Research Report
High-Perfomance Computing in Hessen

20. August 2007

Inhaltsverzeichnis

1 Vorwort

Der hier vorliegende Forschungsbericht gibt Rechenschaft darüber ab, wie die an den Universitäten des Landes Hessen installierten Computerkapazitäten in den Jahren 2004 - 2006 für die Forschung in den Bereichen der Natur- und Ingenieurwissenschaften genutzt wurden. Die beeindruckende Liste der mehr als 125 Publikationen, die in international führenden Zeitschriften veröffentlicht wurden, sind ein Beleg für das hohe Niveau der Forschungsleistungen und der Produktivität der Arbeitsgruppen an den hessischen Universitäten, die sich weltweiter Konkurrenz stellen können. Die auszugsweise vorgestellten Forschungsarbeiten weisen auf das breite Spektrum unterschiedlicher Themen hin, für deren Bearbeitung der Zugang zu Hoch- und Höchstleistungsrechnern unabdingbar ist. Wir legen diesen Bericht nicht ohne Stolz auf die hier dokumentierten wissenschaftlichen Leistungen vor, die in den vergangenen drei Jahren erbracht wurden. Sie wurden durch die schöpferische Kreativität und den engagierten Einsatz der daran beteiligten Wissenschaftler und Studenten ermöglicht, die auf die vorhandene Infrastruktur an den Rechenzentren und die Computerkapazitäten an den hesssischen Universitäten zurückgreifen konnten. Das Zusammenspiel beider Komponenten machte es möglich, daß die im folgenden vorgestellten wissenschaftlichen Ergebnisse erzielt werden konnten. Der Forschungsbericht ist ein eindrucksvoller Beleg für das hohe Forschungsniveau an den hessischen Hochschulen. Die beteiligten Wissenschaftler legen den Bericht als Beleg dafür vor, daß die nicht unerheblichen Investitionen in Computerkapazitäten eine dokumentierbare und nachhaltige Stärkung des Forschungsniveaus an den hessischen Universitäten nach sich ziehen. Die sich daraus ergebene Stärkung der Qualität in der Lehre liegt auf der Hand.

Prof. Gernot Frenking, Marburg, 19.8.2007
Vorsitzender des Hessischen Beirats für Hochleistungsrechnen

2 Einleitung

Die Bedeutung des Wissenschaftlichen Rechnens als einer Schlüsseltechnologie für nahezu alle Bereiche von Wissenschaft und Technik ist heutzutage unumstritten. Trotz der enormen Fortschritte im Bereich der Rechnertechnologie ist hierbei in vielen Anwendungsfällen der Einsatz von Hochleistungsrechnern unerlässlich, nicht zuletzt auch aufgrund der stetig wachsenden Komplexität der Problemstellungen. Das Hochleistungsrechnen trägt entscheidend zur Reduktion von Entwicklungszeiten neuer Methoden und Technologien bei und es können Probleme angegangen werden, die aufgrund der hohen Anforderungen an die Rechenleistung anderweitig einer numerischen Simulation nicht zugänglich sind.

Der Verfügbarkeit einer adäquaten Hochleistungsrechnerkapazität kommt damit für den Wissenschaftsstandort Hessen eine überaus wichtige Bedeutung zu, da dies die Grundlage für eine national und international konkurrenzfähige Forschung im Bereich des Wissenschaftlichen Rechnens darstellt. Der Erfolg von Sonderforschungsbereichen, Forschergruppen, Graduiertenkollegs und einer Vielzahl unterschiedlicher Einzelprojekte hängt entscheidend davon ab.

Der Hochleistungsrechenbedarf in Hessen wird durch zentrale Rechenkapazitäten auf Landesebene gedeckt. Aufgrund unterschiedlicher Anforderungen der Nutzer werden zwei größere Systeme mit unterschiedlichen Architekturen betrieben:

- Ein SMP-Cluster an der TU Darmstadt für Anwendungen mit feingranularer Parallelität mit vergleichsweise hohen Anforderungen an die Kommunikationsleistung, wie z.B. Strömungssimulationen oder Strukturrechnungen komplexer Quantensysteme.
- Ein MPP-Cluster an der Universität Frankfurt für Anwendungen mit grobgranularer Parallelität mit vergleichsweise geringen Anforderungen an die Kommunikationsleistung, wie z.B. Vielteilchendynamik in Stoßprozessen.

Dem Darmstädter Forschungszentrum CE und dem Frankfurter CSC kommt die Funktion von Kompetenzzentren im Bereich des Hochleistungsrechnens zu. Die notwendige fachübergreifende Kompetenz ist durch die interdisziplinäre Zusammensetzung der beiden Zentren, sowie durch entsprechende Aktivitäten der Mitglieder in Forschung und Lehre gewährleistet. Damit leisten beide Zentren einen Beitrag zu den folgenden Aufgaben:

- Entwicklung bzw. Weiterentwicklung von Anwendungssoftware für den Hochleistungsrechner in den verschiedenen Anwendungsbereichen,
- Unterstützung von Nutzern bei der Portierung von Anwendungssoftware.
- Ausbildung von wissenschaftlichem Nachwuchs im Bereich des Wissenschaftlichen Rechnens durch entsprechende Lehrangebote,
- Technologietransfer in die Industrie im Rahmen von Kooperationsprojekten,
- Organisation von regelmäßigen Benutzer-Kolloquien, die den Erfahrungsaustausch zwischen allen Nutzern des Rechners ermöglichen,

- Kontaktpflege und Zusammenarbeit mit anderen im Bereich des Hochleistungsrechnens tätigen Arbeitsgruppen im In- und Ausland (z.B. Workshops, Forschungsprojekte).

Die Rechenzentren der hessischen Universitäten betreiben den Rechner gemeinsam unter Federführung der Rechenzentren der TU Darmstadt und der Universität Frankfurt, an denen die Rechner installiert sind. Zu den Aufgaben der Rechenzentren an den beiden Standorten gehören:

- Bereitstellung von Räumlichkeiten und der zugehörigen Infrastruktur,
- Administration und Operating (24-Stunden-Betrieb),
- Betriebssteuerung und Überwachung der Betriebsvorgaben,
- Fehlerverfolgung und -behebung,
- Benutzerverwaltung,
- Datensicherung.

Die Rechner sind für Nutzer aller hessischen Universitäten zugänglich. Die einzelnen Rechenzeitkontingente richten sich nach den finanziellen Beteiligungen der Hochschulen, Fachbereiche bzw. Fachgebiete. Dies wird durch eine entsprechende Prioritätenvergabe erreicht.

3 Technik und Organisation

3.1 Linux-Cluster am Center for Scientific Computing (CSC) der Uni Frankfurt

Das Center for Scientific Computing (CSC) der Goethe-Universität betreibt einen der beiden hessischen Hochleistungsrechner. Das CSC wurde im Jahr 2002 als gemeinsame Initiative von 15 Forschungsgruppen der naturwissenschaftlichen Fachbereiche der Universität Frankfurt ins Leben gerufen. Ausgangspunkt für seine Gründung war die Erkenntnis, dass in den modernen Naturwissenschaften die Bewältigung komplexer numerischer Aufgaben eine zentrale Rolle einnimmt.

Das CSC bietet daher neben der Bereitstellung einer umfangreichen Rechenkapazität für die Projekte der beteiligten Forschergruppen ein fachübergreifendes Forum auf dem Gebiet Computational Science in Form von interdisziplinären Vorträgen. Darüber hinaus bietet das CSC einen zweijährigen, englischsprachigen Masterstudiengang in Computational Science an. Der Studiengang ist in modularer Form konzipiert, so dass alle Studienleistungen in Form von international anerkannten Credit Points gemäß dem European Credit Transfer System bewertet werden. Die durchweg in englischer Sprache gehaltenen Kurse eröffnen auch ausländischen Studierenden eine interdisziplinäre Ausbildung in allen Bereichen der Computer Simulation.

Die Forschungsaktivitäten der am CSC arbeitenden Wissenschaftlern umfassen eine große Zahl von Projekten mit hohem numerischen Aufwand. Die Projekte, die auf dem CSC-Cluster bearbeitet werden, umfassen eine weite Spanne aktueller Themenbereiche. Sie erstrecken sich über so unterschiedliche Gebiete wie die Untersuchung der Strukturen von Proteinen in der Biochemie und die Eigenschaften von Kristallen unter höchstem Druck in der Geophysik. Die Dynamik der Grundbausteine der Materie, den Quarks und Gluonen, im Urknall und bei Hochenergieexperimenten werden in der theoretischen Physik auf dem CSC simuliert. Wissenschaftler des Frankfurt Institute for Advanced Studies modellieren komplexe atomare Strukturen und untersuchen die Möglichkeiten der Krebstherapie mit Schwerionenstrahlen.

Der Hochleistungsrechner des CSC besteht aus 3 Linux MPP-Cluster, die über das schnelle universitätsweite Netz (10Mb/s) verbunden sind.
CSC I wurde im Jahr 2003 beschafft und besteht aus 70 Knoten mit jeweils 2 Intel Xeon, 2.4 GHZ, CPUs. Jeder Server ist mit 2 Gigabyte Hauptspeicher ausgerüstet. Eine Partition mit 32 Knoten (70 Prozessoren) ist über ein latenzarmes Myrinet-Netz verbunden, um schnelle Kommunikation für parallele Programme zu ermöglichen.
CSC II wurde 2004 in Betrieb genommen. Die Anlage besteht aus 10 wassergekühlten Racks, die 282 Rechenknoten enthalten, die mit jeweils 2 64bit Opteron CPUS mit einer Taktrate von 1.8 GHz bestückt sind. Die Knoten sind standardmäßig mit 4 GByte Hauptspeicher ausgerüstet. 15 Knoten wurden auf 8 Gbyte, weitere 15 auf 16 GByte Speicher aufgerüstet. 64 Knoten sind mit Myrinet schnell vernetzt, die übrigen Knoten mit Gigabit Ethernet verbunden. Das RAID-System verfügt

über 10 TByte Plattenplatz.
Der dritte Cluster CSC III wurde in 2006 zur Benutzung freigegeben. Er besteht aus 251 Knoten, die jeweils mit 2 Dual-Core 2GHz Opteron CPUs ausgestattet sind. Jeder Knoten verfügt über 8 GByte Hauptspeicher, zusätzlich sind 44 Knoten auf 16 GByte aufgerüstet worden. 64 der Knoten sind mit Myrinet vernetzt. Ein Raid-System stellt 25 TByte Speicherplatz zur Verfügung.
Durch den stetigen Ausbau verfügt das CSC damit über ein MPP-System aus insgesamt 1708 Prozessoren mit einer theoretischen Rechenleistung von etwa 6.4 TFlop/s. Es werden eine Vielzahl von Softwarepaketen und Compilern zur Verfügung gestellt. Die Datensicherung aller Systeme erfolgt über das Backup-System des Hochschulrechenzentrums der Universität.
Mehr als 360 Nutzer in über 60 Arbeitsgruppen aus dem Bereich der Naturwissenschaften, Mathematik und Informatik sorgen für eine vollständige Auslastung des Rechners über das ganze Jahr. Etwa ein Drittel der verfügbaren Rechenzeit wird von Gruppen aus Darmstadt, Marburg, Gießen und Kassel verbraucht.

Die Finanzierung der Anlage erfolgte überwiegend durch Beiträge Frankfurter Hochschullehrer und -Institutionen, sowie Zuschüsse des Landes Hessen und des Bundes (im Rahmen des Hochschulbau-Förderungsgesetzes). Über den Verbund der Hessischen Hochleistungsrechner (HHLR) haben Wissenschaftler aller hessischen Hochschulen Zugang zu den Computersystemen des CSC.

3.2 Der HHLR am Forschungszentrum Computational Engineering (CE) in Darmstadt

3.2.1 Systemaufbau

Der Hessische Hochleistungsrechner besteht aus 64 SMP-Knoten unterschiedlicher Leistungsfähigkeit mit insgesamt 520 Power-Prozessoren. Der Zugang erfolgt über einen speziellen Loginknoten. Auf diesem kann der Nutzer seine Programme vorbereiten, sowie Daten analysieren und abholen. Compute-Knoten im Backend sind für den Nutzer nicht direkt zugänlich, sonder werden über ein Queuing-System angesprochen. 60 dieser Rechen-Knoten sind mit, jeweils acht Power5 CPUs ausgestattet zwei weiter verfügen über je 16 Power5+ Prozessoren. Die Power5-Prozessoren sind in der Lage vier Floatingpoint-Operationen pro Tackt auszuführen und haben einen Cache von 36MB im Prozessor integriert. Damit eignen sie sich besonders gut für HPC-Andendungen.

Als Shared Memory Rechner (SMP) sind die Maschinen besonders gut für parallele Probleme mit hohem Kommunikationsbedarf geeignet. Um auch Programme, die mehr als einen SMP-Knoten benötigen, effektiv verarbeiten zu können, sind die Rechner untereinander mit einem schnellen internen Netzwerk verbunden (IBM High Performance Switch (HPS)).

Das Hochschulrechenzentrum (HRZ) der TU Darmstadt betreibt das Rechnersystem im Auftrag des HHLR-Beirats sowie der Kompetenzgruppe wissenschaftliches Hochleistungsrechnen im Forschungszentrum Computational Engineering (CE).

3.2.2 Auslastung des HHLR

Der Rechner wurde im November 2005 ausgebaut. Bereits im Januar 2006 wurde von den Nutzern mehr Rechenzeit abgerufen, als vor dem Ausbau verfügbar war. In der ersten Jahreshälfte ist die Nutzung kontinuierlich angestiegen. In der zweiten Hälfte 2006 ist sie jedoch wieder etwas zurück gegangen. Seit Dezember 2006 ist ein erneuter Anstieg der zu erkennen. Der Einbruch im Februar 2007 ist auf eine 14-tägigen Ausfall des Systems (Ausfall der Klimatisierung) zurückzuführen.

Seit März 2007 ist das System mit 300.000 CPUh/Monat defakto an der Auslastungsgrenze. Theoretisch könnte das System zwar 374.400 CPUh im Monat abgeben, in der Praxis ist es auf einem System mit dieser Jobstruktur aber nur schwer möglich eine deutlich besser Auslastung als 80% zu erreichen.

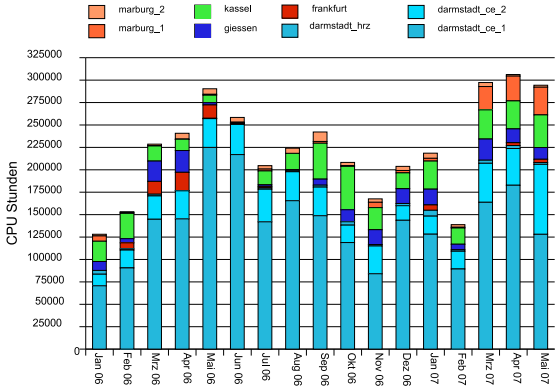

Abbildung 3.1: *Verteilung der Rechnezeit auf die einzelnen Universitäten*

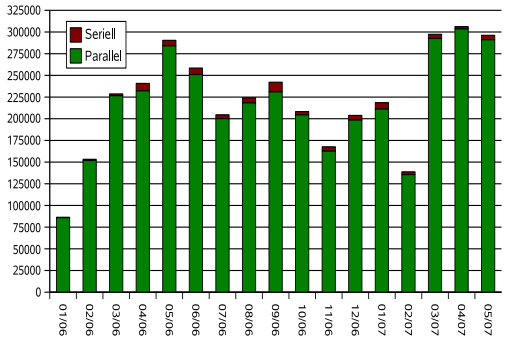

Abbildung 3.2: *Verteilung der Rechenzeit auf Serielle- und Parallelejobs*

Jobprofil des HHLR

Der HHLR ist speziell für die effektive Verarbeitung von parallelen Job konzipiert. Durch den Aufbau aus Mehrprozessorrechnern (8-Wege SMP mit hoher Memorybandbreite) können auch Problem mit starker Kopplung effektiv auf dem System verarbeitet werden. Ein Teil der Knoten ist untereinander nochmal mit einem sehr schnellen Netzwerk (HPS) gekoppelt. Auf dieser HPS-Partition können Job mit bis zu 128 CPUs effektiv laufen. In Abbildung 3.2 ist zu erkennen, dass diese Auslegung des Systems durch die Nutzung des Rechners voll bestätigt wird. Auf dem Rechner laufen fast ausschließlich parallele Rechnungen. 2006 wurde die meiste Rechenleistung am HHLR für 8-fach-parallele Jobs aufgewendet. 65% der Rechenzeit wurde für sie aufgewendet. Fast 19% der Rechenzeit ging an Jobs mit 16 oder mehr Prozessoren. Dabei ist jedoch zu berücksichtigen, dass durch den Aufbau des Rechners Jobs die maximal 8 CPUs benutzen im Scheduling und bei der Verarbeitung im Vorteil sind. Die Nachfrage nach stärker parallelen Jobs kann durch die begrenzen Ressourcen am HPS nicht immer befriedigt werden. Es ist aber ein klarer Trend zu stärkerer Parallelisierung zu erkennen.

4 Projektberichte

4.1 Chemie

4.1.1 Molecular Dynamics Simulations of Potassium Channels

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S. M. Kast, S. Tayefeh, G. Thiel

Potassium channels are membrane-bound proteins enabling the cell to selectively exchange potassium ions with the environment. Exploring the relation between amino acid sequence and channel functionality is important for understanding design principles of channel proteins, which will be relevant, e.g., for creating novel biosensors. The Kcv channel from the plant virus PBCV-1 represents the smallest functional channel known and therefore serves as an ideal model system for studying structure-functions relationships. Ion conduction characteristics can be tuned by site-directed mutagenesis, but since the experimental crystal structure is unknown, an interpretation on an atomic scale is impossible.

Microscopic insight is gained computationally by classical molecular dynamics simulations of Kcv mutants and of hybrids of Kcv with the bacterial KirBac1.1 channel for which an experimental crystal structure is known. Various systems are constructed, comprising the channel pore embedded in a fully solvated lipid bilayer (see Fig. 1). Simulations are performed over several tens of nanosecond for each mutant system. The resulting trajectories are evaluated with respect to structural (see Fig. 2), thermodynamical and dynamical properties reflecting ion permeation capabilities.

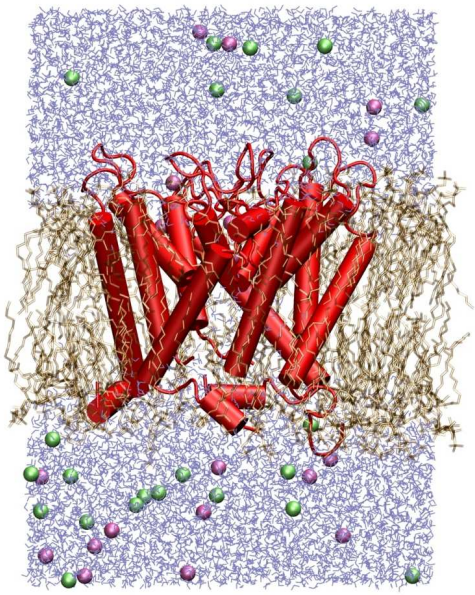

Fig. 1: Snapshot of a typical simulation system

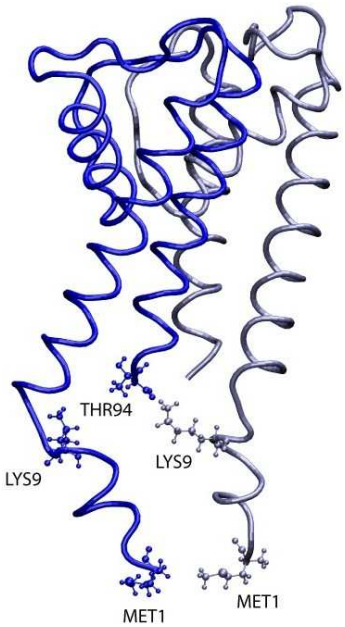

Fig. 2: Salt bridge pattern of a KirBac1.1 mutant structure

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[2] B. Hertel, S. Tayefeh, M. Mehmel, S. M. Kast, J. L. Van Etten, A. Moroni, and G. Thiel: Distortion of the First Transmembrane Domain Alters Gating of Miniature K+ Channel Kcv, *J. Membrane Biol.* 210, 1-9, 2006.

4.1.2 Eliminating Truncation Effects in Molecular Simulations

Physikalische Chemie, TU Darmstadt
S. M. Kast, B. Schilling, J. Brickmann

The limiting step in molecular simulations is the computation of long-range forces acting between the particles in a system, particulary those arising from Coulomb interactions between partially charged atoms. The performance can be dramatically increased by applying truncation to the interaction potentials at a given distance, however at the price of introducing severe errors in structural, dynamical and thermodynamical observables that are calculated from the simulation trajectories.

By combining integral equation theory, an approximate analytical treatment of the statistical mechanics of soft-matter systems, with molecular simulations we are able to compensate quantitatively for various truncation artifacts. Structural predictions like for instance radial distribution functions can be corrected (see Fig. 1) as well as the solvation free energy (see Fig. 2) which is strongly influenced by a modification of the potential. Future aspects of the present project involve the application of the methodology to force field parametrization work.

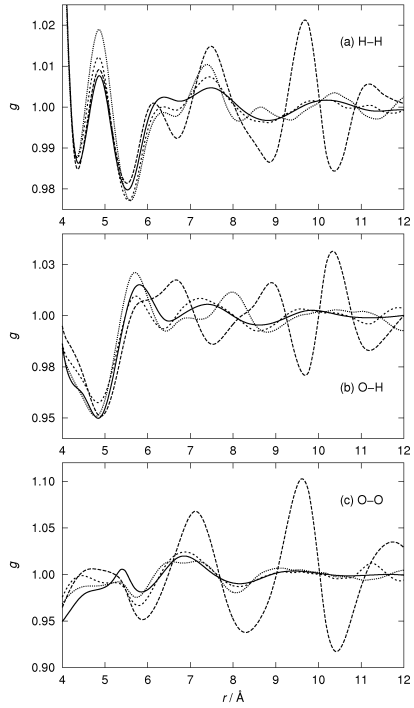

Fig. 1: Original (long dashed) and corrected radial distribution functions for liquid water

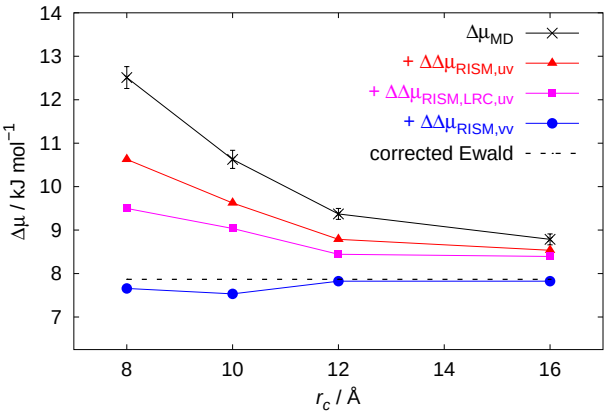

Fig. 2: Original and corrected free energy of hydration for argon

[1] D. Zahn, B. Schilling, and S. M. Kast: Enhancement of the Wolf Damped Coulomb Potential: Static, Dynamic, and Dielectric Properties of Liquid Water from Molecular Simulation, *J. Phys. Chem. B* 106, 10725-10732, 2002.

[2] S. M. Kast, K. F. Schmidt, and B. Schilling: Integral Equation Theory for Correcting Truncation Errors in Molecular Simulations, *Chem. Phys. Lett.* 367, 398-404, 2003.

[3] B. Schilling, J. Brickmann, and S. M. Kast: Hybrid Integral Equation/Simulation Model for Enhancing Free Energy Computations, *Phys. Chem. Chem. Phys.* 8, 1086-1095, 2006.

4.1.3 Thermal Conductivity of Polymers by Non-Equilibrium Molecular Dynamics

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The thermal conductivity is an important physical quantity of polymers for practical applications, above all because they are processed thermally. At present, though, relatively few data are available and the underlying physical mechanisms are unclear. The reasons are the severe difficulties encountered in describing properly thermal properties of polymers on a theoretical ground and in performing experiments in ëxoticconditions (e.g., very high or very low temperature, high pressure), like in the case of synthesis and processing. In this context, molecular dynamics simulations can make an important contribution.

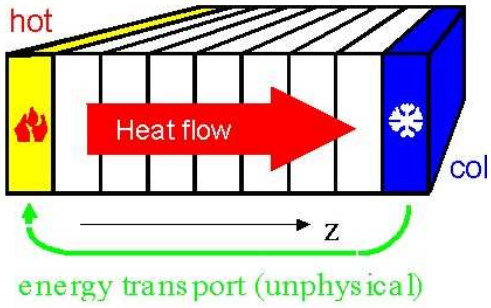

Abbildung 4.1: *Schematic representation of the basic idea applied in the Reverse Non-Equilibrium Molecular Dynamics*

Technical and conceptual difficulties often arise with traditional methods. This is why a non-equilibrium method, called Reverse Non-Equilibrium Molecular Dynamics, has been conceived and developed. The main goal of this project consists in adapting and extending it from simple models of fluids, for which it has proved successful [1], to more complex ones, specifically polymers. Not less important is providing a better physical comprehension of heat transfer in polymers, which can be done through targeted simulations. For example, it is important to understand what the relative contribution of collisions through polymer chains is and, respectively, of energy transport through phonons along the chains; from polymers with a high degree of crystallinity information can be extracted with regard to privileged directions of heat transfer.

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4.1.4 Vapor-Liquid Equilibria in Solvent-Polymer Systems

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Grand Canonical Ensemble Simulation

The chemical potential is a fundamental property in studying many physical phenomena of interest such as phase equilibria, solubilities, the study of interphases, flow in pores, and diffusion in multicomponent mixtures. There are many methods for the calculation of chemical potentials, like thermodynamic integration, Widomâs test particle method and so on. In these methods the chemical potential is calculated at the end of the run. In the simulation in the grand canonical ensemble we can set a target value of the chemical potential. In this method we assume that our physical system is composed of N real particles plus one â scaled particle and is coupled to a temperature reservoir and a particle reservoir. The scaled particle is a fractional particle whose potential and (or) its kinetic energies are scaled by a variable n which varies from zero to one. The inclusion of the scaled particle in the system provides a variable number of particles in a dynamical way. By comparing the potential energy of the scaled particle at each time step with the target value of the chemical potential, we may grow up or delete that particle. Below you can see a schematic representation of the simulation box.

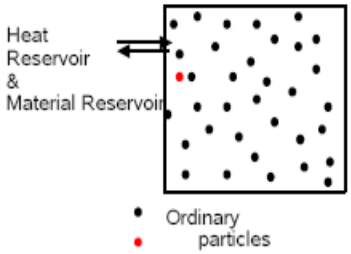

Abbildung 4.2: *Lamellar structure*

4.1.5 Molecular Dynamics Simulations of Platinum(111)/Isopropanol Interface

Konstantin B. Tarmyshov and Florian Müller-Plathe
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Technische Universität Darmstadt, Darmstadt The solid/polymers interface are the subject of numerous applications in both science and our every-day-life. Some examples are coating, packaging of microelectronics, composite materials, â colloidal dispersionâ, and many others. Metal surface and bulk are of particular interest due to their specific electronic structure and microscopic and macroscopic properties driven by this structure (as opposed to any usual solid). More specifically â the transition metals like platinum or gold are used for catalytic purposes. Other (cheaper) metals are employed in current carrying wires or for screening from the external or internal fields (e.g. to perform an experiment). Metals have these features (ability to carry current and screen the electrostatic field) owing to the socalled free band (or conduction band) electrons that appear in the metal bulk and surface. The presence of these features, however, complicates enormously the studying of metal surface / organic adsorbate (in particular polymers) interfaces, as the final interaction is an interplay of all different kinds of interactions: chemical, quantum (very weak chemical), electrostatic, dispersive attraction. In our group we are developing a model and a parameterization procedure, in order to study such interfaces by means of Molecular Dynamics simulations (particularly Pt(111)/isopropanol(poly-vinyl-alcohol) interface.

4.1.6 Investigation of thermal diffusion in molecular fluids and polymer solutions

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Thermal diffusion, or Soret effect, describes the coupling between a temperature gradient and a resulting mass flux in a multicomponent fluid. It is the side-effect when the thermal conductivity is measured in mixture fluids. And it is also the fundament of the technique that the components of mixtures can be separated by a temperature gradient. Since the mechanism of thermal diffusion in liquid mixtures is not completely understood[1], it is hard to predict the thermal diffusion coefficient DT and the Soret coefficient ST, which measure the thermal diffusion. Therefore, we are interested to study the hydrodynamic mechanism of the thermal diffusion in liquids with reverse non-equilibrium molecular dynamics (RNEMD). The RNEMD has been successfully employed to investigate the Soret effect in single site Lennard-Jones fluids[2], etc. The advantages of the molecular dynamics over the experiments in thermal diffusion studies are mainly from two sides: First, in molecular dynamics, each parameter that affects the thermal diffusion, such as mass, size, moment of inertia, and interaction potential, can be tuned independently and even unphysically; second, molecular dynamics helps to understand the mechanism of thermal diffusion microscopically. Our first goal is to study the contributions of the mass and the momentum of inertia of the molecules to the thermal diffusion in binary molecular fluids. Tetrahedral models are used to represent two kinds of molecules, for they have only one component of moment of inertia. Thus it is easier to tune the magnitude of the moment of inertia. Our second aim is to investigate the thermal diffusion in dilute polymer solutions which own two typical thermal diffusion behaviours: the (in)dependence of DT on the degree of the polymerization;[3] and the sign change of ST due to the change of the solvent quality[4, 5]. In our case, the polymer chains will be represented by a generic bead-spring model. How the interactions between the solvent and the local structure of the polymer affect the thermal diffusion behaviour of the entire chain will be investigated.

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4.1.7 Multiscale simulations of dendrimers

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Dendrimers are a special class of branched polymers characterized by a multifunctional core from which relatively short chains (called branches or dendrons) emanate. Each branch end is characterized by a specific functional group which, reacting with another monomer, builds the new generation; this iterative procedure leads to a molecule that resembles a Cayley tree. The branching units flexibility is connected to their chemical constitution: stiff building blocks, such as phenylene groups, lead to rigid dendrimers with structural features and potential applications completely different than flexible ones. Moreover, the use of several chemical groups to functionalize the chain ends and the almost full control over the synthetic process make this class of macromolecules suitable for the design of novel nanostructured materials and for several possible applications. [1]

Several theoretical approaches are used to study the intra and inter-molecular conformations of dendrimers, explaining at molecular scale the properties observed macroscopically. The best compromise for a computational study of dendrimers would be a coarse-grain method that reduces the size of the system while taking into account the atomistic details. Based on the polymeric nature of dendrimers a coarse-grain method used to describe the polymers is the natural choice. Then a mesoscale model usually applied on polymers and that reproduces very well the structural and dynamic properties of the melt, is chosen to study the dynamic behavior of dendrimer solutions and melts. [2] This project is focused on studying with a multiscale modeling method the conformational and dynamical behaviour of the [ethylene-di-amina core]-polyamidoamine (PAMAM) dendrimers (see Figure 4.3). The availability of a sufficient amount of experimental data especially on the PAMAM solutions, will permit to confirm the suitability of the approach, but the developed coarse grain procedure will allow to simulate a larger family of polyamidoamine dendrimers.

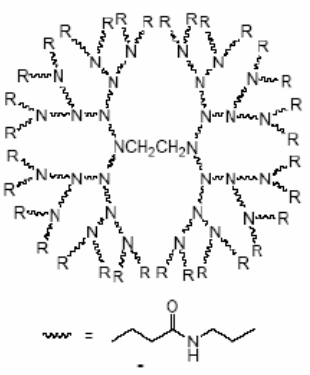

Abbildung 4.3: *[ethylene-di-amina core]-polyamidoamine*

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4.1.8 Mesoscale Simulations of the Fuel Cell Membrane

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Technische Universität Darmstadt, Darmstadt

Block co-polymers are one of the potential candidates to be used as the fuel cell membrane due to its flexibility in designing the structural and mechanical properties as one requires in various extreme fuel cell conditions.

In this work, mesoscale simulations for the experimentally developed diblock copolymers are carried out to explore the phase morphologies and the dynamics of the formation of the bi-continous phases. For mesoscale simulations dissipative particle dynamics(DPD) [1] method has been used where polymers are represented as strings of beads made of 100s atoms to gain a longer time and larger length scale. These melts form an ordered structure after long time simulation depending on the ratio of two blocks and on the Flory-Huggins solubility χ -parameter. We have developed and implemented the DPD algorithm and used it to study linear di-block copolymers with different fractions of two different blocks (A_nB_m). We have reproduced the lamellar, gyroid and cubic bi-continuous phases for A_5B_5 (fig.1), A_3B_7 and A_2B_8 systems respectively. We also carried out several test calculation to check the validation of the code with respect to the temperature and the pressure control for various systems. We are presently involved in studying the dynamics of the different phase formation and the morphologies of the mixture of different types of block co-polymers with different ratios.

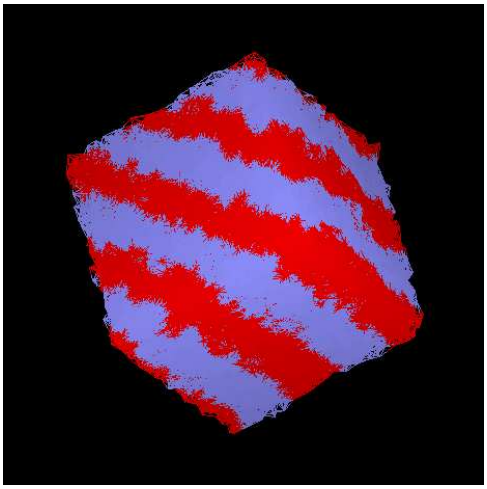

Abbildung 4.4: *Lamellar structure*

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4.1.9 Molecular Dynamics Simulations of Fuel Cell Membrane Material

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Technische Universität Darmstadt, Darmstadt

Polymers are one of the potential candidates to be used as the fuel cell membrane due to their flexibility in designing the structural and mechanical properties as required in various extreme conditions. Particulary poly vinyl phosphonic acid compound is one of the candidate material because of relatively high conductivity and its mechanical, chemical and physical stability.

In this work, atomistic simulations of the proton conductivity-polymer phase are carried out to explore the mechanism of proton transfer in these materials to improve the understanding and the use of polymers as fuel cell membrane.

In the molecular dynamics simulations, the model for the membrane material polyvinyl phosphonic acid has been built based on density and diffusion coefficients at different temperatures, taken from the experiments with heptyl phosphonic acid (In the picture one snapshot from the simulation of the Heptylphosphonic acid is seen). By use of this model, structural properties of the heptyl phosphonic acid material obtained. With the help of this data, a simulation model of poly (vinyl phosphonic acid) has been obtained and the structural properties of this polymer material are investigated. The mechanism of proton conductivity and its relation to the structural properties are being evaluated.

In the future it is possible to include different compound simulations as a candidate membrane material.

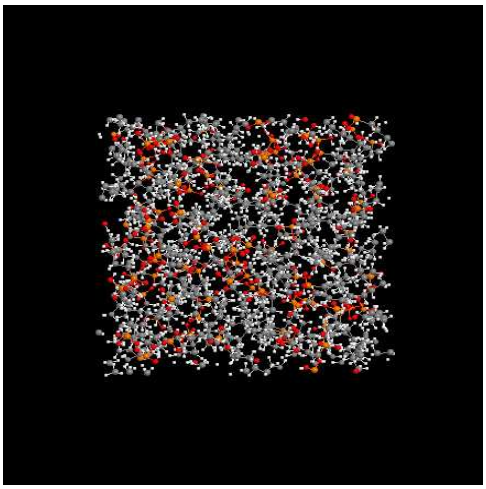

Abbildung 4.5: *100 Heptyl Phosphonic Acid molecules in a simulation box*

4.1.10 Effects of Additives on Lipid Membrane Fluidity Investigation by Molecular Simulation

Thomas J. Mueller and Florian Müller-Plathe
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Technische Universität Darmstadt, Darmstadt

Since the major goal of my PhD thesis is to study The Effects of Additives on lipid membrane fluidity, three of the four topics I m investigating at the moment are related to molecular simulation of bilayer systems. More precisely the membrane of interest consists of DPPC (Dipalmitoylphosphatocholine). All the simulations are calculated with YASP, the simulation package of the group. Transport properties of lipid molecules within a biological cell membrane system have already been studied by several groups. Nevertheless, the methods are very diverse and we add a new one to the list. The Reverse Non-Equilibrium Molecular Dynamics (RNEMD) method, which was introduced by Florian Müller-Plathe is applied for the first time to an inhomogeneous system to calculate the shear viscosity. Other properties like self diffusion and other benchmark parameters for the DPPC system are derived from equilibrium simulations. Transport of chemical agents within or through cell membranes is still one of the most frequent tasks of bilayer simulations. In this subproject we chose to investigate the differences in the physicochemical transport behaviour of heptane and mustard gas. Since these molecules can be considered similar in shape and size but not in the dipole moment and therefore in partial charges, this is also an investigation of the influence of charged particles within the membrane. Molecular simulation allows to study orientation and distribution not only in the equilibrium case but also in a case where the molecules are forced to traverse the membrane. The RNEMD technique can also be used to calculate heat transport and thus thermal diffusion coefficients. For heat transport through the membrane the system is highly inhomogeneous. Therefore the RNEMD technique allows no accurate calculation of diffusion coefficients. Nevertheless, preliminary results show that there are interesting asymmetries in ability to transfer heat in the different layer of the membrane which we try now to map to transport mechanism.

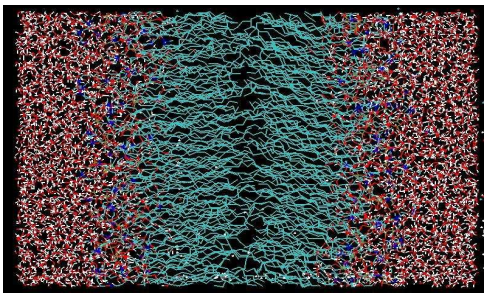

Abbildung 4.6:

4.1.11 Molecular-dynamics simulation of the liquid-vapor interface of aqueous solutions of salts and sugars

Volker Weiss, Daniel dos Santos, Florian Müller-Plathe
Theoretische physikalische Chemie, TU Darmstadt

Recent simulations of electrolyte solutions and their liquid-vapor interfaces [1] have cast doubt on the Onsager–Samaras picture of a depletion layer near the interface, which is considered to be responsible for the increase of the surface tension upon dissolution of salt [2]. By detailed molecular-dynamics simulations using the software packages YASP and GROMACS, we study the importance of the contributions of ionic charge, size, and polarizability of different solutes in an aqueous environment. Of particular interest are the sodium halides, NaF and NaI being the extreme cases featuring particularly hard and very soft anions, respectively. In the early simulations, Jungwirth and Tobias found the concentration of iodide ions to be enhanced near the interface, despite their ionic charges [1]. This accumulation of ions near the interface is of importance in atmospheric chemistry, since water droplets provide reaction sites for atmospheric processes. A similar behavior of the different sodium halides was found near hydrophobic solid surfaces [3]. In our work, we try to reconcile the molecular picture with the requirements that the laws of thermodynamics impose on the relation between negative adsorption and an increase of the surface tension, i.e., we will try to explain why the surface tension of aqueous NaI solutions is higher than the one of pure water, even though there is an apparent positive adsorption of iodide ions.

In a closely related project, solutions of sugars — glucose, to begin with — are simulated. For glucose, one also observes an increase of the surface tension; due to the neutrality of the molecule, this increase cannot be explained by charge repulsion from the interface, and the importance of polarizability effects and other dielectric properties can be examined. For sucrose, there is evidence of a repulsive van der Waals interaction, which keeps the sugar molecules from the interface and, thus, leads to an increase of the surface tension [4]. In addition to these theoretical insights, the molecular simulation can provide us with detailed information on the local structure of the solvent near the sugar molecule and help us to assess the significance of hydrogen bonds in these systems, which are of great importance in nearly all aspects of molecular biology.

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4.1.12 Shear Viscosity Studies in Polymer Melt Through Reverse Non- Equilibrium Molecular Dynamics Simulation

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Technische Universität Darmstadt, Darmstadt

The shear viscosity has been investigated by experiments. It is worth developing a numerical method, which can determine the shear viscosity of a large range of materials: (1), under normal conditions in order to avoid experiments and (2) under extreme conditions, which cannot be reasonably created experimentally in order to check theories and to predict the behavior of commercial materials. The existing simulations for the studies of viscosity are carried out through the two approaches: 1. using equilibrium molecular dynamics calculation based on the Einstein or Green-Kubo relations; 2. using Non-equilibrium molecular dynamics: reproducing the experimental setup by applying an external force on the system to perturb it out of equilibrium and measuring the resulting flux. Both approaches have their problems when it comes to practical calculation. A new method called Reverse non-equilibrium Molecular Dynamics (RNEMD) has been successfully applied to predict the viscosity of Lennard-Jones liquids and atomistic model of molecular liquids. This method has been proved as a very competitive method: they conserve, under certain condition, total energy and total linear momentum and, hence, need no thermostatting; they do not introduce artificial walls into the system and compatible with the usual periodic boundary conditions; the resulting raw data are well-defined, rapidly converging, and easily analyzed gradients.

Although RNEMD has successfully to predict the viscosity of Lennard Jones liquids which relaxation time is very short, it will encounter the typical limitations when it is implemented on polymeric systems by the inherent time scales in polymer. This cited limitation can be circumvented by coarsening the models and keeping the only those degrees of freedom that are deemed relevant for the particular range of interest. MD simulation software GMQ has been modified by our group in order to implement RNEMD method by the Coarse-Grained model. The system of Polystyrene and Polyamide 6,6 are in testing.

Application examples: Calculation of the shear viscosity of hexane by RNEMD.

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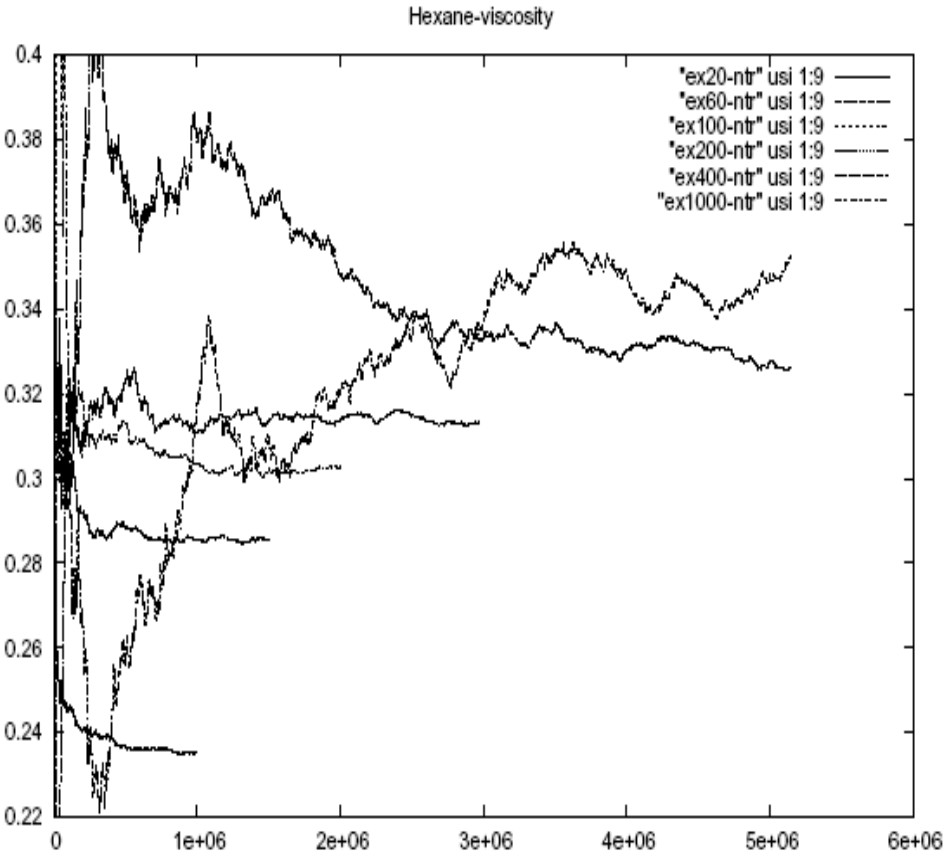

Abbildung 4.7: *Lamellar structure*

4.2 Physik

4.2.1 Self-consistent calculations of nuclear matter properties at nonzero temperature and density

Institut für Theoretische Physik, J.W. Goethe Universität Frankfurt
Christian Beckmann, Dirk H. Rischke, Dirk Röder, Jörg Ruppert

Relativistic heavy-ion collisions as studied at experimental facilities like GSI, BNL and CERN can provide insight into the modification of nuclear matter properties at nonzero density and/or temperature. At sufficiently large energies and system sizes they can therefore even offer the opportunity to study the deconfining and chiral phase transitions of QCD matter. We investigate such problems in an effective field-theory framework using many-body approximations. Since the coupling constant is not small, many-body resummation techniques have to be employed. A thermodynamically consistent framework is provided by Baym's Φ-functional approach. We use it in the form of the approach of Cornwall, Jackiw and Tomboulis, in which self-consistently coupled (Dyson-Schwinger) integral equations for the spectral functions of the physical degrees of freedom are derived. Their iterative solution requires considerable parallel computing power which is provided by the CSC. We have completed various projects along this line of work: broadening of the spectral function of the ρ-meson [1,2], studying chiral symmetry restoration in a linear sigma model with $O(N)$ symmetry beyond the Hartree-Fock approximation [3,4,5], and a self-consistent study of the Walecka model at nonzero density and temperature [6].

Examples of our results are shown in Fig. 1 and Fig. 2.

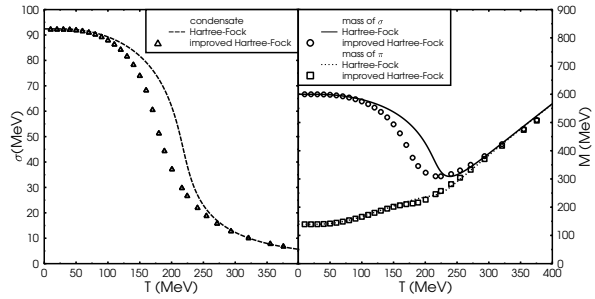

Fig. 1: The chiral condensate σ as a function of temperature as obtained for the standard and the improved Hartree-Fock approximation [4].

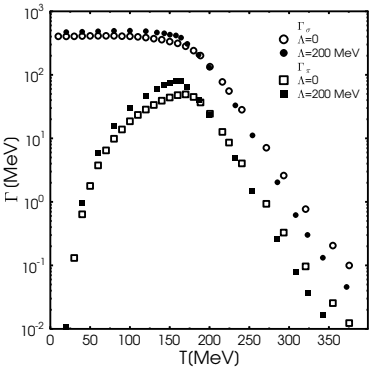

Fig. 2: The decay width of the pion and the sigma meson as a function of temperature [4].

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4.2.2 Plasminos in Superconductors

Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, Frankfurt am Main
B. Betz and D. H. Rischke

Hot and/or dense, normal-conducting systems of relativistic fermions exhibit a particular collective excitation, the so-called plasmino. Computing the dispersion relation and the spectral density for a model where fermions interact via attractive boson exchange, we show that such excitations also exist in superconductors at zero temperature. This is a question of general interest, independent of the specific nature of the superconductor.

The dispersion relation is given by the poles of the propagator

$$\mathcal{G}^{\pm} = \left([G_0^{\pm}]^{-1} + \Sigma^{\pm} - \Phi^{\mp} \left\{ [G_0^{\mp}]^{-1} + \Sigma^{\mp} \right\}^{-1} \Phi^{\pm} \right)^{-1} , \tag{4.1}$$

where $[G_0^{\pm}]^{-1}(P)$ is the inverse free propagator for (charge-conjugate) particles, $\Sigma^{\pm}$ is the self-energy for (charge-conjugate) particles and $\Phi^{\pm}$ is the (charge-conjugate) order parameter for condensation. The real parts of the self-energies (see Fig. 4.1), the roots of the propagator and the spectral density have to be computed numerically.

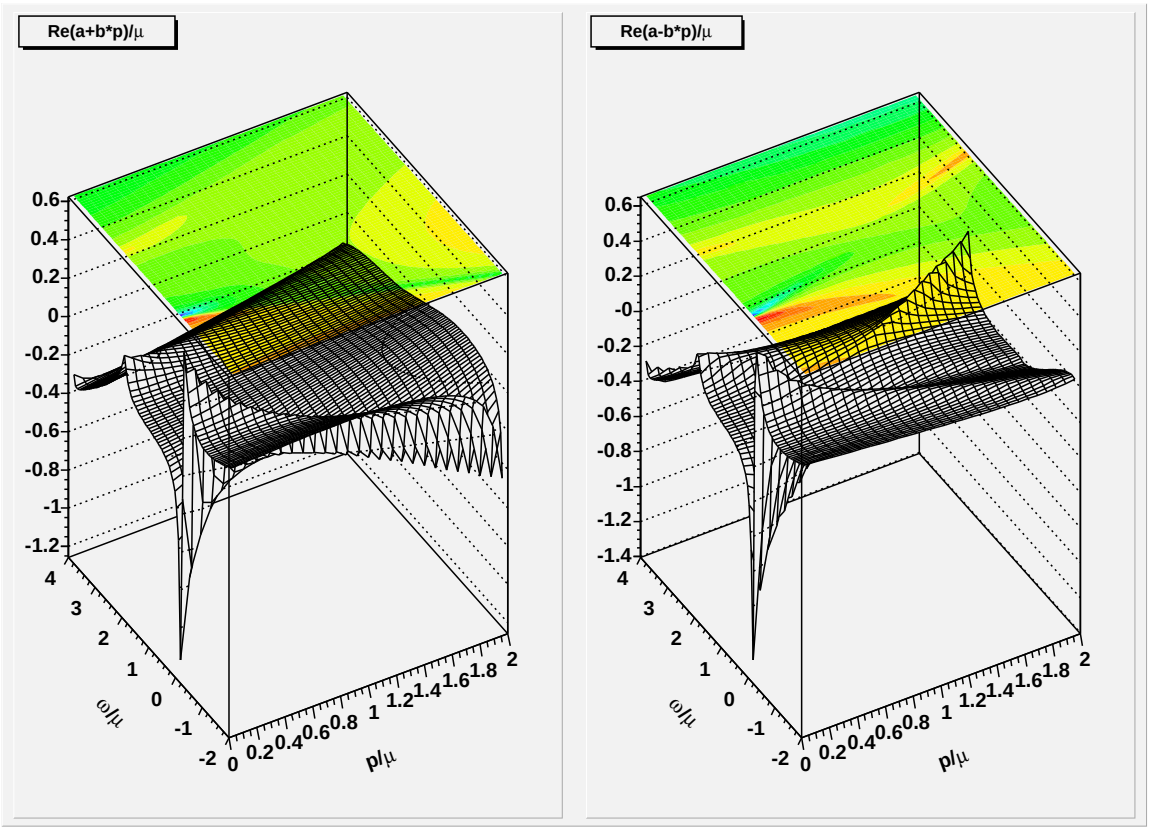

Abbildung 4.8: *The real parts of the self-energy for massless superconducting fermions (left panel) and antifermions (right panel), at $T = 0$, for $\phi_+ = 0.25\,\mu$ and $\phi_- = 0$.*

[1] Barbara Betz and Dirk H. Rischke: *Are there plasminos in superconductors?*, to be published.

4.2.3 Numerical Simulation of the hadron-string dynamics in heavy ion collisions

Institut für Theoretische Physik, Goethe Univ. Frankfurt
M. Bleicher et al.

At RHIC, measurements of the elliptic flow v_2 and the nuclear modification factor $R_{AA,CP}$ for identified particles have led to the conclusion that hadrons ought to be formed via the coalescence or recombination of massive quarks. A cornerstone of this conclusion is the observed number-of-constituent-quark (NCQ-) scaling of the flow of baryons vs. mesons. Because this interpretation addresses key issues in high-energy nuclear collisions such as deconfinement and chiral symmetry restoration, it is of utmost importance to conduct a systematic study of other possible explanations for the observed particle type dependencies.

For these analysis we employed two independent hadron-string transport models RQMD(v2.4) and UrQMD(v2.2) to study the effect of hadronic cross sections, kinematics etc. on the particle type dependence of v_2. These model solve a set of many thousand coupled integro-differential equations to yield the phase space dynamics of hadrons and color flux tubes (strings).

Fig. 1 shows the result of the calculations of the (scaled) elliptic flow of various hadron species. Note that the hadron mass hierarchy is qualitatively well reproduced in the low p_T region. Rescattering is the key that leads to the quasi-ideal hydrodynamic appearance in $v_2(p_T)$. Also in the intermediate p_T region, the hadron type dependence (number-of-constituent-quark scaling) is predicted by both hadronic transport models.

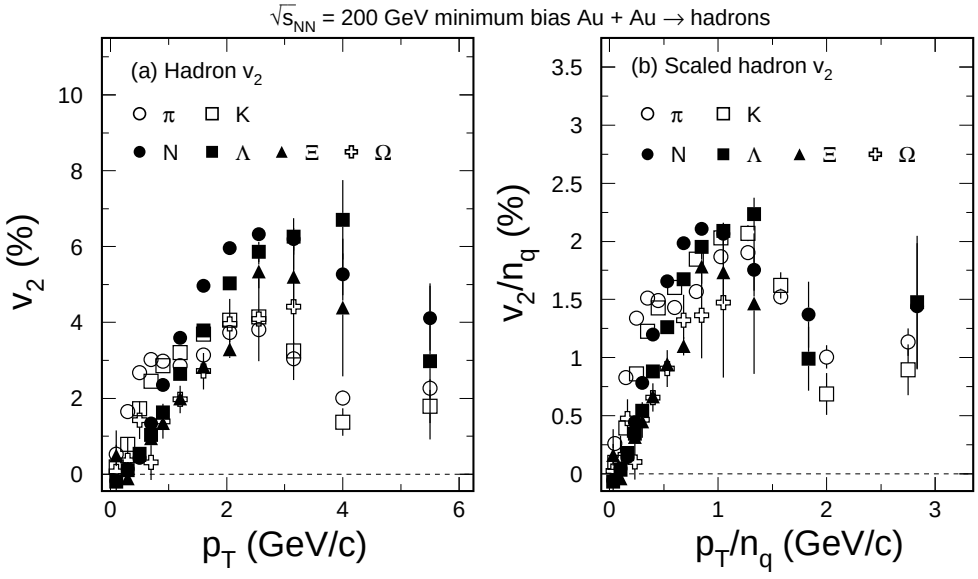

Abbildung 4.9: *(a) Hadron v_2 from minimum bias Au+Au collisions at $\sqrt{s_{\rm NN}} = 200$ GeV; (b) Scaled hadron v_2 results are shown. The n_q refers to the number of constituent quarks. Symbols represent results from the UrQMD (v2.2) model for various hadron species. At low $p_T/N_q \leq 0.5$ GeV/c, π does not follow the scaling perhaps caused by the resonance decay. In higher p_T region, K meson seems to fall off the scaling curve due to the comparatively small hadronic cross sections in the model.*

1. **"Anisotropic flow at RHIC: How unique is the number-of-constituent-quark scaling?"**

Y. Lu *et al.*
arXiv:nucl-th/0602009

2. **"Elliptic flow analysis at RHIC with the Lee-Yang zeroes method in a relativistic transport approach"**
X. l. Zhu, M. Bleicher and H. Stoecker
arXiv:nucl-th/0601049

3. **"Radial and elliptic flow in high energetic nuclear collisions"**
X. Zhu, H. Petersen and M. Bleicher
AIP Conf. Proc. **828**, 17 (2006)

4.2.4 Outer crust of nonaccreting cold neutron stars

Institut für Theoretische Physik, J. W. Goethe-Universität Frankfurt
Stefan B. Rüster, Matthias Hempel, and Jürgen Schaffner-Bielich

We investigated the outer crust of nonaccreting cold neutron stars [1]. In order to obtain the sequence of nuclei in the outer crust, we applied the model of Baym, Pethick, and Sutherland [2]. In constrast to earlier works, we used modern nuclear data and theoretical mass tables in order to update previous works and show the influences of pairing, deformation, and relativity, and the resulting differences in the sequences of nuclei in the outer crust. We show our main results in Fig. 1, the sequences of nuclei which are obtained by using the five most modern of all 21 investigated nuclear models.

Each nuclear mass table of every model contains *thousands* of nuclei and their corresponding data, which was processed in our source code. As the ground state nucleus is density dependent, it was necessary to perform the calculation at every single density, beginning at the surface and ending at the neutron drip point. Especially the computation of the phase transitions, the exact points, where the jumps from one nucleus to another take place, see Fig. 2, demanded a lot of computer resources. We used the XEON cluster of the Center for Scientific Computing (CSC) of the Johann Wolfgang Goethe-Universität for our project.

The authors are grateful for using the CSC of the Johann Wolfgang Goethe-Universität.

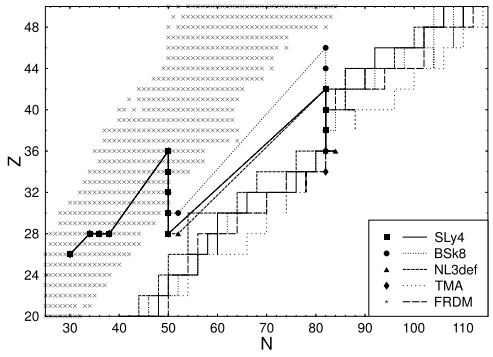

Abbildung 4.10: *Sequences of nuclei of the outer crust of nonaccreting cold neutron stars by using the five most modern nuclear models.*

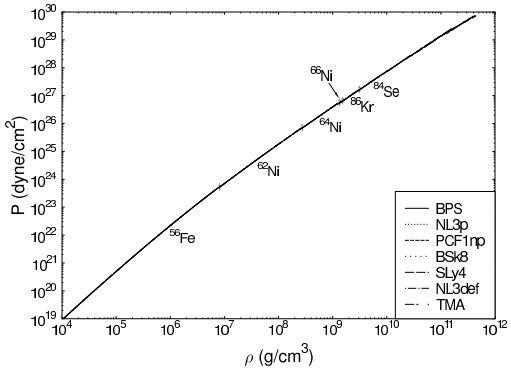

Abbildung 4.11: *Equations of state of the crust of nonaccreting cold neutron stars by using various nuclear models in the BPS model. The crosses mark the phase transitions to another nucleus.*

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4.2.5 DFT-Studies on the Oxygen Reduction Reaction in PEM-Fuel Cells

Fachgebiet Theoretische Physik, Universität Kassel
T. Jacob, J. Anton, W.-D. Sepp, B. Fricke

Nowadays most of the daily energy comes from burning fossile energy resources such as oil, natural gas, or coal. Besides the problems arising from an enormous amount of CO_2 emitted during this process, estimates for the finish of these non-renewable power resources range from one to only a couple of hundred years.

In this context fuel cells should be seen as possibility to directly convert chemical in electrical energy without being limit by the Carnot effect. However, there still exist a variety of problems regarding a better mechanical stability, improved water management, and most important enhanced efficiency. Especially the last aspect requires a deep knowledge about the processes occurring in a fuel cell under operating conditions on the atomic scale.

While the overall fuel cell reaction ($^1/_2$ O_2 + 2 H^+ + 2 e^- $\xrightarrow{Pt}$ H_2O) seems to be rather simple, the exact mechanism of this oxygen reduction reaction (ORR) is still unknown. Therefore a series of density functional theory (DFT) calculations with a parallelized program-code were performed on all possible intermediates that could be present during the ORR on Pt catalysts [1,2]. After calculating binding energies and structures, we also studied various dissociation processes, which allowed for bridging between the intermediates. On the basis of these calculations we were finally able to draw the full reaction pathway (Fig. 4.12). The lowest reaction barriers were obtained for a mechanism in which after adsorption of H_2 and O_2, adsorbed H_2O_2 is formed by two hydrogenation processes. Then the O-O bond dissociates to form two OH molecules on the surface, which then use an adsorbed hydrogen to form water (see dashed arrows in Fig. 4.12).

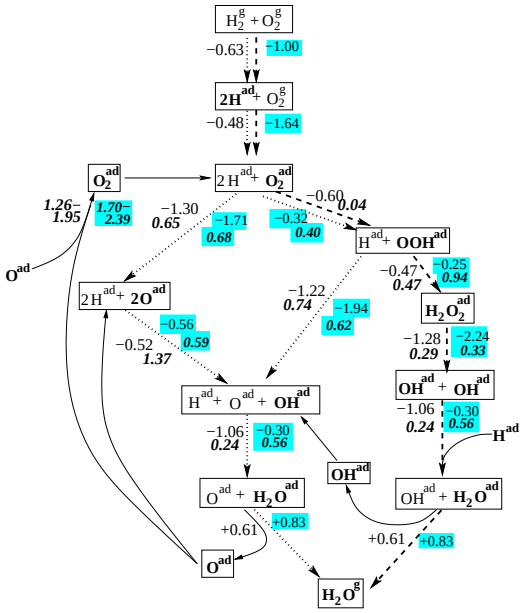

Abbildung 4.12: *Reactions Pathways for the ORR. Dashed arrows mark the mechanism in gas-phase, and dotted arrows after including the surrounding water (energies are highlighted by boxes). All energies and barriers (italic) are in eV.*

Since in the realistic fuel cell the cathode is always hydrated, we afterwards included the water environment to the calculations by a self-consistent reaction field approach (SCRF). In contrast to the gas-phase mechanism, we found that the pathway involving H_2O_2 is blocked, but now the mechanisms in which O_2 either dissociates directly or first forms OOH, which then dissociates to O + OH, are preferred (see dotted arrows in Fig.4.12) [2]. This shows that using gas-phase results is not necessarily appropriate for realistic systems.

Summarizing, these results are most relevant for understanding the ORR under realistic conditions, but also for the development of new and better catalysts [3].

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4.2.6 Orbital-dependent correlation energy functionals

Inst. für Theor. Physik, J.W.Goethe-Universität Frankfurt
H. Jiang and E. Engel

The success of density functional theory relies on the quality of the standard approximation for the exchange-correlation (xc) energy functional, the generalized gradient approximation (GGA). However, the GGA fails for some interesting problems, as highly correlated solids and dispersion forces. A systematic improvement over the GGA is offered by xc-functionals depending on the Kohn-Sham (KS) orbitals. In this formalism, the exchange energy can be treated exactly, which solves the long-standing self-interaction problem. However, neither the complete neglect of correlation nor the combination of the exact exchange with a conventional correlation functional is adequate. In this project, we investigate orbital-dependent correlation functionals E_c derived from perturbation theory on the basis of the KS Hamiltonian. The resulting lowest (second) order functional $E_c^{[2]}$ (MP2) is the first approximation for which the associated potential shows both the correct asymptotic behavior and the correct shell structure [1-3]. However, the magnitude of the exact v_c is significantly overestimated. Moreover, $E_c^{[2]}$ is variationally unstable, which shows up for systems for which the highest occupied (HOMO) and lowest unoccupied KS states are energetically close. Higher order correlation contributions can be included by partial resummation of the perturbation series to infinite order. Already the simplest resummation scheme, the hole-hole Epstein-Nesbet (HHEN) resummation, resolves the variational instability problem for all practical purposes and leads to a significant quantitative improvement [4].

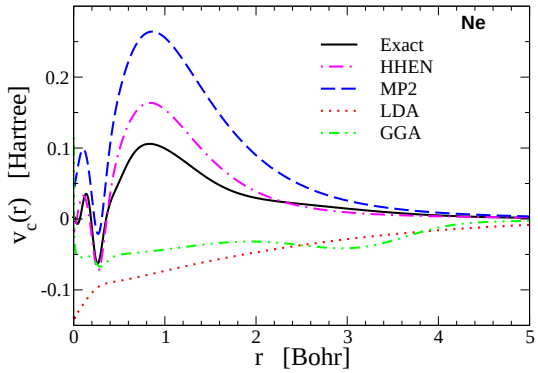


Fig. 1: Correlation potentials of Ne obtained from different E_c versus exact v_c.

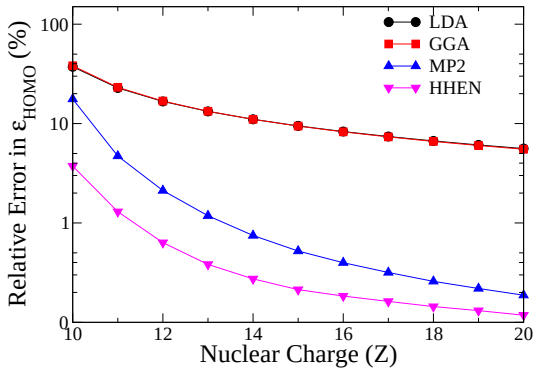


Fig. 2: Percentage errors of HOMO eigenvalues of the Ne isoelectronic series.

[1] E. Engel and H. Jiang, Solubility of the OPM integral equation for finite systems, *Phys. Rev. A* **72**, 052503 (2005)

[2] H. Jiang and E. Engel, Second Order Kohn-Sham Perturbation Theory: Correlation Potential for Atoms in a Cavity, *J. Chem. Phys.* **123**, 224102 (2005)

[3] E. Engel and H. Jiang, Orbital-dependent representation of the correlation energy functional: Properties of second order Kohn-Sham perturbation expansion, *Int. J. Quant. Chem., in press* (2006).

[4] H. Jiang and E. Engel, Kohn-Sham Perturbation Theory: Simple Solution to Variational Instability of Second Order Correlation Energy Functional, *subm. to J. Chem. Phys.* (2006).

4.2.7 Description of hadrons in the high density phase

Institut für Theoretische Physik, Universität Frankfurt
G. Martens, C. Greiner

It is a common belief that Quantum Chromodynamics (QCD) should be able to describe all systems ruled by strong interactions. These cover a wealth of different regimes ranging from the dynamics of quasi free quarks and gluons in a quark gluon plasma (QGP) at high temperatures or densities, over the formation of hadrons out of quarks to the interactions between those color neutral hadrons. However, in this latter region of small relative momenta, where the confinement phenomenon plays a dominant role, no convincing analytical techniques have been established yet.

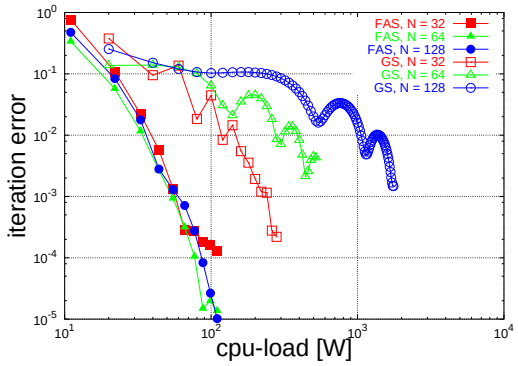


Abbildung 4.13: *Numerical efficiency of the FAS-algorithm compared to Gauß–Seidel-relaxation (GS).*

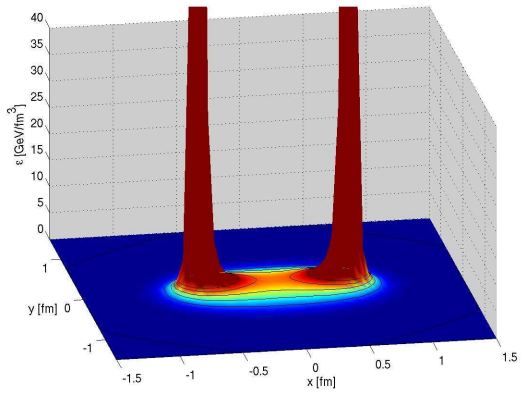


Abbildung 4.14: *Electric flux tube of a quark-antiquark-pair.*

We use the chromodielectric model to simulate the interaction between color charged quarks. The resulting equations of motion of the quarks and both the color electric field and the confinement field are solved with the Full-Approximation-Storage multigrid algorithm (FAS) (see Fig. 4.13).

The aim of our studies is twofold. First we compare our results to those obtained in QCD lattice calculations where possible, e.g. in the analysis of a quark-antiquark-pair (see Fig. 4.14) or the interaction between two of these pairs. There the characteristics of the system are well reproduced even quantitatively. Second we describe the transition of a system of well isolated hadrons to a system of dense quark matter (see Fig. 4.15). The melting of the hadrons into quark matter is observed at an energy density of about 1 GeV/fm^3.

[1] G. Martens, C. Greiner, S. Leupold and U. Mosel: Interactions of multi-quark states in the chromodielectric model *Phys. Rev. D 73*, 096004, 2006

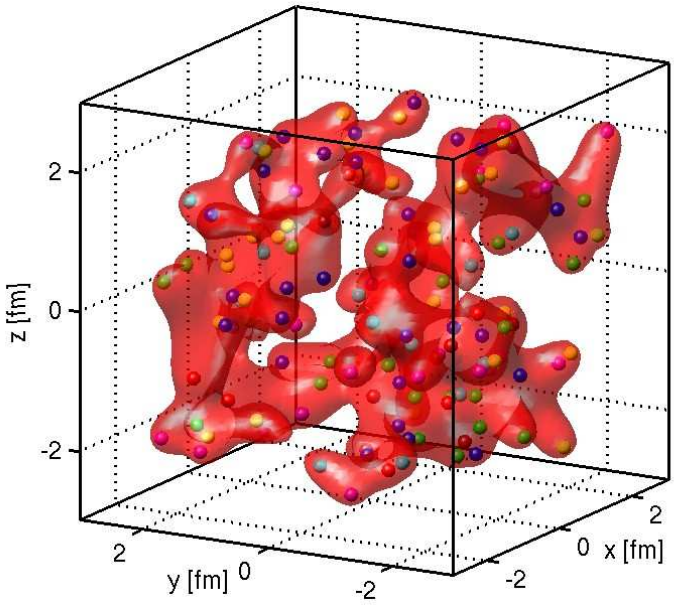


Abbildung 4.15: *High density phase of a quark-system.*

4.2.8 TDHF Simulations of Low-Energy Nuclear Collisions

Institut für Theoretische Physik, Universität Frankfurt
J.A. Maruhn, P.-G. Reinhard[1], P.D. Stevenson[2], M.R. Strayer[3]

The time-dependent Hartree-Fock method allows a microscopic description of heavy-ion reactions that is fully quantal and contains a good description of nuclear ground states when employing modern two-body interactions of the Skyrme type. The method was originally developed in the '70s but could not be fully explored owing to the limited capabilities of computers of that time. We have now written a code that allows for general Skyrme forces, complete three-dimensional treatment and also fully contains the spin degrees of freedom.

An investigation of collisions of ^{16}O on ^{16}O at energies between 50 and 150 MeV yielded the surprising result that the spin-orbit force causes an azimuthat spin excitation as depicted in Fig. 4.16. The energy stored in such an excitation is of the order of 2 MeV after reseparation and depends only weakly on impact parameter, so that it could well be observable in the final states.

In additional test it was shown that if the original, non-Galilei invariant version of the Skyrme density functional is employed, enrgy from collective translation of a nucleus is lost through just such a spin excitation, although it is spurious in this case.

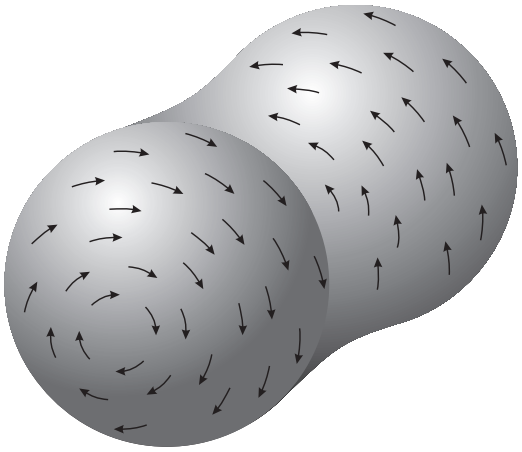


Abbildung 4.16: *Artist's impression of the spin excitation generated in heavy-ion collisions. Based on actual calculations.*

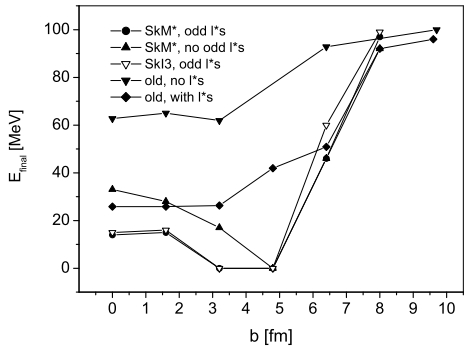


Abbildung 4.17: *Final energy in ^{16}O on ^{16}O collisions for various Skyrme forces.*

Fig. 4.17 shows the final energy of collisions at various impact parameters for 100 MeV initial center-of mass energy. Compared to "old" results it appears that quantitatively there is some convergence as more degrees of freedom are included and more modern, better Skyrme forces employed.

[1] J.A. Maruhn, P.-G. Reinhard, P.D. Stevenson, M.R. Strayer: *Spin-Excitation Mechanisms in Skyrme-Force Time-Dependent Hartree-Fock*, Phys. Rev. C, 2006 (accepted for publication).

[1] Institut für Theoretische Physik, Universität Erlangen
[2] University of Surrey, Guildford, UK
[3] Department of Energy, Washington DC

4.2.9 Alpha Cluster Structure and Exotic States in Light Nuclei

Institut für Theoretische Physik, Universität Frankfurt
J.A. Maruhn, M. Kimura[4], S. Schramm, P.-G. Reinhard[5], H. Horiuchi[6], A. Tohsaki[7]

We examined to what extent traces of α clustering can be found in mean-field ground states of $n\alpha$-nuclei from ^{8}Be through ^{36}Ar as well as in some superdeformed states in ^{32}S, ^{36}Ar, and ^{40}Ca. For this purpose we calculate the overlap of the Skyrme-force mean-field Slater determinant with one containg pure Gaussians and perfect spin and isospin symmetry, optimizing the overlap by varying the α-particle positions and radii. In some cases a coherent sum over different configurations is also employed. We find quite large overlaps for some of the lighter systems that diminish for nuclei above ^{20}Ne but again strong clustering in ^{36}Ar.

In most cases a systematic search for the α-configuration that produced maximum overlap of the many-body wave functions yielded optimal results. Fig. 4.18 shows the geometric configurations obtained in each case. In many cases, though, the separation of α-particles was very small, indicating that neighboring Gaussians serve to generate higher shell-model orbitals through anti-symmetrization.

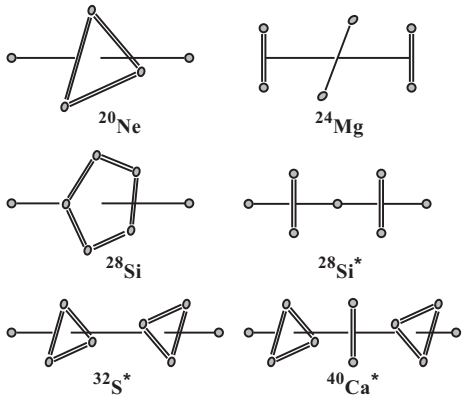


Abbildung 4.18: *Visualization of the cluster geometry present in the Mean–Field ground or excited superdeformed states (denoted by asterisks). The figures only illustrate the topology; no attempt was made to reproduce correct scale lengths. Double links between particles indicate very small distances. The triangles and pentagon are perpendicular to the linear links.*

[1] J.A. Maruhn, M. Kimura, S. Schramm, P.-G. Reinhard, H. Horiuchi, A. Tohsaki: *Alpha Cluster Structure and Exotic States in a Self-Consistent Model for Light Nuclei*, Preprint nucl-th/0606053, 2006.

[4] Yukawa Institute for Theoretical Physics, Kyoto, Japan
[5] Institut für Theoretische Physik II, Universität Erlangen
[6] Physics Department, Kyoto University, Kyoto, Japan
[7] Suzuki Corporation, 46-22 Kamishima, Kadoma, Japan

4.2.10 Optimization of Multiple Response Processes - Inversion of Geodynamic and Seismic Constraints for Models of Large-scale Viscous Flow in the Earth's Mantle

Institut für Geowissenschaften, Facheinheit Geophysik, Goethe-Universität Frankfurt
K. Niehuus, H. Schmeling

Numerical simulation of viscous flow in the Earth's Mantle requires assumptions about rheology and density anomaly distributions which may be inferred, with large uncertainties, from mineralogical, seismic and geodynamic constraints. A model's validity is constrained by globally observable quantities (plate velocities, gravity, dynamically induced topography, surface heat flux, seismic velocity anomalies from global tomography).

In order to determine distributions of thermally vs. chemically induced seismic velocity anomalies and to test appropriate assumptions of variable rheology, in this study models of global viscous flow are optimized to render predictions consistent with observables and to follow mineralogical constraints from laboratory experiments. The multiple responses (observable predictions) of a given forward model and the consistency of its parameters with inferred constraints contribute to its overall quality determined with the desirability function approach (commonly employed in Design of Experiment) in various search methods applied to optimize overall quality: classic Monte-Carlo (MC), Downhill Simplex (DS), Neighbourhood Algorithm (NA).

The instantaneous system response (forward model) is determined analytically for radially variable viscosity. The equations for thermal convection in a sphere (continuity, Navier-Stokes) are transformed to a set of quadratic first-order ordinary differential equations suitable for analytical integration with repsect to radius using a classical propagator matrix technique: A closed expression for the product-sum conversion of spherical harmonics and their derivatives to any order is applied to the quadratic terms arising from advection, dissipation and linear temperature-dependence of viscosity.
For laterally variable viscosity, each mode is still treated separately under assumption of an averaged radial viscosity. The addition of a viscous-load term on the right-hand side of the ODEs accounts for the mode coupling and now requires an iterative solution.

Any optimization method requires calculation of large quantities of forward models if the search is undirected (MC) or local minima are to be avoided (NA, repeated reinitialization of randomly perturbed optimized simplex (DS)). Therefore, optimizations involving an iterative solution of the system's responses are computationally expensive, while for various search methods (MC, NA) computation is readily parallelized and is thus performed time-effectively on the CSC cluster.

4.2.11 Probing the late stage of heavy ion reactions using resonances

Institut für Theoretische Physik, J.W.Goethe-Universität Frankfurt am Main
Sascha Vogel and Marcus Bleicher

One of the most interesting topics of today's research in physics is the study of properties of nuclear matter under extreme conditions, i.e. very high temperatures and densities. One expects several phase transitions for highly excited nuclear matter, one of them is the chiral phase transition, where chiral symmetry is expected to be (partially) restored. One of the key observables for the restoration of the chiral symmetry is the expected change of the spectral function of the ρ meson and thus the changed mass-spectrum compared to a Breit-Wigner-distribution.
However, one has to consider kinematical effects which do not imply chiral symmetry restoration and still change the mass distribution of the ρ meson. In order to disentangle kinematical effects from effects originating from chiral symmetry restoration one has to apply a transport model approach to describe the dynamics of the system and to investigate binary hadron hadron collisions. The model used in Frankfurt is the Ultra Relativistic Molecular Dynamics (UrQMD) model, which has been developed over the past decade.
In order to study resonance effects one has to handle complex array structures and large output files, which is impossible without a dedicated scientific computer cluster. In order to compare with experimental results several thousand events for intermediate energies or several million events for low energies are necessary to draw definite and stringent conclusions.
One recent result is depicted in figure 1. Shown is the mass spectrum of the ρ^0 meson for a carbon-carbon collision at 2 AGeV and the corresponding production channels of the ρ meson. One observes that the $N^*(1520)$ decay chain $N^*(1520) \rightarrow N + \rho$ contributes strongly into the low mass region, whereas pion pion absorption feeds into the expected pole mass region of 770 MeV.

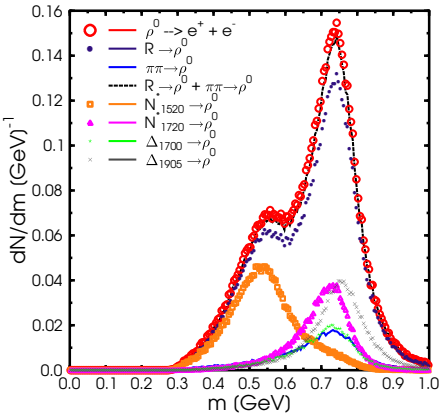


Fig. 1: Mass spectrum of the ρ^0 meson and the corresponding production channels. One observes that the ρ meson originating from a high mass baryon resonance decay or from ππ annihilation contribute to the high mass part of the spectrum, whereas ρ mesons originating from $N^*(1520)$ decays contribute to the mass regime of about 500 - 600 MeV.

[1] S. Vogel and M. Bleicher, Reconstructing ρ^0 and ω mesons from non-leptonic decays in C+C collisions at 2 GeV/nucleon in transport model calculations, Phys. Rev. C
[2] S.Vogel and M. Bleicher, Resonance Dynamics in Heavy Ion Collisons - what can we learn from RHIC?, Heavy Ion Physics
[3] D. Schumacher, S. Vogel and M. Bleicher, Theoretical Analysis of Dilepton Spectra in Heavy Ion Collisions at GSI-FAIR Energies, to be published

4.2.12 Quantum-mechanical Calculations of Inorganic Solids

Institut für Mineralogie, Abteilung Kristallographie, J W Goethe Universität, Frankfurt
B. Winkler, D. J. Wilson, S. Lowitzer

As part of the MaterialsGrid project [1], we have been performing accurate density functional theory calculations on a wide range of inorganic crystal structures. The CSC and HHLR computing facilities have been used for calculations that concentrate on the following areas.

Hydrogen-bond containing minerals

We have performed extensive calculations on hydrogen-bond containing minerals, from relatively simple structures such as beryllium hydroxide ($Be(OH)_2$) and diaspore (α-AlOOH), up to much larger structures such as mozartite ($CaMnO(SiO_3(OH))$, in order to examine the existing empirical relationships between observed vibrational frequencies and H···O bond lengths [2] (Fig. 1). While the agreement is in general fairly good, deviations have been observed in the low frequency-small hydrogen bond length region.

Defect properties of Mercurian minerals

The feldspar group of minerals have been implicated in the formation of the exosphere of the planet Mercury. Although models exist that attempt to explain these processes, the energy required to remove cations from these minerals has not been known.

We have calculated the point defect energies, and the Schottky defect formation energy, for albite ($NaAlSi_3O_8$), a typical feldspar mineral. In order to obtain accurate results, these calculations required very large supercells containing over 200 ions (Fig. 2). As such, the use of large-scale computing facilities was a necessity.

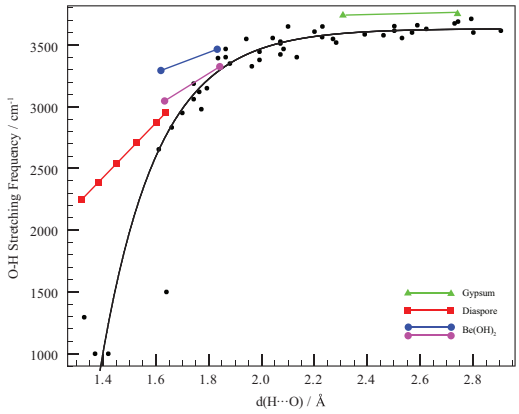


Fig. 1: Calculated O-H stretching frequencies for a number of minerals, as a function of hydrogen-bond length, superimposed upon the experimental results reported by Libowitzky.

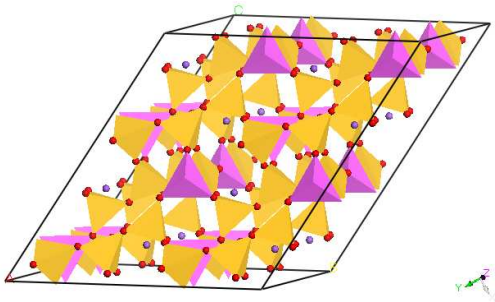


Fig. 2: Supercell of albite ($NaAlSi_3O_8$). Orange and pink tetrahedra represent SiO_4 and AlO_4 units respectively, while purple spheres represent the sodium ions.

[1] http://www.materialsgrid.org

[2] E. Libowitzky: Correlation of O-H Stretching Frequencies and O-H···O Hydrogen Bond Lengths in Minerals, *Monat. Chemie*, **130**, 1047-1059 (1999)

4.2.13 Optical properties of semiconductor photonic crystals

AG theoretische Halbleiterphysik, Philipps Universität Marburg
B. Pasenow, M. Reichelt, T. Stroucken, T. Meier, and S.W. Koch

Various aspects of light matter interaction can be modified in suitably designed semiconductor photonic crystal systems. To analyze such effects, we use a microscopic theory which is capable to describe the optoelectronic properties of hybrid systems. This leads us to the Maxwell semiconductor Bloch equations, i.e. the coupled system of the Maxwell and microscopic semiconductor Bloch equations, which have to be solved in a self-consistent way.
The repeated unit of one of our model systems is shown in fig. 1. The structure is a one dimensional photonic crystal. As active material semiconductor quantum wires are placed in a homogeneous substrate below the photonic crystal. Such structures allow for investigations on the transverse (e.g. coupling to photonic crystal modes) as well as on the longitudinal properties (e.g. Coulomb interaction) of the photonic crystal.
Due to self induced surface polarizations the Coulomb interaction between the charged particles is modified. These modifications lead to the appearance of several spatially inhomogeneous excitonic resonances instead of one homogeneous resonance (fig. 2). With an optical light field superpositions of these excitonic resonances can be excited which lead to interesting wavepacket dynamics of the electron densities in the quantum wires (fig. 3).
As a consequence of the spatial inhomogeneity of the dynamic variables such calculations are very time and memory demanding. Depending on the structure size the light field propagation (using FDTD algorithm) has to be parallelized.

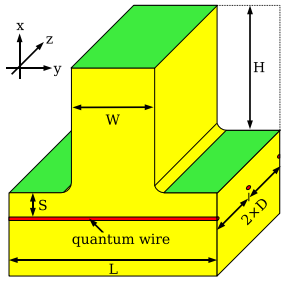


Fig. 1: Schematic picture of the semiconductor photonic crystal

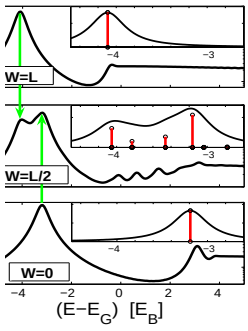


Fig. 2: Inhomogeneous excitonic resonances and the two limiting homogeneous cases

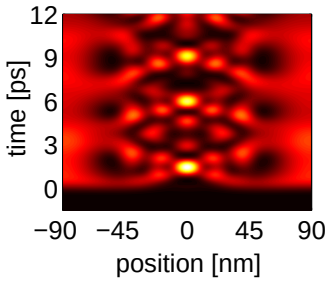


Fig. 3: Coherent electron density dynamics inside the quantum wires

[1] B. Pasenow, M. Reichelt, T. Stroucken, T. Meier and S.W. Koch: *"Excitonic wave packet dynamics in semiconductor photonic-crystal structures*, Physical Review B, 71:195321, 2005

[2] M. Reichelt, B. Pasenow, T. Meier, T. Stroucken and S.W. Koch: *Spatially inhomogeneous optical gain in semiconductor photonic-crystal structures*, Physical Review B, 71:035346, 2005

[3] R. Eichmann, B. Pasenow, T. Meier, T. Stroucken, P. Thomas and S.W. Koch: *Semiconductor excitons in photonic crystals*, Physica Status Solidi B, 238:439-442, 2003

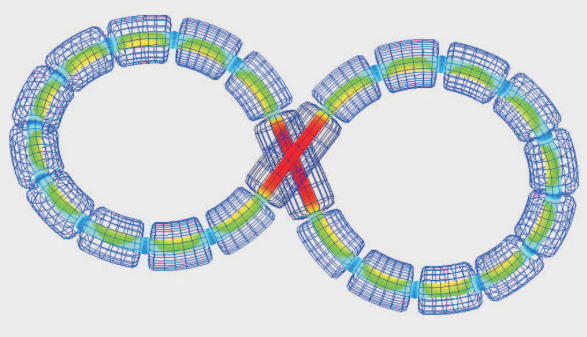
4.2.14 Design Studies on High Current Storage Ring

Institut für Angewandte Physik, J.W. Goethe Universität, Frankfurt am Main
M. Droba, N. Joshi, U. Ratzinger, R. Tiede

A novel type of a high current storage ring for the accumulation of proton and ion beams from the 150kV high current injector is under investigation at Frankfurt University. The configuration is based mainly on a toroidal magnetic field for the storage of intense low energy ion beams.

Due to the 3D-geometry of the ring and to the occurrence of torsion, the magnetic field lines are not simply closed. They lie on folded surfaces and show along the ring circumference the poloidal rotation ι. The collective behaviour of the beam including in some cases space charge compensating electrons additionally, is being studied using in-house developed codes running on the parallel computer cluster of the Center for Scientific computing (CSC), Frankfurt University.

Using 64 Opteron processors of the CSC parallel cluster the magnetic field is mapped in a special manner through the whole structure and the magnetic coordinate system (Ψ - toroidal flux enclosed by surface and actual radial coordinate, θ - poloidal angle, ξ - toroidal angle) is calculated. The figure shows one closed magnetic surface inside the ring by a colour coded B-field profile.



The metric coefficients for the Poisson solver are calculated. A FDTD symplectic solver with drift approximation is used to calculate the new position of the particles in given fields within the coordinate system. Here up to 10^7 macro particles of different species are possible. 10 processors are used for the Poisson solver, with 20x60x100 mesh points each. In every step the boundary data are exchanged and the potential profile is solved by an iteration method (BiCGSTAB - Bi- Conjugate Gradient Method - Stabilized). To save computational memory the sparse matrix format is used. At present the code is tested and prepared for first studies.

1. M. Droba, et. al., “High Current Ion Beams at Frankfurt University”, EPAC’04, Lucerne, July 2004, p. 1198, http://www.jacow.org.

2. M. Droba, et. al., “Design Studies on a Novell Stellarator type High Current Ion Storage Ring”, EPAC’06, Edingurgh, June 2006,accepted.

4.2.15 Phase Diagram of Neutral Quark Matter

Institut für Theoretische Physik, J. W. Goethe-Universität Frankfurt
Institut für Kernphysik, TU Darmstadt
S. B. Rüster, V. Werth, M. Buballa, I. A. Shovkovy, and D. H. Rischke

At sufficiently high densities and sufficiently low temperatures, quark matter is a color superconductor. In nature, such conditions could be found in the interior of compact stars. Quark matter in compact stars is neutral with respect to electric and color charges. In Refs. 1 and 2, we investigated the phase diagram of neutral color-superconducting quark matter as a function of temperature, quark chemical potential, and lepton chemical potential.

We find a multitude of different phases, see Fig. 1: besides the normal quark matter phase (NQ) and the phase where chiral symmetry is spontaneously broken (χSB), there is color-superconducting quark matter with two- (the 2SC phase) and three-quark flavor pairing (the color-flavor-locked, or CFL, phase). Furthermore, requiring electric and color neutrality forces the Fermi surfaces of quarks of different flavor and color apart and leads to so-called gapless phases (g2SC, gCFL) where some quasiparticle excitations do not exhibit a gap at the Fermi surface. Finally, there is also a superconducting phase where up quarks pair with down and with strange quarks (the uSC/guSC phase), but where down and strange quarks do not pair.

A nonzero lepton chemical potential favors the 2SC phase and disfavors the CFL phase, see Fig. 2.

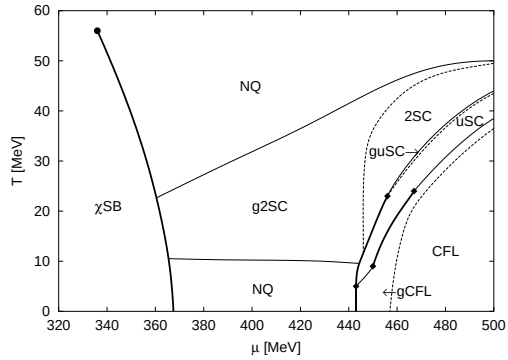


Fig. 1: The phase diagram of neutral quark matter at zero lepton chemical potential.

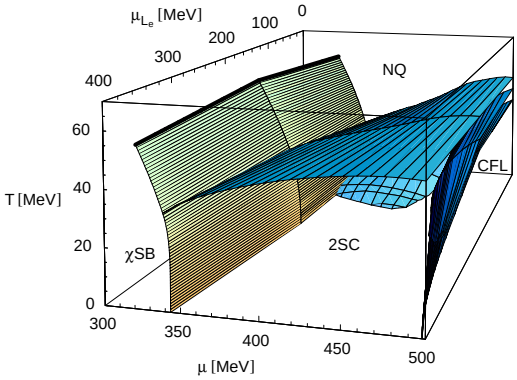


Fig. 2: The phase diagram of neutral quark matter at nonzero lepton chemical potential.

[1] Rüster, V. Werth, M. Buballa, I. A. Shovkovy, and D. H. Rischke, Phys. Rev. D **72**, 034004 (2005).

[2] Rüster, V. Werth, M. Buballa, I. A. Shovkovy, and D. H. Rischke, Phys. Rev. D **73**, 034025 (2006).

4.2.16 Adsorption of Element 112 on a Au (100) surface

Fachgebiet Theoretische Physik, Universität Kassel
C. Sarpe-Tudoran, B. Fricke, J. Anton

Element 112 is located in the Periodic system at the end of the 6d-series having a closed 6d and 7s shell [1]. This structure probably leads to a chemical behaviour which is expected to be somewhere between that of its homologue Hg and that of the noble gas Rn [2]. A summary of the state of the art of superheavy elements is given in Ref. [3]. There are a number of different methods which allow to calculate the adsorption energy of one element on a specific surface. We calculate the problem of the adsorption of element 112 on a Au surface with our relativistic molecular density-functional code [4]. We simulated the surface by a cluster which contains the metal atoms located around the adsorption position, which as an example is shown in Fig. 4.19 for a Au_{14} inner cluster surrounded by 113 environmental atoms plus an adatom.

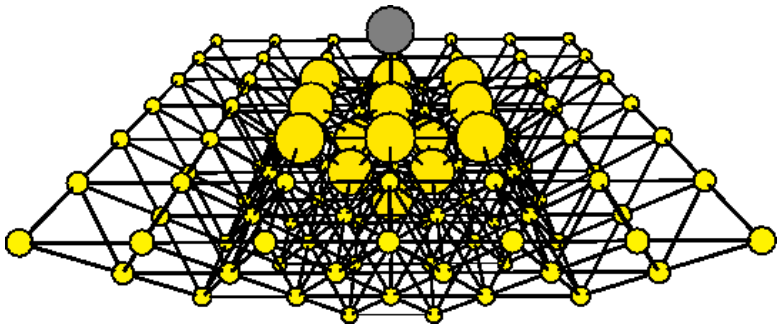


Abbildung 4.19: *Structure of the atoms in an* $Au_{14}(9,4,1)$ *embedded cluster*

Tabelle 4.1: *Adsorption energy of Hg and Element 112 on a (100) gold surface, for different adsorption sites.*

top		bridge		hollow	
System	En. [eV]	System	En. [eV]	System	En. [eV]
$Au_{14}Hg$	1.64	$Au_{20}Hg$	1.31	$Au_{21}Hg$	0.86
$Au_{14}112$	1.47	$Au_{20}112$	0.96	$Au_{21}112$	0.82
$Au_{34}Hg$	1.02	$Au_{36}Hg$	1.52	$Au_{29}Hg$	0.84
$Au_{34}112$	0.65	$Au_{36}112$	1.14	$Au_{29}112$	0.74

The results of our calculations are shown in Table4.1 for the three possible adsorption sites on a Au (100) surface: top, bridge and hollow. The absolute values of the adsorption energies in eV of the elements Hg and 112 calculated in the GGA approximation (with B88 functional for exchange and P86 for correlation) are given. As a consequence of these calculations we conclude that the adsorption energy of element 112 on a gold surface will be 0.54 eV in the bridge position.

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4.2.17 Exotic hadrons from cluster hadronisation

Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, Frankfurt am Main
S. Scherer, H. Stöcker

An outstanding open problem of the physics of heavy ion collisions is the microscopic treatment of the hadronisation transition from a cooling, expanding quark-gluon plasma to a gas of hadrons. Due to the complexity of QCD at low energies, the use of simplified models is currently the only viable option to tackle this issue. One such model is the quark molecular dynamics qMD, where the essential feature of colour confinement is modelled by the use of a colour-dependent potential pair interaction between quarks, which is raising linear with distance. The dynamical evolution of the classical N-body problem of quarks subject to this long-range interaction yields colour neutral clusters that can be identified as hadrons. Calculations are numerically involved, and the raise of computation time as $N(N-1)$ with the number of particles makes the use of computing centres as the CSC mandatory.

Whereas known hadrons consist of three quarks (baryons) or quark-antiquark pairs (mesons), there have been speculations about the existence of larger clusters (exotic hadrons) right from the beginning of the quark model. The search for such exotic hadrons got a boost with the recent hints a the existence of the pentaquark state Θ^+. This has motivated our model study of exotic hadronic clusters emerging at the hadronisation stage heavy ion collision at SPS and RHIC energies, which may provide ideal environments for the formation of exotica. As a result of our simulation, we find a substantial amount of exotic hadrons, most of which, however, do not correspond to stable particles. Moreover, realistic number estimates require a proper treatment of rescattering. However, rapidity distributions as shown in the figure are important as a guidance for experimental search programs.

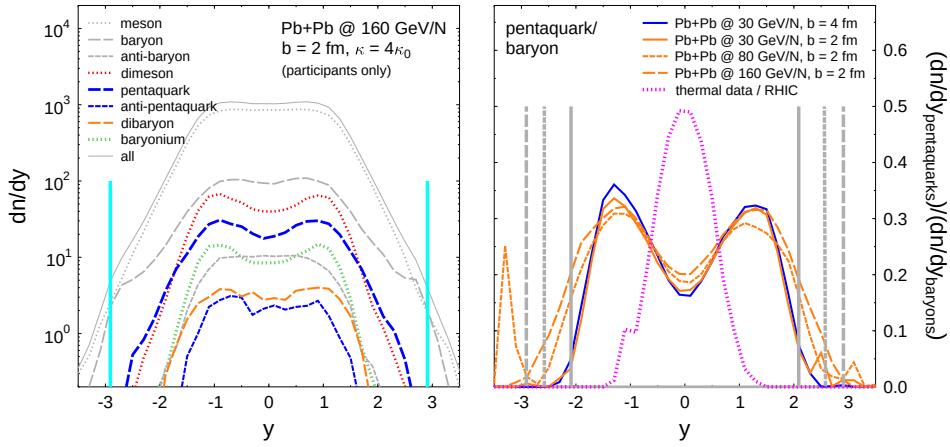

Fig. 1: Rapidity distribution of different types of quark clusters at upper SPS energies (left figure). Pentaquark clusters are represented by the thick doted line. Rapidity distribution of pentaquark clusters, normalised to the total baryon distribution, for different colliding systems (right figure).

[1] S. Scherer: Exotic hadrons from dynamical clustering of quarks in ultra-relativistic heavy ion collisions, *J. Phys.* **G31**, (2005) S1199–S1202, hep-ph/0411296.

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4.2.18 Phase Structures in a Chiral Hadronic Model

Institut für theoretische Physik and Center for Scientific Computing, Universitiät Frankfurt/M.
D. Zschiesche, G. Zeeb, S. Schramm, H. Stöcker

Lattice calculations and effective models are used as complementary approaches to investigate the properties of QCD, the theory of strong interactions. We employ a non-linear σ–ω-model with spontaneously broken chiral SU(3) symmetry and scale invariance to describe interacting baryons and mesons on the mean-field level [1]. The corresponding set of non-trivially coupled field equations are numerically solved via an accelerated gradient iteration method (see Refs. in [1]).

The model can not only describe properties of groundstate nuclear matter, finite nuclei and rotating neutron stars but also observables from heavy ion experiments as the measured particle ratios [2].

To investigate the *QCD phase diagram* within this model demands wide-ranged parameter studies. Qualitative agreement with lattice QCD predictions but also more diverse phase diagram structures can be obtained [3]. A semi-quantitative agreement with the critical endpoint as predicted by lattice calculations can be achieved by introducing further 'effective' degrees of freedom ('test resonances') [4], see the black bar and the black line in Fig. 1, respectively. The figures 1 and 2 show the paths of adiabatic expansion as expected in heavy ion collsions after the initial state of high compression. The beam energies investigated here ($E_{\mathrm{Lab}}/A = 5 - 25$ GeV) correspond to the planned experiments μ-RHIC at RIKEN-BNL and CBM at the upcoming GSI-FAIR facility.

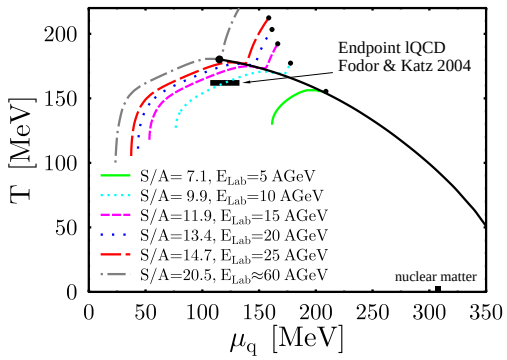

Fig. 1: Phase diagram with adiabatic paths in the temperature vs. chemical potential plane

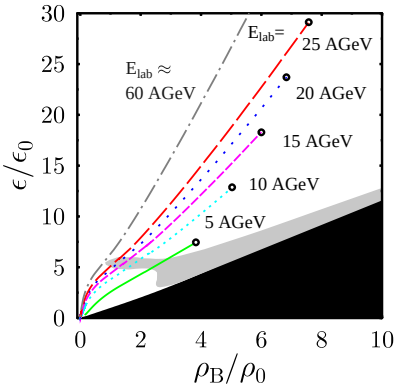

Fig. 2: Same as Fig. 1 in the energy density vs. baryonic density plane

[1] P. Papazoglou, D. Zschiesche, S. Schramm, J. Schaffner-Bielich, H. Stöcker, W. Greiner: Nuclei in a chiral SU(3) model, in *Phys. Rev.* C **59** (1999) 411 [arXiv:nucl-th/9806087].

[2] D. Zschiesche, G. Zeeb, K. Paech, H. Stöcker, S. Schramm: Particle ratios from AGS to RHIC in an interacting hadronic model, in *J. Phys.* G **30** (2004) S381.

[3] D. Zschiesche, G. Zeeb, S. Schramm, H. Stöcker: Impact of baryon resonances on the chiral phase transition at finite temperature and density, in *J. Phys.* G **31** (2005) 935 [arXiv:nucl-th/0407117].

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4.2.19 3d Particle-in-Cell Simulations of a Nonequilibrium Gluon Plasma

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Frankfurt Institute for Advanced Studies

Adrian Dumitru, Yasushi Nara, Michael Strickland

For this project we numerically solve for the time evolution of non-abelian SU(2) gauge fields in the presence of a hard particle background which is anisotropic in momentum-space. This involves real-time solution of the non-abelian Boltzmann-Vlasov/Yang-Mills equations. Our approach goes beyond the standard hard-loop (HL) approximation which results when the Boltzmann-Vlasov equation is linearized in small fluctations about the initial state. As a result of linearization the HL approach implicitly assumes that the hard particles move along straight line (eikonal) trajectories. In our case, solution of the coupled particle-field equations without linearization includes the effect of back-reaction of the self-consistently generated fields on the particle's motion. Algorithmically, we used a system of "smeared" test particles and solve the resulting Wong-Yang-Mills (WYM) differential equations for the time evolution of both particles and fields self-consistently on a lattice. The simulations are run by initializing the system with random SU(2) background fields and

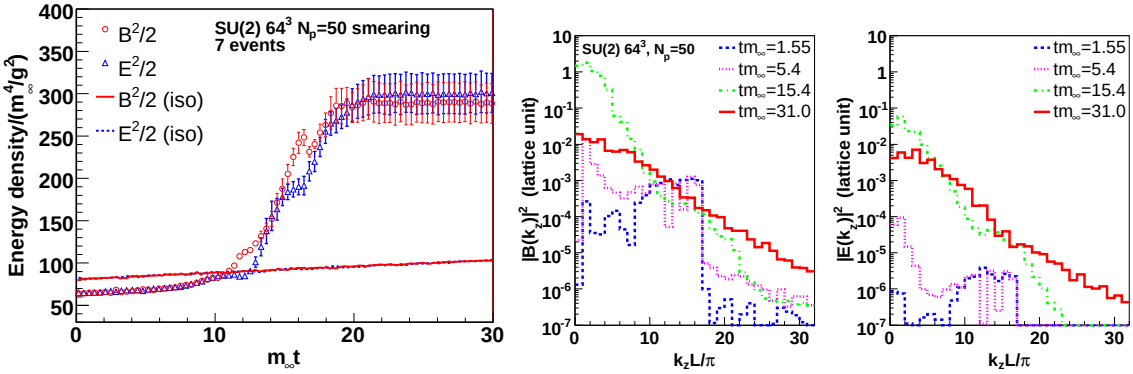

Abbildung 4.20: *Left: Field energy densities as a function of time. Right: Field spectra at four different times.*

taking a particle distribution which is anisotropic in momentum-space. The Figure shows the time evolution of the electric and magnetic energy densities as a function of time averaged over seven 64^3 runs as well as the corresponding fourier transformation at four different simulation times. One sees that after an initial latency period there is a rapid growth in both magnetic and electric field energy densities which stops when what was initially an instability to soft momentum "avalanches" to the ultraviolet causing the growth to cease.

Note that even after significant algorithmic improvement the code is highly memory intensive due to that fact that it must be run with the largest lattice sizes possible due to an observed "avalanche" of soft modes from soft to the smallest lattice scales (corresponding to the lattice spacing a). This project has resulted in one paper (see below) with a sequence of papers planned which will require further dedicated computational resources.

[1] A. Dumitru, Y. Nara, M. Strickland: "Ultraviolet avalanche in anisotropic non-Abelian plasmas," *submitted to Physical Review D*, Apr 2006, 22pp. [hep-ph/0604149]

4.2.20 Numerical Computation of Highly Doubly Excited Resonant *S* Electron States of Helium Atom

CAMTP Center for Applied Mathematics and Theoretical Physics, University of Maribor, Maribor, Slovenia
in cooperation with the group of Prof. Stöckmann,
Fachbereich Physik, Philipps-Universität Marburg, Marburg, Germany
via the university partnerships between Maribor and Marburg
M. Vraničar

Since the work of Poincaré over 100 years ago it has been known that the classical Kepler (also Coulomb) three body problem is nonintegrable which typically implies the mixture of the regular and chaotic classical dynamics in the system phase space. Again, the very same system has played an important role in the development of theoretical physics in 1920s as a catalyst for the quantum theory, since Bohr and others failed to calculate the ground state of helium atom within the concepts of the old quantum mechanics. Today, helium (like other three body Coulomb systems) remains an interesting system in context of quantum chaos dealing with the problem of finding the universal properties of classically chaotic systems in quantum mechanics.

The statistical properties of energy quantum spectra are one of the places where the fingerprints of the underlying classical dynamics are believed to be found in quantum mechanical systems as the manifestation of classical-quantum correspondence with regard to the semiclassical approximations.

In order to achieve the validity of the semiclassical approximations and thus to observe the correspondence one needs to enter the region high enough in the energy spectrum where a large number of excited states need to be accurately calculated to reach the significance and relability of the statistical analysis.

Highly doubly excited states of helium are not bound states but resonant states with finite life times instead. The standard method of computing resonant states is the diagonalization of the complex symmetric non-Hermitian Hamiltonian matrix as representation of the Hamiltonian operator in the appropriate – in case of Coulomb problem the so called Sturmian basis with complex scaling parameters ($\alpha_i e^{-i\theta}$) of the system coordinates [1,2,3]. The physical effect of the applied complex scaling (rotation) is that continua of the Hamiltonian originating from the single electron ionization thresholds and continuing into positive infinity are rotated from the real axis by an angle 2θ into the lower complex energy half plain around the ionization thresholds uncovering the resonances as complex eigenenergies-eigenvalues of the corresponding representation matrix. These eigenvalues are (theoretically) independent of rotation angle θ. Due to the basis truncation the rotated continua are also discretized (fig 1), so only a small fraction of all numerically computed complex eigenvalues of the matrix represents resonances.

The complex symmetric matrix to be diagonalized is sparse and banded due to the known coupling rules between the Sturmian basis functions and the non-zero matrix elements are expressed analytically. The numerical computation – diagonalization is performed in three steps. In a first step (*TVU2M) the basis is set, truncated and ordered in a way that minimizes the matrix band width, matrix element parts independent of θ are computed and stored. In the second step (*ZCBEV) the matrix is diagonalized for a chosen and fixed value of θ using the ARPACK library as implementation of Implicitly Restarted Arnoldi Method. The iterative method is very efficient for computing a portion of (complex) eigenvalues (only) near selected central position in each run

which also prevents us from spending additional CPU time on needless computation of discretized continuum energies. From results of the second step repeated at various values of rotation angle θ the candidates for resonances are set as eigenvalues independent of θ. The candidates enter the third step (*ZOPTEF) where the resonant eigenenergies are optimized with respect to the complex scaling parameters $\alpha_i e^{-i\theta}$. For each resonant state the parmeters are iteratively determined such that the resonance energy becomes stationary. An inverse iteration method on a *LU* decomposition of the complex Hamiltonian matrix is used to compute (update) the energy eigenvalue at each iteration. At the same time expectation values of various observables as well as the eigenvectors being the expansion coefficients of resonance eigenstate expansion in the corresponding Sturmian basis set are also computed providing additional source material for our future work (like studies of energy level dynamics, statistical and structural properties of two-electron wavefunctions,...) in the context of quantum chaos.

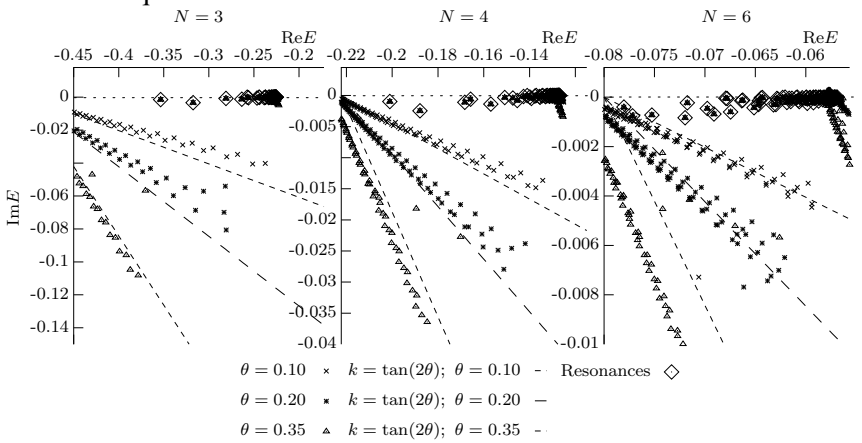

Fig. 1: A part of a complex resonance spectrum of He atom after diagonalization of the Hamiltonian operator in finite Sturmian basis with complex coordinate scaling parameters. Results of diagonalization at three different rotation angles $\theta = 0.1\ , 0.2\ , 0.35$ *are shown in energy regions below 3rd, 4th and 6th ionization threshold. The discretized continua are rotated around the thresholds by* 2θ *uncovering a set of eigenvalues which are independent of the rotation angle. The latter represent good candidates for He atom resonant states.*

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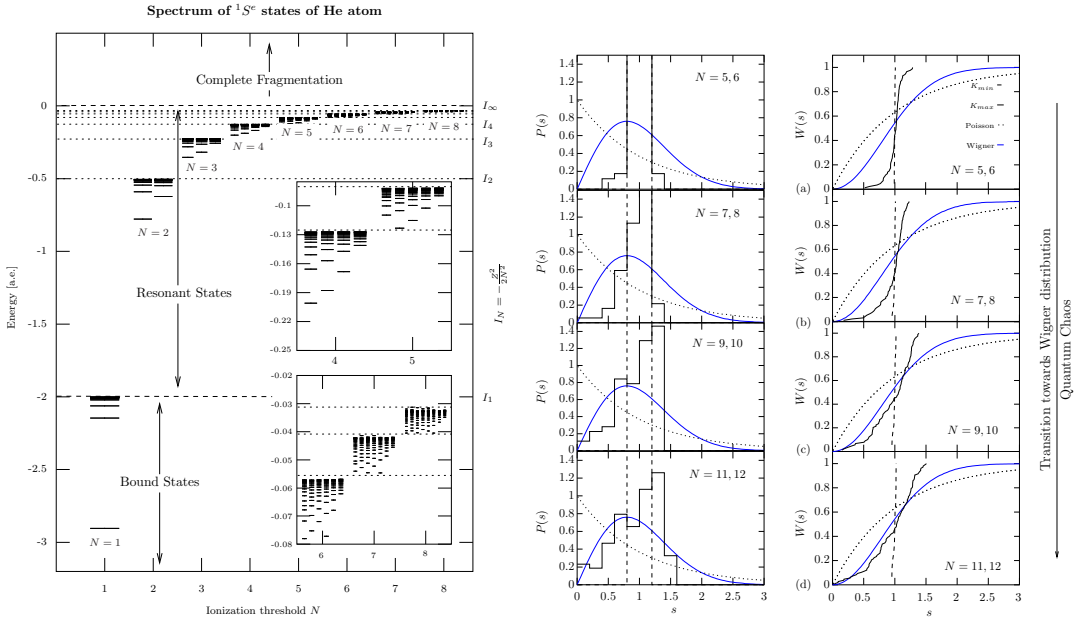

Fig. 2: (left) Exact (numerically computed) energy spectrum of He atom singlet resonant states at zero angular momentum. A spectrum consists of infinite parts converging to single electron ionization thresholds. Spectral lines below each (nth) threshold I_n are further divided into (n) subseries according to the approximate Herrick quantum number K (Herrick 1983). A regularity of Rydberg spectral structure in the subspectra starts to get spoiled in a part of the spectral lines converging to the 5th threshold energy where the energetically lowest state (according to the Rydberg pattern) of the leftmost subseries falls below the 4th ionization threshold and couples to the states of the leftmost subseries converging to the 4th ionization threshold. From this point on, in the direction of an increasing energy (as semiclassical limit is approached) the possibility of quantum chaos is expected to exists and to be observed in statistical properties of the He atom energy spectrum. (right) Nearest neighbor spacing distributions $P(s)$ and Cumulative nearest neighbor spacing distributions $W(s)$ for the energetically lowest and energetically highest unfolded[a] subspectra (leftmost and rightmost approximate subspectra as displayed in the left panel figure) of the complete $^1S^e$ He resonant spectrum are presented at four different energy intervals: (a) from 4th to 6th ionization threshold energy, (b) from 6th to 8th ionization threshold energy, (c) from 8th to 10th ionization threshold energy and (d) from 10th to 12th ionization threshold energy. Numerically computed results are plotted with solid line for energetically lowest subspectrum (K_{max}) and with dashed line for energetically highest (K_{min}) subspectrum. The results are compared to the theoretical prediction of the quantum chaos theory assuming Poisson distribution (doted line) for integrable systems and Wigner distribution (smooth solid blue line) for classically chaotic systems (basic result of the random matrix theory). Approaching the semiclassical limit (increasing the energy) a gradual transition towards Wigner distribution can be observed for K_{max} subspectrum which can indeed be linked to a classically completely chaotic collinear motion with the electrons on opposite sides of the nucleus (eZe collinear configuration). At the same time K_{min} subspectrum can be associated with a classically nearly integrable however highly correlated Zee collinear configuration with both electrons on the same side of the nucleus showing nearly uniform-equidistant structure in the unfolded spectrum significant for 1d regular spectrum like Rydberg series.

[a] To unfold the spectrum means to map the specrum on to the series of levels with mean nearest neighbor spacing equal to 1.

4.2.21 Parton Cascade simulating ultrarelativistic heavy ion collisions

Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität Frankfurt
Z. Xu, A. El, O. Fochler, J. Friedler and C. Greiner

We have developed a new 3+1 dimensional relativistic Monte Carlo cascade solving the kinetic on-shell Boltzmann equations for quarks and gluons including the elastic as well as the inelastic $gg \leftrightarrow ggg$ pQCD processes. With this tool we simulate the space time evolution of partons and explore the important issue whether a Quark-Gluon-Plasma (QGP), a thermal system of quarks and gluons, exists in an ultrarelativistic heavy ion collision. There are strong hints for the formation of such a new state of matter from experiments at RHIC at BNL (USA). However, many details have to be investigated.

Although the initial conditions of partons just after their production in a heavy ion collision are not known yet, speculations show that they are definitely far from thermal distribution. Transport calculations give a transparent way to look at the dynamical processes which drive system to thermal equilibrium. Our present results show that the pQCD Bremsstrahlung process and its back reaction ($gg \leftrightarrow ggg$) make the dominant contribution to thermalization, compared with the contribution from the elastic scatterings. The time scale of full thermalization is about $1-2$ fm/c in a simulation of a central Au+Au collision at RHIC energy. Since the cross section of the pQCD Bremsstrahlung process is smaller than that of the elastic scattering, the inelastic processes seem very efficient for momentum isotropization. The detailed analyses are in progress.

From the numerical results we also see the hydrodynamical behavior of the already equilibrated system. The elliptic flow v_2, which is calculated in noncentral Au+Au collisions, has a large value, which is comparable with the experimental data. This indicates that the viscosity must be small. We are trying to extract the viscosity from the simulations. A pioneering work has been done. Detailed implementations are still in progress.

Also the way thermalization occurs has been investigated and compared with the famous "Bottom-Up" scenario, which suggested that soft gluons thermalize first and harder gluons later. It turns out that whether the "Bottom-Up" scenario is justified depends strongly on the initial conditions. The detailed balance of the inelastic scatterings moderates the suggested scenario. Especially, for an oversaturated initial condition the hard gluons thermalize first and soft gluons later.

Since the Quark-Gluon-Plasma has a large geometrical size, high energy particles will lose their energy when travelling through the medium. This phenomenon is named "Jet-Quenching" and manifested by the experimental measurement. We have investigated this phenomenon applying the parton cascade. The results imply a stronger energy loss of factor 3 compared with the experimental data. A detailed study of the dependence of the pQCD Bremsstrahlung process on the Landau-Pomeranchuck-Migdal suppression has to be done. This is one of our future projects.

[1] Z. Xu and C. Greiner: *Thermalization of gluons in ultrarelativistic heavy ion collisions including three-body interactions in a parton cascade*, Phys.Rev.C71:064901,2005

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4.3 Ingenieurwissenschaften

4.3.1 Combustion Noise Predictions by a LES/CAA Hybrid Approach

Institute for Energy and Powerplant Technology, TU Darmstadt
F. Flemming, A. Sadiki, J. Janicka

In general, technical combustion systems, as for example in gas turbines for power generation applications, exhibit low Mach numbers, since a stable flame localization is advantageous with respect to reduced emissions of pollutants. Therefore, the propagation of acoustic waves is clearly separated from the convective transport processes. The corresponding characteristic velocities are at least an order of magnitude apart $Ma = U/c < 0.1$. The current LES/CAA hybrid approach exploits this difference in scales, by applying specialized techniques and solvers to either problem. The description of the turbulent reacting flow is performed by a large eddy simulation using FLOWSI, while the acoustic propagation is conducted by solving the wave equation applying CLAWPACK with the appropriate sources extracted from the LES. Such an approach is capable of predicting noise levels of turbulent flames fully three dimensional and temporally resolved, as for example for a non-premixed jet flame (see Fig. 1). In Fig. 2 a comparison of the numerical results with experimental measurements is presented, showing a generally good agreement in the frequency range of interest. The computational cost of the current combination of tools amounts to approximately twice the cost of the LES alone. For future applications, this hybrid approach will be extended in order to predict thermoacoustic instabilities. In that case, the acoustics couple back to the turbulent flame and excite resonant modes of the combustion chamber. Such instabilities are a major problem for modern gas turbine combustors, burning fuel in a lean premixed mode and can lead to the destruction of the combustor.

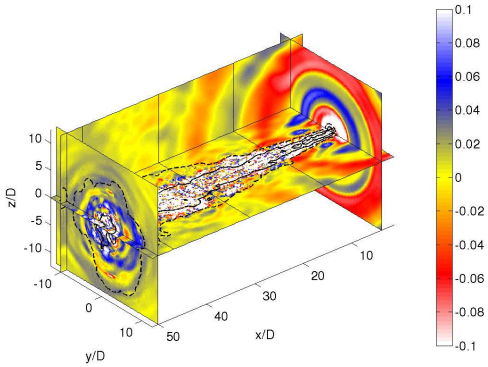

Fig. 1: Instantaneous acoustic pressure distribution of a turbulent non-premixed flame.

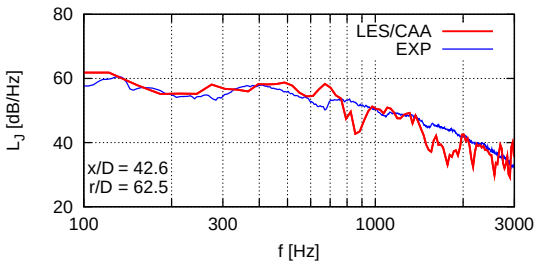

Fig. 2: Spectral comparison of the simulated noise intensity and measurements.

[1] F. Flemming, C. Olbricht, B. Wegner, A. Sadiki, J. Janicka, F. Bake, U. Michel, B. Lehmann, I. Röhle: Analysis of Unsteady Motion with Respect to Noise Sources in a Gas Turbine Combustor: Isothermal Flow Case. In *Flow Turb. Combuts.*, 75: 3–27, 2005

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4.3.2 Large Eddy Simulation of Premixed Combustion

Fachgebiet Energie und Kraftwerkstechnik Maschinenbau, TU Darmstadt
M. Freitag, J. Janicka

A world wide increasing demand for energy, a decline of available resources and compelling environmental requirements make the development of reliable predicting tools for combustion processes a must. The desire in terms of combustion engines and gas turbines is to enhance the thermal output and, at the same time, reduce specific fuel consumption and thereby also the amount of pollutants. Recently the numerical simulation of combustion processes has shown its capability compared to expensive experimental investigations.
The aim of this work was to predict the behavior of a complex, unconfined, premixed swirling flame in a temporary resolved manner. Beside the Navier Stokes equations, which describe the fundamental physics of fluid motion, a set of additional equations are solved, which mimic the dynamical behavior of the flame and its integration with the gaseous fluid. The so called G-equation, used in this work, is considered to be one the most challenging models and requires advanced numerical tools, such as the level set method.
A fundamental requirement in the concept of Large Eddy Simulation (LES), is to resolve most of the kinetic energy on the computational grid. Due to this demand parallel computations become a must. The parallelization of the code is accomplished to achieve maximum efficiency on small and medium parallel architectures. The results, plotted in Fig. 1 and 2, demonstrate the possibilities of the method.

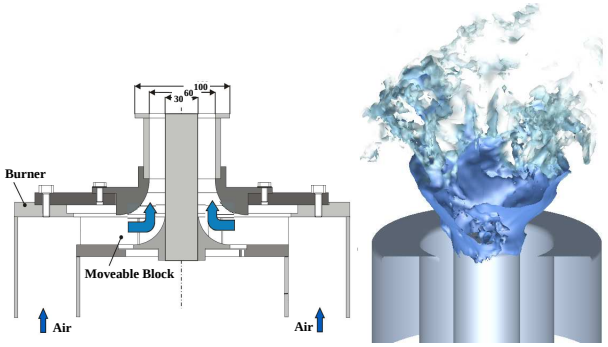

Fig. 1: Sketch of the swirler device (left) and snapshot of the calculated, turbulent flame front (right).

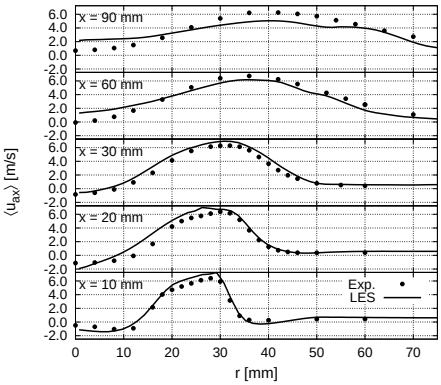

Fig. 2: Predicted mean axial velocity, comparison with experimental results.

[1] M. Freitag and J. Janicka. Investigation of a strongly swirled unconfined premixed flame using les. *Proc. Comb. Inst.*, 31, 2006.

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4.3.3 Large-Eddy-Simulation of Multiphase Flows

Fachgebiet Energie- und Kraftwerkstechnik, TU Darmstadt
F. Hahn, A. Sadiki, J. Janicka

Multiphase flow phenomena are common in nature and technology. One subset of these flow phenomena is the condition where small particles or droplets interact with the gaseous carrier phase. Characteristically for this type of flow is that only one of the (fluid) phases is continously connected. Technical examples are cyclone dust separators and all kinds of spray systems. Due to the strong interaction of both phases, it is evident to accurately calculate the transient behavior of both phases simultaneously. Especially the correct prediction of the carrier phase turbulence and its modulation is essential.

The focus of the present project is on the prediction of liquid fuel combustion in gas turbines. Therefor, the existing flow solver FASTEST is expanded with a Lagrangian particle tracking module. In this Euler/Lagrangian called approach the gaseous phase is calculated using an Eulerian description whilst for the dispersed phase the paths of all particle are computed individually based on Newton's second law. The approach is suited for multiphase flows with dilute or medium dispersed phase loadings. Flow phenomena occurring in those cases are strongly affected by continuous/dispersed phase interactions. The approach is limited in practice, even though it leads to a very detailed description of physical phenomena, due to the fact that numerical effort scales with the number of tracked Lagrangian particles. In combination with the standards of LES concerning resolution in space and time the method is not only accurate, it as well requires high computing power. To retain the performance of FASTEST and to fulfill these needs, the Lagrange module is parallelized by means of domain decomposition.

In the following two application examples are shown which are computed using the previously described methodology. The first example (see Fig. 1) shows the instantaneous velocity field in a cutting plane through a cyclone dust separator. One can observe the capability to represent highly unsteady phenomena, and high velocity gradients which are essential for the functionality of the separator. The second example (see Fig. 2) shows the spatial instantaneous distribution of polydisperse particles for a swirling jet streaming into a pipe. This is a generic case, comparable with liquid fuel driven combustors. Clearly unsteady phenomena like separation and clustering with strong impact on the chemical reaction occur.

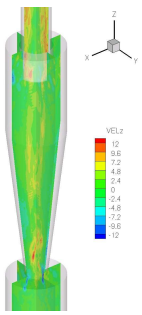


Fig. 1: Axial velocity profile inside a cyclone separator

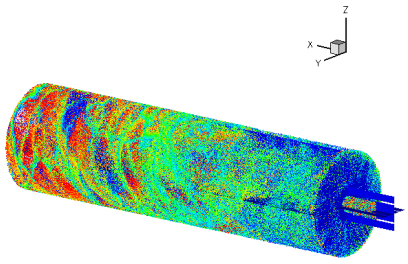


Fig. 2: Particle distribution in a swirling co-annular jet, color represents particle size

4.3.4 Heat and Mass Transfer in Complex Mixing Devices

Fachgebiet Energie- und Kraftwerkstechnik im Maschinenbau, TU Darmstadt
C. Olbricht, A. Sadiki, J. Janicka

Regarding technical and industrial flow application developments an accurate prediction of turbulent heat and mass transfer processes is necessary. A time-resolved approach to determine mixing on all scales is provided by the hybrid LES-Monte-Carlo method (LES, *large eddy simulation*). Hereby, large flow structures are resolved at the computational grid of the LES. Whereas the scalar joint probability density function (*JPDF*) within the subgrid can be achieved by an ensemble of stochastic Monte-Carlo particles. Both methods are coupled using the velocity information and the fluid properties.
Currently, three different mixing configurations have been simulated using this hybrid approach. Beside a simple turbulent mixing layer, two complex mixing devices were considered, Olbricht *et. al.* [1]. By means of a jet-in-crossflow configuration (*JIC*, [1] and [2]) at moderate Reynolds-Number the consistency feature and the statistical convergence of the used Eulerian Monte Carlo approach has been demonstrated. The obtained results could reproduce the experimental data adequately. It has been shown that the instantaneous error decreases with the square root of the particle number.
An investigation of the more complex multi jet-in-crossflow configuration (*MJIC*, [1]) at a higher Reynolds-Number has been carried out. In particular the time-resolved SGS mixing and the evolution of the SGS normalized temperature PDFs has been investigated. The hybrid LES-MC method has been proved to be a reliable tool for the investigation and the prediction of mixing processes, also in complex configurations. The task of consideration of chemical reactions or combustion is left for future work.

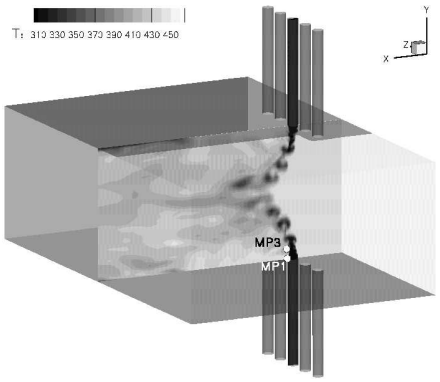


Fig. 1: Instantaneous filtered temperature field of the multi jet-in-crossflow.

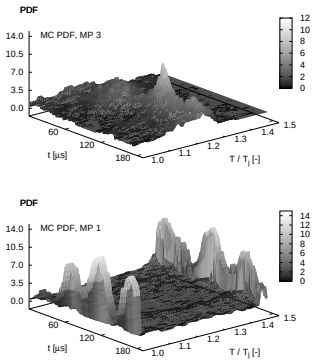


Fig. 2: Evolution of the probability density function of the normalized temperature.

[1] C. Olbricht, A. Sadiki, J. Janicka, and J.-Y. Chen: Study of heat and mass transfer in complex mixing devices using a hybrid LES-Monte-Carlo PDF method, *Turbulence, Heat and Mass Transfer, 5*, Dubrovnik, Croatia, 2006

[2] B. Wegner, Y. Huai, and A. Sadiki: Comparative study of turbulent mixing in jet in cross-flow configurations using LES, *International Journal of Heat and Fluid Flow Selected papers from the 4th International Symposium on Turbulence Heat and Mass Transfer*, 25:767-775, 2004

4.3.5 Large Eddy Simulation of Non-Premixed Combustion

Fachgebiet Energie und Kraftwerkstechnik Maschinenbau, TU Darmstadt
B. Wegner, J. Janicka

To reduce pollutant emissions and increase the efficiency of combustion devices, simulation techniques are required that do not only offer a reliable prediction accuray, but also offer insight into the complex physico-chemical processes taking place in turbulent combustion. The large eddy simulation technique has evolved over the last years from a purely academic method to a tool being applied to semi-academic and even full-scale industrial problems [1]. The current work deals with the simulation and analysis of non-premixed combustion in a model aero-engine combustor. Simulations performed so far have already revealed a strong flow-mixing interaction due to swirl flow instabilities [2]. Ongoing work focuses on a comparative analysis of different combustion models for the configuration under consideration.

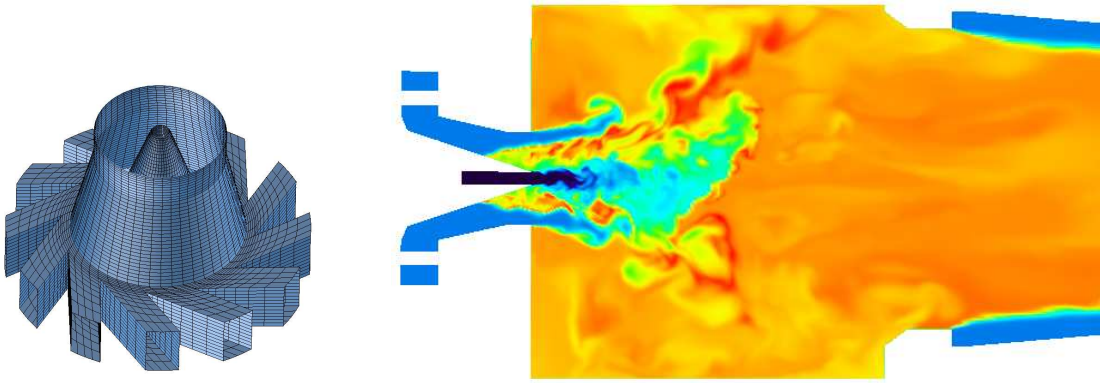


Fig. 1: Left: Fuel injector nozzle being investigated; Right: Snapshot of instantaneous temperature distribution in the combustion chamber

[1] B. Wegner, B. Janus, A. Sadiki, A. Dreizler, and J. Janicka. Study of flow and mixing in a generic GT combustor using LES. In *ETMM6, 6th International Conference on Engineering Turbulence Modelling and Experiments*, 6:731-740, Sardinia, 2005.

[2] J. Janicka and A. Sadiki. Large Eddy Simulation of turbulent combustion systems. *Proc. Comb. Inst.*, 30:537–547, 2005.

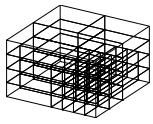
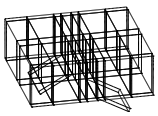
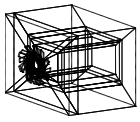
4.3.6 Optimal Grid Partitioning for Block Structured Grids

D. Junglas, A. Martin, Fachgebiet Diskrete Optimierung, TU Darmstadt
M. Schäfer, D. Sternel, Fachgebiet Numerische Berechnungsverfahren, TU Darmstadt

In order to efficiently perform simulations based on block-structured grids on multiprocessors the computational load must be equally balanced over the available processors. The traditional approach for finding a good balancing is to partition the grid into as many partitions as there are processors and to map each partition to one processor. This is usually done in such a way that each processor bears the same number of grid points or control volumes respectively. Among all mappings that satisfy this constraint one attempts to pick the mapping with the minimal number of data exchanges between processors. This is done according to the assumption that communication overhead is proportional to the number of data exchanges performed during simulation.

In this project we took a refined approach to the grid mapping problem. Along with the grid mapping we determined an optimal communication schedule that requires minimal time to satisfy all data dependencies between processors. Moreover, we refrained from requiring that all processors have the same number of computations mapped to them. Instead, we attempted to find mappings in which the sum of arithmetic computation time and communication time is minimal.

The aim of this project was to find a way to model this problem for certain hardware architectures and afterwards use this model to partition real-world grid instances. We formulated the optimization problem as an integer programming model by representing the grid as a graph and phrasing the communication schedule as an edge-colouring problem in multigraphs. Table 4.2 shows three grids to be simulated on a four-processor machine and the time required for one iteration in the simulation. The underlying mappings are optimal for the traditional assumptions (first line) and for our new model (second line), respectively. In the last line Table 4.2 shows the amount of simulation time that the new mappings save over the traditional ones.

traditional	1000.0225	1807.6160	2379.2161
new	750.0450	1594.4800	1746.7200
saved	25.00 %	11.80 %	26.58 %

Tabelle 4.2: *Milliseconds per iteration in simulation.*

These results and the fact that the new mappings could be obtained within only a few seconds prove that it is feasible to employ complicated optmization models and strategies in order to find better mappings and thus save up to 25 percent of simulation time.

[1] D. C. Sternel, D. Junglas, A. Martin, M. Schäfer: *Optimisation of Partitioning for Parallel Flow Simulation on Block Structured Grids*, Proceedings of the Fourth International Conference on Engineering Computational Technology (eds. B. H. V. Topping and C. A. Mota Soares), Civil-Comp Press, 2004

4.3.7 Numerical Simulation of Fluid-Structure Interactions

Fachgebiet Numerische Berechnungsverfahren im Maschinenbau, TU Darmstadt
M. Schäfer, D. Sternel, M. Heck, S. Yigit

Many engineering problems involve interactions between fluids and structures. Examples can be found, for instance, in machine and plant building, engine manufacturing, turbomachinery, heat exchangers, offshore structures, chemical engineering processes, microsystem techniques, biology, or medicine. A possibility to investigate such problems is to solve the corresponding field equations in the continuum mechanical settings in a fully coupled way. Due to the coupling and the dynamics such kinds of computations are rather challenging.

The aim of this project is the development and application of an efficent fully-implicit partitioned solution algorithm for fluid-structure interaction problems. For the fluid and structural parts the finite-volume solver FASTEST and and the finite-element solver FEAP, respectively, are employed. The coupling is provided by the library MpCCI ensuring high flexibility. An arbitrary Lagrangian-Eulerian description together with algebraic and elliptic grid adaption tools are employed to handle the movement of the flow domain. The solver is integrated in a global multigrid method to achieve a high numerical efficiency (see Fig. 1).

Application examples (see Fig. 2) have shown that the approach allows for an efficient and reliable study of the complex mechanical behavior of practical fluid-structure interaction processes.

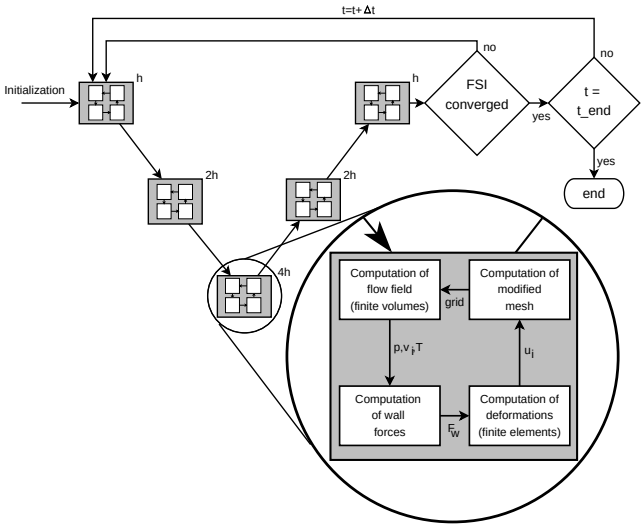


Fig. 1: Implicit partitioned coupled solver within global multigrid method

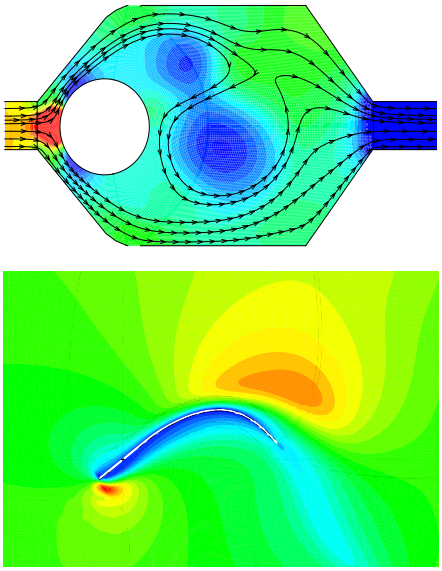


Fig. 2: Application examples: fluid excited flag and sphere valve

[1] H.-J. Bungartz and M. Schäfer (Editors): *Fluid-Structure Interaction*, Springer, LNCSE 53, Berlin, 2006

[2] S. Yigit, M. Schäfer, and M. Heck: Numerical Investigation of Structural Behaviour During Fluid Excited Vibrations, *Europ. J. Comp. Engrg.*, accepted, 2006

[3] M. Schäfer, M. Heck, and S. Yigit: An Implicit Partitioned Method for the Numerical Simulation of Fluid-Structure Interaction, in *Fluid-Structure Interaction* (eds. H.-J. Bungartz and M. Schäfer), Springer, LNCSE 53, Berlin, 2006

4.3.8 Large Eddy Simulation of Complex Turbulent Flows

Fachgebiet Numerische Berechnungsverfahren im Maschinenbau, TU Darmstadt
M. Schäfer, D. Sternel, M. Kornhaas

The knowledge about turbulent flow fields plays an important role in the industrial design process. Large Eddy Simulation (LES) is a promising way to get reliable results with acceptable computational effort. The method is well tested for simple academic test cases. However, technically relevant flows often occur in very complex geometrical configurations. Computations of such flows require fine discretizations in space and time which leads to a high computational effort. Highly efficient algorithms for solving such problems have to be developed and investigated, also with respect to achieve "best practice guidelines" to reach the best possible accuracy within minimum computational effort.

For solving the governing partial differential equations a parallelized finite-volume code is used that works in a specially adapted multi-grid environment. For LES subgrid modeling the Smagorinsky model together with the dynamic Germano procedure is implemented. Parallel computing requires the distribution of the blocks to the given processors with respect to the load balancing. An algorithm is implemented which optimizes this partitioning process has been developed. Systematic investigations of the influence of numerical parameters, like grid spacing, time steps, and convergence criteria, are carried out. Test cases of different complexity are investigated (see Fig. 1) and the simulation results are compared with experimental and other numerical data (see Fig. 2).

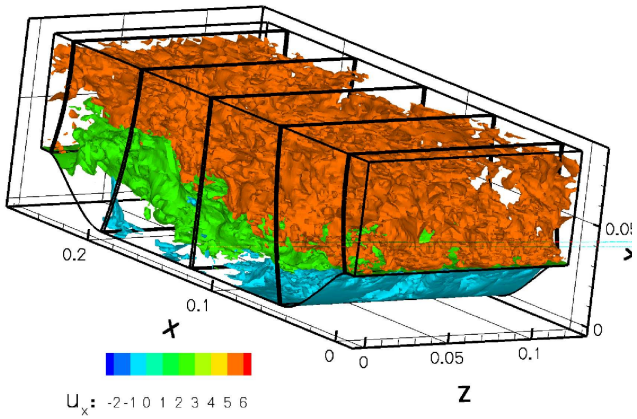


Fig. 1: Instantaneous velocity component in turbulent flow over wavy hill

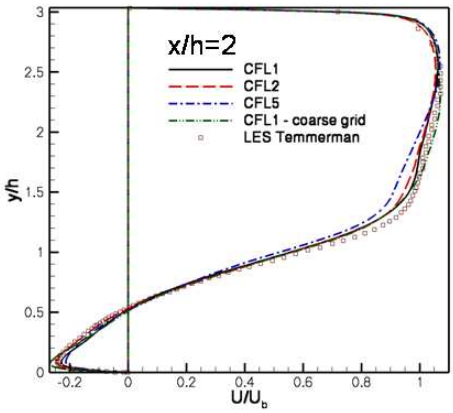


Fig. 2: Comparison of time averaged velocity components

[1] S. Ertem-Müller. Numerical Efficiency of Implicit and Explicit Methods with Multigrid for Large Eddy Simulation in Complex Geometries. PhD thesis, Department of Numerical Methods in Engineering, TU Darmstadt, 2003.

[2] D.C. Sternel, D. Junglas, A. Martin, M. Schäfer. Optimisation of Partitioning for Parallel Flow Simulation on Block Structured Grids. In *Proc. 4th Int. Conf. on Engrg. Comp. Techn.* (eds. B.H.V. Topping, C.A. Mota Soares), Stirling, Civil-Comp Press, 2004.

[3] D. Sternel. Effiziente und zuverlässige Grobstruktursimulation in komplexen Geometrien mit Mehrgitterverfahren. PhD thesis, Department of Numerical Methods in Engineering, TU Darmstadt, 2005.

4.3.9 Numerical Shape Optimization of Flow Geometries

Fachgebiet Numerische Berechnungsverfahren im Maschinenbau, TU Darmstadt
M. Schäfer, Z. Harth, H. Sun

The numerical simulation of fluid flow applications has reached a level, regarding efficiency and accuracy of computation, which permits optimization of technical systems. Engineering optimization can be defined as the process of finding the best conditions that give the minimum or maximum value of a quality function. In practice, the quality function may be, e.g., reducing the dissipation in channels or hydraulic valves, minimizing the drag force of airplanes or vehicles, etc. Our research concentrate on developing and improving optimization techniques in real applications.

For such an approach various distinct modules are combined, i.e. geometric modelling, mesh generation, non-linear analysis of the fluid flow, sensitivity analysis, mathematical programming, and shape optimization (see Fig. 1). In the context of numerical flow simulation there is often no gradient information of the objective function available, or is very difficult to obtain, such that it is advantageous to use an optimization technique which do not directly depend on the derivative information. Genetic Algorithms (GAs) and Newton based derivative free methods are adequate for these kind of optimization applications. Further, highly efficient and parallel algorithms are investigated due to the large number of function evaluations needed.

Both methods have been implemented and investigated for various application examples. The parallelization of the genetic algorithm is based on a master-slave model (see Fig. 2), while the Newton based method is parallelized by domain decomposition within the flow solver. As a multi-objective example, the diameters of the 8 pipes of a heat exchanger configuration are optimized with respect to the pressure drop between inlet and outlet channel, the maximum temperature, and the total area occupied by the fluid. Two optimal states, i.e. with low pressure drop and low heat transfer as well as with high pressure drop and high heat transfer are shown in Fig. 2.

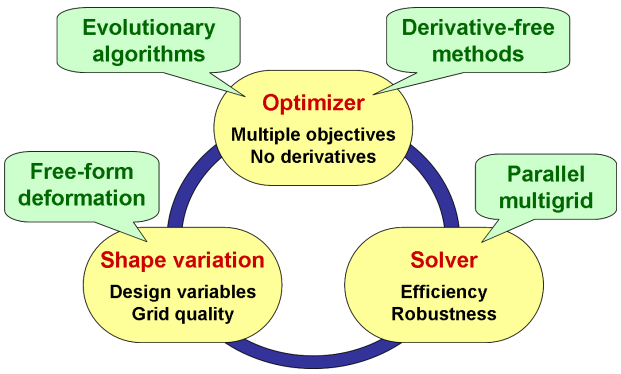


Fig. 1: Methodologies for automated multi-objective shape optimization of flow processes

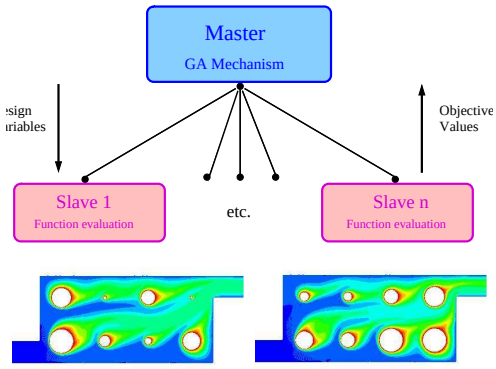


Fig. 2: Parallel master-slave model and optimized heat exchanger configurations

[1] K. Hirschen and M. Schäfer. A Study on Evolutionary Multi-Objective Optimization for Flow Geometry Design, *Computational Mechanics*, 37:131-141, 2006.

[2] T. Lehnhäuser and M. Schäfer. A Numerical Approach for Shape Optimization of Fluid Flow Domains, *Computer Methods in Applied Mechanics and Engineering*, 194:5221-5241, 2005.

4.4 Mathematik

4.4.1 Constructive Galois Theory

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J. Klüners

Let $f \in \mathbf{Z}[x]$ be an irreducible polynomial of degree n with integral coefficients. To such a polynomial we associate a so-called Galois group, which is a permutation group acting on the complex roots $\alpha_1, \ldots, \alpha_n$ of f. Using the Galois group we can derive many useful properties. E.g. all roots of f are expressible as iterated root expression (are solvable by radicals) if and only if the Galois group is solvable. Computationally one can ask the following two questions:

1. Given a polynomial f. Compute its Galois group (Direct problem).

2. Given a group G. Compute a polynomial which has G as Galois group (Inverse problem).

During the last years the author [1] has developed algorithms to compute Galois groups of polynomials up to degree 15. Recently, in a not published joint work with Claus Fieker, Sydney, this problem can be now solved degree independent.

It is not known, if one can find a polynomial for every finite group. In a joint work with Gunter Malle [3] we created a database, where we computed at least one polynomial for each group up to degree 15. This database can be accessed via:
http://www.mathematik.uni-kassel.de/∼klueners/minimum/minimum.html.

In order to compute those polynomials it was necessary to perform huge computations. The algorithms we used for it are described in [3]. Depending on the group we want to realize these algorithms are deterministic or probabilistic.

During the last weeks we were able to finish degree 16 and 18. Especially degree 16 was very difficult since we had to realize 1954 different groups. In degree 17 we explicitly realized all groups but one. For this group it is even theoretically not known if it can be realized by a polynomial.

Our database was already used by many other mathematicians in order to contradict conjectures (by finding a counter example in our database) or by creating new conjectures considering the data in our database. E.g. in the habilitation thesis [2] of the author we proved conjectures which were made using the examples in our database.

[1] K. Geissler and J. Klüners: Galois Group Computation for Rational Polynomials, J.Symb.Comput., 30, 2000, 653-674

[2] J. Klüners: Über die Asymptotik von Zahlkörpern mit vorgegebener Galoisgruppe, Universität Kassel, Shaker-Verlag, 2005

[3] J. Klüners and G. Malle: A Database for Field Extensions of the Rationals, LMS J. Comput. Math., 4, 2001, 182-196

4.5 Sonstiges

4.5.1 Cosmic Ray Air Shower Simulations

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Frankfurt am Main
H.J. Drescher

Highest energy cosmic rays present many unsolved questions in physics. The acceleration mechanisms are essentially unknown as well as possible candidates for their sources. The propagation of these particles through the cosmic microwave background should lead to an absorption at energies above 10^{19} eV, the so-called GZK cutoff.

Cosmic rays can only be studied indirectly via air showers which they induce upon entering the atmosphere. A cascade of secondary particles produced by sequential collisions is sweeping through the atmosphere and detected by ground arrays or fluorescence telescopes. Essential for the interpretation of the data is the modeling of air showers, with which one tries to deduce properties of the primary cosmic ray. The simulation of the air shower itself presents a highly computationally difficult task, since one has to trace 10^{11} particles or more. Here, we rely on hybrid simulations, in which a part of the shower is treated numerically by a transport equation. Computing power is therfore crucial in this field.

Since energies are much higher than reached in any terrestrial accelerator, known physics has to be extrapolated.The cosmic ray group in Frankfurt is working on hadronic interaction models used in such air shower simulation tools. The figures seen below show how these models influence directly air shower properties. Fig. 1 shows the ratio of lateral distribution functions (LDF) solely due to different low energy interaction codes (below 100 GeV). The UrQMD model from Frankfurt, which describes accelerator data at these energies much better, shows a flatter LDF. This is of great importance, since the LDF is used to deduce the energy of the primary cosmic ray. Fig. 2 show the results for the mean shower maximum due to high energy hadronic models. The model BBL, developed in Frankfurt, implements suppression of forward scattering due to high density QCD. The resulting penetration depth is therefore decreased.

This kind of physics can only be done with a great amount of computing power. The calculations involve physics models which are realized with Monte Carlo techniches and sophisticated, but numerically exigent algorithms.

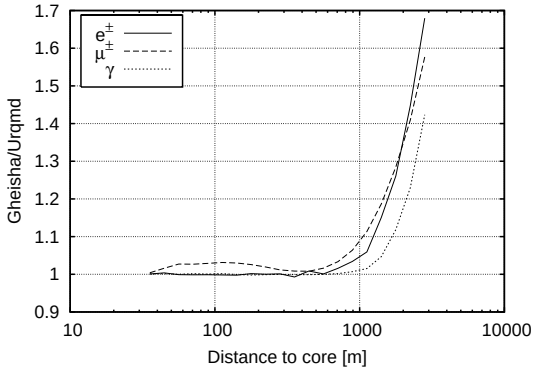


Fig. 1: Ratio of lateral distribution functions for different low energy hadronic models.

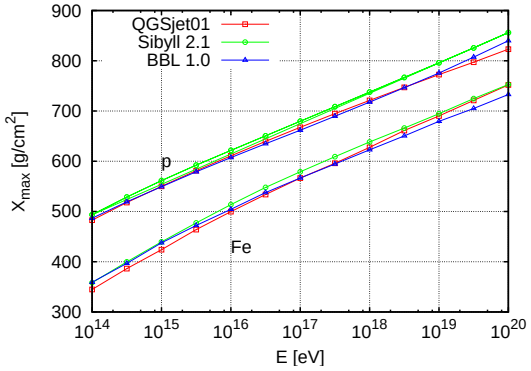


Fig. 2: Mean X_{max} for different high energy hadronic models.

[1] H. J. Drescher, G. R. Farrar, M. Bleicher, M. Reiter, S . Soff, H. Stöcker: Proceedings of the

28th International Cosmic Ray Conferences (ICRC 2003), Tsukuba, Japan, 31 Jul - 7 Aug 2003, 507-510; arXiv:astro-ph/030542

[2] H. J. Drescher, M. Bleicher, S. Soff, H. Stöcker; Astropart. Phys. **21**:87, 2004

[3] H. J. Drescher, A. Dumitru, M. Strikman: Phys.Rev.Lett.94:231801,2005

[4] H. J. Drescher: Proceedings of 29th International Cosmic Ray Conference (ICRC 2005), Pune, India, 3-11 Aug 2005.

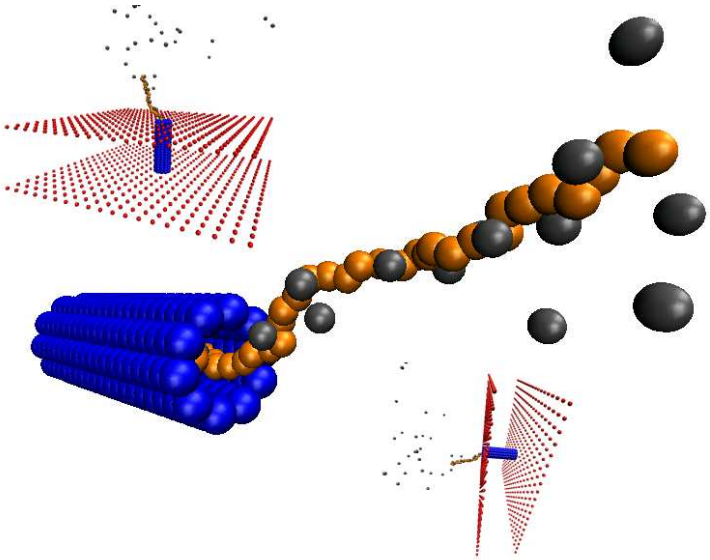
4.5.2 Dynamics of charged biomolecules under electro-hydrodynamic effects

Frankfurt Institute for Advanced Studies, JWG-U Frankfurt
C. Holm, S. Tyagi, M. Suzen, K. Grass

Biomolecules like DNA and proteins are usually charged, and predominantly exist in aqueous solution. The dynamics of biomolecules in such an environment is determined by an interplay of various factors: External forces, the local flow of the medium, short-range interactions, and long-range electrostatic and hydrodynamic interactions. Externally applied flow or external electric fields are used to manipulate and separate biomolecules in bioanalytic devices.

In order to understand these processes from a theoretical point of view, the biomolecules must clearly be modeled on a molecular level. However, a full simulation of a microchannel, which accounts explicitly for every single water molecule, is not only a formidable task, but also unnecessarily inefficient. Since typical channel sizes are still much larger than the size of small molecules, a solvent treatment on the level of a continuum theory is perfectly sufficient.

We study the electro-hydrodynamic effects of charged macromolecules with a combination of analytical theories and sufficiently coarse-grained numerical models. The models are simulated with algorithms that still accurately include the key mechanisms such as electrostatic and hydrodynamic interactions, but which are still sufficiently fast to achieve system size and timescales that can resolve the underlying microscopic physical mechanisms. A better understanding of these mechanisms will prove valuable for developing microfluidic devices for biosensing and gene sequencing applications.



Polymer translocation through a nanopore.

[1] K. Grass: Electro-hydrodynamic effects on polyelectrolyte dynamics, *PhD thesis in preparation*

[2] M. Suzen: Generic polyelectrolyte translocation through polarizable nanopores, *PhD thesis in preparation*

4.5.3 Interplay of electrostatic and van der Waals forces in dimer of coronene

Frankfurt Institute for Advanced Studies
O. I. Obolensky, V. V. Semenikhina, A. V. Solov'yov, W. Greiner

Studying properties of polycyclic aromatic hydrocarbon clusters presents an important problem in astrophysical research of interstellar medium. The current knowledge of structure, properties and ways of formation of such clusters is very limited. We have studied an interplay of electrostatic and van der Waals forces in formation of dimer of coronene. Our results show that the dimer's lowest energy configuration is not necessarily a stack, as it might had been expected *a priori*. This is a surprising result for the dimer of such a large polycyclic aromatic hydrocarbon (PAH) as coronene ($C_{24}H_{12}$). The energy of the T-shaped configuration at all highest feasible levels of density functional theory (B3LYP,PBE/6-31+G(d),D95,cc-pVDZ,cc-pVTZ) is lower than the energies of the three plausible stack configurations (superimposed stack - „sandwich" (SS), twisted stack (TS) and parallel-displaced (PD) stack, see Fig. 1). This is the first comparative study of the different configurations of the coronene dimer within the *ab initio* approach. A simple model is proposed which is useful for qualitative understanding of possible geometries of the coronene dimer and larger coronene clusters. The model represents coronene dimer as two sets of charged rings interacting via Coulomb and Lennard-Jones potentials. The model provides an intuitively clear explanation why the T-shaped dimers can be of importance even for some of moderately large PAHs such as coronene and, may be, for circumcoronene. The unexpectedly strong competetiveness of the T-shaped configuration is connected to the round shape of the coronene molecules. Indeed, rotation or parallel-displacement of the non-round monomers result in significantly smaller Coulomb repulsion as compared to the face to faceßandwich configurations. On the other hand, for the stacked round molecules rotation and/or displacement are much less effective. Therefore, the round shape of the coronenes leads to an increased role of the electrostatic repulsion in the stack configurations. The proposed model can be easily generalized to other polycyclic aromatic hydrocarbons, DNA bases, etc.

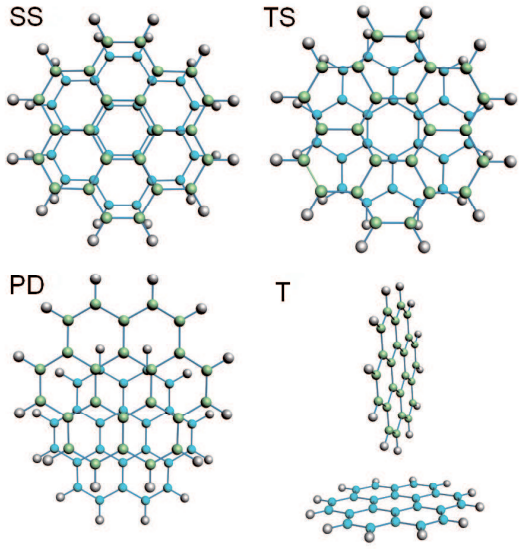


Fig. 1: T-shaped and stacked configurations of coronene dimer

4.5.4 Structure, stability and fission of metal clusters

Frankfurt Institute for Advanced Studies
A. G. Lyalin, O. I. Obolensky, I. A. Solov'yov, A. V. Solov'yov, W. Greiner

One of the most important and challenging tasks in physics of atomic clusters is to study cluster's stability, structure and electronic properties. In this project we investigate the optimized ionic structure, stability and the electronic properties of neutral and charged metal clusters. The evolution of metal clusters properties with their size governs by an interplay of the electronic and geometry shell closures. That fact implies using computer time demanding direct *ab initio* molecular dynamics simulations methods rather than simple jellium model approaches when exploring electronic properties and stucture of metal clusters. In the current project we calculate binding energies per atom, ionization potentials, dissociation energies and energy gaps between the highest occupied and the lowest unoccupied molecular orbitals for clusters of alkali, alkaline earth and rare earth metals. We study how the excessive charge influence on the optimized geometry and other properties of metal clusters and demonstrate that ionization of the small metal clusters results in the alteration of the sequence of magic numbers. Fission and dissociation of charged Na, Mg and Sr clusters have been studied by means of *ab initio* DFT methods. Energetics of the process, fission barriers, and fission pathways, were analyzed. The impact of cluster structure and its rearrangement on the fission process was elucidated. The importance of rearrangement of the cluster structure during fission has been demonstrated. An impact of the cluster geometry on the change of the system's entropy due to fission was studied. Stability, structure and properties of electron-positron droplets of different sizes were investigated. Our calculations are based on *ab initio* theoretical methods invoking the density-functional theory and molecular dynamics simulations. The results obtained are compared with the available experimental data and the results of other theoretical works.

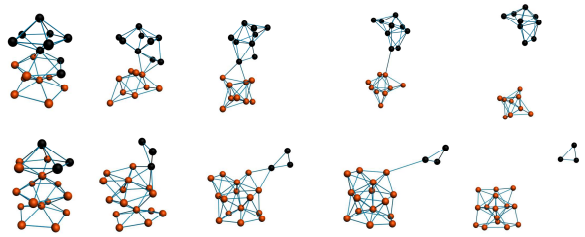


Fig. 1: Rearrangement of the cluster structure during the fission processes $Na_{18}^{2+} \rightarrow 2Na_{9}^{+}$ *(upper row) and* $Na_{18}^{2+} \rightarrow Na_{15}^{+} + Na_{3}^{+}$ *(lower row).*

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4.5.5 Magnetic properties of atomic clusters

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The properties of atomic clusters are very different from those of the bulk materials and change drastically with increasing cluster size. This fact gives a unique opportunity to form new materials by properly assembling selected clusters. One of the most exciting developments in the physics of clusters relates to their magnetic behavior. The study of evolution of magnetic properties from atoms to the bulk is important for the development of magnetic nanomaterials and understanding the fundamental principles of spin coupling in finite and low dimensional systems.

In this project we perform a systematic theoretical investigation of optimized ionic structure, electronic and magnetic properties of *La* clusters within the size range $N \leq 14$. The cluster geometries have been determined by finding local minima on the multidimensional potential energy surface. With increasing cluster size, such calculations become computer time demanding. We focus our study on emergence of magnetic properties in *La* clusters and found a giant enhancement of magnetism in La_4, La_6 and La_{13} clusters. We also found that the ground states of La_2, La_3, La_5, La_7, La_9–La_{11}, and La_{14} clusters possess non zero magnetic moment, that ranged from ~ 0.1 to 1.0 μ_B per atom, clearly indicating that small *La* clusters display magnetic behavior, even thought bulk *La* has no magnetic ordering.

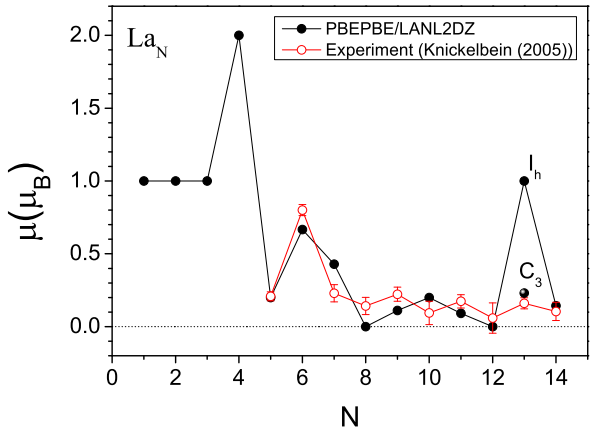

Abbildung 4.21: *Magnetic moments per atom of La clusters as a function of cluster size. Filled circles represent the magnetic moments per atom calculated within PBEPBE/LANL2DZ method. For La_{13}, the ground state structure I_h and the first low-lying isomer C_3 are presented. Open circles present the results of experiment by Knickelbein (2005)*

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4.5.6 Theoretical study of structure and dynamics of polypeptide chains

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Proteins consist of amino acids whose number may vary in the range from hundreds up to tens of thousands. Small fragments of proteins are usually called polypeptide chains or polypeptides. This project is devoted to a study of the conformational properties of alanine polypeptide chains. We have investigated the potential energy surfaces for alanine chains consisting of three and six amino acids. For these molecules we have calculated potential energy surfaces as a function of the Ramachandran angles φ and ψ, which are widely used for the characterization of the polypeptide chains. These particular degrees of freedom are essential for the characterization of proteins folding process. Calculations have been carried out within *ab initio* theoretical framework based on the density functional theory and accounting for all the electrons in the system. We have determined stable conformations and calculated the energy barriers for transitions between them. Using a thermodynamic approach, we have estimated the times of characteristic transitions between these conformations. We have also investigated the influence of the secondary structure of polypeptide chains on the formation of the potential energy landscape. This analysis has been performed for the sheet and the helix conformations of chains of six amino acids. From theoretical viewpoint, investigation of small polypeptides is of significant interest because they can be treated by means of *ab initio* methods which allow accurate comparison of theoretical predictions with experiment. The results of *ab initio* calculations can be then utilized for the development of model approaches applicable for the description of larger and more complex protein structures. It is worth noting that for some conformations of alanine hexapeptide the angles φ and ψ change significantly when the relaxation of all degrees of freedom in the system accounting for. This means that the potential energy surface of the alanine hexapeptide in the vicinity of the mentioned minima is very sensitive to the relaxation of all degrees of freedom. However, calculation of the potential energy surface with accounting for the relaxation of all degrees of freedom is unfeasible task. Indeed, one needs about 2000 hours of computer time (single processor Pentium Xeon 2.4 GHz) for the calculation of the potential energy surface for the alanine hexapeptide. To perform an analogues calculation with accounting for the relaxation about 5 years of computer time would be needed. Nevertheless, the potential energy surface calculated without accounting for the relaxation carries a lot of useful information. Thus, one can predetermine stable conformations of polypeptide, which then can be used as starting configurations for further energy minimization.

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