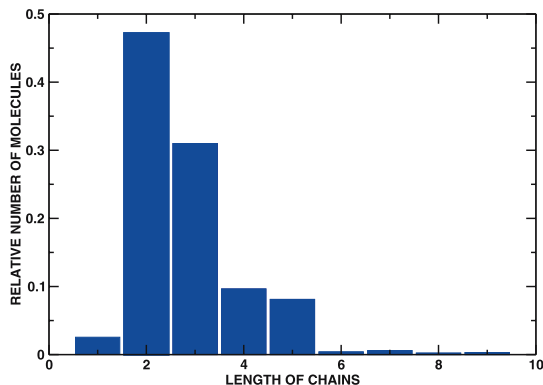


Fig. 5. Probability of different chain length for the PBE simulation.

we considered, using a simple geometrical criteria, namely the Al-Al distance, the length of the chains that were build in the simulation of the liquid.

Figure 5 shows the relative number of molecules plotted against the length of chains.

It is apparent from its peak hight of less than 0.05 that our liquid contains almost no monomers. The dimers are the most frequent species followed by trimers. There are also 10 per cent of each, tetramers and pentamers, but higher species such as hexamers become less probable. A picture of a pentamer is given in Fig. 6. In general we can say that most molecules are incorporated into units greater than the monomer but smaller than a hexamer.

We also calculated the distribution of the Al-Cl-Al angle. It is apparent from Fig. 1 that this angle can be used to distinguish the edge- versus corner-sharing configuration of the clusters. Figure 7 depicts the relative probability to find a particular angle.

Again the dominance of the edge-sharing dimer rather than the corner-sharing dimer is indicated in Fig. 7, as we observe a high peak at angles of 90 degrees. However, a small percentage of clusters provide higher angles that fit to the corner-sharing configuration.

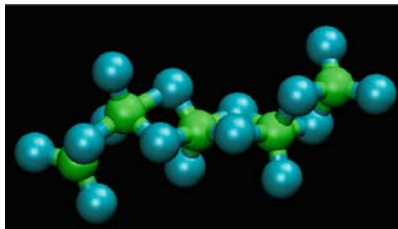


Fig. 6. A pentamer cluster as found in the simulation.

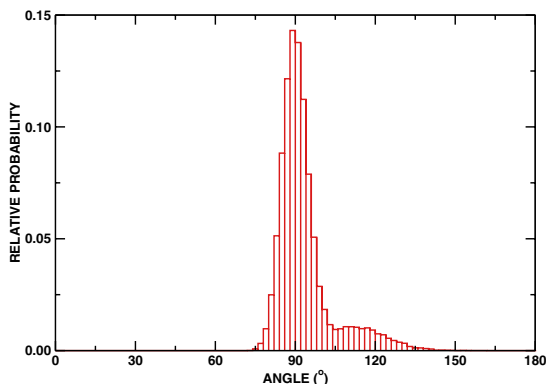


Fig. 7. Cl-Al-Cl Angular distribution for the PBE simulation.

4 Conclusions

We simulated the AlCl_3 liquid and found mainly dimers that are connected in the edge-sharing configuration. However, there were also other configurations such as trimers, tetramers and pentamers. The simulated data will be further analyzed to see whether the small amount of larger angles is due to the monomers or due to a small amount of corner-sharing dimers or even larger clusters such as trimer, tetramers or pentamers.

Acknowledgments

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Miscellaneous Topics

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This section is an outgrowth of the section *Earth Sciences* of the Transactions of the High Performance Computing Center 2004. Although the two articles published last year under this heading find their continuation in the present volume, it was thought to be useful to broaden the scope of the heading so that more singular topics can be included. The four articles that follow clearly indicate the necessity of the use of high performance computers in new fields of science, and also the spreading tendency of computing into fields which until now relied on other than numerical techniques.

The first article is a continuation of the work reported in the volume of last year. The investigation is concerned with a numerical study of the influence of viscous fluid forces on the wave propagation in porous media, as it is observed in many rocks, caused by a complex interaction between heterogeneous solids and viscous fluids. The work is carried out as a cooperative investigation of the Free University Berlin, Germany, the Stanford Rock Physics Lab., and Stanford University, USA. The numerical technique used is based on a displacement-stress rotated staggered finite-difference scheme, with which the elastodynamic wave equation is solved. The results enable the authors to compare effective elastic properties of dry and viscous fluid filled three-dimensional porous media. All three distinct coupling mechanisms of fluid-solid interactions can be studied: The inertial coupling, the Biot coupling, and the Squirt flow. The article describes the numerical method and summarizes the most recent results obtained with the method proposed.

The second contribution is in part also a continuation of previous work, originated at the university of Jena in Germany, and now continued together with the Department of Earth & Planetary Science of the University of California at Berkeley. So far a thermo-chemical model for the description of the evolution of the mantle of the earth, together with its numerical implementation were described. In the last year the model could substantially be improved: The temporal development of the radial viscosity profile caused by the cooling of the earth could be taken into account in a more accurate manner. Also, the laterally averaged heat flow and the time dependence of the

volume-averaged temperature used now compare better to other evolution models. With these and other improvements the dynamic model presented for the description of the evolution of the earth mantle is reported to generate a good self-consistent plateness of the oceanic lithosphere and a proper approximation of the thermal evolution as a function of time. The method of solution is based on a three-dimensional finite-element discretization of the system of differential equations describing convection in a compressional spherical shell. The results shown comprise the computed temperature distribution and creeping velocities for various depths and also the evolution of the laterally averaged surface heat flow among other data.

The third article is a new investigation of the Geodetic Department of Stuttgart University. The investigation is aimed at using data of geoscientific satellites to analyze the gravity field of the earth. Three satellites will be used to obtain the data required: The CHAMP (CHAllenging Minisatellite Payload), the GRACE (Gravity Recovery And Climate Experiment), and the GOCE (Gravity field and steady-state Ocean Circulation Explorer). It will be possible to determine the physical shape of the earth, spatial and temporal variations, global sea level variations, ocean circulation, ocean mass and heat transport, ice mass balance, the global water cycle, and other phenomena. The solution of the system of equations which has to be solved for such an analysis involves the determination of up to a hundred thousand unknown coefficients of an existing series expansion model, which can only be achieved with the aid of high performance computing. So far the work was concentrated on the CHAMP data, which were used in an existing analysis procedure, involving direct normal matrix inversion and other methods. First results of a comparison of two solution techniques implemented on the HLRS machines are reported.

The fourth article deals with a completely different subject: In the Institute of Technical Thermodynamics and Thermo-Chemical engineering at Stuttgart University a new approach is offered for the modeling of vapor-liquid equilibria of pure components and mixtures. It is proposed to enable a more reliable description and prediction of thermo-physical properties with the aid of molecular modeling and simulation. In the article new Lennard-Jones based molecular models for ethanol [SVH05], ammonia [SEV05], and water [Der05] were developed. It is reported, that the excellent agreement of the descriptive mode results for vapor-liquid equilibria confirm that reliable mixture properties can be obtained over a wide range of state points.

Considerations of the Biot Velocity Relations: Viscous Finite-difference Calculations in Combination with Flow Simulations

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Summary. This paper is concerned with numerical considerations of viscous fluid effects on wave propagation in porous media. We apply a displacement-stress rotated staggered finite-difference (FD) grid technique to solve the elastodynamic wave equation. An accurate approximation of a Newtonian fluid is implemented in this technique by using a generalized Maxwell body. With this approach we consider the velocity predictions of the Biot theory for elastic waves in different digital rock samples. To distinguish between the low and the high frequency range we estimate the effective permeabilities by a flow simulation. Our numerical results indicate that the viscous Biot-coupling is visible in the numerical experiments. Moreover, the influences of other solid-fluid interactions (e.g. Squirt flow) are also discussed.

1 Introduction

Although the theory of seismic wave propagation in porous fluid-saturated media has been established 50 years ago [3] there are still many unanswered questions about the origin of attenuation and dispersion in such media. In particular, while it is generally accepted that these dissipative effects can be explained by the presence of wave-induced flow phenomena, there is still no consensus on the mathematical model of these phenomena. Some of the questions about the physics of wave propagation in porous materials can be addressed by numerical simulations performed on the micro-scale, that is, on the scale of individual pores and grains. Having this in mind, Saenger et al (2004b) [14] already have performed such wave propagation simulations based on the rotated staggered grid (RSG) finite-difference (FD) technique [12]. However, they have restricted themselves to determine effective elastic properties of porous media saturated with a non-viscous fluid.

In this paper we extend this approach to a Newtonian (i.e. viscous) fluid. We propose an accurate approximation of a viscous fluid saturating a porous solid using a generalized Maxwell body. This is a well-known rheo-

logical model, which has been previously used to simulate (nearly) constant frequency-independent attenuation by a time-domain FD scheme [4, 7].

In a second part of this paper, we use the proposed method to test the applicability of the Biot velocity relations [3] to porous materials. We explicitly simulate elastic waves in porous solid structures saturated with a viscous fluid. This means that our modeling involves all solid-fluid interactions which are covered by the elastodynamic wave equation. The goal here is to identify explicitly the seismic effect of the viscous Biot-coupling in the numerical experiments.

The flow simulations additionally performed in this paper are carried out for the determination of the reference frequency of the Biot theory. These simulations provide a combined estimate of transport and mechanical properties of the same digital rock sample.

2 Digital rock samples

To generate realistic synthetic microstructures we use an approach described in [11], the so-called open-cell Gaussian random field (GRF) scheme. The porespace is defined by the intersection of two two-cutted Gaussian random fields (i.e. Gaussian A and Gaussian B; see Table 1 for details). To ensure a complete connectivity of the pores we eliminate isolated pores. In this paper we use exact the same GRF's as in [14]. Figure 1 shows one typical realization (GRF3).

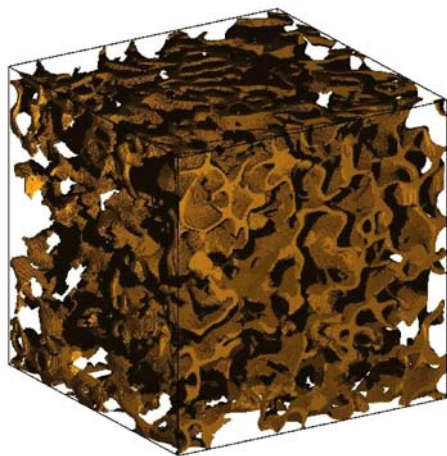


Fig. 1. An open-cell Gaussian random field (GRF3). The structure shown is the porespace, the transparent part is the grain material.

Table 1. Details of the open-cell GRF models (size: 400^3 gridpoints, $\Delta x = 0.0002m$). Every single model (GRF1-5) is build up of the intersection of two two-level cutted Gaussian random fields (Gaussian A and B).

MEDIUM	GRF 1	GRF 2	GRF 3	GRF 4	GRF 5
Porosity ϕ	3.42%	8.77%	13.2%	8.02%	21.6%
Perm. κ [$10^{-4}(\Delta x)^2$]	9.780	151.5	500.6	33.1	647.6
<i>Gaussian A</i>					
corrl. len. [0.0002m]	25	25	25	13	25
cut min.	0.4	0.4	0.4	0.4	0.38
cut max.	0.6	0.6	0.6	0.6	0.62
<i>Gaussian B</i>					
corrl. len. [0.0002m]	30	30	30	15	14
cut min.	0.485	0.48	0.4575	0.4904	0.46
cut max.	0.515	0.52	0.5415	0.5296	0.54

Permeability values were estimated through the Lattice-Boltzmann (LB) flow simulations on the synthetic digital rocks. The biggest advantages of the LB method are that it is readily applied to any arbitrary discrete geometry [6] and that it describes fluid flow in porous media very accurately [8, 5]. We used the time-averaged velocity scheme [8] to avoid artifacts in local velocity fields. The numerical flow simulation was performed with an assigned pressure gradient (∇P) across opposite faces of cubical digital rocks. We imposed no-flow boundary condition on the other four side faces of the cube. From the simulated local flux field, we calculated a volume-averaged flux $\langle q \rangle$. Then, the macroscopic permeability (κ) was estimated using the Darcy's law:

$$\langle q \rangle = \frac{\kappa}{\eta} \nabla P \quad (1)$$

where η is the dynamic viscosity of the fluid. We repeated the LB simulation with 1-D pressure gradient for all three directions and the permeability was estimated by averaging three permeability values (κ_x , κ_y and κ_z). We did not observe any significant anisotropy of permeability in the synthetic digital rocks. With the permeability (Table 1) it is possible to calculate the Biot reference frequency (Table 2).

3 Viscoelastic wave simulations

3.1 Theoretical model of viscoelasticity

We reformulate the approach described by [4] and [7]. Incorporation of viscosity based on the generalized Maxwell body (GMB) means that Hooke's law is modified:

$$\sigma_{ij} = c_{ijkl} \epsilon_{kl} - \sum_{m=1}^n \xi_m^{ij}. \quad (2)$$

In this equation, σ_{ij} , c_{ijkl} , ϵ_{kl} denote the stresses, the elastic tensor and the strains, respectively. The number of relaxation mechanisms is equal to n . The anelastic functions ξ_m^{ij} are determined by:

$$\dot{\xi}_m^{ij} + \omega_m \xi_m^{ij} = \omega_m \tilde{Y}_m^{ijkl} \epsilon_{kl}, \quad (3)$$

with $\tilde{Y}_m^{ijkl}$ as the tensors of anelastic coefficients and ω_m as angular relaxation frequencies. The GMB frequency-dependent viscoelastic modulus $C_{ijkl}(\omega)$ can be derived by inserting the Fourier transform of equation (3) into equation (2):

$$C_{ijkl}(\omega) = c_{ijkl} - \sum_{m=1}^n \tilde{Y}_m^{ijkl} \frac{\omega_m}{i\omega + \omega_m}. \quad (4)$$

Using this formalism it is possible to implement attenuation in a general anisotropic media.

3.2 Implementation of viscoelasticity in a displacement-stress rotated staggered grid scheme

A second-order discretization in time of equation (3) yields (compare with discretization of equation (28) of [4]):

$$\begin{aligned} \xi_m^{ij}(t + 1/2\Delta t) = \\ \frac{2 - \omega_m \Delta t}{2 + \omega_m \Delta t} \xi_m^{ij}(t - 1/2\Delta t) + \frac{2\omega_m \Delta t}{2 + \omega_m \Delta t} \tilde{Y}_m^{ijkl} \epsilon_{kl}(t). \end{aligned} \quad (5)$$

This can be implemented in a displacement-stress finite difference algorithm as shown in [10]. They point out that this is the most efficient FD scheme for incorporating attenuation models. One main feature of the RSG is that all components of one physical property are placed in an elementary cell at one single location. This is also true for the anelastic functions ξ_m^{ij} and the tensor of anelastic coefficients $\tilde{Y}_m^{ijkl}$. These parameters are located at the same position as the stiffness tensor (see Fig. 1(d) of [12]).

3.3 Approximation of a Newtonian fluid using a generalized Maxwell body

A compressible viscous fluid is characterized by the following frequency-dependent elastic moduli [1]:

$$C_{44}(\omega) = \mu(\omega) = i\omega\eta_\mu, \quad (6)$$

$$C_{12}(\omega) = \lambda(\omega) = \lambda(0) + i\omega\eta_\lambda, \quad (7)$$

with $\lambda(\omega)$ and $\mu(\omega)$ as angular-frequency dependent Lamé parameters. For all examples in this paper we assume that $\eta_\mu = \eta_\lambda = \eta$. The key problem is how to approximate the viscous behaviour given by equation (6) and (7) using a GMB. The following strategy (illustrated in Fig. 2) is based on a Taylor-expansion of equation (4) around $\omega = 0$:

- We use one relaxation mechanism ($n=1$).
- $\tilde{Y}_1^{44} = c_{44}$. Only in this case it is possible that $C_{44}(0) = 0$ [compare with equation (6) and (4)].
- In the low frequency range of the GMB, using one relaxation mechanism, the wanted fluid-viscosity can be determined by the following relations:

$$\eta_\mu = \frac{1}{i} \left. \frac{\partial C_{44}(\omega, \tilde{Y}_1^{44} = c_{44})}{\partial \omega} \right|_{\omega=0} = \frac{c_{44}}{\omega_1}, \quad (8)$$

$$\eta_\lambda = \frac{1}{i} \left. \frac{\partial C_{12}(\omega)}{\partial \omega} \right|_{\omega=0} = \frac{\tilde{Y}_1^{12}}{\omega_1}. \quad (9)$$

- From $\eta_\mu = \eta_\lambda$ it follows $\tilde{Y}_1^{12} = c_{44}$. Further, with equation (4), (7) and the known relation $c_{11} = c_{12} + 2c_{44}$ we obtain:

$$c_{11} = \lambda(0) + 3c_{44}. \quad (10)$$

- For FD approaches it is necessary to take into account the stability criterion. For the rotated staggered grid with FD operators of second order in time and space the following relation is valid [12]:

$$\sqrt{\frac{c_{11}}{\rho_{fluid}}} = v_p \leq \gamma, \quad \gamma = \frac{\Delta h}{\Delta t}. \quad (11)$$

- We choose c_{44} from the following range [given by the 'stability criterion'-relation (11) and equation (10)]:

$$c_{44} \leq \frac{\gamma^2 \rho_{fluid} - \lambda(0)}{3}. \quad (12)$$

Together with the choice of the angular relaxation frequency ω_1 one can determine the wanted dynamic viscosity η [compare with equation (8)].

- We choose a source signal in the low frequency range of the applied GMB ($2\pi f_{source} \ll \omega_1$).

3.4 Wave propagation modeling procedure

We apply the 3D RSG-technique with the viscoelastic extension described above to explicitly model wave propagation in fluid saturated porous media. The synthetic porous rock-models are embedded in a homogeneous elastic region. The full models are made up of 804x400x400 grid points with an interval of $\Delta x = 0.0002\text{m}$. In the homogeneous region and for the grain material we set a P-wave velocity of $v_p = 5100\text{m/s}$, a S-wave velocity of $v_s = 2944\text{m/s}$ and a density of $\rho_{grain} = 2540\text{kg/m}^3$. For dry pores we set $v_p = 0\text{m/s}$, $v_s = 0\text{m/s}$ and $\rho_v = 0.0001\text{kg/m}^3$. For the fluid-filled pores we use the parameters given in Table 2. We perform our modeling experiments with periodic boundary

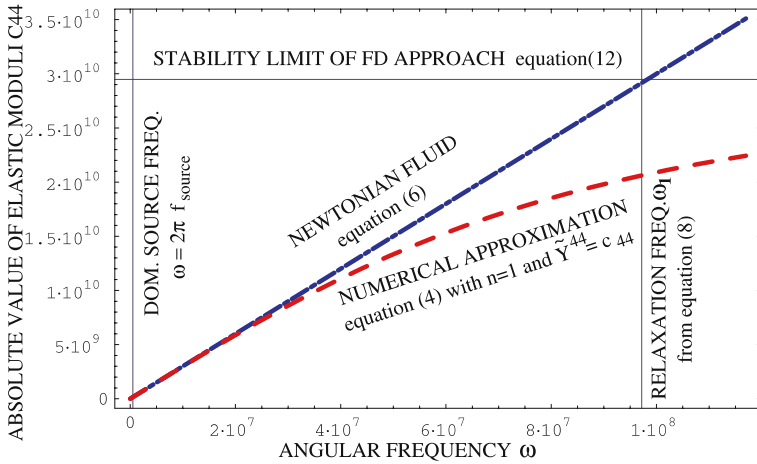


Fig. 2. Absolute values of the shear modulus C_{44} in dependence of the angular frequency ω . In the frequency range of the used source the precision of the numerical approximation of the Newtonian fluid is very high. Parameters are taken from experiment 13 (Table 2).

conditions in the two horizontal directions. To obtain effective velocities in different models we apply a body force plane source at the top of the model. The plane P- or S-wave generated in this way propagates through the porous medium. We measure the time-delay of the peak amplitude of the mean plane wave caused by the inhomogeneous region. Using the time-delay we estimate the effective velocity and, therefore, also the corresponding elastic moduli (see Table 2). The source wavelet is the first derivative of a Gaussian with a dominant frequency of $f_{source} = 8 \times 10^4 Hz$ and with a time increment of $\Delta t = 2.1 \times 10^{-8} s$. All computations are performed with second order spatial FD operators and with a second order time update. A similar numerical setup with a detailed error analysis is discussed in [13].

4 Interpretation of numerical results

4.1 Permeability versus static dry elastic moduli

Experiments No. 1,2,3,9 and 15 (see Table 2) provide the effective dry rock moduli of the digital rock samples GRF 1-5. As expected we observe an increasing permeability with an increasing porosity (Table 1). Also elastic moduli decrease with increasing porosity. We make the following observations: First, the permeability varies over two orders of magnitude whereas the effective elastic moduli varies about 30%. Second, the permeability varies with the poresize (i.e. Δx) whereas the static elastic moduli are scale independent.

Table 2. Normalized effective moduli ($\hat{\mu} = \langle \mu \rangle / \mu_{grain}$, $\hat{K} = \langle K \rangle / K_{grain}$) for the digital rock models GRF1-5 saturated with different types of fluids. The fluid can be characterized by its elastic moduli c_{44} , the fluid viscosity η_{fluid} , the density ρ_{fluid} and the p-wave velocity at zero frequency $v_p(\omega = 0)$. Additionally we give the reference frequency f_{biot} of the Biot approach.

No.	$c_{44} of fluid$ [$10^9 kg/(ms^2)$]	$v_p(\omega = 0)$ [m/s]	ρ_{fluid} [kg/m^3]	η [$kg/(ms)$]	f_{biot} [$10^4 Hz$]	norm. eff. moduli
<i>GRF 1</i> ($\phi = 3.42\%$)						
1	0	0	0.0001	0	- (dry)	$\hat{\mu} = 0.849$, $\hat{K} = 0.790$
<i>GRF 2</i> ($\phi = 8.77\%$)						
2	0	0	0.0001	0	- (dry)	$\hat{\mu} = 0.605$, $\hat{K} = 0.493$
<i>GRF 3</i> ($\phi = 13.2\%$)						
3	0	0	0.0001	0	- (dry)	$\hat{\mu} = 0.472$, $\hat{K} = 0.369$
4	0	1485	1000	0	0	$\hat{\mu} = 0.509$, $\hat{K} = 0.529$
5	29.16	1485	1000	300	314	$\hat{\mu} = 0.532$, $\hat{K} = 0.544$
6	0	1485	15000	0	0	$\hat{\mu} = 0.652$, $\hat{K} = 1.097$
7	6.694	1485	15000	1000	69.9	$\hat{\mu} = 0.602$, $\hat{K} = 1.028$
8	6.694	1485	15000	10000	699	$\hat{\mu} = 0.735$
<i>GRF 4</i> ($\phi = 8.02\%$)						
9	0	0	0.0001	0	- (dry)	$\hat{\mu} = 0.754$, $\hat{K} = 0.695$
10	0	1485	1000	0	0	$\hat{\mu} = 0.759$, $\hat{K} = 0.757$
11	29.16	1485	1000	300	2892	$\hat{\mu} = 0.764$, $\hat{K} = 0.763$
12	0	1485	15000	0	0	$\hat{\mu} = 0.776$, $\hat{K} = 1.005$
13	6.694	1485	15000	1000	643	$\hat{\mu} = 0.770$, $\hat{K} = 0.986$
14	6.694	1485	15000	10000	6427	$\hat{\mu} = 0.851$
<i>GRF 5</i> ($\phi = 21.6\%$)						
15	0	0	0.0001	0	- (dry)	$\hat{\mu} = 0.344$, $\hat{K} = 0.272$
16	0	1485	15000	0	0	$\hat{\mu} = 0.410$, $\hat{K} = 1.058$
17	437.4	1485	15000	1000	88.4	$\hat{\mu} = 0.440$, $\hat{K} = 0.992$

4.2 Viscous versus non-viscous pore fluid

In experiments No. 4,5,10 and 11 (Table 2) we consider effective elastic moduli of GRF3 and GRF4 saturated with a non-viscous and a Newtonian fluid of normal density ($\rho_{fluid} = 1000 kg/m^3$). However, the theoretical differences of the low- and the high-frequency limit of Biot are in these cases not significant enough to clarify unambiguously if the Biot effect is visible in the synthetics (exact formulae can be found e.g. in [9]). This change significantly if we use a fluid with an artificially high density ($\rho_{fluid} = 15000 kg/m^3$):

- Using a non-viscous high-density fluid for pore saturation [experiment 6,12 and 16 of Table (2)] we consider the high frequency limit of Biot ($\Rightarrow$ viscosity $\eta = 0$; hence, the reference frequency f_{biot} can be determined for our rock-models with a non-zero permeability κ using $f_{biot} = \phi\eta/(2\pi\rho_{fluid}\kappa)$ as zero; see e.g. [9]). This enables us to estimate the corresponding tortuosity of the rock models [see Fig. (3) and [14] for details].

- Using a high-density Newtonian fluid with a viscosity of $\eta = 1000 \text{ kg}/(\text{ms})$ for pore saturation [experiment 7,13, and 17 of Table (2)] we consider the low frequency limit of Biot because the dominant frequency of the propagating wave [$f_{\text{source}} = 8 \times 10^4 \text{ Hz}$] is clear below the Biot reference frequency. We observe a reduction of the effective elastic moduli towards the theoretical predicted low-frequency limit of Biot (i.e. Gassmann; derived from the dry case) in comparison to experiment 6,12 and 16. This is shown in Fig. 3 for the effective bulk modulus.

The interpretation of this result is as follows: The seismic effect of the Biot theory is clearly visible in our numerical wave propagation experiments.

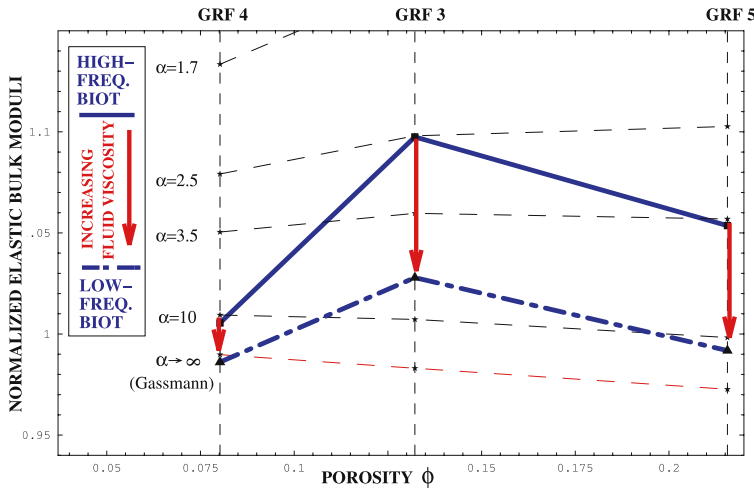


Fig. 3. The normalized effective bulk modulus ($\langle K \rangle / K_{\text{grain}}$) versus porosity for GRF 3,4 and 5 saturated with a non-viscous (thick solid line) and a Newtonian [$\eta = 1000 \text{ kg}/(\text{ms})$; dash-dotted thick line] fluid of artificially high density ($\rho_{\text{fluid}} = 15000 \text{ kg}/\text{m}^3$). The dashed lines display the high frequency limit of the Biot theory calculated from $\langle K_{\text{dry}} \rangle$ using different values for the tortuosity α .

However, we have fixed three physical reasons why we still observe some numerical deviations from Biot's predictions (i.e. for GRF 3 and 5 the observed low-frequency value is not consistent with Gassmann; see Fig. 3):

- The unknown influence of Squirt. The critical frequency of this flow as well as the amount of soft porosity is very difficult to estimate for our used models (for details see [9]).
- The relatively high velocity of shear waves (most significant for experiment 8 and 14) in the fluid ($v_s = \sqrt{i\omega\eta_{\text{fluid}}/\rho_{\text{fluid}}}$) is not included in Biot and Squirt theories; this effect can be roughly estimated by analysing the upper Hashin-Sthrikmann bound (e.g. [9]) using $\mu_{\text{fluid}} = v_s^2 \rho_{\text{fluid}}$ and $\omega = \omega_{\text{source}}$ (see Table 2).

- Local anisotropy in overall isotropic heterogeneous porous media (for details see [2])

Conclusions

In this paper we perform finite-difference simulations on micro-scale to study the effect of viscous Biot-coupling on wave propagation. We implement a generalized Maxwell body [4, 7] into a displacement-stress rotated staggered grid scheme with the result that all viscous parameters are located in the centre of an elementary cell. Using this technique it is possible to saturate synthetic rock models with realistic approximations of Newtonian fluids. This allows us to study all coupling mechanism of fluid-solid interaction which are covered by the elastodynamic wave equation. To estimate the reference frequency for the Biot approach we also determine the permeabilities of our digital rock samples by flow simulations. This gives us the possibility to compare mechanical and transport properties derived for exact the same digital rock samples. The wave propagation experiments in those highly heterogeneous media saturated with viscous fluids indicate that the velocity estimations of the Biot theory are visible in our numerical results.

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Plateness of the Oceanic Lithosphere and the Thermal Evolution of the Earth's Mantle

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Summary. Compared to [33], the model of the thermal evolution of the Earth's mantle is considerably improved. The temporal development of the radial viscosity profile due to cooling of the Earth could substantially be taken into account by numerical progress using a new variant of the temperature- and pressure-dependence of the shear viscosity of the mantle, namely Eq (5). The laterally averaged heat flow, the Urey number, the Rayleigh number and the volume-averaged temperature as a function of time come up to the expectations that stem from the parameterized evolution models. The mentioned evolution parameters of the present paper better approximate the observational data. Contrary to the parameterized curves, these quantities show temporal variations. This seems to be more realistic for geological reasons. Due to the activation enthalpy, the presented viscosity profile has a highly viscous transition layer (TL) with steep viscosity gradients at the phase boundaries. A low-viscosity zone is situated above and below the TL, each. The lithosphere moves piecewise en bloc. Thin cold sheet-like downwellings have an Earth-like distribution.

1 Introduction

The present dynamical model of the Earth's mantle *simultaneously* generates good self-consistent plateness of the oceanic lithosphere and a proper approximation of general thermal evolution parameters as a function of time. This second point of view is often treated by another kind of models. In these parameterized models, the creeping-velocity and the temperature fields are not computed in detail but taken into consideration in the energy balance only by a relation between Nusselt number, Nu , and Rayleigh number, Ra . According to Schubert et al. (1979, 1980), the energy conservation can be expressed in a simplified way:

$$M \cdot c \cdot \frac{\partial \bar{T}}{\partial t} = M \cdot H_0 \cdot e^{-\lambda t} - \frac{A \cdot k \cdot (\bar{T} - T_0)}{d} \cdot \left(\frac{Ra}{Ra_{cr}} \right)^\beta \quad (1)$$

where M is the mass of the Earth's mantle, c is its specific heat, $\bar{T}$ is the volume-averaged mantle temperature, t is the time, H_0 is the specific radiogenic heat production rate at the beginning of the evolution, λ is a generalized decay constant, k is the thermal conductivity, d is the thickness of the mantle, T_0 is the fixed surface temperature, Ra_{cr} is the critical Rayleigh number, A and β are constants. There are different planetary heat transport mechanisms since, due to the dependence of the viscosity on temperature and volatiles, different regimes develop near the surface: mobile regime, plate-tectonic regime and stagnant-lid regime. Separate Nu - Ra parameterizations for each mode have been derived by Solomatov (1995) and Reese et al. (1998, 1999). In the present paper, however, we solve the full set of the equations of mass, momentum and energy in a viscous compressible spherical shell with yield stress. For the special form of the equations see Chapter 3.2 by Walzer et al. (2003a). For the implementation of the yield stress see Walzer et al. (2004a). All equations have been simultaneously solved at 1351746 nodes of the mantle grid for each time step of the 4.49×10^9 years of the mantle evolution. So, the computed evolution starts at a time when the chemical differentiation of the Earth's core was certainly finished. Some runs were made with 10649730 nodes to check

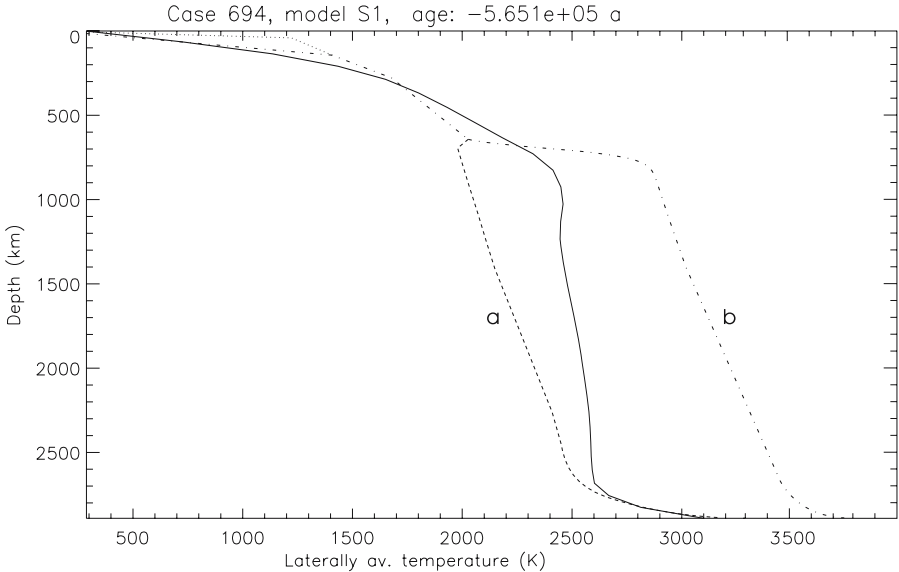


Fig. 1. The solid curve denotes the laterally averaged temperature of the geological present time for the reference run of this paper with $\sigma_y = 135 \text{ MPa}$. The CMB temperature, T_c , is spacially constant but variable in time according to the heat balance of the Earth's core. The range of possible mantle geotherms according to Schubert et al. (2001) is shown for comparison. Label *a* and *b* refer to geotherms of whole-mantle and partially layered convection, respectively. The dotted line represents the ridge geotherm.

the convergence. The focus of this paper is to compare the temporal development of global thermal numbers with those of parameterized models, e.g. Schubert et al. (2001), and to show the general planform of the convection. So, the second main task of this paper is to show the self-consistent generation of oceanic lithospheric plates with Earth-like distribution of the subduction zones. Other authors made other numerical experiments with some kinds of constitutive equations to produce subducting plates, e.g. pseudoplastic yielding, strain weakening (Tackley, 2000a, 2000b), self-lubrication and viscoplastic yielding (Bercovici, 1998; Moresi and Solomatov, 1998; Richards et al., 2001). Trompert and Hansen (1998) used a strongly temperature-dependent viscosity with yield stress and found episodic plate-like motion with long time spans with a stagnant lid. Auth et al. (2003) used 2-D simulations with temperature- and damage-dependent viscosity. In dependence on the damage source term, they found four different convective regimes. The plate-like regime is characterized by focused low-viscosity bands, homogeneous surface velocities, and asymmetric subduction of the slab. Funiciello et al. (2003) used 2-D numerical experiments to investigate how rheology influences slab dynamics and slab-mantle interaction. Regenauer-Lieb and Yuen (2003) studied the slab mechanisms in connection with shear localization and mylonitic shear zones. Morra and Regenauer-Lieb (2004) presented an approach to solve the prob-

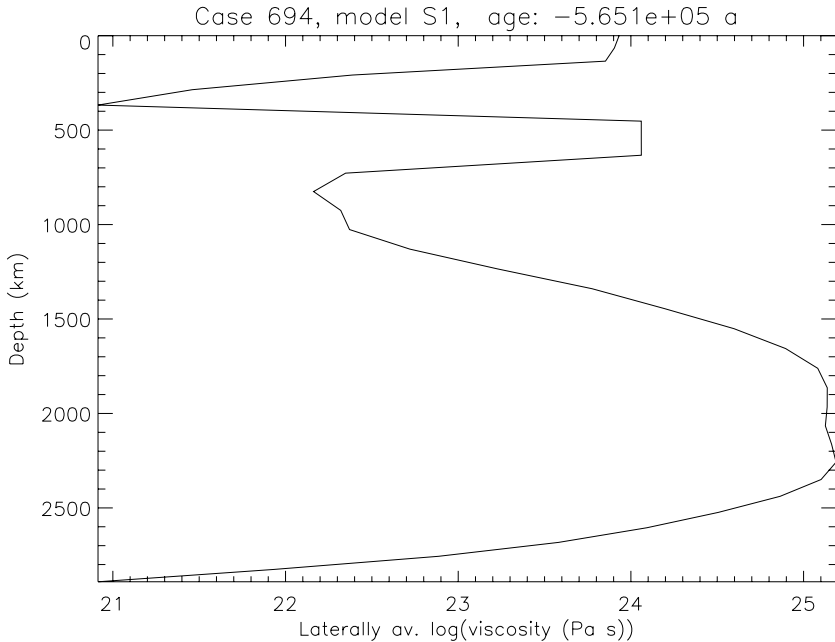


Fig. 2. The laterally averaged viscosity of the reference run for the geological present.

lem of a cold subducting slab into a hot fluid-like mantle. For this purpose, they join the Boundary Element Method and the Finite Element Method. It is evident that the latter three papers cannot be used in our code because of the demanded grid-point density. – In addition, the rheology of the subduction zones has been investigated in considerably more details. Karato et al. (2001) incorporated grain-size, stress, temperature and pressure dependence of the rheology. They studied diffusional creep, dislocation creep and the Peierls mechanism of the relevant minerals and found that the rheological structure of the slab varies laterally and with depth. For the deep slab, they found a weak, fine-grained spinel region wrapped up in a narrow but strong skin. Further details of the mineralogy of the subducting lithospheric slab are given by Weidner et al. (2001) and Bina et al. (2001). At present it is not possible to incorporate these findings in detail into our model because of lack of computing time.

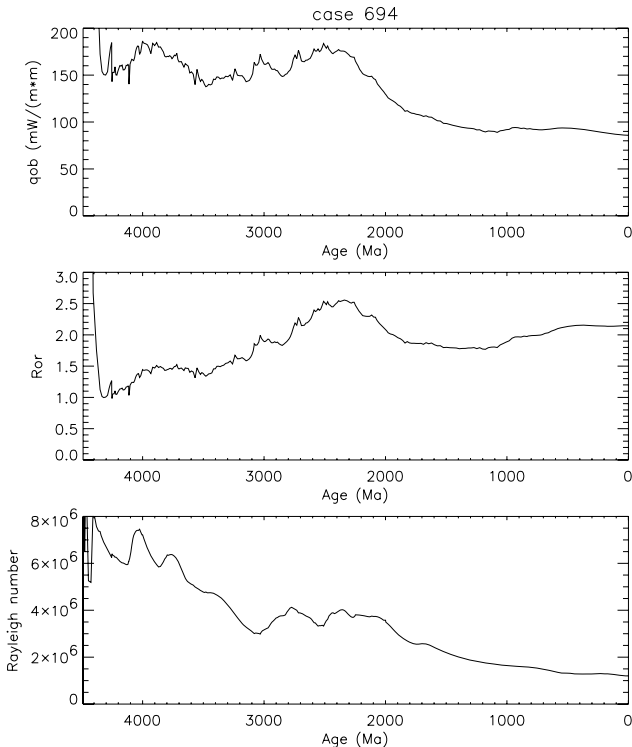


Fig. 3. The evolution of the laterally averaged surface heat flow, q_{ob} , of the ratio of the surface heat outflow per unit time to mantle's radiogenic heat production per unit time, R_{or} , and of the Rayleigh number, Ra .

Stein et al. (2004) explored the self-consistent formation of plates in a 3-D Cartesian box model. For temperature- and stress-dependent rheology, they obtained plates. But the plate motion only exists during short intervals followed by long time spans of an immobile lid. However, adding the pressure dependence of the viscosity and of the thermal expansivity, they found a continuous plate motion and a low-viscosity zone. They varied the parameters and found that plate-like behavior is restricted to a narrow window of parameters.

2 The model

Walzer et al. (2003b, 2004a, 2004b) found the self-consistent formation of slabs and continuous plate motion in a 3-D spherical-shell model. We used a viscous model supplemented by a viscoplastic yield stress, σ_y , for the uppermost 285 km of the mantle. In this upper zone, an effective viscosity, η_{eff} ,

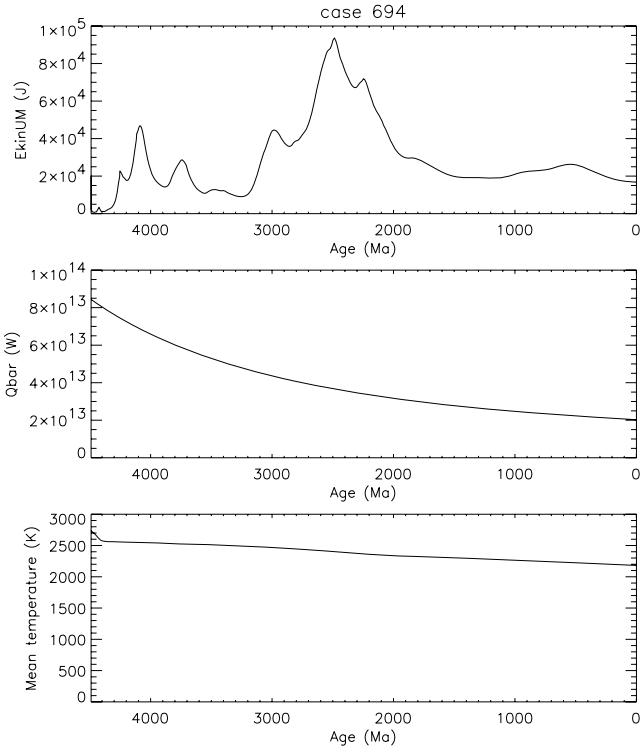


Fig. 4. The evolution of the kinetic energy of upper-mantle convection, E_{kinUM} , the power of the internal heat generation of the mantle, $\bar{Q}$, and the volume-averaged mean temperature of the mantle.

was implemented

$$\eta_{eff} = \min \left[\eta(P, T), \frac{\sigma_y}{2\dot{\epsilon}} \right] \quad (2)$$

and used instead of the shear viscosity, η . The second invariant of the strain-rate tensor is denoted by $\dot{\epsilon}$, P is the pressure, T is the temperature. In [32, 33], the parameters have been varied and a central Rayleigh-number–yield-stress range with continuous plate-like motion was found. However, we use an infinite Prandtl number fluid in a compressible spherical shell. This shell is heated from within by a homogeneous distribution of the major heat-producing elements with the abundances of the primordial mantle according to McCulloch and Bennett (1994). Therefore, the heating power decreases as a function of time. We [31] parameterized the pressure, P , density, ρ , bulk modulus, K , and dK/dP using a Birch-Murnaghan equation of state and PREM (Dziewonski and Anderson, 1981). So, using the Vashchenko-Zubarev (1963) gamma, we are able to directly derive the Grüneisen parameter, γ , from seismic observations. Introducing an experimental thermal expansivity, α , that decreases with increasing pressure, we [31] obtained also the specific heat at constant pressure, c_p , and the specific heat at constant volume, c_v , as a function of depth. We derived a viscosity profile with considerable viscosity gradients at the upper and lower boundaries of the transition layer. We could use it only in [32, 33, 34] and in the present paper because of improvements of the numerics. In [31] only an approximation was applied. The mentioned steep viscosity gradients are caused by jumps of the activation volume, V^* , and of the activation energy, E^* , at the mineral phase boundaries. A second way to derive the radial dependence of the viscosity is to compute the melting temperature, T_m , by Gilvarry's (1956) formulation of Lindemann's law and by

$$\eta = \eta_0 \cdot \exp \left(\frac{k_2 T_m}{T} \right) \quad (3)$$

The direct use of Eq (3) generates big numerical difficulties because of steep viscosity gradients. Therefore, the following approximation of Eq (3) was introduced in [33]:

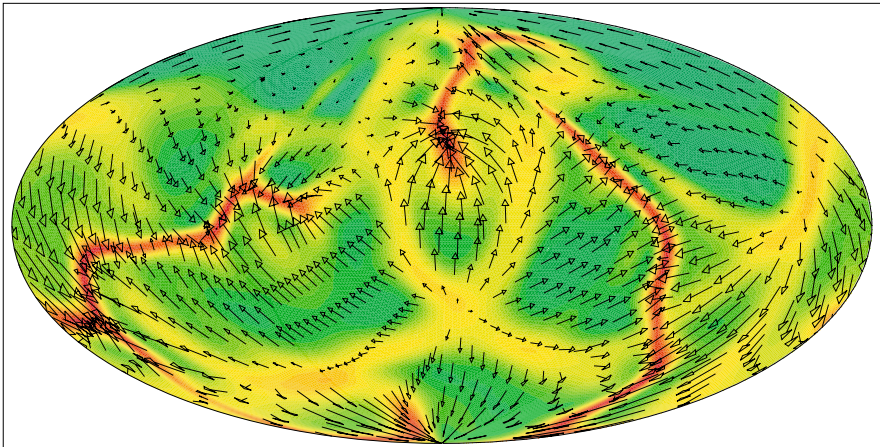
$$\eta(r, \theta, \phi, t) = 10^{r_n} \cdot \eta_3(r) \cdot \exp \left[c_t \cdot T_m(r) \cdot \left(\frac{1}{T(r, \theta, \phi, t)} - \frac{1}{T_{av}(r, t)} \right) \right] \quad (4)$$

where T_{av} is the laterally averaged temperature, r the radius, θ the colatitude, ϕ the longitude, t the time, c_t a constant and r_n the viscosity-level parameter. The quantity r_n is zero for Eq (3). It serves only for the shift of the viscosity profile during the variation of the parameters. Up to now, we had ignored the temporal dependence of η_3 . This fact misrepresented the thermal evolution behavior of the model whereas the general circulation, the generation and distribution of the oceanic lithospheric plates and of the subduction zones showed a good Earth-like behavior. Due to improvements of the code, we are

able to replace Eq (4) by

$$\eta = 10^{r_n} \cdot \frac{\exp(c \overline{T_m/T_{av}})}{\exp(c \overline{T_m/T_{st}})} \cdot \eta_3(r) \cdot \exp \left[c_t \cdot T_m \left(\frac{1}{T} - \frac{1}{T_{av}} \right) \right] \quad (5)$$

in this paper. The bar denotes the radial average, T_{st} the initial temperature profile. By Eq (5), the viscosity profile has rising values with the cooling of the Earth. So, the real thermal evolution is better reflected by the present model than in [33]: The increasing average viscosity of the cooling mantle is essentially taken into account without loss of plateness and other successful features of the previous model. For MgSiO_3 perovskite we should insert $c = 14$, for MgO wüstite $c = 10$ according to Yamazaki and Karato (2001). So, the lower-mantle c should be between 10 and 14. However, for numerical reasons we can use only $c = 7$. The lateral variability of viscosity is described only by the fourth factor of the right-hand side of Eq (5). For the present reference run, we take $c_t = 1$, $r_n = -0.6$ and $\sigma_y = 135 \text{ MPa}$.



Case 694

Tcmb Var. B eta3 ys=135 MPa

Depth = 0.000e+00 km

Time = 4.491e+09 a Age = -5.652e-01 Ma

Max vel = 1.407e+00 cm/a Av hor vel = 6.916e-01 cm/a

log visc (Pa s)

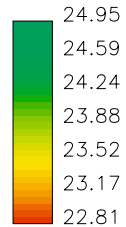


Fig. 5. The surface distribution of log viscosity for a yield stress, σ_y , of 135 MPa. The creeping velocities (arrows) show a good plate-tectonic behavior. Elongated high strain-rate zones have reduced viscosity due to plastic yielding.

3 Results

We anticipate that the features of the presented solution apply for a wider range of the values of temporally averaged Rayleigh number and yield stress. Fig. 1 presents the laterally averaged temperature profile of the geological present. As expected, $T_{av}(r)$ is nearer to the parameterized profile, a , for whole-mantle convection since this kind of convection is hindered by the high-viscosity transition layer of the model but not prevented. The present T_{av} curve lies nearer to the curve a than the corresponding curves of Fig. 3 of [33], mainly in the lower region of the lower mantle since the second factor of Eq (5) allows a stronger, and therefore more realistic, cooling of the mantle. The sharp bend of the T_{av} curve of Fig. 1 reminds one of the scheme of the plate-tectonics isotherm in Fig. 2.1 of Breuer (2003), although the cause of the sharp bend there stems from the thermal lithosphere.

Figure 2 shows the characteristic present-day viscosity profile of the present paper. A highly viscous lithosphere is on top as expected. Below of it, is an asthenosphere. The low-viscosity region of it corresponds to the Haskell (1935) value. New features of this profile are a high-viscosity transition layer with steep viscosity gradients at the boundaries. The latter fact is in contrast with [31]. Further new features are a second low-viscosity layer below the 660-km phase boundary, considerably high viscosity in the thick middle part of the lower mantle with good opportunities to preserve primordial chemical inhomogeneities in that region and a strong decrease of the viscosity down to the D'' layer. We found similar features in our earlier papers but the numerical values of the extreme viscosity values vary. Cf. Table 1.

Table 1. The extreme values of different viscosity profiles of the reference runs

Paper	[32]	[34]	[35], first part	[35], second part	this paper
Figure	1	4	6, fourth panel	15	2
$\sigma_y(MPa)$	∞	135	∞	135	135
Dimensions	3-D	3-D	2-D	3-D	3-D
max log $\eta_{av}(Pa\ s)$					
of lithosphere	22.68	23.71	25.2	23.71	23.92
min log $\eta_{av}(Pa\ s)$					
of asthenosphere	21.0	20.56	20.1	20.56	20.92
max log $\eta_{av}(Pa\ s)$					
of TL	23.7	23.7	25.5	23.7	24.5
max log $\eta_{av}(Pa\ s)$					
of LM	24.6	24.9	24.7	24.9	25.2

Figures 3 and 4 present essential improvements in the model of thermal evolution in comparison with earlier papers. In [31], i.e. the model without yield stress, σ_y , and without plates, the laterally averaged heat flow, qob , decreases as a function of time to $73.98\ mW/m^2$ for the reference run, to values

somewhat below the observed values also for the other runs. In [33], i.e. a model with σ_y and with plates, qob decreases only since an age of $\tau \approx 2400\text{ Ma}$ only very slightly down to 104.4 mW/m^2 that lies above the observed value. However, the first panel of Fig. 3 of this paper shows that, starting with very high values, qob strongly decreases with some temporal variations in the Archean and the Proterozoic down to 85.86 mW/m^2 now. The observed present-day qob is 82 mW/m^2 . This behavior is well matched to parameterized models, e.g. by McGovern and Schubert (1989). According to the design, no temporal variations are possible in parameterized models. But geology teaches that variations are realistic.

The reciprocal value, Ror , of the Urey number of [31] increases during the first half of the Earth's evolution and is nearly constant in the second half. [33] is characterized by continuous rise of Ror during the whole Earth's history. According to parameterized models (see McGovern and Schubert (1989) and Schubert et al.(2001), p. 603), a strong decrease of Ror is to be expected for the earliest history and a gradual rise of Ror in the big rest of the evolution.

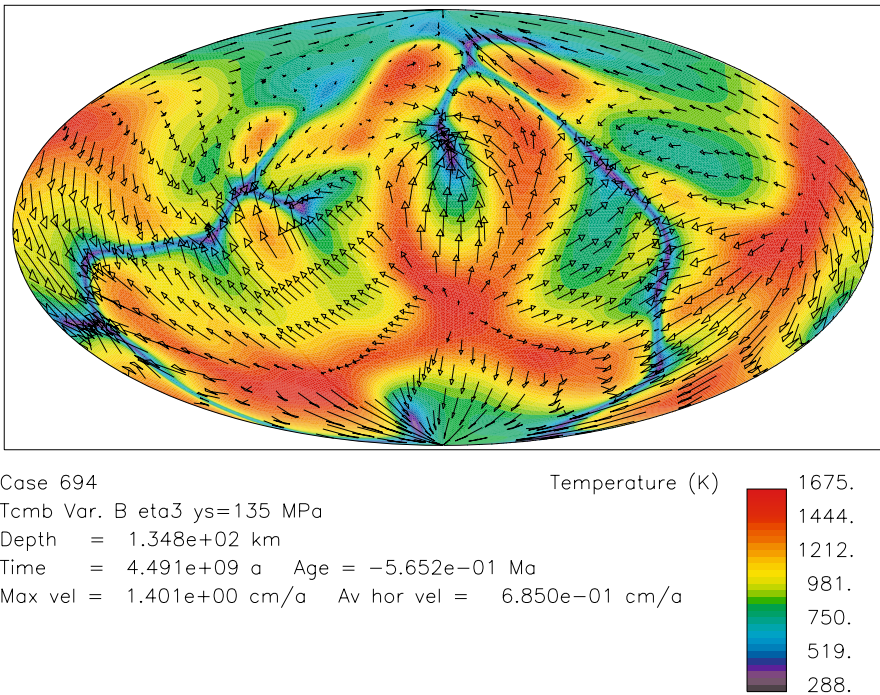


Fig. 6. Temperature distribution (colors) and creeping velocities (arrows) of our reference run for the geological present, for 134.8 km depth and $\sigma_y = 135\text{ MPa}$. The narrow blue downwelling zones can be pursued in the deeper equal-area projections of temperature distribution. The “slabs” are rather narrow in comparison with the broad upwelling zones.

The second panel of Fig. 3 shows that our Ror sharply diminishes at the very beginning, but than Ror gradually increases with some temporal variations. Stacey and Stacey (1999) derived an averaged value of 1.85 for Ror of the last 2000 Ma . We arrive at about 2.00, that is somewhat too high. In summary, $Ror(\tau)$ of this paper seems to be more realistic than that of [31] and [33].

The Rayleigh number, Ra , decreases also in [31] and [33] but essentially less than demanded by parameterized models. The first panel of Fig. 3 presents now an considerably stronger decrease of Ra . The real magnitude of Ra cannot be reached for numerical reasons as in dynamical calculations of other workers, too. So the present model reflects rather well not only plateness and subduction but also the thermal evolution. For numerical reasons, the model is stiffer than the real Earth.

The kinetic energy of the upper mantle, E_{kinUM} , can be considered as a measure of the power transmission to the oceanic lithospheric plates. The first panel of Fig. 4 presents a pronounced maximum at the turn from Archaic to Proterozoic, at $\tau = 2500$ Ma . The radiogenic heating from within of the mantle non-linearly decreases as a function of time. That is depicted in the second panel of Fig. 4. – Although the volume-averaged temperature, T_{mean} , grows down as a function of time in [31], it is somewhat to low.

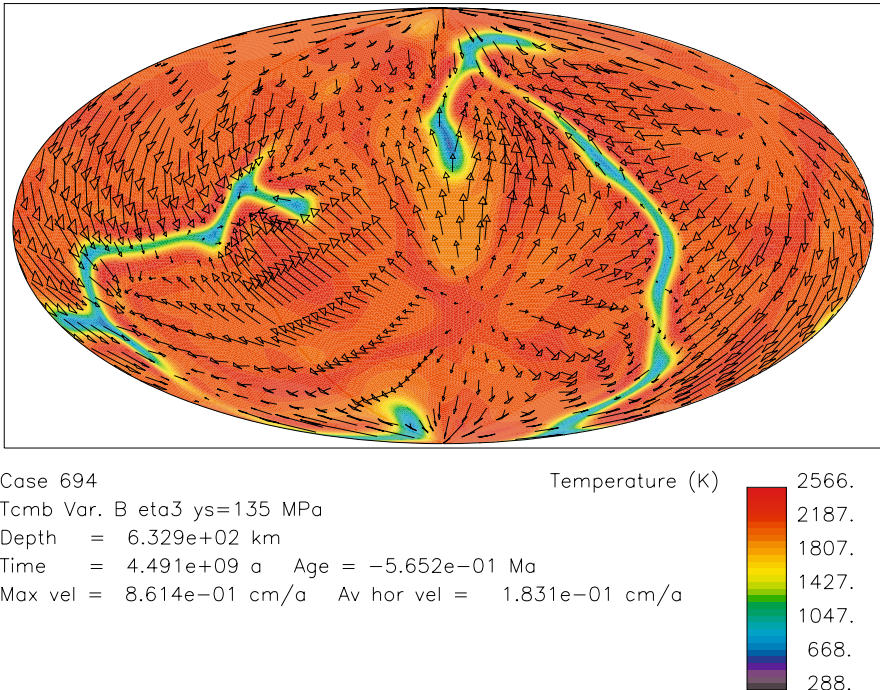


Fig. 7. Temperature distribution and creeping velocities for 632.9 km depth.

In [33], however, T_{mean} is higher but at first it rises slowly until an age of $\tau = 3000 Ma$ is reached. From this time, it decreases until the present time but much less steeply than expected by parameterized models. The third panel of Fig. 4, however, shows that, at first, T_{mean} decreases stronger, then moderately grows down until the present time. T_{mean} descends by $400 K$ during the last $4000 Ma$. These values correspond to the results of komatiite research. Parameterized models give similar results.

Figure 5 reveals that pieces of the surface move with spatially constant angular velocity. So, they flow plate-like. Only relatively small boundary areas don't fit in this simplified picture. But also on the real Earth, some plate boundaries are somewhat extended (Gordon 2000). So, Fig. 5 seems to be rather realistic apart from the missing continents. In our next paper, we want to include the evolution of continents by chemical differentiation. Already [32] and [33], we found plate-like solutions near the Earth's surface. In [31], however, the upwelling currents show star-shaped, divergent flow lines at the surface. That behavior is well-known from purely viscous models.

Figure 6 depicts an equal-area plot of the temperature distribution (colors) and the creeping velocities (arrows) for the geological present in $134.8 km$ depth. The distribution of the arrows reminds one of the plate-tectonic picture of the surface, yet. The downwelling areas are very sharp lines compared with the broad upflow areas. The distribution of this slab-like features is Earth-like and not reticular as in [31], yet. But also [31] was characterized by a very small thickness of the cold sheet-like downwellings. In [33] and Fig. 6, however, we have an Earth-like distribution of thin cold sheet-like downwellings.

Figure 7 shows the temperature and velocity distribution in $632.9 km$ depth, in the transition layer, yet. As in all upper spherical surfaces, the solid creeps toward the slab-like features. Figure 8 is the first shown picture of this kind that is situated in the lower mantle: The cold downwellings are somewhat more diffusely distributed. The material begins to flow divergently away from the cold zone. Figure 9 demonstrates that the mentioned tendencies of Fig. 8 are stronger in $1864 km$ depth. Although the cold zone is at the expected place, yet, its distribution is rather broad as it is observed in the continuations of the slabs in the real lower mantle.

4 Numerical and computational aspects

We solved the system of differential equations of convection in a compressional spherical shell in the special form of [31] and [33] using a three-dimensional finite-element discretization, a fast multigrid solver and the second-order Runge-Kutta procedure. The mesh is generated by projection of a regular icosahedron onto a sphere to divide the spherical surface into 20 spherical triangles or 10 spherical diamonds. A dyadic mesh refinement procedure connects the mid-points of each side of a triangle with a great circle such that each triangle is subdivided into four smaller triangles. Successive grid refinements

produce an almost uniform triangular discretization of the spherical surface of the desired resolution. Corresponding mesh points of spherical surfaces at different depths are connected by radial lines. The radial distribution of the different spherical-surface triangular networks is so that the volumes of the cells are nearly equal. More details are given by Baumgardner (1983, 1985), Bunge et al. (1997) and Yang (1997). For the most runs, we employed a mesh with 1351746 nodes. Some runs were made with 10649730 nodes to check the convergence of the lower resolution runs. The result is that the laterally averaged heat flow, the ratio of heat outflow to radiogenic heat production, the Rayleigh number, and the Nusselt number as functions of time show hardly discernable differences. The calculations were performed on 32 processors of a Cray Strider Opteron cluster. A scalability test showed a scaling degree of nearly 90%. The code was benchmarked for constant viscosity convection by Bunge et al. (1997) with numerical results of Glatzmaier (1988) for Nusselt numbers, peak temperatures, and peak velocities. A good agreement was found. – The conclusions are condensed in the summary.

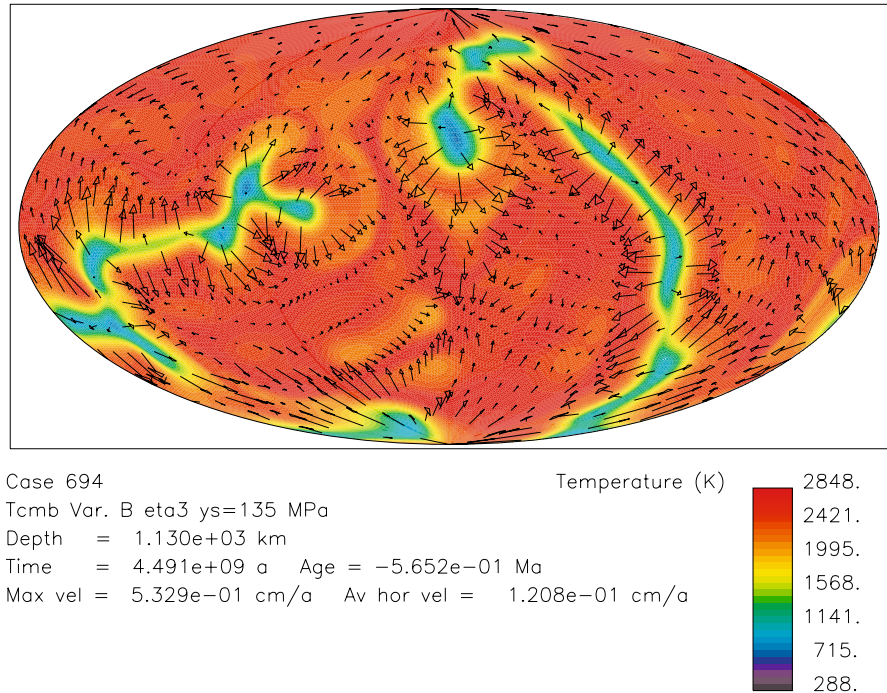


Fig. 8. Temperature distribution and creeping velocities for 1130 km depth.

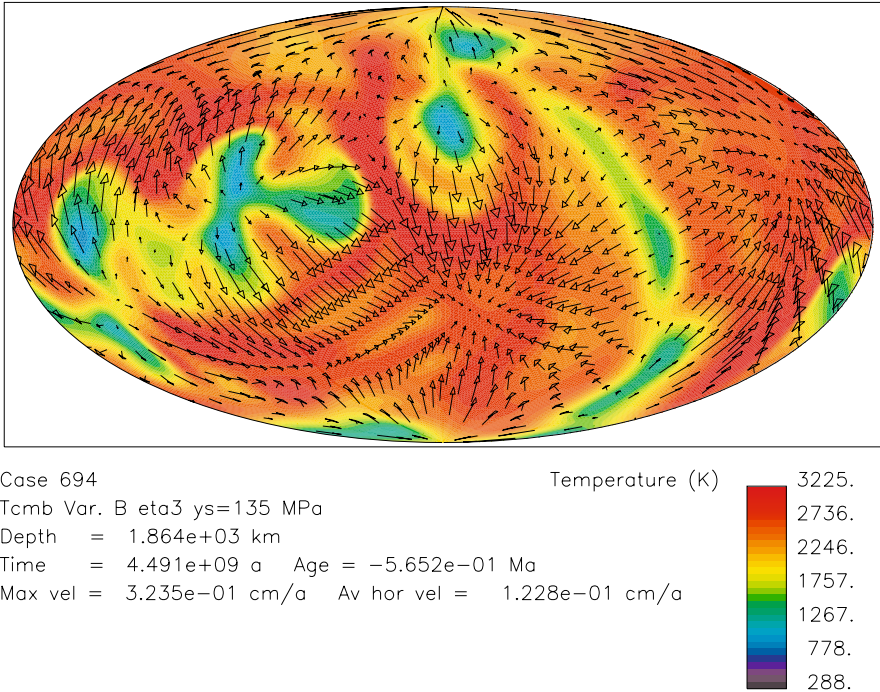


Fig. 9. Temperature distribution and creeping velocities for 1864 km depth.

Acknowledgements

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Use of High Performance Computing in Gravity Field Research

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Summary. In the light of the three geoscientific satellite missions CHAMP, GRACE and GOCE the overall scientific aim is to achieve an automatism for the recovery of the Earth's gravity field respectively the physical shape of the Earth, namely the geoid. Furthermore, an improved understanding of the spatial and temporal variations of the geoid is of great benefit for the study of the dynamics of the Earth's lithosphere and upper mantle, global sea level variations, ocean circulation and ocean mass and heat transport, ice mass balance, the global water cycle and the interaction of these phenomena. This involves the determination of up to a hundred thousand unknown coefficients of the corresponding series expansion model from data sets which amount to several millions of observations provided by the satellites. The resulting system of equations which has to be solved for such an analysis cannot be evaluated without simplistic assumptions or within a satisfying time frame on personal computers due to hardware limitations. Consequently this challenging problem has to be tackled by means of high performance computing strategies. Only adoption of parallel programming standards such as MPI or OpenMP in conjunction with highly efficient numerical libraries allows for successfully accomplishing the demands of gravity field analysis. Indeed, the huge amount of data provided by satellite sensors, together with a high-resolution gravity field modeling, requires the determination of several ten thousands of unknown parameters and leads to the assignment that this problem is a true "challenge of calculus".

1 Field of Research – Introductory Remarks

In the last three decades, geosciences have developed an ever-growing interest in a detailed modeling of the Earth's static and time-variable gravity field to meet the current requirements of geoscientific research but also to stimulate economic progress in technological applications. For gravity modeling on a global scale, this can only be achieved by satellite-geodetic methods. Fortunately, at present we are in the favourable situation that some dedicated satellite missions for gravity field recovery are already operational or in the process of due realization.

1.1 Global Geodetic Satellite Missions – CHAMP, GRACE, GOCE

In July 2000 the CHAMP (CHALLENGING Minisatellite Payload) satellite [GFZ00] has been launched successfully in orbit. Being now more than four years in operational mode the satellite's lifetime is estimated to end in 2008. The CHAMP mission was developed and realized by the German Aerospace Center (DLR) and the GeoForschungsZentrum (GFZ) Potsdam. Its mission objectives range in magnetic field recovery, atmospheric and ionospheric profiling and gravity field recovery. In this contribution we concentrate exclusively on the latter one: the recovery of the gravity field of the Earth using satellite observations. There is an enormous interest in various geoscientific communities concerning the mission products such as in Geodesy, Geophysics, Oceanography and Meteorology. Last but not least this wide spectrum of applications contributes to the great success of contemporary satellite geodesy, which becomes manifested in international media reports and conference programs. The principle of CHAMP-type gravity field recovery is as follows. An on-board Global Positioning System (GPS) receiver tracks the satellite semi-continuously, being almost in free fall around the Earth. At the same time, non-conservative forces acting on the satellite surface are measured by on-board accelerometry. The time series in GPS satellite positions, which can be determined without the help of prior gravity models, is referred to as kinematic orbit. Such orbits have been released to the geodetic community for CHAMP already, and will be computed for following missions. The deviations of the real satellite orbit from a nominal Kepler orbit allow for modeling the anomalous gravity field, induced by the inhomogeneous mass distribution of the Earth. But due to its rapid motion in space (about 8 km/s), the satellite's positioning accuracy is limited to some centimeters. In terms of gravity field recovery this leads to a rather moderate resolution covering the long-wavelength part. In consequence, only the static gravity field is observable using kinematic orbit analysis. The achievable orbit accuracy does not allow detecting time-varying gravity phenomena such as caused by geophysical fluid movement like e.g. continental water storage variations.

To resolve time-variability of the gravity field of the Earth, the GRACE (Gravity Recovery And Climate Experiment) mission [JPL99] was initiated by cooperation of the DLR and the National Aeronautics and Space Administration (NASA). Since March 2002 GRACE is in orbit for at least five years of duration. This twin-satellite mission is composed of two CHAMP-type spacecrafts. One satellite follows his companion in the same orbit (that is why the two satellites are called Tom and Jerry in the media). Like with CHAMP, both spacecrafts are tracked by GPS. In addition, their relative motion is measured precisely by a high sensitive microwave link. Relative variations in range and range-rate reflect the inhomogeneity of the Earth's mass distribution. The analysis of the relative motion allows the resolution of the long-wavelength part of the gravity field with a much higher accuracy as possible

using kinematic orbit analysis only. Time-variable gravity field variations can be detected by analyzing a series of monthly static solutions. Since August 2004, science data is released to the public.

The ESA satellite GOCE (Gravity field and steady-state Ocean Circulation Explorer) [ESA99] is scheduled to be launched in autumn 2006 and to remain 20 months in orbit. Its lifetime is limited by the low satellite altitude (≈ 250 km, CHAMP and GRACE ≈ 450 km), which guarantees an ultra-high sensitivity with regard to the gravity field of the Earth. The prior benefit of GOCE will be the recovery and modeling of the medium- to short-wavelength part of the static terrestrial gravity field, which is not covered by the missions presented above. Its objectives are thus complementary to those of CHAMP and GRACE. To meet this challenge, besides orbit tracking with GPS the technique of three-dimensional satellite gravity gradiometry (SGG) will be realized for the first time. This means, differential acceleration measurements using six accelerometer test masses in a diamond configuration will be analyzed.

1.2 Impact on Earth Sciences

The knowledge of the Earth's gravity field with respect to both high accuracy and high resolution is of fundamental interest for a multitude of scientific communities. Geophysicists, e.g., need this information to constrain realistic density models of the Earth's interior, which in turn allows an improved understanding of the Earth's interior dynamics. In combination with satellite altimetry (measuring the sea surface topography) oceanographers determine the temporal and causal changes in water mass transport by analyzing absolute geostrophic currents, which have a significant influence on local and global climatic phenomena. Monitoring and predicting global sea level variation is another key indicator to assess whether there exists global warming or not. Glaciology examines post-glacial land-uplift movements. Typical geodetic applications deal with the unification of height systems, nivellement with GPS, orbit determination and inertial navigation. Pre-CHAMP satellite-only gravity models (e.g. GRIM5-S1) reflect the long-wavelength static part with a resolution of 500 km (half wavelength) and an accuracy of a few decimeters in terms of geoid heights. Due to innovative techniques such as GPS tracking, intersatellite links, accelerometry and SGG, state-of-the-art satellite geodesy is aiming to provide static gravity field information with an accuracy of 2 cm resolving spatial features down to 70 km in near future. In addition, time-variable phenomena caused by geophysical fluid movements will be detectable. Figure 1 illustrates not only phenomena discussed here but also displays many other examples for physical processes which manifest themselves as changes in the gravity field of the Earth or geoid variations.

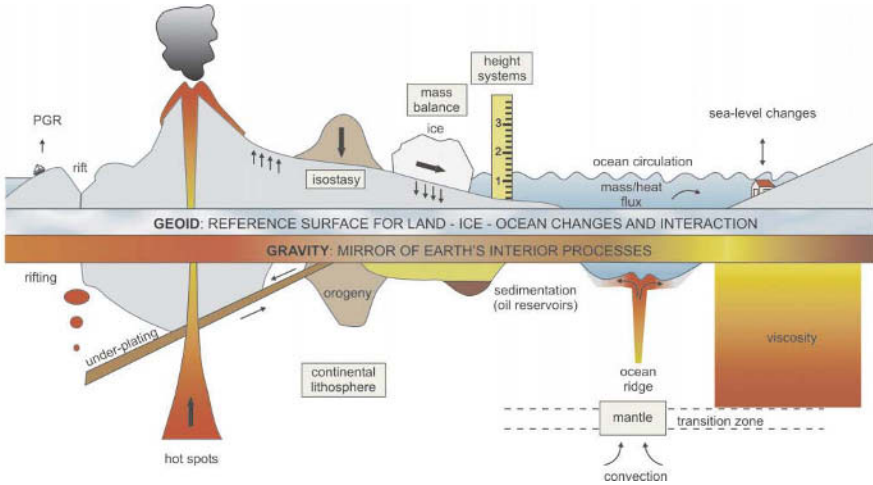


Fig. 1. Geophysical phenomena affecting the geoid (GOCE Project Office, Munich)

1.3 Benefit of High Performance Computing for Satellite Geodesy

Satellite geodesy as a non-typical discipline for high performance computing (HPC) is concerned with the modeling of the terrestrial gravity field based on observation data from space. In the past however, satellite data has been relatively sparse (mainly based on laser observations) and the resolution has been limited. But with the new technologies and new analysis strategies at hand, one has to deal with the fact to resolve many unknown parameters and to process large amounts of data records collected by the satellites during their operation mode. To give an example up to 100 000 unknown parameters required to describe a mathematical model of the terrestrial gravity field have to be estimated by least squares techniques from satellite observations provided by low Earth orbiting GPS tracked satellites such as CHAMP, GRACE or GOCE. On the other hand, to fully assess the problem dimension mission lifetimes and data sampling rates have to be considered. E.g., the GRACE mission with its design lifetime of 5-7 years and a data sampling rate of 5 s will collect up to 40-50 millions of observations. The GOCE mission, with an even higher sampling rate, will deliver in a one-year observation phase approximately twice the number of observations. Therefore, it can be stated that one has to deal with a new challenge arising from the computational point of view. Only the use of high performance computing can overcome this challenge. In future, follow-on satellite missions will be realized for an even more detailed modeling of the gravity field. Thus, we can be confident that satellite geodesy will find its established position regarding HPC in the near future.

2 Gravity Field Parameter Estimation

In the context of gravity field recovery as outlined in the last section we focus on the CHAMP mission principle. As seen before, the positions of the CHAMP spacecraft in space are deduced from GPS measurements between the low orbiting CHAMP satellite and the high flying GPS satellites. This so-called high-low satellite-to-satellite tracking (hl-SST) observation scenario has been chosen here to exemplify the use of HPC technologies for geodetic applications. The achievements made within the scope of this case study for CHAMP can be transferred to the analysis of GRACE and GOCE observation data as well.

In physical geodesy in first order approximation the Earth is considered as a sphere with symmetric mass distribution. In reality this is not true. The shape of the Earth is a very irregular surface and the masses are not distributed uniformly at all. To develop a mathematical model for this anomalous behavior potential theory is applied. Accordingly, the physical shape of the Earth is defined as a special equipotential surface of its gravity field, referred to as the geoid. Its scalar counterpart (if Earth rotation is neglected), namely the terrestrial gravitational potential $U(\lambda, \varphi, r)$, is harmonic outside the gravitation inducing masses, i.e. the Laplace equation (1) holds for each point (λ, φ, r) in the outer space of the Earth, parameterized in spherical coordinates.

$$\Delta U(\lambda, \varphi, r) = \frac{\partial^2 U}{\partial r^2} + \frac{2}{r} \frac{\partial U}{\partial r} + \frac{1}{r^2} \frac{\partial^2 U}{\partial \varphi^2} + \frac{\tan \varphi}{r^2} \frac{\partial U}{\partial \varphi} + \frac{1}{r^2 \cos^2 \varphi} \frac{\partial^2 U}{\partial \lambda^2} = 0 \quad (1)$$

Solving (1) by means of the separation approach yields the terrestrial potential $U(\lambda, \varphi, r)$ in terms of a spherical harmonics series expansion (2), consisting of the attenuation factor $(R/r)^{l+1}$ and the orthonormal base functions $e_{lm}(\lambda, \varphi)$ (3), with the normalized Legendre functions of the first kind $\bar{P}_{lm}(\sin \varphi)$.

$$U(\lambda, \varphi, r) = \frac{GM}{R} \sum_{l=0}^{\infty} \sum_{m=-l}^l \left(\frac{R}{r}\right)^{l+1} e_{lm}(\lambda, \varphi) u_{lm} \quad (2)$$

$$e_{lm}(\lambda, \varphi) = \begin{cases} \bar{P}_{lm}(\sin \varphi) \cos m\lambda & 0 \leq m \leq l \\ \bar{P}_{l|m|}(\sin \varphi) \sin |m|\lambda & -l \leq m < 0 \end{cases} \quad (3)$$

Equation (2) constitutes a typical model of the Earth's gravitational potential. The double sum expression can be understood as a two-dimensional Fourier expansion. In theory an infinite series is necessary to fully characterize the gravitational field, but practically the double sum is truncated at a maximum degree $l_{\max}$ determined by the observation principle of the satellite mission and the desired resolution of the field. Both the geocentric constant GM and the mean Earth radius R are fixed. The Stokes coefficients u_{lm} are unknown parameters, describing the deviation of the terrestrial gravitational potential from its first order spherical approximation. Their estimation can be performed best by globally distributed observation data such as provided by CHAMP. The spacecrafts' orbit is tracked continuously by GPS. Considering the CHAMP satellite free falling around the Earth, the observation

equation can be formulated quite simple. According to (4) the acceleration of the satellite (reduced by all disturbing effects such as tidal forces) is equal to the terrestrial attraction, namely the gradient of the Earth's gravitational potential. The gradient operator in spherical coordinates is given in (5).

$$\frac{d^2}{dt^2}\mathbf{x}(t) = \ddot{\mathbf{x}}(t) = \text{grad } U(\lambda, \varphi, r) \quad (4)$$

$$\text{grad}_{(\lambda, \varphi, r)} = \mathbf{e}_r \frac{\partial}{\partial r} + \mathbf{e}_\lambda \frac{1}{r \cos \varphi} \frac{\partial}{\partial \lambda} + \mathbf{e}_\varphi \frac{1}{r} \frac{\partial}{\partial \varphi} \quad (5)$$

Numerical differentiation techniques provide satellite accelerations $\ddot{\mathbf{x}}(t)$ derived from the observed position information $\mathbf{x}(t)$ [RAG03]. From the numerical point of view (4) constitutes a linear system of equations (6) with the unknown parameter vector $\mathbf{x}$, the vector of observations $\mathbf{y}$ and the design matrix $\mathbf{A}$ describing the functional relationship between them. CHAMP allows for recovering the terrestrial gravitational field in the so-called long-wavelength part, namely up to degree and order $l_{\max} \approx 70$ of its series expansion. This equals to about 5000 unknown parameters to be estimated in a least squares adjustment procedure. The L_2 -norm minimization of (6) leads to the normal equation system, as outlined in (7), for an unbiased estimate $\hat{\mathbf{x}}$ of the unknowns.

$$\mathbf{A}\mathbf{x} = \mathbf{y} \quad (6)$$

$$\mathbf{A}^T \mathbf{A} \hat{\mathbf{x}} = \mathbf{A}^T \mathbf{y} \leftrightarrow \mathbf{N} \hat{\mathbf{x}} = \mathbf{b} \quad (7)$$

$$\mathbf{N} = \mathbf{A}_1^T \mathbf{A}_1 + \dots + \mathbf{A}_j^T \mathbf{A}_j = \sum_{i=1}^j \mathbf{A}_i^T \mathbf{A}_i = \sum_{i=1}^j \mathbf{N}_i \quad (8)$$

For the direct inversion of (7), e.g. by Cholesky decomposition, at least one triangle of the symmetric normal matrix $\mathbf{N} := \mathbf{A}^T \mathbf{A}$ has to be kept in the memory. The setup of $\mathbf{N}$ itself can be achieved by blockwise computation. This is shown in (8), where the dimension k of each block $i = 1, 2, \dots, j$ is small compared to the dimension of $\mathbf{N}$. Table 1 shows the memory requirement for normal matrix storage dependent on the truncation of the series expansion according to (2). The number of unknowns increases approximately quadratic with higher resolution. Whereas the demands for CHAMP data processing with regard to memory availability is nowadays covered by ordinary personal computers (PCs), this doesn't hold for GRACE and especially GOCE data analysis. For the latter, $l_{\max} \approx 300$ holds.

We refer to the direct inversion of (7) as brute-force approach (BFA). Alternatively we implemented an iterative algorithm for solving (6), namely the LSQR algorithm according to [PS82a], [PS82b] and [BA05], a Krylov subspace method, such as the widely used conjugate gradient (CG) methods, cf. [HS52]. Least squares adjustment is performed iteratively by successive QR decomposition of a bidiagonal subproblem of (6) representing the original minimization problem. Furthermore, normal matrix preconditioning is applied

Table 1. memory requirement for normal matrix storage

resolution $l_{\max}$	number of unknowns	memory requirement for $\mathbf{N}$ (MByte)
50	2598	27
70	5038	101
100	10198	416
200	40398	6500
300	90598	33000

to increase the speed of convergence of LSQR considerably. For more details on the technique of preconditioning see e.g. [PS82b], [Ben99], [JHS03] and [BA05]. We denote the LSQR method in its preconditioned version as PC-LSQR. Independent on memory requirements the processing of millions of data with the methods presented can only be performed within a reasonable time frame by using HPC platforms.

3 Results

Within the scope of this contribution we aim to compare the direct BFA and the iterative PC-LSQR method for solving the system of equations associated with the gravity field parameter estimation process and categorize their suitability with respect to different platform architectures. For both solvers parallel implementations with OpenMP and MPI were realized, which allows for the use of the BFA and PC-LSQR on any of the following HLRS platforms: (i) NEC AzusA (ii) NEC TX-7 (iii) NEC SX-6 (iv) Cray Strider. The architecture of platforms (i) and (ii) is ccNUMA, i.e. similar to shared-memory systems. Platform (iii) is, considering only one node, a shared-memory array processor system. Platform (iv) is in principle (disregarding that each single node is in fact a SMP node of 2 CPUs) a distributed-memory cluster. In summary it can be ascertained that we investigated the suitability of the BFA and PC-LSQR for three different architectures: (i) shared-memory (ii) (shared-memory) array processor (iii) distributed-memory.

3.1 Parallelization of the BFA and PC-LSQR

With regard to the BFA setup of the design matrix $\mathbf{A}$ and computation of the normal matrix $\mathbf{N}$ is done blockwise according to (8). This approach is indispensable, given that for a large amount of observations and many unknowns the design matrix can not be kept in the main memory. Indeed, a blockwise procedure even allows for the use of parallel matrix-matrix and matrix-vector routines provided by numerical libraries such as e.g. INTEL MKL to repeatedly compute $\mathbf{N}_i = \mathbf{A}_i^T \mathbf{A}_i$. Additional parallelization is achieved for the setup of each design matrix block $\mathbf{A}_i$ by distributing the observations contributing

to each block to several central processing units (CPUs).

Due to the character of the PC-LSQR method, matrix-matrix and matrix-vector multiplications are avoided by means of repeated vector-vector operations. Since neither the design matrix nor the normal matrix must be kept in the main memory, storage requirements are by far smaller as compared to direct solvers at the expense of an increased number of floating point operations (FLOPs). Fortunately, these multiplications can be done separately for each observation. Additionally, the major computational costs occur within the setup of the design matrix. It is therefore reasonable, as addressed before, to distribute the observations on several CPUs of a multiprocessor computation platform to set up the design matrix line by line, each line referring to a different observation in time.

3.2 Effect of Parallelization

For the evaluation of the parallelization of the BFA and PC-LSQR as outlined in the section before several calculations have been executed on the NEC TX-7 platform. For the BFA gravity field recovery up to degree and order $l_{\max} = 100$ and for PC-LSQR up to degree and order $l_{\max} = 50$ has been performed based on half a million of observations. Table 2 summarizes the runtime results for the BFA, Table 3 the results for PC-LSQR. For the use of up to eight CPUs

Table 2. BFA: effect of parallelization

number of CPUs	wall time (min)	user time (min)
1	639	639
2	300	596
4	149	595
8	76	606
12	53	638
15	48	710

Table 3. PC-LSQR: effect of parallelization

number of CPUs	wall time (min)	user time (min)
1	79	79
2	41	81
4	21	83
8	11	83
12	7	84
15	9	86

a linear scaling can be achieved; the doubling of CPUs results in a bisection of the wall time. When using more than eight CPUs this doesn't hold anymore. This is also detectable in an increased user time measurement. For PC-LSQR even a deceleration from 12 to 15 CPUs turns out. Maybe this is justified in the increased effort for administration and synchronization of the threads. Finally, the performance of parallelization when using both OpenMP and MPI

Table 4. BFA: runtime dependent on number of nodes

number of nodes	wall time (min)
1	50
2	26
4	13
6	9

on a cluster architecture has been investigated. Runtime measurements based on the BFA ($l_{\max} = 50$, half a million of observations) on the Cray Strider cluster are listed in Table 4. Here as well nearly linear scaling is achieved using different numbers of processing nodes. The effort for MPI communication is small.

3.3 Influence of Problem Dimension

In this section we want to assess for both methodologies the impact of different problem dimensions, i.e. recovering the gravity field with increased resolutions. As already listed in Table 1 doubling the maximum degree of resolution $l_{\max}$ is equivalent to solving a system with about four times the number of unknowns.

Influence of Problem Dimension – BFA

Table 5 presents results for various resolutions $l_{\max}$. The computations are based on half a million of observations and are achieved using eight CPUs of the NEC TX-7 platform. Two facts can be pointed out. The time required to compute the inverse of the normal matrix is negligible in comparison to the overall runtime. Secondly, considering an increase of the maximal resolution by a factor of two, respectively an increase of the unknowns by a factor of approximately four, the overall runtime increases even by a factor more than ten. The reason is that the involved design matrices not only enlarge in their number of elements but also the effort to generate a single matrix entry increases considerably. Furthermore, within the course of these studies it turned out that it is not possible to solve problems with resolutions higher than $l_{\max} = 200$. The reason is that the INTEL MKL library uses (so far) 32 bit integers and the number of normal matrix elements exceeds the maximum number which can be represented with 32 bit integers and therefore not all matrix elements can be addressed.

Table 5. BFA: effect of problem dimension on runtime

resolution $l_{\max}$	wall time (min)	user time (min)	time for inversion (sec)
20	1	5	1
50	7	54	2
70	20	156	7
100	78	620	30
150	352	2805	302
200	1120	8686	1304

Influence of Problem Dimension – PC-LSQR

Table 6 provides the results for the iterative method. Computations are performed on the NEC AsuzA with 12 CPUs and 0.5 million observations. It can be stated that an increasing problem dimension results in a higher number of necessary iterations associated with an increased computational effort per iteration. The reason for the last result ($l_{\max} = 100$) exhibiting an extraordinary increase in the number of iterations and respectively in the overall runtime is, that the normal matrix preconditioner represents the simplest but also non-optimal preconditioner.

Table 6. PC-LSQR: effect of problem dimension on runtime

resolution $l_{\max}$	wall time (min)	user time (min)	number of iterations
20	3	34	11
50	18	206	12
70	49	573	22
100	736	8512	274

3.4 Comparison of Different Computation Platforms

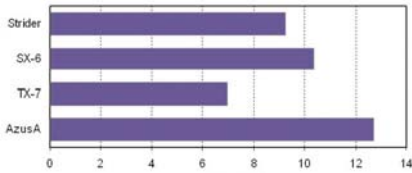
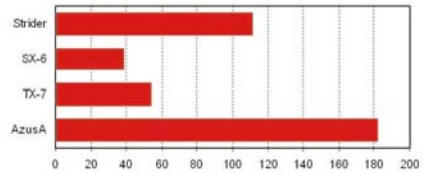
This section deals with comparison studies concerning the four computation platforms introduced at the beginning of this chapter, namely NEC AzusA, NEC TX-7, NEC SX-6 and Cray Strider. Since based on completely different techniques for normal equation inversion both the BFA and the PC-LSQR method are considered. They have been processed with the same problem dimension, namely half a million of observations are used to resolve the terrestrial gravitational field up to degree and order $l_{\max} = 50$. We focus on both the runtime and performance of the algorithms themselves as well as compared to one another dependent on the use of HPC. To come up with a fair comparability of the systems all computations have been performed with approximately the same theoretical peak performance as outlined in Table 7.

Table 7. Settings to achieve comparable theoretical peak performance (TPP)

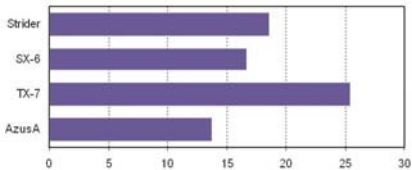
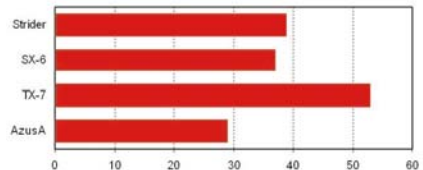
platform	number of CPUs	TPP of one CPU (GFlops)	TPP (GFlops)
NEC AzusA	15	3.2	48
NEC TX-7	8	6	48
NEC SX-6	5	9	45
Cray Strider	6x2	4	48

Comparison of Different Computation Platforms – BFA

The runtime results for the BFA are displayed in the Figs. 2 and 3. The user time for Cray Strider is extrapolated since the `time` command only provides the wall time but not the user time. Figures 4 and 5 illustrate the real performance achieved for the implementation. The platforms AzusA and TX-7

**Fig. 2.** BFA: wall time (min)**Fig. 3.** BFA: user time (min)

have comparable hardware designs, differing mainly in the type of processors (AzusA: Itanium1 - 800 MHz, TX-7: Itanium2 - 1.5 GHz). Obviously, the Itanium2 CPU is by far more efficient. It exploits its huge L3-cache of 6 MByte. Additionally, with an amount of 15 CPUs the hardware limit of the AzusA is almost reached. It turned out that optimal scaling using OpenMP can only be obtained up to eight CPUs (see Sect. 3.2). Probably a comparison study

**Fig. 4.** BFA: performance (GFlops)**Fig. 5.** BFA: efficiency (%)

with a lower theoretical peak performance, i.e. the use of less CPUs, would decrease the discrepancy between the two systems. The SX-6 is more than three minutes slower than the TX-7 and only achieves an efficiency of 37%.

This is surprising since vectorization of the program should increase the performance significantly. Actually, the efficiency of the platform is decreased by comparatively time-consuming data reading. The time for real computations is about seven minutes which corresponds to a performance of 24.6 GFlops, respectively an efficiency of 55%. This is still disappointing but due to the moderate problem dimension. To proof that, an additional calculation has been performed on the SX-6 with a resolution up to $l_{\max} = 100$ for the terrestrial gravitational potential. The impact of vectorization is obviously since the efficiency amounts to 88% which is near to the theoretical peak performance. Thus, the array processor system SX-6 is suited very well for the BFA. Finally, the results for the Opteron cluster Cray Strider range in between the ones of AzusaA and TX-7. This has been expected in advance since compared to the TX-7 the cache of the Opteron CPUs is considerably smaller. Additionally, runtime costs for the communication between the cluster nodes by using MPI has to be accepted.

Comparison of Different Computation Platforms – PC-LSQR

The results for PC-LSQR regarding runtime and performance are displayed in the Figs. 6 to 9. Again the user time for the Cray Strider is extrapolated based on the wall time measurements. For PC-LSQR the results for the

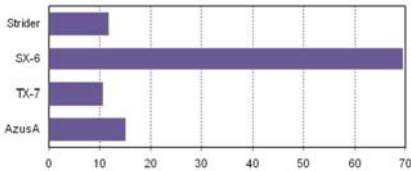


Fig. 6. PC-LSQR: wall time (min)

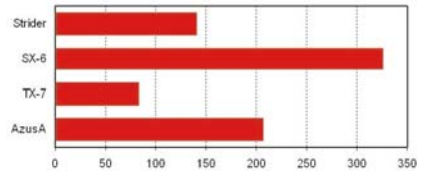
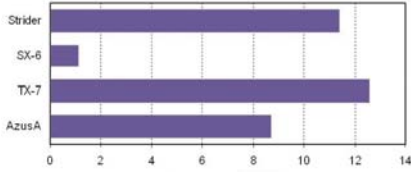
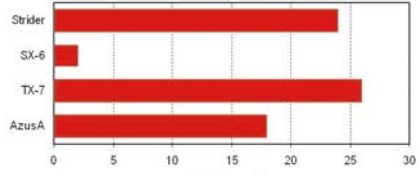


Fig. 7. PC-LSQR: user time (min)

AzusaA and TX-7 don't differ that dramatic than for the BFA. This is due to the principle of the iterative LSQR solver. Matrix-matrix respectively matrix-vector operations are replaced by repeated vector-vector operations of small dimension. Thus, the Itanium2 CPUs can't utilize their advantages, mainly with regard to their large cache. Handling with small vectors, combined with repeated operations from iteration to iteration, the SX-6 is not suited at all for PC-LSQR. Vectorization of the algorithm is nearly not possible. Therefore, the SX-6 performs very bad. The behavior is totally different for the Cray Strider. It performs only a bit worse than the TX-7. Additionally, the time for MPI communication between the nodes is marginal. Have in mind that the TX-7 is limited to 16 CPUs but cluster systems generally come up with a large number of processing nodes. This means, PC-LSQR is well suited for cluster systems such as the Cray Strider.

**Fig. 8.** PC-LSQR: performance (GF1.)**Fig. 9.** PC-LSQR: efficiency (%)

Final Remarks

As seen in Sect. 3.2 for both the BFA and PC-LSQR we achieved a very good scaling when using different numbers of CPUs for calculation. In contrast to that the performance of the BFA is by far better than that one of PC-LSQR. The computational effort for algebraic computations in case of the BFA is entirely accomplished by the use of numerical libraries based on the Lapack standard. Predominately routines for matrix-matrix and matrix-vector multiplications as well as for normal equation inversion are applied. These routines are optimized for parallel use. In contrast to that, the PC-LSQR method is composed of a lot individual calculation steps, each of them has to be repeated for each iteration of the iterative process. That means, only a part of the algorithm can be treated by optimized numerical libraries. Thus, the performance achieved for PC-LSQR is clearly minor than that one for the BFA.

4 Conclusions and Outlook

We investigated the use of HPC for terrestrial gravity field recovery based on satellite observations as provided by CHAMP, GRACE and GOCE. Concentrating on the CHAMP-like mission design we successfully parallelized the analysis procedure, namely based on the brute-force approach (BFA) for direct normal matrix inversion and the iterative preconditioned LSQR (PC-LSQR) method. Parallelization with OpenMP resulted in linear runtime scaling up to the use of eight CPUs. Further, optimal scaling (for a manageable number of processing nodes) was also achieved with MPI programming. Concerning the problem size, namely the dimension of the normal matrix, the BFA for terrestrial gravity field processing is limited so far to a resolution of about $l_{\max} = 200$ when using the INTEL MKL library since it is restricted to 32 bit integers. In terms of PC-LSQR, problems as a consequence of using a non-optimal preconditioning technique occurred for field resolutions beyond degree and order 70. This is at present under further investigation. In fact, preconditioning on the level of the design matrix promises remedy. With respect to vectorization it can be stated that depending on the problem dimension the BFA is well suited for array processors. This doesn't hold for PC-LSQR. For the latter one cluster systems turned out to be perform very well. A higher

level of efficiency and performance for the BFA than for PC-LSQR is clearly observable which is due to the efficient usage of optimized numerical libraries for algebraic operations. Based on the promising experiences and first results achieved using HPC techniques we have now the opportunity to concentrate on large dimensional problems arising with studies on GRACE and GOCE data analysis. This issue will be addressed in the near future.

Acknowledgments

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Molecular Modeling of Hydrogen Bonding Fluids

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1 Introduction

Reliable modeling of vapour-liquid equilibria of pure components and mixtures is essential for many tasks in process engineering. Conventional approaches to model vapour-liquid equilibria of pure components and mixtures with empirical equations of state or lattice-based G^E -models yield in many cases excellent correlations, but often lack in predictive power, especially when the available experimental database for the adjustment of binary parameters is narrow. These models are well developed but hold only little promise for further improvements. Molecular modeling and simulation is a promising route to a more reliable description and prediction of thermophysical properties of pure components and mixtures.

2 Pure Component Molecular Models

New Lennard-Jones based molecular models for ethanol [SVH05], ammonia [SEV05] and water [Der05] were developed. These models account for the hydrogen bonding and the polarity of the molecules by using point charges. In the following, the molecular models and the pure component results are described.

2.1 Ethanol

A new ethanol model was developed with the aim to give accurate vapor-liquid equilibria with low computational and programming effort. It neglects the internal degrees of freedom and uses nuclei off-center Lennard-Jones united atoms for the methyl, methylene and hydroxyl group, accounting for repulsion and dispersion. Point charges are located on the methylene and hydroxyl Lennard-Jones centers, as well as on the nucleus position of the hydroxyl

hydrogen. The Coulombic interactions account for both polarity and hydrogen bonding.

The molecular interaction and geometry of the resulting model is described in the following. The potential energy u_{ij} between two ethanol molecules i and j is given by

$$u_{ij}(r_{ijab}) = \sum_{a=1}^4 \sum_{b=1}^4 4\epsilon_{ab} \left[\left(\frac{\sigma_{ab}}{r_{ijab}} \right)^{12} - \left(\frac{\sigma_{ab}}{r_{ijab}} \right)^6 \right] + \frac{q_{ia}q_{jb}}{4\pi\epsilon_0 r_{ijab}}, \quad (1)$$

where a is the site index of molecule i and b the site index of molecule j , respectively. The site-site distance between molecules i and j is denoted r_{ijab} . σ_{ab} , ϵ_{ab} are the Lennard-Jones size and energy parameters, q_{ia} and q_{jb} are the point charges located at the sites a and b on the molecules i and j , respectively. Finally, ϵ_0 is the permittivity of vacuum. The interaction between unlike Lennard-Jones sites of two ethanol molecules is defined by the Lorentz-Berthelot combining rules

$$\sigma_{ab} = \frac{\sigma_{aa} + \sigma_{bb}}{2}, \quad (2)$$

$$\epsilon_{ab} = \sqrt{\epsilon_{aa}\epsilon_{bb}}. \quad (3)$$

In the following, a few remarks on the model development are given. Jorgensen's investigations on the potential of the internal rotation about the carbon-oxygen bond in an ethanol monomer [Jor81] yield three energetic extremal values in the corresponding configurations: the absolute minimum is reached in the trans configuration, the 0.64 kcal/mol higher local minimum in the gauche configuration and the 2.06 kcal/mol (above trans) higher absolute maximum in the cis configuration. For the present rigid ethanol model, the energetically most likely trans configuration has been chosen. The nuclei positions of all ethanol atoms were computed using the quantum chemistry software package GAMESS (US) [SBB93]. The basis set 6-31G and the Hartree-Fock method were applied for geometry optimization.

Starting from these positions, for the methyl and methylene group the AUA4 parameters of Ungerer et al. [UBD00] were applied. The AUA4 parameters were optimized by Ungerer et al. for vapor-liquid equilibria of linear alkanes. Following the approach of Ungerer et al. [UBD00], a small offset of the Lennard-Jones hydroxyl center (0.1010 Å) in direction to the hydroxyl hydrogen nucleus was allowed for optimization. The five parameters of the hydroxyl group were fitted to yield optimal saturated liquid densities and vapor pressures. The parameters are the two point charges, the Lennard-Jones size and energy parameters as well as the offset of the hydroxyl Lennard-Jones center. These parameters were chosen since they model the strongly interacting hydrogen bond and since the methyl and methylene parameters were already optimized by Ungerer et al. [UBD00]. The point charge on the methylene center was set in such a manner to yield overall neutrality of the molecular model.

The proposed set of charges in the present work yields a resulting dipole moment of 2.47 D. Quantum chemistry calculations (Møller-Plesset level 2 with basis set aug-cc-pVTZ) in a cavity (COSMO with a dielectric constant $\epsilon_r = 25$) and in the vacuum yield dipole moments of 1.99 and 2.10 D, respectively. Note that the higher dipole moment of the molecular model than those from quantum chemistry calculations is not unusual for modeling hydrogen bonding molecules with point charges.

Pure substance vapor-liquid equilibria for the optimization of the ethanol model were calculated using the NpT +test particle method proposed by Möller and Fischer [MoF90]. To determine the residual chemical potential in the liquid phase with high accuracy, the Monte Carlo based gradual insertion method [VKH02] was used. For the residual chemical potential in the vapor phase, standard Monte Carlo simulations with Widom's test particle insertion [Wid63] proved to be sufficient. Simulation details are given in the Appendix.

Figure 1 depicts one of the vapor-liquid equilibria results including the TraPPE-UA simulation data taken from [CPS01]. The agreement between the new model and the experimental data is excellent, even better than that for the more complex and already very good TraPPE-UA ethanol model. The simulation results of the present ethanol model yield mean unsigned errors

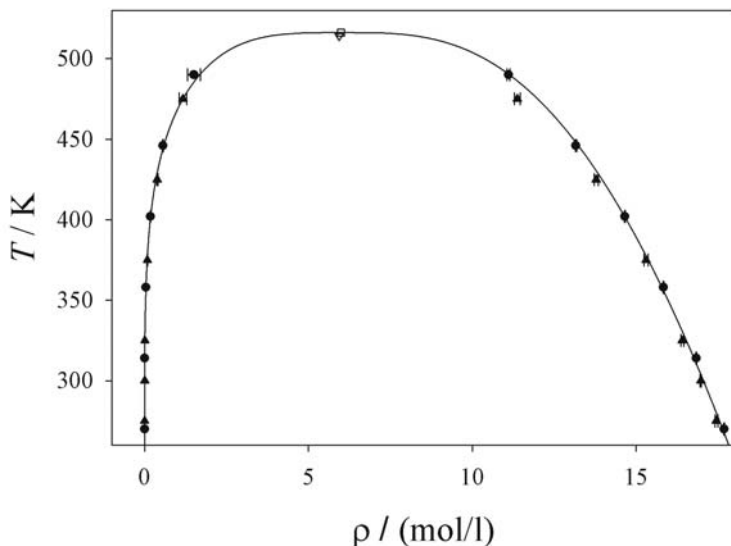


Fig. 1. Saturated densities of ethanol: filled bullet, present simulation; empty triangle down, critical point derived from simulated data; filled triangle up, TraPPE-UA simulation [CPS01]; line, experimental data [DaD84]; empty square, experimental critical point [DaD84].

compared to experimental data [DaD84] in vapor pressure, saturated liquid density and heat of vaporization of 3.7, 0.3, and 0.9 %, respectively, in the temperature range 270 to 490 K, which is about 55 to 95 % of the critical temperature. Following the procedure suggested by Lotfi et al. [LVF92], the critical temperature, density and pressure were determined. The results compare favorably to experimental data (numbers in parenthesis): $T_c = 514.12$ (516.25) K, $\rho_c = 5.94$ (5.99) mol/l and $p_c = 5.89$ (6.38) MPa. The TraPPE-UA molecular model for ethanol yields mean unsigned errors in vapor pressure, saturated liquid density and heat of vaporization of 8.4, 1.4, and 1.6 %, respectively. Critical temperature and density are quoted with $T_c = 514$ K and $\rho_c = 6.1$ mol/l [CPS01].

2.2 Ammonia

The new molecular model of ammonia [SEV05] was developed in a similar way as the ethanol model described in Sec. 2.1. It is also based on rigid Lennard-Jones and point charges sites. Starting with a first model whose nuclei positions and point charges were derived from quantum chemistry calculations and whose Lennard-Jones parameters were taken from the molecular model of Kristóf et al. [KVL99], the present molecular model was obtained by optimizing the point charges and the Lennard-Jones parameters. The quality

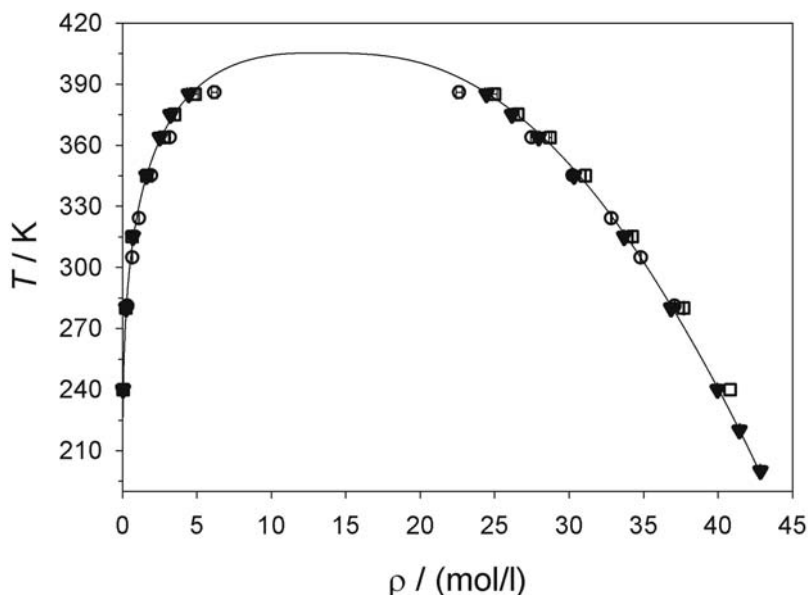


Fig. 2. Saturated densities of ammonia: empty bullet, Kristóf et al. [KVL99]; empty squared, starting model; filled triangle down, present model [SEV05]; line, experimental data [DaD84].

of the new ammonia model to describe thermophysical properties is in the same order of magnitude as from the new ethanol model. As an example, the saturated densities of the starting, present and Kristóf's ammonia molecular models together with experimental data are given in Fig. 2.

2.3 Water

Several molecular models for water based on Lennard-Jones and exponential-6 potentials, rigid and flexible point charges as well as point polarizabilities have been published. None of them describes thermophysical properties over a wide range of state points favorably. Starting from the molecular water model of Jorgensen et al. [JCM83], which uses Lennard-Jones sites and three off-center point charges, this model type was reparameterized [Der05]. The predictive power of the present model is overall not as accurate as the new molecular models of ethanol (Sec. 2.1) and ammonia (Sec. 2.2). However, it yields better results than the best molecular model describing vapor-liquid equilibria proposed by Errington and Panagiotopoulos [ErP98]. Figure 3 shows saturated densities of the new water model compared to the Errington and Panagiotopoulos molecular simulations as well as experimental data [DaD84].

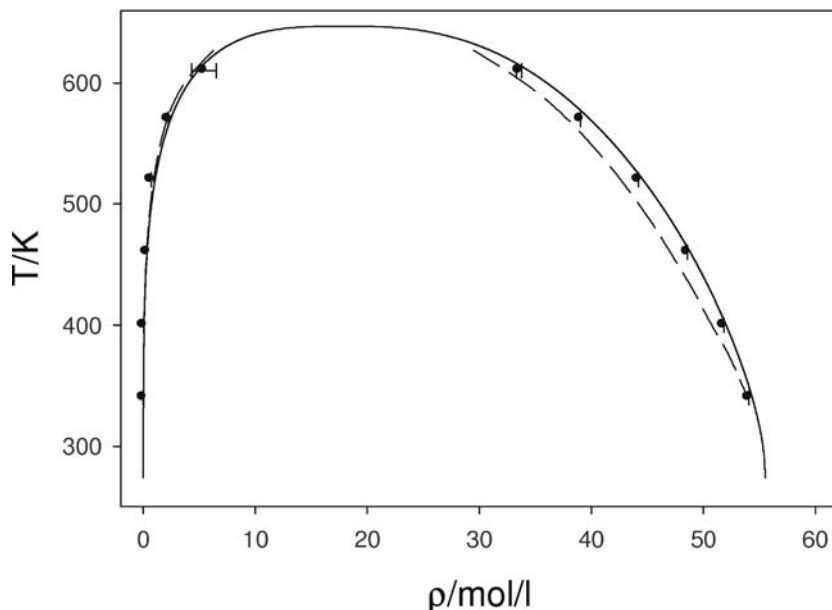


Fig. 3. Saturated densities of water: full bullet, present model [Der05]; dashed line, model of Errington and Panagiotopoulos [ErP98]; line, experimental data [DaD84].

3 Mixture Properties

Henry's law constants of the solutes methane, nitrogen, oxygen and carbon dioxide in the solvent ethanol are predicted by molecular simulation [SVH05].

3.1 Mixture Modeling

In molecular simulations of binary mixtures with pairwise additive potentials, three different interactions are present: two between molecules of the same component which are fully defined by the pure substance models and the unlike interaction between molecules of different kind. The unlike polar interactions were determined in a straightforward manner without using binary parameters. To define the unlike Lennard-Jones interactions between solvent and solutes methane, nitrogen, oxygen, and carbon dioxide, the modified Lorentz-Berthelot combining rules were used

$$\sigma_{ab} = \frac{\sigma_{aa} + \sigma_{bb}}{2}, \quad (4)$$

$$\epsilon_{ab} = \xi \cdot \sqrt{\epsilon_{aa}\epsilon_{bb}}, \quad (5)$$

where ξ is the binary interaction parameter which accounts for mixture effects.

In the “predictive mode”, the Henry's law constants were computed setting $\xi = 1$, cf. Equation (5).

Simulations of many binary mixtures [SVJ03, VSH05] have shown that the Lorentz-Berthelot combining rules ($\xi=1$) are too crude to predict the unlike Lennard-Jones energy parameter in an accurate way. Therefore, in the “adjusted mode”, ξ was fitted to one experimental Henry's law constant.

3.2 Determination of Henry's Law Constants

Several approaches have been proposed in the literature [MuG00, Sad97] to obtain Henry's law constants on the basis of molecular models. Henry's law constants are related to the residual chemical potential of the solute i at infinite dilution μ_i^∞ [SGL88]

$$H_i = \rho k_B T \exp(\mu_i^\infty / (k_B T)), \quad (6)$$

where k_B is the Boltzmann constant, T the temperature, ρ the density of the solvent.

In order to evaluate μ_i^∞ , molecular dynamics simulations applying Widom's test particle method [Wid63] are sufficient here. This is due to the fact, that the solute molecules are all smaller than ethanol molecules and so acceptable statistics can be achieved. Therefore, test particles representing the solute i were inserted after each time step at random positions into the liquid solvent and the potential energy between the solute test particle and

all solvent molecules ψ_i was calculated within the cut-off radius

$$\mu_i^\infty = k_B T \langle V \exp(\psi_i / (k_B T)) \rangle / \langle V \rangle, \quad (7)$$

where V is the volume and the brackets represent the NpT ensemble average.

The residual chemical potential at infinite dilution and hence, the Henry's law constant is directly attributed to the unlike solvent-solute interaction and indirectly to the solvent-solvent interaction which yields the configurations of the solvent molecules. In these configurations, the solvent test particles are inserted. The mole fraction of the solute in the solvent is exactly zero, as required for infinite dilution, since the test particles are instantly removed after the potential energy calculation. Simulations were performed at specified temperature and the according vapor pressure of pure ethanol.

3.3 Results

Henry's law constants of the four solutes methan, nitrogen, oxygen and carbon dioxide in ethanol were determined from simulation in the predictive mode at temperatures between 273 to 498 K with an increment of 25 K [SVH05]. For all four solutes, reliable experimental data on the Henry's law constants are available at around room temperature. Therefore, in the present work for all four solutes, the binary interaction parameter ξ of the modified Lorentz-Berthelot combining rule, cf. Equation (5), was adjusted to experimental data of the Henry's law constants at 298 K.

As an example, the simulation results of Henry's law constant of oxygen in ethanol for the predictive mode ($\xi = 1$) and the results with the adjusted ξ (descriptive mode) are compared together with experimental data in Fig. 4. Deviations between the predictive mode and the experimental data are mostly within 10 %.

The examination of the experimental data at 300 K shows, that the Henry's law constants differ from about 150 (carbon dioxide) up to 3000 bar (nitrogen), i.e. more than an order of magnitude. Compared to this, the prediction of the gas solubility from pure component data alone are good, especially when taking into account that this property is dominated by the unlike interaction in mixtures. Since the slope of the Henry's law constant as a function of temperature $H(T)$ is related to the heat of solution, this means that also that caloric property is predicted well.

The excellent agreement of the descriptive mode results for both the Henry's law constants and the vapor-liquid equilibria over the whole composition range confirm that reliable mixture properties can be obtained over a wide range of state points with simple molecular models when the unlike interactions are adjusted to a small experimental data basis.

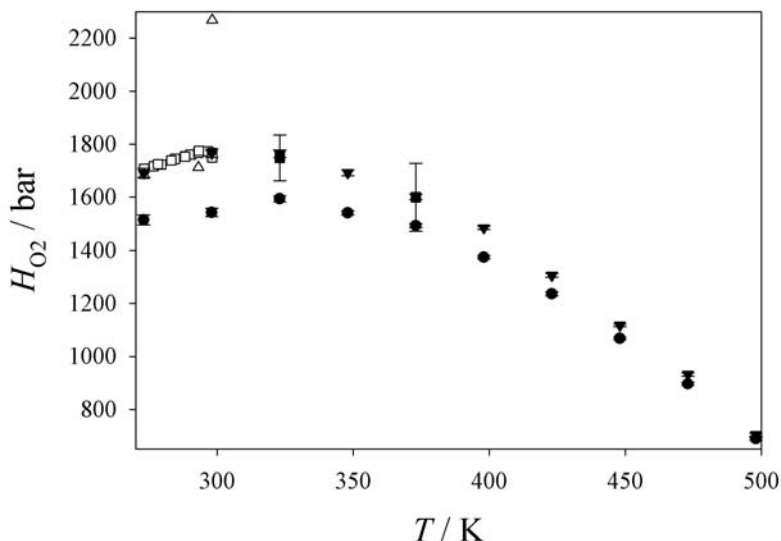


Fig. 4. Henry's law constants of oxygen in ethanol: empty square, confirmed experimental data; empty triangle up, other experimental data; filled bullet, predictive ($\xi = 1$) simulation data; filled triangle down, simulation data with adjusted ξ ; filled square, recommended experimental data recently published after the Simulation Challenge.

4 Computing Performance

The computing of the Henry's Law constants described in Sec. 3.2 was carried out on the NEC SX-6 since the molecular dynamics simulation code together with the calculation of the residual chemical potential by using Widom's test particle method is highly suitable for vectorization. However, the simulation code works not in parallel, and hence, single processor jobs were employed. Vectorization rates for this code are usually higher than 99%. For each binary system, ten jobs were needed for the predictive mode, about 5 jobs to adjust the binary interaction parameter and 10 jobs for the predictive mode. Thus, about 100 single processor jobs were calculated on the NEC SX-6 whereas one job lasted normally 20 hours.

The computing of the vapor-liquid equilibria of ethanol, ammonia and water as described in Sec. 2.1, Sec. 2.2 and Sec. 2.3 is based on Monte Carlo methods. For the development and new parameterization of the new molecular models, several calculations of the vapor-liquid equilibria are necessary. Since the methods applied are not appropriate for vector computers, these simulations were carried out on the Cray-Opteron Cluster. The core loop in the Monte Carlo code was parallelized with OpenMP and scales up to 1.35

on the double processor shared memory node on this cluster was obtained. Approximately 300 jobs were calculated whereas each job lasted about 40 hours.

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Benchmarking MPI One-sided Communication with SKaMPI-5

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Summary. SKaMPI is now an established benchmark for MPI implementations. Two important goals of the development of version 5 of SKaMPI were the extension of the benchmark to cover more functionality of MPI, and a redesign of the benchmark allowing it to be extended more easily (thus matching requests from SKaMPI users). In the present paper we give an overview of the extension of SKaMPI-5 for the evaluation of one-sided communication and present a few selected results of benchmark runs, giving an impression of the breadth and depth of SKaMPI-5.

A look at the source code, which is available under the GPL, reveals that it was extremely easily to extend the SKaMPI with benchmarks for one-sided communication using the infrastructure of version 5.

1 Introduction

“The MPI standard defines a set of powerful collective operations useful for coordination and communication between many processes. Knowing the quality of the implementations of collective operations is of great interest for application programmers. In particular, one has to decide, whether to use predefined collective operations, [...]” This text [Worsch et al.(2003)] describes one of the major motivations for the development of SKaMPI, the Special Karlsruher MPI-Benchmark [Reussner et al.(2002)].

SKaMPI (<http://liinwww.ira.uka.de/~skampi/>) measures the performance of an MPI implementation on a specific underlying hardware. By providing not simply one number, but detailed data about the performance of each MPI operation, a software developer can judge the consequences of design decisions regarding the performance of the system to be built.

The text also indicates, and benchmark results from a wide variety of machines indeed show, that more often than it should be there is for example a collective operation which is implemented in a suboptimal way, asking for self-made replacements. The development of new implementations for collective operations covered by MPI and for more complex collective operations not

covered by MPI is thus a natural next step. The same holds for the possibility to explore the influence of virtual topologies.

The rest of this paper is organized as follows: In Section 2 we give a short overview over SKaMPI-5 and related work. The main part are Sections 3 to 5. Section 3 discusses some measurements for determining synchronization costs. Section 4 is devoted the standard latency and bandwidth measurements using the pingpong pattern. Less trivial communication patterns are the topic of Section 5. This part is based on the diploma thesis of the second author [Straub(2004)]. We conclude this paper in Section 6.

This paper is an extended version of a paper accepted for EuroPVM/MPI 2005.

2 Overview

SKaMPI-5 offers more than 60 different functions for investigating different performance aspect of one-sided communication routines in an MPI-2 library. Several groups of functions can be identified; many of them accept an `MPI_Info` and/or an `assert` parameter which can be used to investigate their influence.

1. Functions for measuring the amount of time needed for calls to synchronization functions like `MPI_Win_fence`. This includes more complicated cases where for example `MPI_Win_wait` is delayed by a specified amount of time after another process has called `MPI_Win_complete`.
2. Functions for measuring the amount of time needed for calls to communication functions like `MPI_Win_Put`. Latency and bandwidth of for example simple pingpong communications implemented with one-sided communication are also easily determined.
3. Functions for measuring the amount of time needed for more complex communication patterns, e.g. the shift and exchange patterns mentioned above, one-sided implementations of broadcast, alltoall and (all)reduce, exchange of “ghost cells” etc.

Of course, it is impossible to discuss all facets of SKaMPI-5’s one-sided measurements in this paper. We have chosen a few aspects with an emphasis on those *not* covered by other benchmarks, e.g. those mentioned next.

2.1 Related other MPI benchmarks

There are some benchmarks which allow to do some (in particular latency and bandwidth) measurements. The following ones are available on the WWW and similar in the sense, that they produce data with running times for message exchange operations. Benchmarks like PPerfMark [Mohror and Karavencic(2004)] take a different approach.

MBL

The MBL library [Uehara et al.(2002)] allows to make measurements for the following communication patterns: ping, pingpong, shift and exchange. The first two are used in the obvious way with two processes; one can choose between `MPI_Get`, `MPI_Put` and `MPI_Accumulate` for the communication.

In the shift pattern each process i sends to $i + 1 \bmod P$ (where P is the size of `MPI_COMM_WORLD`). Thus a total of P messages is exchanged.

The exchange pattern realizes a kind of `MPI_Alltoall` with a total of $P(P - 1)$ messages. In one version all processes first send to 0, then all send to 1, etc., while in another version process i first sends to $i + 1 \bmod P$, then to $i + 2 \bmod P$, etc. MBL always uses `MPI_Win_fence`; dedicated and passive synchronization are not considered.

NetPIPE

NetPIPE [Scalable Computing Laboratory(2004)] is a benchmark measuring latency and bandwidth for a variety of communication mechanisms, including MPI2's one-sided communication. As with IMB one can choose between uni- or bi-directional communication and between `MPI_Put` and `MPI_Get`.

The end of the communication is usually ensured using `MPI_Win_fence`. When using `MPI_Put` one can alternatively request, that the target process watches the last memory location to be written for a specific byte to arrive. This violates the requirements of the MPI standard. In fact it may lead to a never ending program run, because an MPI implementation is free to postpone all communication until calls of `MPI_Win_fence` happen.

PMB/IMB

More comprehensive than the above was the Pallas MPI benchmark (PMB). Since Intel bought part of Pallas, that benchmark has been more or less replaced by the Intel MPI benchmark (IMB) [Intel(2004)].

For the benchmarking of one-sided communication a variable number of M messages are sent. One can choose whether `MPI_Win_fence` is called after each message or only after the last one. In the latter case it is ensured that for each message a different part of the target buffer is accessed. Furthermore the user may select `MPI_Get` or `MPI_Put` and uni- or bi-directional communication.

There are also possibilities to measure one call to `MPI_Accumulate` on all processes (followed by `MPI_Win_fence`) and the sequence `MPI_Win_create`; `MPI_Win_fence`; `MPI_Put(1 byte to same proc)`; `MPI_Win_free`; It is possible to change the `MPI_Info` argument in some calls, but then the benchmark has to be recompiled. Measurements using dedicated or passive synchronization are not possible.

2.2 Related papers

Gabriel et al. [2003] report latency and bandwidth numbers for several MPI implementations. They also show the influence of using `MPI_Alloc_mem`. The authors sound somewhat reluctant when it comes to recommending one-sided communication. On the other hand Matthey and Hansen [2001] show that there are situations where significant speedups can be obtained by replacing two-sided by one-sided communication.

Träff et al. [2000] differs from the above mentioned papers by emphasizing that pingpong measurements are definitely not the only way to assess the quality of an implementation of one-sided communication, but more complex communication patterns should be considered, too. SKaMPI-5 does that.

In the paper by Luecke et al. [2004] compare implementations of collective operations using SHMEM and MPI-2 one-sided communication. The broadcast algorithm in this paper violates the MPI-2 standard: data retrieved with `MPI_Get` are accessed locally without closing the communication epoch before.

The same problem is present in the paper by Desplat [2001]. It describes the differences between SHMEM and MPI-2 one-sided communication (blocking versus non-blocking) and how to make the transition from the first to the second. But again some code is not correct: Data retrieved with `MPI_Get` are accessed locally without closing the communication epoch before; similarly a remote location is accessed using `MPI_Get` as well as `MPI_Accumulate` without closing the epoch in between.

In the following three sections we will report on some findings from benchmark runs of SKaMPI-5. Of course it is possible to do the standard latency and bandwidth measurements. But in order to stress the much greater breadth and depth of what is possible with SKaMPI-5 we will spend most of the space on results which can (to the best of our knowledge) not be obtained with the other benchmarks mentioned above. We want to emphasize that

SKaMPI-5 allows to provide and use such measurements very easily.

3 Synchronization costs

We start with some simple measurements throwing some light on the performance of the synchronization calls for one-sided communication. SKaMPI-5 offers routines for checking collective (`MPI_Win_fence`) as well as dedicated (`MPI_Win_start`, etc.) and passive (`MPI_Win_lock`, etc.) synchronization. The times needed by those functions depending on possible assertions and the relative timing on different processors can be investigated. Below we exemplarily discuss two selected topics in a little bit more detail.

All data shown in this and the following sections have been obtained on a NEC SX6 of the HLRS in Stuttgart (Germany) and on the IBM SP of the computing center of the University of Karlsruhe (Germany). The NEC has nodes with 8 processors each, the IBM has two-processor nodes.

3.1 Influence of assertions on MPI_Win_fence

Figure 1 shows, how the assertions `MPI_NO_PRECEDE` and `MPI_NO_SUCCEED` may have an influence on the time needed by an `MPI_Win_fence` call. While this is true on the NEC SX6, there seems to be no influence on the IBM SP (for which we show no diagram).

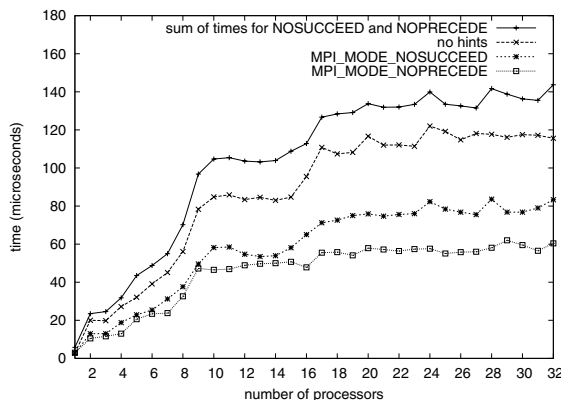


Fig. 1. Influence of assertions `MPI_NO_PRECEDE` and `MPI_NO_SUCCEED` on `MPI_Win_fence` on a NEC SX6.

3.2 MPI_Win_unlock

SKaMPI basically uses the following code for measuring the time needed by `MPI_Win_unlock`. A shared as well as an exclusive lock can be used. The `MPI_Put` can optionally be switched off is there to prevent the implementation to possibly detect and exploit the special case of no real communication.

```
MPI_Win_lock(lock_type,...)
MPI_Put(...,rank,...);
sleep(delay);
t1 = start_synchronization();
MPI_Win_unlock(rank, win);
time = stop_synchronization() - t1;
```

The last action of `start_synchronization()` is calling `MPI_Wtime` and returning that time. In addition it makes sure that all processes start at about the same global time. This is the same method that is now used by SKaMPI for the measurements of collective operations [Worsch et al.(2003)]; it gives better results than any other method we know. Similarly the first action of `stop_synchronization()` basically is calling `MPI_Wtime` and returning that time at the end (unless something went wrong). In addition some bookkeeping is done for our synchronization method.

Figure 2 shows the results for an IBM SP and Fig. 3 for an NEC SX6. A possible explanation of the very big variance of the times measured on the

IBM may be the following: IN the case of passive synchronization there has to be some kind of agent at the target which “reacts” to remote `MPI_Win_lock` and `MPI_Win_unlock` calls. If it is implemented as control thread, it is subject to the scheduling strategy. If the thread was inactive for a while, it is not clear how fast it gets the CPU again.

On the NEC there is a clear distinction between the processes on the same node (communication via memory) and the processes on other nodes (communication via network). We have no explanation for the higher times for 8 of the distant processors. It might be produced by the OS or the network load at the time of the measurement.

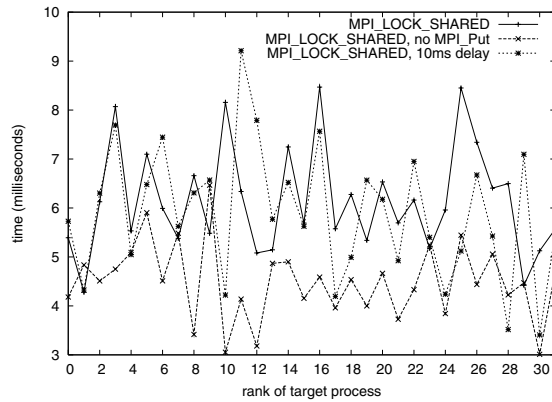


Fig. 2. Time needed `MPI_Win_unlock` on an IBM SP for varying target rank.

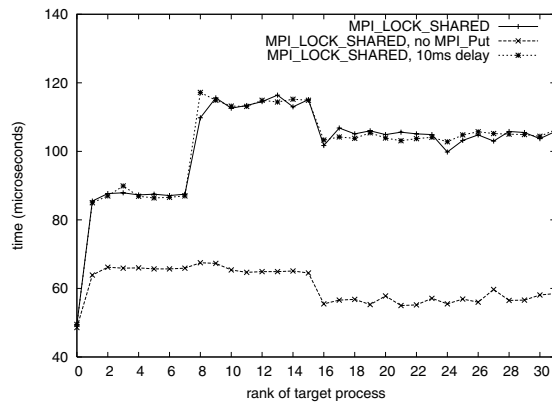


Fig. 3. Time needed for `MPI_Win_unlock` on a NEC SX6 for varying target rank.

4 Latency and bandwidth

Though it is probably not the most important aspect of one-sided communication [Träff et al.(2000)], what almost all benchmarks do is determining latency and bandwidth achievable in simple pingpong measurements using `MPI_Win_fence`; see Section 4.1 below. But SKaMPI-5 allows to do much more. For one example see Subsection 4.2.

4.1 Pingpong using `MPI_Put`

The code for the standard bandwidth benchmark looks like this:

<pre> Process 0 MPI_Win_fence(...); t1=start_synchronization(); MPI_Put(...,1,...); MPI_Win_fence(...); MPI_Win_fence(...); time=stop_synchronization()-t1; </pre>	<pre> Process 1 MPI_Win_fence(...); t1=start_synchronization(); MPI_Win_fence(...); MPI_Put(...,0,...); MPI_Win_fence(...); time=stop_synchronization()-t1; </pre>
--	--

Putting the calls to `MPI_Put` in above code in `if` statements checking the rank of the process already gives the complete code one has to write in order to have SKaMPI-5 provide the measurement (see [Augustin et al.(2005)] for more details on how easily SKaMPI-5 can be extended). All the rest is provided by the SKaMPI-5 framework.

Figure 4 shows some results on a NEC SX6. Figure 5 shows the results for the same measurement on an IBM SP. In the latter case it is surprising that in particular for small medium sized messages the transmission times depend on the specific ranks of the processes inside a node and that staying inside a node is *slower* than going outside.

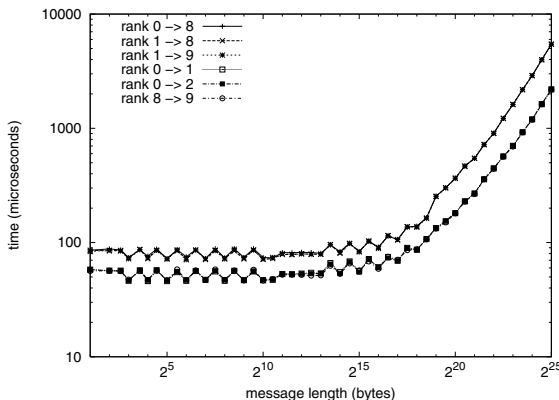


Fig. 4. Time needed for pingpong of messages using `MPI_Put` on a NEC SX6 (nodes with 8 processors). Clearly there are only two cases: if source and target are on the same node (faster) or not (slower).

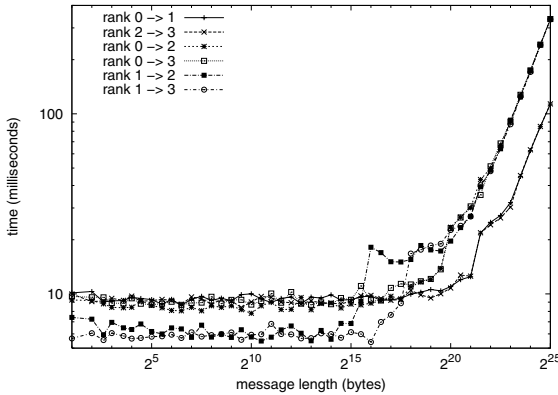


Fig. 5. Time needed for pingpong of messages using `MPI_Put` on an IBM SP (nodes with 2 processors). It is generally slower than the NEC. For large messages one has the same two cases as above; for smaller messages the situation is more involved.

4.2 Call duration of `MPI_Put`

The code for determining the duration of a call to `MPI_Put` is basically a

```
t1=MPI_Wtime(); MPI_Put(...,1,...); time=MPI_Wtime()-t1;
```

on process 0. Results for an NEC SX6 are shown in Figs 6 and 7. In the first case processes with rank 0 and 1 communicate, which are on the same node, in the second case processes with rank 0 and 8, which are on different nodes. In each figure there are four lines: `MPI_Put` is compared with `MPI_Isend` for the cases where messages buffers were allocated using `MPI_Alloc_mem` and where they were allocated using `malloc`. In Fig. 7 the large variations of times spent in calls to `MPI_Put` for different message lengths (with `MPI_Alloc_mem`) can be explained as follows: If the message length is exactly a multiple of 4, `MPI_Put` blocks and immediately does the communication; if the message length is different, `MPI_Put` only makes some arrangements for the transmission to be carried out later. (This explanation can be confirmed by additional measurements.) This characteristic may hurt a user who wants to hide communication times behind computations. And it might be hidden by a benchmark which only uses message lengths which are a power of two.

5 More complex measurements

In the last main section we deal with measurements which are more complicated than those in the previous sections. SKaMPI-5 includes functions for investigating the following questions:

- Does the MPI implementation delay the actual data transfer triggered by e.g. an `MPI_Put` and when? Does it try to combine several small messages into a larger one and transmit that?

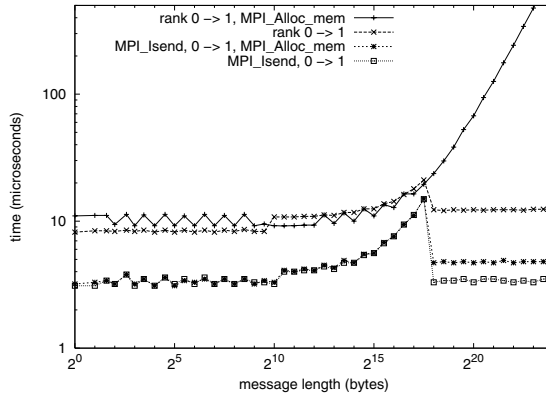


Fig. 6. Time needed for calling `MPI_Put` on a NEC SX6 compared to `MPI_Isend`, for intra-node communication. Data are shown for the case of message buffers allocated using `MPI_Alloc_mem` and the case when that was not done.

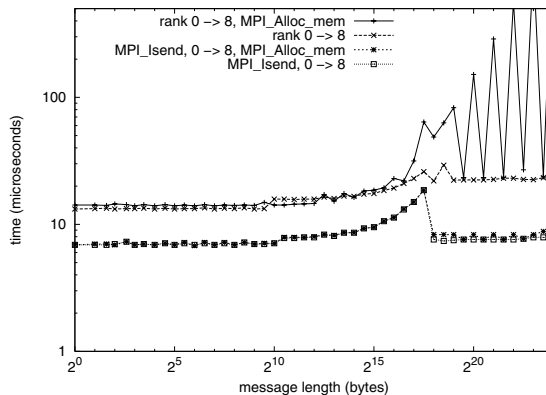


Fig. 7. The same measurement as in Fig. 6, but this time two processes on different nodes communicate. See the text for an explanation of the outliers.

- How do simple self-made “one-sided collective operations” perform compared to the built-ins like `MPI_Bcast`?
- What happens in the case of high network load? How much bandwidth per processor is still available?
- What happens if several processes want to access the same window and request an `MPI_LOCK_EXCLUSIVE`?
- How is the performance of one-sided (vs. two-sided) communication in applications, where dynamic load balancing is to be achieved by splitting the local work and giving part of it to other processors upon request?
- How fast can the exchange of border (“ghost” or “halo”) cells in one- or higher-dimensional grid decompositions be realized using one-sided (versus two-sided) communication?

From this list we have picked two topics for which some interesting results are discussed in some detail below.

5.1 Delayed sending for MPI_Put

Assume that process 0 executes the following codesegment:

```
start_synchronization();
MPI_Win_fence(...);
for(rank = 0; rank < P; rank++)
    MPI_Put(..., rank, ...);
sleep(delay);
t1 = MPI_Wtime();
MPI_Win_fence(...);
time = stop_synchronization() - t1;
```

All other processes only call `MPI_Win_fence` twice. If an MPI implementation delays sending messages until the `MPI_Win_fence`, the `delay` for which process 0 is sleeping, has no influence on the time measured. If messages are *not* delayed, larger delays should lead to smaller times measured for the `MPI_Win_fence`. Figure 8 shows what happens on an IBM SP. The MPI implementation allows to specify the size of a cache using `IBM_win_cache` in an `MPI_Info`. By default the size is 4 kilobytes. The sending of messages of (in fact, up to) this size is postponed to the call of `MPI_Win_fence`. As a consequence the times measured for that call are more or less independent of the length of the delay. On the other hand, for larger messages, or when the cache size is set to 0, messages are sent immediately. Consequently larger delays lead to shorter times spent in the `MPI_Win_fence` call.

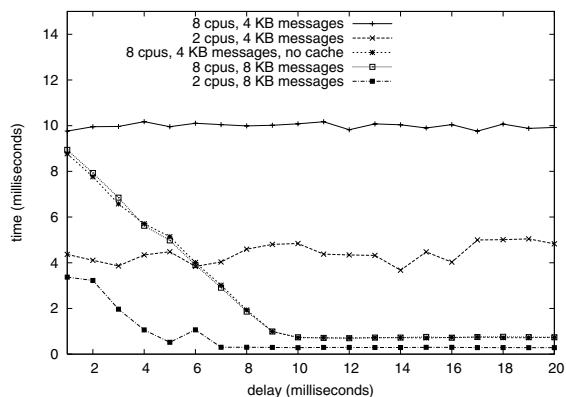


Fig. 8. Postponed sending of messages on an IBM SP. See the text for explanations.

5.2 Self-made “one-sided collective” operations

Sometimes it is clear, that there will be a communication epoch for some one-sided communication operations. If in addition there is the need for an alltoall exchange of data whose results will only be needed after the end of the epoch,

it may be feasible not to use the built-in `MPI_Alltoall` but realize it using one-sided communication, too.

For example, a simple variant of one-sided alltoall might be implemented like this:

```
void onesided_alltoall(void* buffer, int count, MPI_Datatype datatype,
                     int displacement, MPI_Win win) {
    MPI_Group group;
    void* rank_buffer;
    int size, i, rank, myrank, displacement, datatype_size;

    MPI_Win_get_group(win, &group);    MPI_Group_rank(group, &myrank);
    MPI_Group_size(group, &size);      MPI_Group_free(&group);
    MPI_Type_extent(datatype, &datatype_size);

    displacement = displacement + myrank * count;

    for(i = 1; i <= size; i++) {
        rank = (myrank + i) % size;
        rank_buffer = buffer + rank *
                        (count * datatype_size);
        MPI_Put(rank_buffer, count, datatype,
                rank, displacement, count,
                datatype, win);
    }
}
```

Figure 9 shows the running times for this operation on a NEC SX6 for different sizes of the communicator and for four lengths of the chunks exchanged between any two processes. For comparison the time needed by `MPI_Alltoall` for 1 kb chunks is also presented. As one can see the self-made implementation is faster if the communicator is larger than one node (with 8 processors).

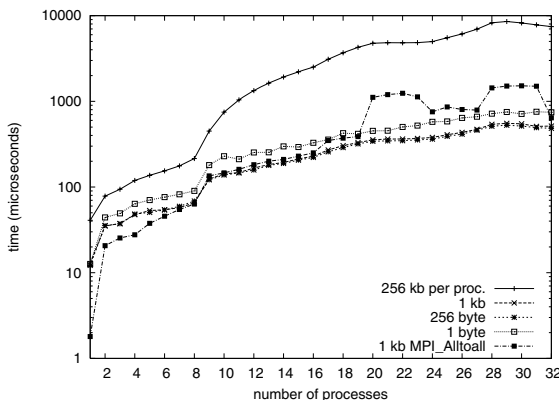


Fig. 9. Measurements of an implementation of the alltoall pattern using one-sided operations, and the running time of `MPI_Alltoall` for comparison.

6 Conclusion

The use of the machines at the HLR Stuttgart is an inevitable and invaluable help for the development of portable software. The widespread use of SKaMPI all over the world can be attributed to the fact that it compiles and runs everywhere where MPI is available.

All parts of SKaMPI are available under the GPL and we are accepting contributions to SKaMPI-5 wherever we see them fit.

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