UNIVERSITÄT PADERBORN
Die Universität der Informationsgesellschaft

Annual Report 2008/2009

PADERBORN
CENTER FOR
PARALLEL
COMPUTING

University of Paderborn
Paderborn Center for Parallel Computing
Fürstenallee 11, D-33102 Paderborn

www.upb.de/pc2

Table of Contents

Foreword

The Paderborn Center for Parallel Computing PC² is a central scientific institute at the University of Paderborn, serving as a research and service center for parallel and distributed computing. PC² develops and provisions innovative parallel computer systems for universities in North-Rhine Westphalia. Scientists at PC² investigate methods and architectures for the efficient use of parallel and distributed systems. This research includes classical high-end computing as well as datacenter administration and storage.

After the withdrawal of the managing director Professor Dr. Odej Kao and the chairman of the board Professor Dr. Burkhard Monien, far reaching changes took place. In the last two years, 2008 and 2009, the tasks and facilities of PC² where consolidated and the collaboration with other research facilities were extended. An important step was the appointment of Dr. André Brinkmann as junior professor at the institute of computer science, associated with the position of managing director at PC². His professorship “Virtualization in High-End Computing Systems” is closely related with the current aims of PC². Jun.-Prof. Dr. Brinkmann took over these tasks on August 1st 2008. He influenced the work at the PC² within a short time and was extraordinarily successful in project acquisition. We wish Dr. Brinkmann similar success also for the future.

The PC²’s management structure also changed even more in 2008 and 2009. Most notably, the PC² has an advisory board since 2009. We were able to win as board members Karsten Beins, Fujitsu Technology Solutions Paderborn, Dr. Horst Joepen, Searchmetrics Berlin, Prof. Thomas Lippert, Forschungszentrum Jülich, Prof. Alexander Reinefeld, Humboldt University and managing director of the Zuse Institute Berlin, Prof. Michael Resch, High Performance Computing Center Stuttgart, Prof. Nikolaus Risch, President of the University of Paderborn and Dr. Werner Sack, Miele Gütersloh. We were happy to recruit new members for our management board as well, even though we had to say good-bye to long-time board members as well.

Dr. Kerstin Voß and Dr. Stefan Lietsch had successfully finished their dissertations at the end of 2008. Miss Tanja Müller finished her apprenticeship and became an IT-specialist in June 2009.

New projects were acquisitioned, enabling PC² to increase the number of employees to 26. During this reporting period, the EU projects SCALUS (Marie Curie Actions – Networks for Initial Training) and OneLab2 as well as the participation in the EU project HYDRA have started. The new projects DGSI and MoSGrid are supported by the BMBF. MoSGrid makes it possible to further improve the working relationship

with colleagues from the Paderborn department of chemistry. Additionally, the PC² was very successful in obtaining BMWi projects like RECS, which deals with new computer architectures, as well as the custom computing projects Prostheses Shaft, Tumor Diagnosis and ProAdapt-2. Furthermore Intel suports the project Intel-AAP and Microsoft Research the project GOmputer. The BMBF projects BiS-Grid and Tandem have continued in 2009. The EU-projects HPC4U and AccessGrid, the DFG projects Move-2 and ReconOS-2 as well as the BMBF project D-Grid/DGI were successfully completed.

These projects, as well as other research at the university, took advantage of the service role of PC². A main service was the provision of the computing power of the "Arminius"-cluster. Altogether a utilization of 90% was reached in 2008 and 2009, which is an excellent value for a computing center of this class. The importance of this system is not only limited to Paderborn, as nearly 55% of the computing power is consumed by research institutes outside of Paderborn, 17% alone by the University Bielefeld. This shows in particular the importance of high performance computing in our part of North Rhine-Westfalia. Nevertheless, Arminius is reaching its end of life and needs to be replaced in the near future. Therefore, some experimental systems were introduced and tested, paving the way for the procurement of a new high performance computer. The prospect of such a new procurement is good, especially as the University of Paderborn just started constructing a new building for PC2 (and other purposes) in January 2010. With this building the required technical infrastructure (electrical supply, cooling, admission control) is created to allow the growth of the PC² and enables it to deploy new, innovative parallel computing systems.

At the "International Supercomputing Conference" 2008 in Dresden, the initial agreement for the Gauss Alliance was signed. The 12 German supercomputing centers had herewith created a globally unique network of HPC centers; PC² was and is involved as a founding associate member.

Members of the PC² won several awards during the period under report. Jun.-Prof. Dr.-Ing. André Brinkmann (together with Dr. Herres-Pawlis, TU Dortmund) has received the research award 2008 of the University of Paderborn for the project "Theoretical Analyses of Lactid-Polymeristion in a Virtualized Surrounding". In 2009, this research award was given to Dr. Christian Plessl and Dr. Förster (department of physics) for the project "Custom Computing Architectures for Nanophotonics". A graduate award for the best German diploma thesis in the context of open source computing went to Dominic Eschweiler, a former student of PC² and supervised by Jun.-Prof. Dr.-Ing Brinkmann.

Altogether we can look back at two successful years. The initiated structural change of the years 2006 and 2007 showed first success. We confidently believe that this can be continued in the next years.

Prof. Dr. Holger Karl
Chairman of the PC² board
May 2010

Vorwort

Das PC^2 ist eine zentrale wissenschaftliche Einrichtung der Universität Paderborn und arbeitet als Forschungs- und Dienstleistungszentrum im Bereich des parallelen und verteilten Rechnens. Die wesentlichen Aufgaben des PC^2 liegen in der Entwicklung und Bereitstellung innovativer paralleler Rechnersysteme für die Hochschulen des Landes Nordrhein-Westfalen sowie in der Entwicklung von Methoden und Verfahren zur effizienten Nutzung paralleler und verteilter Systeme, insbesondere auch über die klassischen Anwendungen des Hochleistungsrechnens hinausgehend für Anwendungen der Datencenter-Verwaltung oder der Speicherung von Informationen.

Nachdem in den Jahren 2006 und 2007 durch das Ausscheiden des geschäftsführenden Leiters Prof. Dr. Odej Kao und des Vorsitzenden des Vorstandes Prof. Dr. Burkhard Monien tief greifende Veränderungen stattfanden, gelang in den letzten beiden Jahren 2008 und 2009 eine Konsolidierung und Arrondierung der Tätigkeitsfelder und Forschungsrichtungen des PC^2 und eine Ausrichtung auf moderne Anwendungsfelder des verteilten Rechnens. Wesentlich war dazu die Berufung von Herrn Dr.-Ing. André Brinkmann auf eine Juniorprofessur im Institut für Informatik, verbunden mit der geschäftsführenden Leitung des PC^2. Der Titel der Professur „Virtualisierung in Hochleistungssystemen“ steht dabei in engem Einklang mit den fortgeschriebenen Zielen des PC^2. Jun.-Prof. Dr.-Ing. Brinkmann übernahm diese Aufgaben zum 1. August 2008 und hat in der kurzen Zeit bereits prägenden Einfluss auf das PC^2 gehabt und kann bereits außerordentliche Erfolge in der Akquisition von Projekten vorweisen. Wir wünschen Herrn Brinkmann auch weiterhin viel Erfolg!

Neben diesen Änderungen gab es auf weiteren Feldern eine Fortentwicklung des PC^2. Seit 2009 verfügt das PC^2 über einen Beirat, der durch Herrn Beins von Fujitsu Technology Solutions, Dr. Horst Joepen von Searchmetrics, Prof. Thomas Lippert vom Forschungszentrum Jülich, Prof. Reinefeld vom Zuse-Institut Berlin, Prof. Resch vom Hochleistungsrechenzentrum Stuttgart, Prof. Risch von der Universität Paderborn und Dr. Sack von der Miele hochrangig besetzt ist. Diverse Änderungen gab es auch im PC^2 Vorstand zu verzeichnen. Wir sind sehr froh, das wir neue Mitglieder für unseren Vorstand dazu gewinnen konnten, mussten uns aber auch leider von einigen langjährigen Mitgliedern verabschieden.

Frau Dr. Kerstin Voß und Herr Dr. Stefan Lietsch haben Ende 2008 erfolgreich ihre Promotion abgelegt und Ihre Ausbildung zur Fachinformatikerin hat Frau Tanja Müller im Juni 2009 erfolgreich abgeschlossen.

Durch den Zuwachs an neuen Projekten konnte das PC^2 auch eine Reihe an neuen Mitarbeitern einstellen und somit auf 26 Mitarbeiter wachsen. In der Berichtsperiode sind dies die EU-Projekte SCALUS (Marie Curie Actions – Networks for Initial Training (ITN)) und OneLab2 sowie eine Beteiligung am EU-Projekt HYDRA. Durch

das BMBF wurden die Projekte DGSI und MoSGrid gefördert; letzteres ermöglichte insbesondere eine Vertiefung der Zusammenarbeit mit Kollegen der Chemie. Zusätzlich war das PC^2 sehr erfolgreich bei der Einwerbung von Projekten des BMWi mit den Projekten RECS, Prothesenschäfte, ProAdapt-2, und Tumordiagnose. Weiterhin wurden durch Intel das Projekt Intel-AAP und durch Microsoft Research das Projekt GOmputer gefördert. Das BMBF-Projekt BiS-Grid und das Projekt Tandem liefen weiter; die EU-Projekte HPC4U und AccessGrid, die DFG-Projekte Move-2 und ReconOS-2 sowie das BMBF-Projekt D-Grid/DGI wurden in der Berichtsperiode erfolgreich beendet.

Diese Projekte wie auch andere in der Universität durchgeführte Forschungsarbeiten profitieren dabei auch von der Dienstleistungsrolle des PC². Diese wird insbesondere durch die Bereitstellung von Rechenleistung im „Arminius"-Cluster wahrgenommen. Zwar ist dieses System noch das Arbeitspferd des PC² und vollbringt diesen Dienst, arbeitet inzwischen verlässlich und steht einfach nutzbar zur Verfügung. Insgesamt wurde im vergangenen Jahr eine hohe Auslastung von ca. 90% erzielt; ein für Rechenzentren dieser Klasse ausgezeichneter Wert. Die Bedeutung dieses Systems ist dabei nicht auf Paderborn beschränkt: Ca. 55% der Rechenleistung wurde für nicht in Paderborn arbeitende Forscher zur Verfügung gestellt, davon alleine 17% für die Universität Bielefeld. Dieses zeigt eindrucksvoll die Bedeutung des Hochleistungsrechnens für die gesamte Region Ostwestfalen-Lippe. Allerdings ist der „Arminius-Cluster" inzwischen deutlich in die Jahre gekommen und bedarf in absehbarer Zeit der Ablösung. Um dies vorzubereiten, wurden im Jahr 2009 einige experimentelle Systeme aufgebaut und getestet, die als Vorläufer der neuen Rechnergeneration angesehen werden können. Die daraus resultierenden Erfahrungen werden in die Beschaffung eines neuen Hochleistungsrechners einfließen. Die Perspektiven für eine solche Neubeschaffung sind sehr gut, da die Universität Paderborn durch den im Januar 2010 erfolgten Spatenstich für einen Neubau die Grundlagen gelegt hat; mit diesem Neubau wird die gebäudetechnische Infrastruktur (Stromversorgung, Kühlung, Zugangskontrolle) geschaffen, die dem PC^2 ein Wachstum in neue, innovative und größere Systeme über die bisherigen Beschränkungen hinaus ermöglichen wird.

Am Rande der Internationalen Supercomputing Konferenz 2008 in Dresden wurde die Vereinbarung zur Gründung der Gauss Allianz unterzeichnet. Damit schaffen die 12 beteiligten Supercomputerzentren in Deutschland einen weltweit einzigartigen Rechnerverbund. Das PC^2 war an dieser Initiative beteiligt.

Preise und Auszeichnungen gab es für PC^2 selbstverständlich auch zu verzeichnen. Der Forschungspreis 2008 wurde für das Projekt „Theoretische Analyse der Lactid-Polymeristion in einer virtualisierten Umgebung" an Jun.-Prof. Dr.-Ing. Brinkmann (gemeinsam mit Dr. Herres-Pawlis der TU Dortmund) vergeben. Den Forschungspreis 2009 gab es für Dr. Christian Plessl und Dr. Förster (Physik) für das Projekt „Custom Computing Architectures for Nanophotonics". Auch der Absolventenpreis der Univention ging an einen ehemaligen Studenten des PC^2 –

Dominic Eschweiler. Dessen hervorragende Diplomarbeit wurde durch Jun.-Prof. Dr.-Ing. Brinkmann betreut.
Insgesamt können wir damit auf zwei erfolgreiche Jahre zurückblicken. Der in den Jahren 2006 und 2007 eingeleitete Strukturwandel hat erste Erfolge gezeigt. Wir sind zuversichtlich, dass dies auch in den nächsten Jahren fortgesetzt werden kann.

Prof. Dr. Holger Karl
Vorsitzender des Vorstandes PC²
Im Mai 2010

2 Inside PC²

2.1 Board

The PC² is headed by an interdisciplinary board comprising professors from various working groups. The following people were assigned to the PC^2 board in the reporting period.

2.2 Members of the Board

Prof. Dr. Holger Karl (Chairman)
Faculty of Electrical Engineering, Computer Science and Mathematics

Jun.-Prof. Dr.-Ing. André Brinkmann (Managing Director)
Faculty of Electrical Engineering, Computer Science and Mathematics

Prof. Dr. Wilhelm Dangelmaier (until August 2009)
Faculty of Business Administration and Economics

Prof. Dr. Michael Dellnitz
Faculty of Electrical Engineering, Computer Science and Mathematics

Prof. Dr. Gregor Fels (since 2009)
Faculty of Science

Prof. Dr. Hans-Ulrich Heiß (until 2009)
Institute for Telecommunication Systems, Technical University Berlin

Prof. Dr. Joachim Lückel (until 2008)
Faculty of Mechanical Engineering

Prof. Dr. Burkhard Monien
Faculty of Electrical Engineering, Computer Science and Mathematics

Prof. Dr. Marco Platzner
Faculty of Electrical Engineering, Computer Science and Mathematics

Prof. Dr. Franz Josef Rammig
Faculty of Electrical Engineering, Computer Science and Mathematics

Prof. Dr. Ulrich Rückert
Faculty of Electrical Engineering, Computer Science and Mathematics

Prof. Dr. Otto Rosenberg (until 2008)
Faculty of Business Administration and Economics

Prof. Dr. Wolf Gero Schmidt
Faculty of Theoretical Physics

Prof. Dr. Hans-Joachim Warnecke
Faculty of Science

Dr. Jens Simon
Paderborn Center for Parallel Computing
Assistant researchers´ representative

Dipl.-Inform. Sabina Rips (until 2008)
Faculty of Electrical Engineering, Computer Science and Mathematics
Assistant researchers´ representative

Dipl.-Inform. Axel Keller
Paderborn Center for Parallel Computing
Non researchers´ representative

Patrick Koch (until 2009)
Student representative

2.3 PC² Advisory Board

Karsten Beins
Senior Director Portfolio & Technology
Fujitsu Technology Solutions, Paderborn

Dr. Horst Joepen
CEO
Searchmetrics GmbH, Berlin

Prof. Dr. Dr. Thomas Lippert
Director of Institute for Advanced Simulation, Head of Jülich Supercomputing Centre,
Jülich Supercomputing Centre, Jülich

Prof. Dr. Alexander Reinefeld
Head of Computer Science, Zuse-Institut Berlin
Humboldt Universität Berlin

Prof. Dr.-Ing. Michael Resch
Director of the High Performance Computing Center Stuttgart
HLRS Höchleistungsrechenzentrum Stuttgart

Prof. Dr. Nikolaus Risch
Präsident der Universität Paderborn
Universität Paderborn

Dr. Werner Sack,
Leiter Konstruktion/Entwicklung, Head of Product Engineering and Development
Miele & Cie. KG, Gütersloh

2.4 PC² Staff

The following people were assigned to the PC² for the period of time covered by this report.

Dipl.-Inform. Bernard Bauer
M.Sc. Tobias Beisel (since June 2008)
Dipl.-Inform. Georg Birkenheuer
Jun.-Prof. Dr.-Ing. André Brinkmann
Dipl.-Inform. Sascha Effert (since January 2009)
Birgit Farr (Secretary)
Dipl.-Inform. Yan Gao (since February 2009)
M.Sc. Mariusz Grad (associated with since October 2007)
M.Sc. Matthias Grawinkel (since November 2009)
Dipl.-Inform. Dipl.-Math. Paul Kaufmann
Dipl.-Inform. Axel Keller
Dipl.-Inform. Matthias Keller (Since October 2009)
Michaela Kemper (Secretary)
Dipl.-Inform. Tobias Kenter (since October 2008)
Dipl.-Ing. Andreas Krawinkel
Dipl.-Inform. Stefan Lietsch (until December 2008)
Dipl.-Inform. Jens Lischka
Dipl.-Ing. Enno Lübbers
Nils Lücking (Trainee since August 2008)
M.Sc. Dirk Meister (since January 2009)
Dipl.-Ing. Björn Meyer (since December 2009)
Tanja Müller (until December 2009)
Dipl.-Inform. Oliver Niehörster
Holger Nitsche
Dr. Christian Plessl
Dipl.-Inform. Lars Schäfers (since March 2009)
Dipl.-Inform. Tobias Schumacher
Dr. Jens Simon
Dipl.-Inform. Kerstin Voß (until December 2008)

Within the reporting period additional support was provided by students and graduate assistants who were engaged part time (9.5 h/week and 19 h/week) in tasks, which included programming, user support, system administration, etc.

Zahra Aghayary	Alexander Kujat	Adrian Wilke
Andreas Agne	Dominik Leibenger	Jakob Wisor
Alexander Boschmann	Robert Meiche	
Holger Bürger	Dirk Meister	
Martin Dräxler	Marc Östermann	
Matthias Frye	Kai-Uwe Renken	
Matthias Grawinkel	Alexander Rittler	
Christoph Kleineweber	Jörn Schumacher	
Tobias Kniepe	Elmar Weber	
Christoph Konersmann	Jannis Weide	
Alexander Krieger	Tobias Wiersema	

In the year 2008/2009 the PC² employed two trainees to learn the trade of a “computer specialist” (Fachinformatiker) in the field of system integration. With the source required to employ trainees provided by the North Rhine-Westphalia government, the PC² was able to oversee this priority assignment.

3 Research and Projects

3.1 Research Areas

Research interests of the PC² are parallel and distributed large scale systems.
The focus of research is on

- Custom Computing & Many Cores
- Middleware & system software
- Scalable Storage Systems
- Testbeds & Benchmarking

Current information is also presented on the web pages of the PC²
(http:/www.upb.de/pc2).

Computer Architecture
Application-specific coprocessors can significantly accelerate many high-performance computing (HPC) applications. Designing fast accelerators and optimizing their performance remains a difficult task requiring significant hardware design expertise.
The PC² has a long-term experience with innovative cluster systems based on commodity as well as on specialized hardware components. Different techniques to accelerate compute nodes are considered, like multi-core processors, graphical processing units (GPUs), and acceleration cards equipped with field-programmable gate arrays (FPGAs). Hence, vendors of supercomputers and high-performance workstations are beginning to integrate reconfigurable accelerators in their products, which makes this custom computing technology available to a broader user group. One of our missions is to make the potential of custom computing more accessible to users. To this end, we work on basic infrastructure for reconfigurable computers, specifically we work on flexible and portable communication infrastructures and on runtime systems that support dynamic reconfiguration. In several application projects we are exploring the applicability of these infrastructures by building scalable accelerators for HPC applications that exploit the performance of FPGAs and standard CPUs.

Maximizing the performance of an application consisting of many tasks is challenging, since the hardware accelerator cores affect each other when accessing

shared resources. Hence, meticulous care has to be taken to avoid bottlenecks in an implementation. To support the designer with performance optimization, we are working on estimating the application's performance with a model-based approach. By combining a model of the application and a model of the execution architecture, we can study the influence of various system parameters, such as communication bandwidths and latencies, and can use this information for performance optimization

Research Topics	***Contact***	***Email***
Multi-Objective Intrinsic Evolution of Embedded Systems	Paul Kaufmann	paul.kaufmann@upb.de
Reconfigurable hardware Operating Systems	Enno Lübbers	enno.luebbers@upb.de
High performance custom computing	Dr. Christian Plessl	christian.plessl@upb.de
Reconfigurable architectures	Tobias Schumacher	tobe@upb.de
Computer system architecture	Dr. Jens Simon	simon@upb.de

Middleware & system software

The PC²'s research focuses on the problem of how to guarantee Service Level Agreements (SLA) in Cloud and Grid environments. This research includes fault tolerance mechanisms like checkpointing and migration of jobs and the assessment of the likelihood of SLA violations. The combined instruments, risk assessment and fault tolerance mechanisms, allow a powerful risk aware management of cluster, cloud, and grid jobs. This improves the guaranteed service quality of the resource management.

In addition, the PC² works on the integration of Web service based Enterprise Application Integration (EAI) into Grid and Cloud environments. Our aim is to combine the strengths of the two areas, loosely coupled services and secure and easy to deploy grid infrastructures. The result will be the ability to create secure business workflows in distributed infrastructures.

Resource Management Systems (RMS) are needed for the grid as well as for compute clusters. They allow users and system administrators to access and manage various computing resources like processors, memory, networks, or storage. PC² has developed an expandable and modular RMS, called Computing Center Software (openCCS), which uses a planning based job scheduler. OpenCCS is used in several projects and its features are continuously extended.

Research Topics	*Contact*	*Email*
Risk Assessment / Management, Service Level Agreements,	Georg Birkenheuer	birke@upb.de
Grid and Cloud Computing	Matthias Keller	mkeller@upb.de
Grid-based integration and orchestration of business information systems	Holger Nitsche	hn@upb.de
Computing Center Software (OpenCCS)	Axel Keller	kel@upb.de

Scalable Storage Systems

Data has become one of the most valuable assets in all businesses and one of the most volatile. With all businesses, today, the growth of data needed to operate is increasing at 67% per year at current business practices. To worsen the data storage problem, many new regulations require that much data and electronic records and emails be readily available. For these reasons, the requirement for storage continues to grow at a phenomenal pace. Complexity and the proprietary nature of storage systems have meant and continue to mean high investment and management costs.

The Paderborn Center for Parallel Computing develops parallel storage algorithms, integrates them in scalable storage architectures and leverages their usage by new management concepts.

Research Topics	*Contact*	*Email*
Scalable Storage Systems	Sascha Effert	fermat@upb.de
Parallel Data Deduplication	Dirk Meister	dmeister@upb.de
Reliability in scalable environments	Yan Gao	yan.gao@upb.de
Archiving	Matthias Grawinkel	grawinkel@upb.de

Testbeds & Benchmarking

The development of software components for highly complex networked systems requires, besides analytical and simulation-based evaluation methods, more and more experiments in large real live traffic environments. One method to build a new system on top of an existing system is to use virtualization. Virtualization of resources can be found in all areas of computing. Also in the domain of networking, virtualization is used to hide the characteristics of network resources (like routers,

switches, etc.) from the way in which other systems interact with them. The PC² is engaged in investigating how virtualization can be utilized as a concept in the context of building new network testbeds.

The PC² benchmarking center is specialized in evaluating the performance of high-speed networks and parallel computer systems. Typically, these are based on cluster technology. We evaluate functional parts or complete systems with the help of so-called low-, system-, and application-level benchmarks. Derived from this evaluation new system architectures will be developed. In addition, the PC² offers assistance with running existing parallel applications in a cost efficient way and with porting applications to high performance parallel computers.

Research Topics	***Contact***	***Email***
Testsbed for network virtualization	Jens Lischka	jens.lischka@uni-paderborn.de
System Evaluation, Benchmarking, Experimental Cluster Systems	Dr. Jens Simon	simon@uni-paderborn.de

3.2 Projects

Projects started in 2008 and 2009

Funding agency	*Projectname*	*Start of the Project*	*End of the Project*
EU	Hydra	October 2008	June 2010
EU	OneLab2	September 2008	November 2010
EU	SCALUS	December 2009	November 2013
BMBF	DGSI	May 2009	April 2012
BMBF	MoSGrid	September 2009	August 2012
BMWi	RECS	January 2009	July 2010
BMWi	Prothesengeschäfte	April 2009	March 2011
BMWi	ProAdapt-2	July 2009	October 2011
BMWi	Tumordiagnose	July 2009	June 2011
Intel	Intel-AAP	September 2008	December 2009
Microsoft Research Ltd.	GOmputer	March 2009	February 2012

Ongoing Projects

Funding agency	*Projectname*	*Start of the Project*	*End of the Project*
BMBF	BIS-Grid	May 2007	April 2010
BMBF / IHP	Tandem	July 2007	December 2010

Projects finished in 2008 and 2009

Funding agency	*Projectnamen*	*Start of the Project*	*End of the Project*
EU	HPC4U	June 2004	February 2008
EU	AssessGrid	June 2006	March 2009
DFG	Move-2	September 2007	August 2009
DFG	ReconOS-2	January 2008	December 2009
BMBF	D-Grid (DGI)	September 2005	February 2008
Fujitsu Siemens Computer		July 1999	December 2009

For current information about our projects please refer to our website.

3.3 Publications, Grants, and Awards

Papers 2009

Tobias Schumacher, Christian Plessl, Marco Platzner
IMORC: Application Mapping, Monitoring and Optimization for High-Performance Reconfigurable Computing
In: 7th IEEE Symposium on Field-Programmable Costum Computing Machines

Georg Birkenheuer, André Brinkmann, Holger Karl
The Gain of Overbooking
In: Proceeding of the 14th Workshops on Job Scheduling Strategies for Parallel Processing (JSSPP)

Dirk Meister, André Brinkmann
Multi-Level Comparison of Data Deduplication in a Backup Scenario
In: Proceedings of SYSTOR 2009 – The Israeli Experimental Systems Conference

André Brinkmann, Dominic Eschweiler
A Microdriver Architecture for Error Correcting Codes inside the Linux Kernel
In: Proceedings of Supercomputer (SC)

Stefan Gudenkauf, Andre Höing, Guido Scherp, Dirk Meister, André Brinkmann
An Orchestration as a Service Infrastructure using Grid Technologies and WS-BPEL
In: Proceedings of the 7th International Joint Conference on Service Oriented Computing

Jens Lischka, Holger Karl
A virtual network mapping algorithm based on subgraph isomorphism detection
In: Proceedings of the 1st ACM workshop on Virtualized infrastructure systems and architectures

Mariusz Grad, Christian Plessl
Poster Abstract: Woolcano - An Architecture and Tool Flow for Dynamic Instruction Set, Extension on Xilinx Virtex-4 FX
Proc. IEEE Symp. on Field-Programmable Custom Computing Machines (FCCM)

Matthias Woehrle, Christian Plessl, Lothar Thiele
Rupeas: Ruby Powered Event Analysis DSL
In: TIK-Report 290, ETH Zürich, Computer Engineering and Networks Lab

Tobias Schumacher, Tim Süß, Christian Plessl, Marco Platzner
Communication Performance Characterization for Reconfigurable Accelerator Design on the XD1000
In: Proc. Int. Conf. on ReConFigurable Computing and FPGAs (ReConFig)

Jan Beutel, Stephan Gruber, Andreas Hasler, Roman Lim, Andreas Meier, Christian Plessl, Igor Talzi, Lothar Thiele, Christian Tschudin, Matthias Woehrle, Mustafa Yuecel
Demo Abstract: Operating a Sensor Network at 3500m Above Sea Level
In: Proc. ACM/IEEE Int. Conf. on Information Processing in Sensor Networks (IPSN)

Jan Beutel, Stephan Gruber, Andreas Hasler, Roman Lim, Andreas Meier, Christian Plessl, Igor Talzi, Lothar Thiele, Christian Tschudin, Matthias Woehrle, Mustafa Yuecel
PermaDAQ: A Scientific Instrument for Precision Sensing and Data Recovery in Environmental Extremes
In: Proc. ACM/IEEE Int. Conf. on Information Processing in Sensor Networks (IPSN)

Tobias Schumacher, Christian Plessl, Marco Platzner
An Accelerator for k-th Nearest Neighbor Thinning Based on the IMORC Infrastructure
In: Proc. Int. Conf. on Field Programmable Logic and Applications (FPL)

Matthias Woehrle, Christian Plessl, Lothar Thiele
Poster Abstract: Rupeas - An Event Analysis Language for Wireless Sensor Network Traces
In: Adjunct Proc. of European Conf. on Wireless Sensor Networks (EWSN)

Mariusz Grad, Christian Plessl
Woolcano: An Architecture and Tool Flow for Dynamic Instruction Set Extension on Xilinx Virtex-4 FX
In: Proc. Int. Conf. on Engineering of Reconfigurable Systems and Algorithms (ERSA)

Paul Kaufmann, Christian Plessl, Marco Platzner
EvoCaches: Application-specific Adaptation of Cache Mapping
In: Proc. NASA/ESA Conference on Adaptive Hardware and Systems (AHS)

Georg Birkenheuer, Arthur Carlson, Alexander Fölling, Mikael Högqvist, Andreas Hoheisel, Alexander Papaspyrou, Klaus Rieger, Bernhard Schott, Wolfgang Ziegler
Connecting Communities on the Meta-Scheduling Level: The DGSI Approach!
In: Proceedings of the Cracow Grid Workshop (CGW)

Oliver Niehörster, Georg Birkenheuer, André Brinkmann, Brigitta Elsässer, Sonja Herres-Pawlis, Jens Krüger, Julia Niehörster, Lars Packschies
Providing Scientific Software as a Service in Consideration of Service Level Agreements
In: Proceedings of the Cracow Grid Workshop (CGW)

Papers 2008

André Brinkmann, Sascha Effert
Redundant Data Placement Strategies for Cluster Storage Environments
In: 12th International Conference on Principles of Distributed Systems (OPODIS 2008)

Marcin Bienkowski, André Brinkmann, Miroslaw Korzeniowski
Degree 3 Suffices: A Large-Scale Overlay for P2P Networks
In: 12th International Conference on Priniciples of Distributed Systems (OPODIS 2008)

Björn Griese, André Brinkmann, Mario Porrmann
SelfS - - A Real Time Protocol for Virtual Ring Topologies
In: 16th International Workshop on Parallel and Distributed Real-Times Systems (WPDRTS ´08)

André Brinkmann, Sascha Effert
Data Replication in P2P Environments
In: 20th ACM Symposium on Parallelism in Algorithms and Architectures (SPAA)

Georg Birkenheuer, André Brinkmann, Hubert Dömer, Sascha Effert, Christoph Konersmann, Oliver Niehörster, Jens Simon
Virtual Supercomputer for HPC and HTC
In: Proceedings of the “Gemeinsamer Workshop der GI/ITG Fachgruppen Betriebssysteme und KuVS”: Virtualized IT infrastructures and their managment

André Brinkmann, Stefan Gudenkauf, Wilhlem Haselbring, André Höing, Holger Karl, Odej Kao, Holger Nitsche, Guido Scherp
Employing WS-BPEL Design Patterns for Grid Service Orchestration using a WS-BPEL Engine and a Grid Middleware
In: Proceedings of the Cracow Grid Workshop (CGW)

André Brinkmann, Sascha Effert
Storage Cluster Architectures
In: Proceedings of the 1.GI/ITG kuVS Fachgespräch Virtualisierung

André Brinkmann, Holger Karl
Proceedings of the 1. GI/ITG KuVS Fachgespräch Virtualisierung

André Brinkmann, Roger Chamberlain
Proceedings of the 5th IEEE Workshop on Storage Network Architecture and Parallel IO (SNAPI)

Stefan Lietsch, Henning Zabel, Christoph Laroque
Computational Steering of Interactive Material Flow Simulations
In: ASME CIE08: Proceedings of the 28th ASME Computers and Information in Engineering Conference

Stefan Lietsch, Paul Hermann Lensing
CUDA-based, parallel JPEG Compression for Remote Rendering
IN: ISIVC08: Proceedings of the 4th International Symposium on Image/Video Communications over fixed and mobile networks

Stefan Lietsch, Paul Hermann Lensing
GPU-Supported Image Compression for Remote Visualization – Realization and Benchmarking
In: ISVC08: Proceedings of the International Symposium of Visual Computing

Christoph Laroque, Stefan Lietsch, Henning Zabel
Computational Steering verteilter, interaktiver Materialflusssimulationen
In: Augmented & Virtual Reallty in der Produktentstehung

Matthias Woehrle, Christian Plessl, Roman Lim, Jan Beutel, Lothar Thiele
EvAnT: Analysis and Checking of event traces for Wireless Sensor Networks
In: IEEE Int. Conf. on Sensor Networks, Ubiquitos, and Trustworthy Computing (SUTC)

Tobias Schumacher, Christian Plessl, Marco Platzner
IMORC: An infrastrcture for performance monitoring and optimization of reconfigurable computers
In: Many-core and Reconfigurable Supercomputing Conference (MRSC)

Tobias Schumacher, Robert Meiche, Paul Kaufmann, Enno Lübbers, Christian Plessl, Marco Platzner
A Hardware Accelerator for k-th Nearest Neighbor Thinning
In: Proceedings Int. Conf. on Engineering of Reconfigurable Systems and Algorithms (ERSA)

Kerstin Voss
Recursive Evaluation of Fault Tolerance Mechanisms for SLA Management
In: International Conference on Networking and Services (ICNS)

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Increasing Fault-tolerance by Introducing Virtual Execution Environments
In: Fachgespräch Virtualisierung

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Virtual Execution Environments for ensuring SLA-compliant Job Migration in Grids
In: SCC 2008: International Conference on Services Comouting, Honolulu, Hawaii

Tobias Beisel, Stefan Lietsch, Kris Thielemans
A method for OSEM PET reconstruction on parallel architectures using STIR
In: Nuclear Science Symposium Conference Record

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Increasing Fault-tolerance by Introducing Virtual Execution Environments
In: Proceedings of the Fachgespräch

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Germany, Belgium, France, and Back Again: Job Migration using Globus
In: Proceedings of the 2008 International Conference on Grid Computing and Applications (GCA´08), Las Vegas, USA

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Virtual Execution Environments for ensuring SLA-compliant Job Migration in Grids
In: Proceedings of the IEEE International Conference on Services Computing (SCC 2008)

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Job Migration and Fault Tolerance in SLA-aware Resource Management Systems
In: Proceedings of the The 3rd IEEE International Conference on Grid and Pervasive Computing

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Implementation of Virtual Execution Environments for improving SLA-compliant Job-Migration in Grids
In: Proceedings of the SRMPDS ´08, Fourth International Workshop on Scheduling and Resource Management for Parallel and Distributed Systems, Portland, USA

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Quality Assurance of Grid Service Provisioning by Risk Aware Managing of Resource Failures
In: Proceedings of the 3rd international Conference on Risks and Security of Internet and Systems, Tozeur, Tunisia

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Virtual Execution Environments and the Negotiation of Service Level Agreements in Grid Systems
In: 2nd International DMTF Academic Alliance Workshop on Systems and Virtualization Management: Standards and

Dominic Battré, Matthias Hovestadt, Odej Kao, Axel Keller, Kerstin Voss
Enhancing SLA Provisioning by Utilizing Profit-Oriented Fault Tolerance
IN: Proceedings of the 20th IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS 2008)

Georg Birkenheuer, Matthias Hovestadt, Odej Kao, Kerstin Voss
Overbooking in Planning Based Scheduling Systems
In: Proceedings of the 2008 International Conference on Grid Computing & Applications, GCA 2008, Las Vegas, Nevada

Dominic Battré, Georg Birkenheuer, Vikas Deora, Matthias Hovestadt, Omer Rana, Oliver Wäldrich
Guarantee and Penalty Clauses for Service Level Agreements
In: Proceedings of the Cracow Grid Workshop (CGW)

Dominic Battré, Georg Birkenheuer, Matthias Hovestadt, Odej Kao, Kerstin Voss
Applying Risk Management to Support SLA Provisioning
In: Proceedings of the Cracow Grid Workshop (CGW)

W. Richert, O. Niehörster, M. Koch
Layered understanding for sporadic imitation in a multi-robot scenario
In: Proceedings of the IEEE/RSJ International Conference on Intelligent Robots and Systems (IROS´08)

W. Richert, F. Klompmaker, O. Niehörster
Guiding exploration by combining individual learning and imitation in societies of autonomous robots
In: IFIP Conference on Biologically Inspired Cooperative Computing - BICC

Dissertations 2008

Stefan Lietsch
A Novel Approach to Interactive, Distributed Visualization and Simulation on Hybrid Cluster Systems, Universität Paderborn, 2008

Kerstin Voss
Supporting SLA Provisioning in Grids by Risk Management Processes, Universität Paderborn, 2008

Organization of Workshops

Fachgespräch Virtualisierung, Fachgruppe Kommunikation und Verteilte Systeme (KuVS) der GI/ITG, Februar 2008

5th IEEE Workshop on Storage Network Architecture and Parallel IO (SNAPI), Baltimore, USA, September 2008

Participation at Fairs

ISC 2009 in Hamburg

Awards

André Brinkmann and Sonja Herres-Pawlis: „Theoretische Analyse der Lactid-Polymerisation in einer virtualisierten Grid-Umgebung“, Forschungspreis der Universität Paderborn / Research Award of the University of Paderborn, 2008

Christian Plessl and Jens Förstner: „Custom Computing Architectures for Nanophotonics“, Forschungspreis der Universität Paderborn / Research Award of the University of Paderborn, 2009

Dominic Eschweiler: „Barracuda – eine Microdriver-Architektur für fehlerkorrigierende Codes im Linux-Kernel“, Univention-award for an outstanding master thesis in the area of Open-Source research, Berlin, 2009

4 Services

4.1 Operated Parallel Computing Systems

In 2008 and 2009 the PC² operated 11 high performance computing systems and one parallel file system. 7 of the HPC systems were dedicated to specific projects and/or working groups. 4 HPC systems were available for all internal and external researchers of the University

4.1.1 Publicly Available Systems

Arminius Cluster

With the financial support of the state North Rhine-Westphalia and the federal republic of Germany, the PC² established 2005 the ARMINIUS cluster. In co-operation with Fujitsu-Siemens Computers we designed the system consisting of 200 compute and 8 visualization nodes. The official opening with a ceremonial inauguration was at June, 21st 2005.

Hardware	***Description***
200 dual processor Intel Xeon	400 processors, each node with 3.2 GHz, 1 MByte L2-cache 4 GByte DDR2 main memory 4x InfiniBand PCI-e HCA
8 dual processor AMD Opteron	16 processors, each node with 2.4 GHz, 1 MB L2-cache 12 GByte DDR main memory 4x InfiniBand PCI-e HCA nVidia Quadro FX 4500G PCI-e graphics card
216 port InfiniBand switch Fabric	central switch fabric with 18 switch modules each with 12 ports
7 TByte parallel file system	Accessible from all nodes
1 login node	Nodes are used for compiling and starting user applications
Stereoscopic rear projection	1.80m x 2.40m screen 2 D-ILA projectors 3D tracking system

Table 1: Hardware specification of the Arminius Cluster

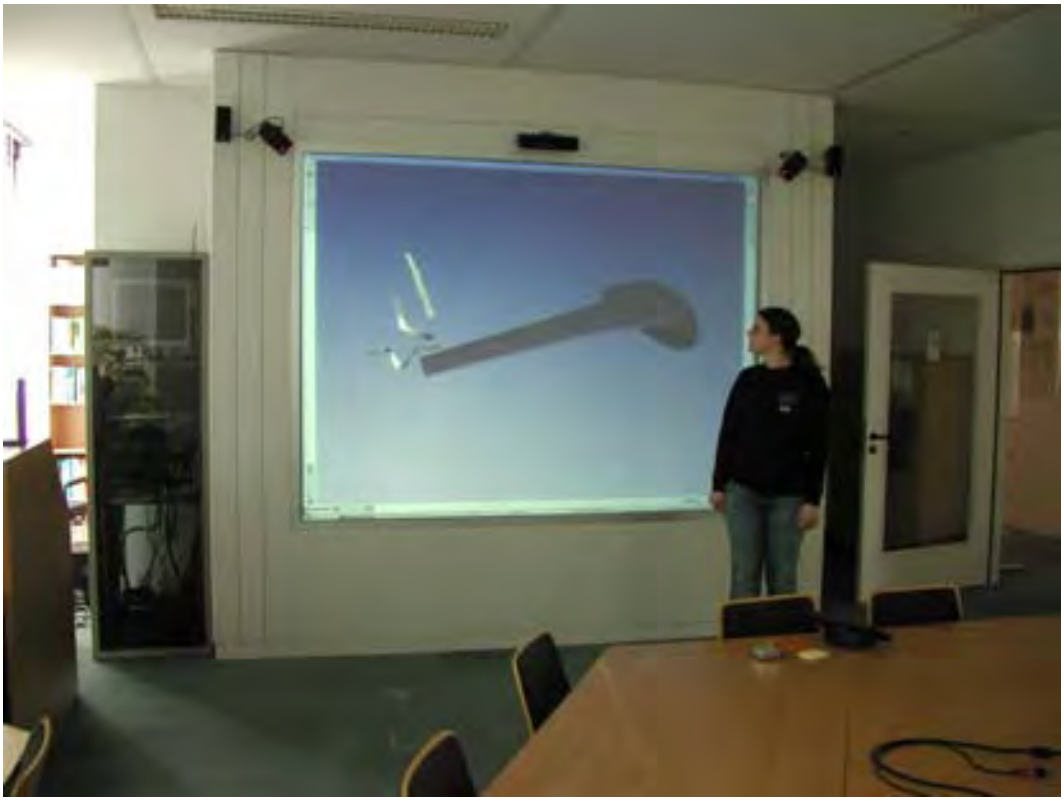


Fig. 1 The stereoscopic rear projection of the Arminius cluster

The Arminius cluster with 416 processors has a peak performance of 2.6 TFlop/s. This compute performance needs about 70 kWatt electrical power which leads to a nearly equal amount of thermal energy. Our computing center is not able to get that much energy out of the room with the installed air conditioning system. Therefore a special fluid based cooling system is used inside the system. All processors of the compute nodes have special heat sinks which are connected via a heat exchanger to the cooling system of the building. This technique is able to move 50 to 60 percent of the thermal energy directly out of the room. The rest is cooled with the air conditioner.

We provide standard system software for cluster systems. A Linux operating system with its software development tools is installed. Additionally, some MPI message passing libraries thereunder, three MPI versions optimized for InfiniBand are available. Scientific libraries for numerical applications are provided and the Intel compiler suite optimized for the Intel Xeon processor can be used. The software environment of the Arminius cluster is shown in the following table:

Software	***Description***
RedHat Advanced Server Release 5	Linux operating system 2.6.9 kernel
GNU Tools	e.g. gcc
Intel compiler	C/C++, Fortran
Scali-MPI-Connect	MPI 1 compliant, fail-over from IB to GbE
MvAPICH	MPICH on VAPI from Ohio State University
MPICH-vmi	MPICH for VMI from NCSA
Intel MKL	Math Kernel Library

Table 2: System Software of the Arminius Cluster

Company	***Components***
Fujitsu-Siemens Computers GmbH	general contractor cluster system
ICT AG	housings, system integration
SilverStorm Technologies	InfinIO 9200 switch fabric 216 ports (max 288 ports)
SilverStorm Technologies Mellanox Inc.	InfiniBand Host Channel adaptor PCI-E IB 4x
nVidia GmbH	graphics cards
Rittal AG	heat exchanger,racks, controlling and management of cooling system
Atotech GmbH	fluid based heat sinks
Intel GmbH	INTEL Xeon EM64T processors HPC software tools
Scali Inc.	MPI Connect
UNITY AG	general contractor visualization equipment
3-Dims GmbH	Integrator of visualization equipment

Table 3: Companies involved in the development of the Arminius Cluster system.

The system is able to sustain 1.978 TFlop/s out of 2.6 TFlop/s peak performance. Based on the Linpack benchmark for supercomputers, the Arminius cluster achieved rank #205 and rank #13 of the german supercomputers in the 25th Top-500 list. The Arminius system is embedded in the German D-Grid and in two worldwide used Grid Computing environments: Globus and UNICORE.
In 2009, we dismounted 50 nodes from the ARMINIUS cluster. This was done for two reasons:

1. In 2010, we will install a new cluster system. It should bridge the performance gap between the “outdated” ARMINIUS and its successor which is planned for 2012.
2. In cooperation with working groups from the physics faculty, we installed a new cluster system which uses the 50 InfiniBand network interface dismounted from the ARMINIUS cluster.

Utilzation

Figure 2 depicts the utilization of the system in 2008.
The average load was 91.22%. Table 4 depicts the outage dates in 2008 (marked with numbers in Figure 2) the system was not accessible.

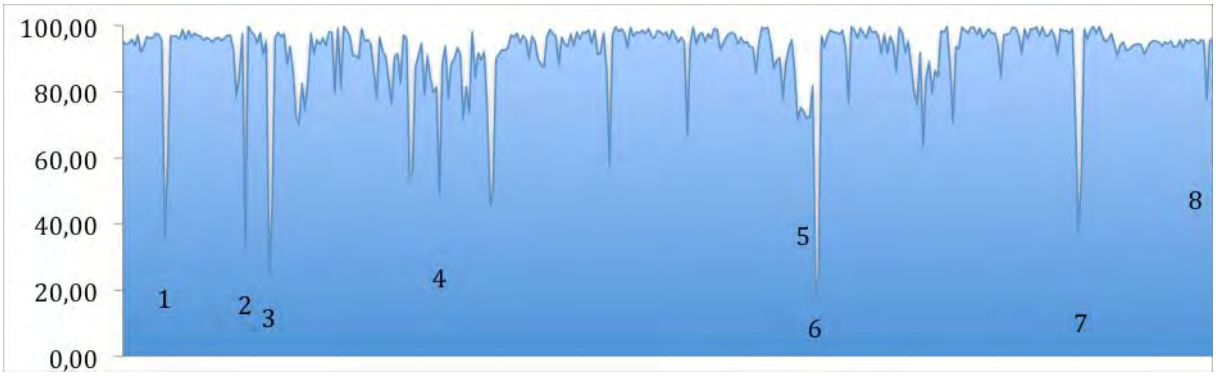


Figure 2 Utilization of the Arminius cluster in 2008 (24 hours per day).

Event	Date	Reason
1	14.01.08 – 15.01.08	General Maintenance
2	11.02.08 – 12.02.08	GPFS Maintenance
3	19.02.08 – 20.03.08	GPFS Maintenance
4	17.04.08 – 22.04.08	GPFS Failure
5	18.08.08	Power Failure in the whole building
6	20.08.08 – 21.08.08	GPFS training
7	15.11.08 – 17.11.08	Air Condition Failure
8	29.12.08	Maintenance

Table 4 Times in 2008 were the system was not fully usable.

Figure 3 depicts the utilization of the system in 2009. The average load was 79.90%. Table 5 depicts the outage dates in 2009 the system was not fully accessible.

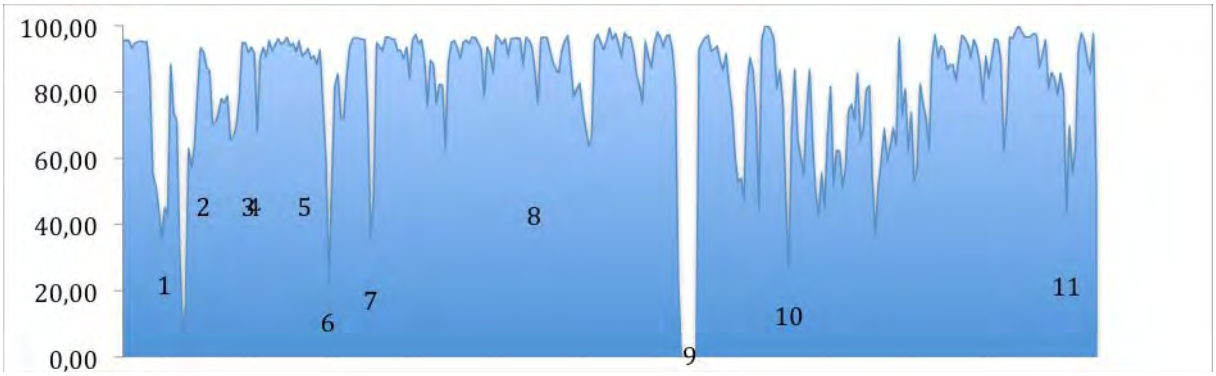


Figure 3 Utilization of theArminius cluster in 2009 (24 hours per day).

Event	Date	Reason
1	15.01.09 – 16.01.09	RAID-Controller Failure
2	28.01.09 – 29.01.09	Heat-Exchanger Failure
3	12.02.09	Power Failure in 4 of 14 cabinets (Cooling problem)
4	14.02.09 – 15.02.09	Power Failure in 4 of 14 cabinets (Cooling problem)
5	03.03.09	Fluid cooling compressor failure
6	11.03.09	Repair of the fluid cooling system
7	25.03.09 - 26.03.09	Maintenance
8	19.05.09 – 20.05.09	Power failure in Paderborn
9	06.07.09 – 13.07.09	Installation of new cooling and power supply
10	12.08.09	Dismounting of 50 nodes
11	13.11.09	Maintenance
12	29.12.09 – 30.12.09	PC^2 Firewall maintenance

Table 5 Times in 2009 the system was not fully usable.

Itanium2 / InfiniBand Cluster

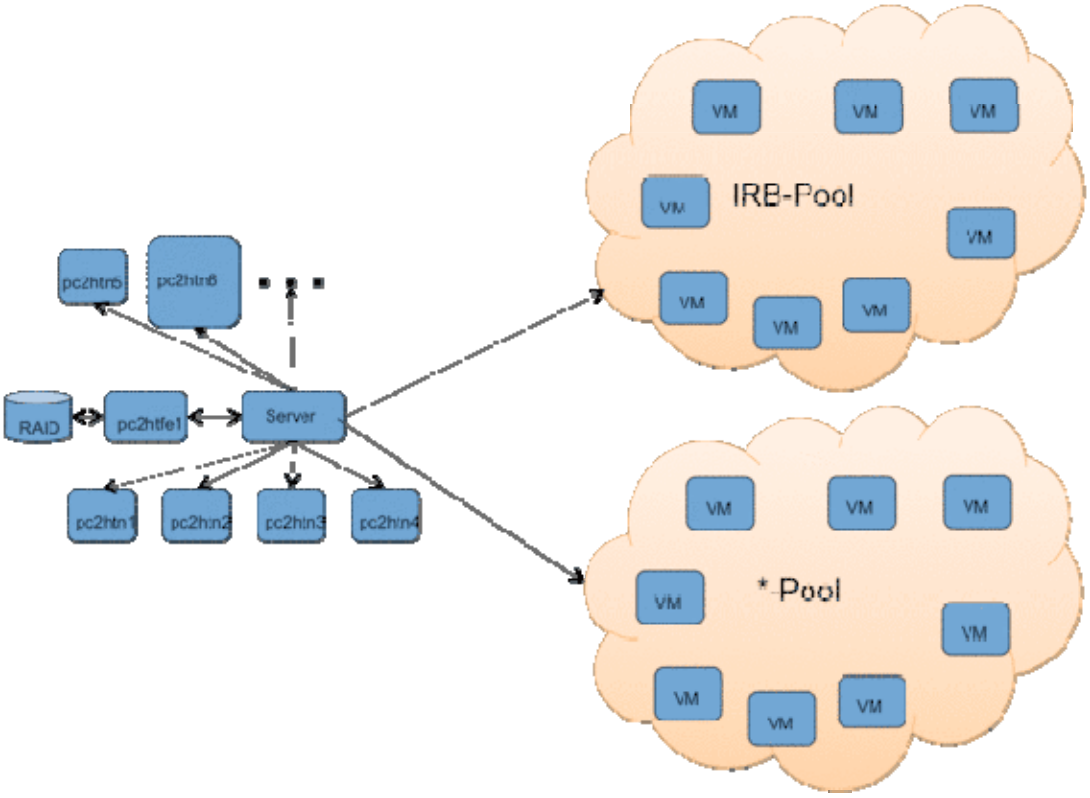
Installed	2002
Vendor	Hewlett-Packard
Number of nodes / CPUs	4 / 8
Node type	HP ZX6000 (2x Intel Itanium-2, 1GHz)
Node memory	12 MByte
System memory	48 GByte
Node peak performance	8 GFlop/s
System peak performance	32 GFlop/s
High speed network type	Infiniband
High speed network topology	switched
Infiniband performance (MPI)	Bandwidth: 446 MByte/s, Latency: 7.79 µs
Myrinet performance (MPI)	Bandwidth: 270 MByte/s, Latency: 11.81 µs
Operating system	Linux
Compiler	GNU, Intel
Message Passing SW	MPICH, ScaMPI

The Itanium system was accessible via the Globus Toolkit and was dedicated to the members of the German D-Grid initiative. It has been switched off in 2009.

SMP Compute Server

Installed	2009
Vendor	Intel, Fujitsu-Siemens
Number of nodes / cores	1 / 24
Node type	4x Intel X7460
Node Memory	128 GByte
Operating system	Linux (CentOS)

High Throughput Cluster (HTC)



This system has been established in 2009 and is intended to run sequential jobs with no timeout (i.e. sequential throughput computing) only. The HTC provides access to about 200 CPUs. Most of them are running as virtual machines on the student pools of the computer science faculty.

The HTC comprises:

- **A frontend node**
  - pc2htfe1
  - accessible via ssh from 131.234.
  - 4* Intel Xeon 2.4 GHz
  - 4GB main memory
  - CentOS 5.2
  - Linux-Kernel 2.6.18-92

- **A server (admin node)**
  - hosting the batch system (Torque)

- **The physical worker nodes**
  - pc2htn*
  - Up to 8GB main memory
  - accessible only via Torque
  - CentOS 5.2
  - Linux-Kernel 2.6.18-92

- **The virtual worker nodes hosted on machines in the IRB- and other pools**
  - accessible only via Torque
  - 1GB main memory
  - CentOS 5.2
  - Linux-Kernel 2.6.18-92
  - The master RAID hosting the cluster local homes and the pre-installed software

The following software is installed on the frontend and the worker nodes

- Matlab 7.7.0 (R2008b)
- Gcc 4.1.2
- Java 1.4.2
- Java 1.6.0
- Valgrind 3.2.1
- DDD 3.3.9
- Perl 5.8.8
- Python 2.4
- automake 1.9
- autoconf 2.59
- Emacs 21.4.1
- Vim 7.0.237

The HTC is dedicated to members of the University Paderborn only.
To be able to use the HT-Cluster one has:

- to have an IMT account and an AFS home
  - (AFS home can be activated by using the "IMT Benutzerverwaltung").
- to be member of a special group
  - Send an email to your local support-team to apply for using the HTC.

4.1.2 Dedicated Systems

Physics InfiniBand Cluster (Pling2)

Hardware	***Description***
49 Fujitsu RX200S5 Intel Xeon E5540	392 processor cores, each node with 2.53 GHz, dual socket, quad-core, 24 GByte DDR3 main memory 4x InfiniBand SDR PCI-e HCA
8 Fujitsu RX200S5 Intel Xeon X5570	64 processor cores, each noode with 2.93 GHz, dual socket, quad-core, 12 GByte DDR main memory 4x InfiniBand SDR PCI-e HCA
InfiniBand switch	216 port Fabric shared with the ARMINIUS cluster
48 TByte file system	NAS storage shared with all major HPC systems
1 login node	Nodes are used for compiling and starting user applications

BisGrid Cluster

Installed	2008
Vendor	AMD, Fujitsu-Siemens
Number of nodes / cores	8 / 32
Node type	4x Opteron, 2.8 GHz
Node Memory	64 GByte
System memory	512 GByte
Node peak performance	45 GFlop/s
System peak performance	360 GFlop/s
Operating system	Linux

The cluster consists of a frontend system and 8 compute nodes. All nodes are connected via InfiniBand HCAs to a 24 port InfiniBand 4x DDR switch, via Gigabit Ethernet to a control network, and via FibreChanel to a Storage Area Network. The Storage Area Network consists of a switched 4Gbit/s Fibre Channel fabric and 10 TByte disk storage. The parallel file system GPFS is used for high performance disk access.
The system is operated for the German D-Grid project BIS-Grid. It is available as a D-Grid resource.

Available Software

- Gaussian
- Gromacs
- NWChem
- TurboMole
- FlexX

RECS – Resource Efficient Cluster System

The system is dedicated to the project “Resource efficient cluster system”**.**

Hardware	***Description***
CPU	2x Intel(R) Core(TM)2 Quad Q9300 @ 2.50GHz
System Memory	8 Gbyte
Gigabit Ethernet switch	1x GBit-Ethernet (Intel Corporation 82567LM-3)
HDD	300 GB (Western Digital WDC WD3000GLFS-01F8U0)
TByte file system	NAS storage
1 login node	Nodes are used for compiling and starting user applications

WinCCS - Paderborner Windows Compute Cluster

Installed	2006
Vendor	FSC
Number of nodes / CPUs	6/ 12
Node type	4x Intel Xeon 5160, 3.0 GHz
Node type	2x AMD Opteron 270, 2.0 GHz
Node Memory	8 GByte
System memory	48 GByte
Node peak performance	96/32 GFlop/s
System peak performance	128 GFlop/s
High speed network type	Infiniband
High speed network topology	Switched
Operating system	Windows HPC Server 2008

The WindowsCCS cluster is able to execute 32-bit and 64-bit applications. An MPI version optimized for the highspeed interconnect InfiniBand is available.

Available Software

- Intel Compiler Suite C/C++ / Fortran
- MS MPI
- Matlab
- ANSYS V11.0
- Altera Quartus II 7.1
- Xilinx ISE 9.2i

Paderborn SCI Cluster-2 (PSC2)

Installed	1999
Vendor	Fujitsu-Siemens
Number of nodes / CPUs	96 / 192
Node type	Primergy Server (2x Pentium III, 850 MHz)
Node memory	512 MByte
System memory	48 GByte
Node peak performance	850 MFlop/s
System peak performance	163 GFlop/s
High speed network type	SCI (Scalable Coherent Interface)
High speed network topology	12x8 torus
SCI performance (MPI)	Bandwidth: 84 MByte/s, Latency: 5 µs
Operating system	Linux
Message Passing SW	PVM, MPICH, ScaMPI
Compiler	GNU, Intel, PGI, Lahey-Fujitsu
Debugger	Totalview
Performance Analyzer	Vampir

The PSC2 system was dedicated to research projects e.g. HPC4U or VDrive and has been switched off in 2009.

Paderborner Linux Cluster Next Generation (PLING)

Installed	2003
Vendor	Hewlett-Packard
Number of nodes / CPUs	32 / 64
Node type	HP RX-2600 (2x Itanium-2 1.3 GHz)
Node memory	4 GByte
System memory	128 GByte
Node peak performance	10.4 GFlop/s
System peak performance	332 GFlop/s
High speed network type	Infiniband
High speed network topology	switched
Infiniband performance (MPI)	Bandwidth: 751 MByte/s, Latency: 6.51µs
Operating system	Linux
Message Passing SW	MPICH, ScaMPI
Compiler	GNU, Intel

The system is owned by and dedicated to the working group of Prof. Dr. Gero Schmidt. It has been switched off in 2009 and replaced by a new system.

FPGA Test Cluster

Installed	2003
Vendor	MEGWARE
Number of nodes / CPUs	4 / 8
Node type	2x Intel Xeon, 2.8 GHz
Node Memory	2 GByte
System memory	8 GByte
Node peak performance	5.6 GFlop/s
System peak performance	22 GFlop/s
High speed network type	Myrinet
High speed network topology	Switched
Operating system	Linux

The system was owned by the SFB 376 “Massive Parallelität, Algorithmen, Entwurfsmethoden, Anwendungen”. It has been switched off in 2008.

KAO Cluster

Installed	2003
Vendor	Dell
Number of nodes / CPUs	4 / 8
Node type	2x Intel Xeon, 2.4 GHz
Node Memory	1 GByte
System memory	4 GByte
Node peak performance	4.8 GFlop/s
System peak performance	19.2 GFlop/s
High speed network type	Myrinet
High speed network topology	Switched
Disks	365 GByte SCSI-RAID
Operating system	Linux

The system was dedicated to the EU projects AssessGrid and HPC4U. The system has been switched off in 2009.

4-way Opteron Cluster

Installed	2004
Vendor	AMD, Fujitsu-Siemens
Number of nodes / CPUs	2 / 8
Node type	4x Opteron, 2.2 GHz
Node Memory	32 GByte
System memory	64 GByte
Node peak performance	4.6 GFlop/s
System peak performance	18.4 GFlop/s
Operating system	Linux

The system is used for dedicated purposes.

The PC² provides an environment for IT systems operated by other research groups or institutes of the University of Paderborn. For these systems only floor space, electrical power, and cooling is provided. In the years 2008 and 2009 the following systems were hosted by the PC²:

- FPGA-Cluster, Research Group of Prof. Dr.-Ing. Ulrich Rückert
- Server for Unified Collaboration, Research Group of Prof. Dr. Reinhard Keil
- Network Infrastructure, Zentrum für Informations- und Medientechnologien (IMT)

4.1.3 System Access

The access to the systems at the PC² is free of charge for all users coming from the academic world e.g. universities or colleges. Users from commercial sites are also welcome but may have to pay a fee for using the systems. Please contact the PC² administration phone number +49 5251 606291 for more information.

Access to systems dedicated to specific user groups may be denied depending on the requirements of the owner.
To apply for an account for the PC² systems one has to fill in small application forms available on our web server. Refer to http://www.upb.de/pc2/services/access.
After processing the application all necessary information will be sent via email within one or two days.
The registration information is kept private and will not be disclosed to third parties. It helps us to keep track about the usage of our parallel systems.
To register for a new project one has to provide:

- A project description.
- The name and office address of the research manager and the project leader.
- The name and office address of each project member using the system.
- Additionally needed requirements like disk space or special software packages.

Specialist counseling is available for the following fields:

- Compiler
- Debugging
- Grid Computing
- MPI
- Optimization
- Performance Profiling
- System Access
- System-Benchmarking and -Evaluation

For detailed information about how to use our systems please also refer to this URL:
http://www.ubb.de/pc2/services/systems

Please report your problems to:
pc2-gurus@upb.de or call our service number +49 5251 606303.

Available Software

Software	Purpose	Licence
Abaqus	Finite element analysis	Dedicated
Ansys	3D FEM solvers	Dedicated
Fluent	Computational fluid dynamics	Dedicated
FFTW	library for computing the discrete Fourier transform (DFT)	None
Gaussian	Electronic Structure	PC²
Gromacs	Molecular dynamics	None
MKL	Intel Math Kernel Library	PC²
MOE	Molecular operating environment	Dedicated
Matlab	Technical computing	Campus
MPICH	MPICH 1 and 2 for Ethernet	None
MPICH-vmi	MPICH for VMI from NCSA	None
MvAPICH	MPICH on VAPI from Ohio State University	None
OpenMPI	MPI for Ethernet and Infiniband	None
NWChem	High Performance Computational Chemistry	PC²
OpenFoam	Finite element analysis	None
Padfem2	Finite element analysis	None
ORCA	Electronic Structure Program Package	None
Siesta	Electronic Simulations	PC²
ScaMPI	MPI 1 compliant, fail-over from IB to GbE	PC²
StarCD	Finite element analysis	Dedicated
VMD	Visualization	Dedicated
VASP	Ab-initio quantum-mechanical molecular dynamics	PC²
Xilinx	FPGA design software	Dedicated

4.2. Collaborations

4.2.1 Ressourcenverbund – Nordrhein-Westfalen (RV-NRW)

Project coordinator:	Dr. Jens Simon, PC², University of Paderborn
Project Members:	Axel Keller, PC², University of Paderborn

The Ressourcenverbund – Nordrhein-Westfalen (RV-NRW) is a network of university computer centers of the state North Rhine-Westphalia which provides a network of excellence and cooperative resource-usage of high performance compute systems [1]. Targets of this network are:

- Outsourcing of work besides the main focus of each computer center.
- Providing access to short and expensive resources.

Active member organizations of the RV-NRW are:

- RWTH Aachen
- University Köln
- University Paderborn
- University Münster
- University Siegen
- University Dortmund
- University Duisburg-Essen
- Ruhr-University Bochum
- Open University Hagen

In generally, all systems and services of the Ressourcenverbund are available for all scientists of RV-NRW members. The use of the resources is free of charge for this community.

The RV-NRW excellence network provides different kind of services to researchers of universities and institute of the state North Rhine-Westphalia.

Consulting HPC users: The RV-NRW provides a primary point of contact for users for all resources provided within the network. Expert advice will be provided by the appropriate compute center staff responsible for the requested resources. PC²

provides all technical services and user support for its systems. Additionally, courses and material concerning high performance computing are offered to increase the skills and qualifications of the users.

HPC systems and application software:
Several high-performance computer systems are available for the users of the RV-NRW. The *Rechen- und Kommunikationszentrum* of the RWTH Aachen provides a cluster system with 60 nodes, each 2 quad-core processors and a cluster system with 64 nodes, each with 4 processors. The *Paderborn Center for Parallel Computing* of the University Paderborn provides the ARMINIUS cluster system with 200 nodes, each node with two Intel Xeon processors. The University Siegen operates a 128 nodes cluster with two AMD Opteron processors per node.
The following centers are providing resources to RV-NRW, but they are up to now not integrated in the unified user management: The *Zentrum für Informationsverarbeitung* of the University Münster operates an InfiniBand connected cluster system with 20 nodes, each with 2 quad-core processors. The *Zentrum für Angewandte Informatik* of the University Köln provides a 128 nodes cluster system with AMD Opteron dual processor nodes. Finally, 384 blade nodes with 8 cores each are provided by the University Dortmund.
Interested scientists apply for access to the RV-NRW compute resource at their local compute center.

Certificate Registration Authority: The Open University Hagen provides a Public Key Infrastructure (PKI) for an automatically issue of X.509v3 certificates. Members of the RV-NRW are free to use the dedicated certificate-server.
The University Paderborn, PC² is a registration authority for Grid certificates. In Germany two Certificate Authorities (CAs), Karlsruhe GridKa and Hamburg DFN, are established for grid services. The standard DFN certificates, used for the encryption of e-mails, can not be used for grid services.

Resource Usage
PC² provides about 30 percent of the compute resources of the Arminius cluster to users of universities and institutes of North Rhine-Westphalia. Researchers from University Münster, RWTH Aachen, and Ruhr-Universität Bochum are currently using RV-NRW accounts to access the PC² cluster system.
Further information about the RV-NRW network of excellence is available on the web-pages of the Ressourcenverbund-NRW [1].

References
[1] Ressourcenverbund Nordrhein-Westfalen (in German), http://www.rv-nrw.de

4.3. Teaching

4.3.1 Theses and Lectures in PC²

Lectures

- Operating Systems (WS08/09, WS09/10 – Jun.-Prof. Dr.-Ing. André Brinkmann)
- Compact Course on Theoretical Aspects of Storage Systems Research (WS09/10 – Jun.-Prof. Dr.-Ing. André Brinkmann)
- Architektur Paralleler Rechnersysteme (WS08/09, WS09/10 – Dr. Jens Simon)
- Software-Praktikum für Ingenieur-Informatiker (WS09/10 – Jun.-Prof. Dr.-Ing. André Brinkmann)
- Storage Systems (SS09 - Jun.-Prof. Dr.-Ing. André Brinkmann)
- Hardware/Software Codesign (SS09 – Dr. Christian Plessl)

Project Groups

- Virtualized Supercomputer (2008/2009 – Jun.Prof. Dr.-Ing. André Brinkmann, Georg Birkenheuer, Oliver Niehörster, Dr. Jens Simon)

Master´s Theses

- Baron, David: Computational Steering von verteilten, interaktiven Simulationen - Konzeption, Implementierung und Evaluation, 2009
- Dickehage, Felix: Aufbau dynamischer Speichersysteme auf basis von p2p-Technologien, 2009
- Eschweiler, Dominic: Barracuda – eine Microdriver-Architektur für fehlerkorrigierende Codes im Linux-Kernel, 2009
- Grawinkel, Matthias: Efficient Database Driven Metadata Management for Petabyte Scale File Systems, 2009
- Groppe, Dennis: GPU-basierte Beschleunigung neuer Bildrekonstruktionsalgorithmen in der Tomographie aus MATLAB, 2009
- Kenter, Tobias: Automatische Koregistrierung von kardinalen CT und PET Volumendaten, 2008
- Lensing, Paul: File Systems Optimized for Small File Accesses, 2009
- Meister, Dirk: Daten-Dediplizierung mit Hilfe von Flash-basierten Indizes, 2008
- Schäfers, Lars: Analyse neuer Spielbaumsuchverfahren, wie sie im Computer-Go angewendet werden, 2008

Bachelor´s Theses

- Bürger, Holger: Vermessung, Analyse und Bewertung von parallelen Dateisystemen, 2008
- Dömert, Hubert: Vermessung der I/O Leistung von Blockgeräten in virtualisierten Umgebungen, 2008
- Frye, Matthias: Entwicklung einer webbasierten Oberfläche für Virtualisierungslösungen am Beispiel von V:Drive, 2008
- Konersmann, Christoph: Leistungsbewertung unterschiedlicher Virtualisierungslösungen im HPC-Umfeld, 2008
- Lensing, Paul Hermann: GPU-basierte, verlustbehaftete Bildkompression für Remote Rendering, 2008
- Lüken, Frank: Analyse von GridBeans für Unicore6 und Implementierung für Gaussian, 2008
- Sievers, Michael: Beschleunigung von Bildrekonstruktionsverfahren in der Positronen-Emissions-Tomographie unter Einsatz der Cell Broadband Engine, 2008
- Vogelsang, Andreas: Konzeption und Bewertung von Integrationen des Windows Server 2008 Active Directory im Umfeld von Branch Offices, 2008
- Weber, Elmar: Design anf Implementation of Services to Use OpenCCS in Commercial Grids, 2008
- Welp, Daniel: Analyse der Netzwerkperformanz in virtualisierten Systemen, 2009
- Wiersema, Tobias: Integration einer netzwerkgestützten Interaktionskomponente in ein Framework für Remote Rendering, 2008

PhD Theses

- **Dr. Stefan Lietsch**
  A Novel Approach to Interactive, Distributed Visualization and Simulation on Hybrid Cluster Systems, Universität Paderborn, 2008

- **Dr. Kerstin Voss**
  Supporting SLA Provisioning in Grids by Risk Management Processes, Universität Paderborn, 2008

PC² Colloquium 2008

- Beisel, Tobias und Steinke, Thomas: Medical Imaging und Parallelverarbeitung, 2008
- Korzenlowski, Miroslaw: Degree 3 Suffices: A Large-Scale Overlay for P2P Networks, 2008
- Projektgruppe PC^2: PG-vSC Seminar, 2008
- Sievers, Michael: Beschleunigung von Bildrekonstruktionsverfahren, 2008
- Tönne, Andreas: Smalltalk als Vertreter dynamischer Programmiersprachen, 2008

PC² Colloquium 2009

- Nehring, Dirk: XenSource – Eine Lösung zur Servervirtualisierung, 2009
- Baron, David: Computational Steering von verteilten, interaktiven Simulationen, 2009
- Dickehage, Felix: Aufbau dynamischer Speichersysteme auf Basis von P2P-Technologien, 2009
- Grawinkel, Matthias: Efficient Driven Metadata Management for Petabyte Scale File Systems, 2009
- Groppe, Dennis: GPU-basierte Beschleunigung neuer Bildrekonstruktionsalgorithmen in der Tomographie aus MATLAB, 2009
- Welp, Daniel: Analyse der Netzwerkperformanz in virtualisierten Systemen, 2009

4.3.2 PhD at PC²

Dr. Stefan Lietsch: "A Novel Approach to Interactive, Distributed Visualization and Simulation on Hybrid Cluster Systems**"**

Abstract

The introduction of hybrid cluster systems, which consist of several heterogeneous groups of homogenous nodes (e.g. computing nodes, visualization nodes, hardwareaccelerated nodes) marks a paradigm shift in the usage of cluster systems. For the first time, the powerful hardware is open to applications other than classical high performance computing (HPC) applications, such as number crunching and massively parallel simulations. Various new fields of science and industry could use it as a powerful new tool for simulation and visualization. Interactive simulations and their visualization as well as Virtual Reality applications are areas where HPC on hybrid cluster systems can bring significant benefit in many aspects, as for example realism, multiple comparative simulations, multiuser-support etc.. But, to enable and to lateron ease the utilization of the complex cluster systems for such simulations, tools to orchestrate and access these resources are needed. Existing applications should be quickly able to run on and to benefit from the new hardware with only little effort and changes in source code. Currently there are only few systems that (partially) fulfill these tasks. Most of the existing ones for traditional HPC applications lack important features to provide the desired interactivity and flexibility. This thesis addresses two main aspects of this problem and introduces concepts for the computational steering (CS) and the remote visualization (RV) of interactive simulations and Virtual Reality (IS/VR) applications on hybrid cluster systems. The main focus is to conserve the interactivity and user-integration of these applications and, at the same time, dramatically extend their features by harvesting the power of the hybrid cluster architecture. Thus, the main contribution of this thesis is the introduction of two new subsystems, one for the steering and orchestration of the application's distributed components (CS) and one for the remote access to the interactive graphical applications running on the cluster (RV). The concept for the CS framework bases on three new models for the steering of IS/VR applications that significantly differ from the model used for traditional CS. Besides the original idea that a running simulation is observed and controlled by a connected visualization, many parts of traditional CS needed to be redesigned and adapted to the needs of IS/VR. Especially interactivity and flexibility play a big role during the conceptual design of the system. The 1 proposed framework and its implementation is tested and evaluated by realizing distributed versions of two existing IS/VR applications and is further showing that these applications greatly gain on flexibility, performance and quality for the users. Thereafter, the introduction of a framework for RV gives

the users graphical access to the applications running on the cluster system. Again, the developed system takes the idea of traditional RV (e.g. for remote administration purposes) and transfers it to the domain of IS/VR, where interactivity and high quality are of highest importance. To achieve these goals, the developed system, as the first of its kind, makes use of powerful graphics cards for image compression. Until now, these GPUs (Graphics Processing Unit), built into most of the existing hybrid clusters, were almost exclusively used for the rendering of the results of HPC simulations. But, only recently these processors have become available for general purpose computing through the introduction of new and universal APIs. By different benchmarks it is shown that the performance of the remote visualization is thereby improved in many cases. Additionally, the framework is able to use the flexibility that clusters provide, to allow the remote access to multiple, simultaneously running applications on the cluster by multiple users. All in all, a novel approach to effectively use hybrid clusters for interactive simulations and VR applications is presented, and the findings are manifested by exemplary applications and various benchmarks.

Dr. Kerstin Voß: Supporting SLA Provisioning in Grids by Risk Management Processes

Abstract:
Grid technologies have reached a high level of development, however core shortcomings have been identified relating to security, trust, and dependability of the Grid which reduce its appeal to potential commercial adopters. Users require a job execution with a desired priority and quality. In order to stipulate such requirements, Service Level Agreements (SLA) can be negotiated. These are a powerful instrument enabling the specification of the business relationship between service provider and service user in detail. However, providers are aware of the unreliability of Grid resources and are therefore reluctant to adopt a mechanism which requires them to meet strict requirements and to guarantee associated quality constraints.
If strict guarantees cannot be agreed by contract, many users prefer to operate their own resources instead of using the Grid. This is more expensive but they control their applications, which removes the issues of trust and ensures dependability concerning its successful completion. To establish a commercial Grid environment ,it is essential that Grid providers are prepared to accept an approach involving SLAs with associated guarantees.

In order to enable providers to accept such SLAs, they need estimates of the likelihood that they are unable to fulfill an SLA, i. e. Risk Assessment. Furthermore the resource management should take into account such estimations when allocating resources or initiating fault-tolerance mechanisms, i. e. Risk Management. This work integrates risk awareness in the provider's processes which are involved in SLA provisioning: During SLA negotiation they evaluate which resources can be used for service provisioning and estimate the Probability of Failure (PoF) of resources and of fulfilling the SLA. If the estimated PoF is too high then by applying risk reduction the provider may be able to reduce it sufficiently to accept the SLA. The estimated PoF will also be considered by the service provider and service consumer when determining the revenue and the contractual penalty. Compared to a service request requiring a relatively low quality of service, providing a more reliable service requires to receive a higher price since more guarantees have to be ensured. If a more reliable service is provided, the consumer might also define a higher contractual penalty. Thus, the PoF is an additional decision making element in the SLA negotiation since it enables end-users to compare different SLA offers by an objective measurement. When providers have accepted an SLA, they have to be able to compensate for resource failures in order to prevent SLA violations. The usage of fault-tolerance mechanisms combined with risk awareness support Grid providers in this task. The Risk Management processes are interlaced with the resource management and thereby transparent for Grid service consumers. An

important aspect of the Risk Management developed for the Grid are self-organising mechanisms, which initiate a fault-tolerance action or a chain of them, in order to manage resource instabilities or resource outages. Decisions are made on the basis of financial considerations, such as the profit margin, the cost for performing fault-tolerance, and the expected profit when executing a job. Taking into account such financial factors is of high importance for commercial Grid providers.

In conclusion, the integration of Risk Management in the processes of Grid providers is the initial step towards a risk aware Grid. It will increase transparency, reliability, and trust and provides an objective basis for decision processes in the resource management. Risk Management is integrated to address the SLA negotiation as well as the post-negotiation phase and thereby improves the SLA provisioning process in general.

4.3.3 Project Group: Virtualized Supercomputer

Project coordinator	Jun.-Prof. Dr. André Brinkmann, PC², University of Paderborn
Project members	Dr. Jens Simon, PC², University of Paderborn Georg Birkenheuer, PC², University of Paderborn Oliver Niehörster, PC², University of Paderborn Axel Keller, PC², University of Paderborn

The Project Group Virtualized Supercomputer (Pg-Vsc) is engaged in virtualization of high performance computers (HPC). Our goal is to study how the benefits of virtualization can be used to compensate the performance loss, caused by hypervisor overhead. Furthermore we develop a sophisticated solution to manage several hypervisors in a common way.

End Users

Our target groups are companies, universities and research centers, which are interested in a persistent, scalable, flexible and easy to use technology to monitor and manage a heterogeneous hypervisor infrastructure. This innovative technology provides maximum flexibility and minimizes the performance losses by clever load balancing strategies and the administration overhead at the same time.

The end users are also developers of Resource Management Systems (RMS), who need a well arranged API to deal with virtual machines (VMs). This API is a great platform for research and testing of load balancing strategies and can be interesting for proofs of theoretical concepts.

Virtualization in HPC

In high performance computing (HPC), virtualization holds many possibilities to break the classical space sharing, where resources are statically assigned to Jobs. At this, the smallest resource unit is a node with possibly multiple CPU cores and a large amount of RAM. So if a non-parallel job that can only use one core and does not need much RAM space has to be executed, a waste of resources occurs. Due to virtualization, resources can be arbitrarily partitioned and assigned to a Job. Thus, such waste of resources can be avoided. Furthermore, more resources can be saved by migrating jobs to more utilized nodes for a short period of time while these jobs do not use much CPU time (e.g. while doing I/O). Another problem, which we solve, is the inflexibility of a cluster system. In many cases clusters run special

operating systems adjusted to the clusters. This leads to recompilation of jobs to make them run on the cluster. By using virtualization every job obtains an isolated, customized environment in the form of a VM. The VM image, where this environment is installed can be created by customers themselves.

Features

The Virtualized Supercomputer Project provides following features:

- Support of Xen, VMware, Hyper-V
- Well-arranged API to manage virtual machines
- Monitoring utility for VMs and hosts
- User Interface to deploy VMs
- Live migration of VMs
- Job scheduler with exchangeable scheduling algorithms
- Steering interface to VMs for application control and monitoring
- Authentification proxy within a HPC cluster

References

[1] Web-page PG VSC:
http://pc2.uni-paderborn.de/research-projects/projects/pg-vsc

4.3.4 Project Group: CSI PC² - Biometric Computing

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Dr. Jens Simon, PC², University of Paderborn
	Tobias Schumacher, PC², University of Paderborn
Supported by:	TST Biometrics

General Problem Description

Identification of individuals by biometric properties is a topic of major interest in many different areas today. For example, fingerprints or iris scans can be used by the police for identifying offenders. Another field of application for these techniques is to control access to rooms, buildings or computer systems. All these systems roughly work in the same way. First, a fingerprint or iris scan is taken from a person. Several identification features are extracted from this scan and saved to a database. When someone now wants to enter a room that is controlled by such a biometric system, his fingerprint or iris scan is taken again, the features are extracted and compared to those in the database. Several challenges arise in this step:

- The scans can include a certain noise, so one cannot expect an exact match to the features stored in the database. The algorithms used must take this into account and provide a good hit ratio while minimizing the number of false positives.
- Depending on the area of application, the database can become very large, which directly impacts the performance. In most application areas, it is desirable to get the results fast. For example, if one wants to enter a room or building, he does not want to wait for minutes until the system checked his authorization.

These problems directly lead to the goals of this project. We want to implement a biometric system that maximizes the hit ratio while minimizing the number of false positives returned. Additionally, the system should provide a small response time.
These goals shall be achieved by using a parallel computer for the database matching, where the database will be stored on a parallel file system. An additional speedup for the matching algorithm will be gained by using reconfigurable hardware for the matching. The initial implementation will be done on the Arminius cluster operated at PC². This machine provides a parallel file system, powerful compute nodes, a fast communication network and several nodes equipped with additional

FPGA boards. Therefore, it is an ideal platform for development. However, the system will be designed as portable as possible.
The user frontend to the system will be a separate PC providing a graphical user interface that communicates with the cluster via a socket based protocol. The frontend is equipped with a fingerprint sensor and an iris camera.

Problem Details and Work Done

The project group is still ongoing. Conforming to the project plan, the first milestone was successfully achieved. For the frontend side this means that the fingerprint sensor and the iris camera can be accessed. The data received can be processed, and relevant features are extracted. The GUI is also operational and the system can send the features extracted to the cluster for matching them against the database. A screenshot of the GUI is shown in Figure 1. Work that still needs to be done consists of improving the algorithms for feature extraction as well as parameter and performance tuning.

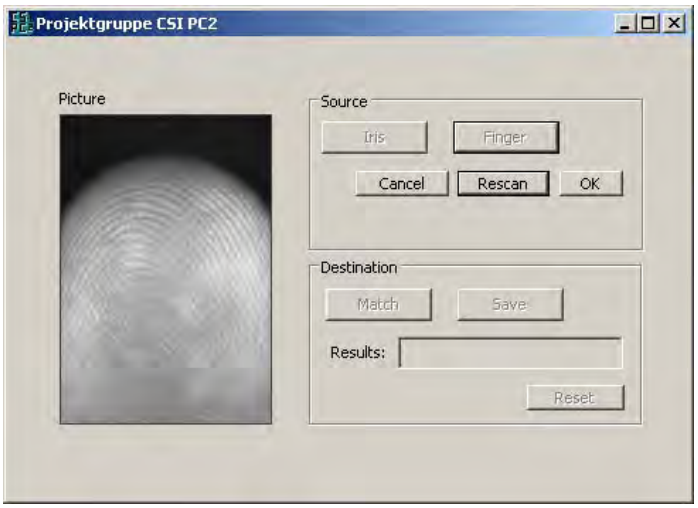


Figure 1 The graphical user interface

The central parts of the parallel database matching are also operational. The database format has been defined; methods exist for efficiently reading from and writing to the database. A cluster control daemon exists receiving connections from the frontend and distributing the work to be done. A first version of the matching algorithms has also been implemented. The next steps will include the FPGA implementation of the matching algorithms. Here we hope to achieve great speedups, because FPGAs can perform lots of feature comparisons in parallel as

opposed to the sequential nature of a general purpose CPU. To sum up, the complete system is already in an initial working state.

Resource Usage

The main work of the project group is done on the Arminius cluster. Most of the features this machine provides are utilized, for example the high speed network, the parallel file system and the FPGA boards available in four of the compute nodes. The communication between the compute nodes is implemented using MPI. For testing purposes, two other machines (ic13 and ic14) are also used, which provide an Infiniband network and two FPGAs per node.

The frontend is a dedicated computer running Microsoft Windows. Connected to this machine are a fingerprint sensor and an iris camera. To simplify user interaction, the system provides a touch screen.

Additionally, the project group will likely use the Windows CCS computer cluster for generating artificial fingerprints needed for performance benchmarks. The program used for this task is not a parallel application and therefore cannot directly utilize multiple processors or even multiple compute nodes and a high speed network, but it is possible to start the program with different initial parameters on different processors.

The project was partially supported by TST biometrics who donated a fingerprint sensor and the APIs available.

References

[1] http://www.csipc2.de

5 Research Projects

5.1 Computer Architecture

5.1.1 RECS – Resource Efficient Cluster System

Project coordinator	Jun.-Prof. Dr. André Brinkmann, PC², University of Paderborn
Project members	Dr. Jens Simon, PC², University of Paderborn Tobias Schumacher, PC², University of Paderborn Axel Keller, PC², University of Paderborn Matthias Keller, PC², University of Paderborn Christoph Konersmann, PC², University of Paderborn
Partners:	christmann informationstechnik + medien GmbH & Co. KG University of Paderborn, Department of System and Circuit Technology
Work supported by	BMWi – Zentrales Innovationsprogramm Mittelstand (ZIM)

General Problem Description

In the project *Resource Effienct Cluster System* (RECS) we want to provide supercomputer performance to small and medium-sized enterprises. Typically, these companies do not have large budgets and adequate instructed personal to operate classical supercomputer systems. Our mission is to building affordable and simple administrable computer systems with low operating costs. The systems have to scale from small to large configurations to fit application requirements optimally.

Problem Details and Work Done

A first prototype of a RECS system was built. The Department of System and Circuit Technology developed a new and innovative board design supporting the new cooling concepts. The cluster consists of compute nodes equipped with low power CPUs. Then nodes are connected by a standard Gigabit Ethernet network. The system software consists of a Linux operating system with a resource management layer above. Several application benchmarks have been done. We presented the

system at the CeBIT 2009 and at the International Supercomputer Conference 2009 (ISC) on the exhibition booth of the PC². The ISC with its trade fair is the most important professional conference and exhibition on High Performance Computing, Networking, and Storage in Europe. We evaluated the Kerrighed single system image operating system as a part of the resource management layer

Picture 1: Booth of the PC² at the ISC 2009. Dr. M. Porrmann, T. Schumacher, Dr. J. Simon, Ch. Pohl, S. Mikulski

In the next step we will implement the architecture depicted in Figure 2.

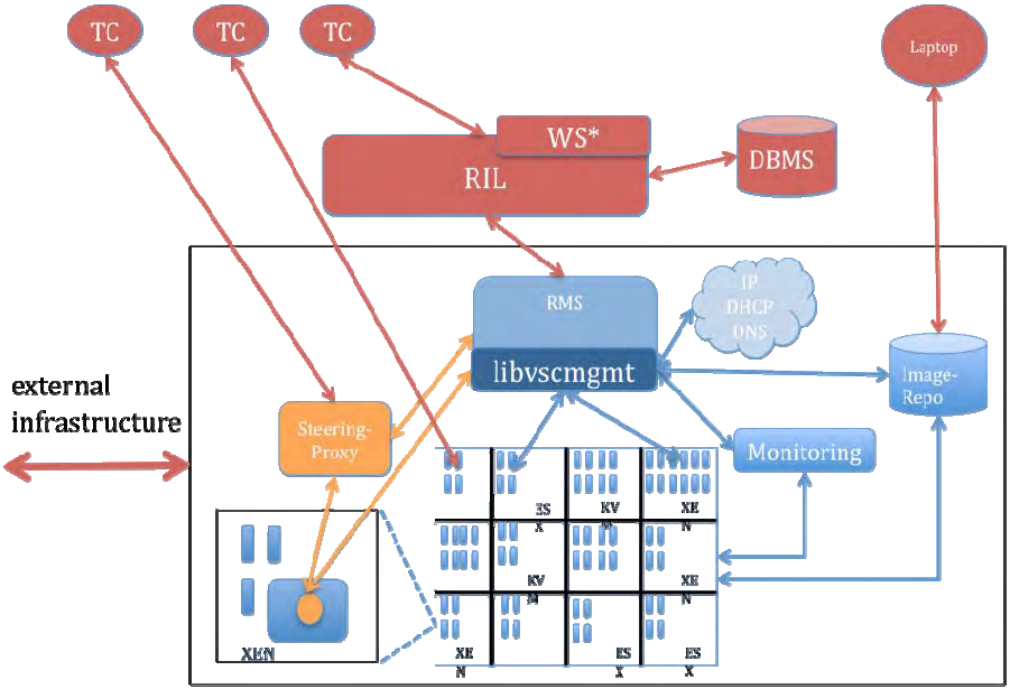


Figure 2: RECS Software Architecture

On the physical nodes virtual machines will run different images provided by administrators and users. This may be for example virtual desktops, specific environments for software development purposes, or on demand extensions for special applications (parallel matlab). Images may be transferred from / to laptops. The resource management layer will allow to reserve resources in advance. For example to provide the environment for a training course.

The system comprises :

- different hypervisors (XEN, ESX, KVM, …) ,
- a monitoring layer, observing the physical nodes and the virtual machines,
- a subnet management layer, allowing to provide IP-subnets on demand,
- an image repository, storing the available images,
- a steering layer, allowing to steer and monitor the applications inside a virtual machine,
- a resource management system controlling the physical nodes and the virtual machines by means of the libvirt library,
- a web based layer (RIL) allowing to setup usage profiles and to handle the connections between the thin clients (TC) and the RECS cluster.

References

[1] ISC2009, http://www.supercomp.de/isc09/
[2] Kerrighed, http://www.kerrighed.org

5.1.2 Project MM-RPU: Multi Modal Reconfigurable Processing Unit

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Tobias Kenter, PC², University of Paderborn
	Dr. Christian Plessl, PC², University of Paderborn
Supported by:	Intel Microprozessor Technology Lab

General Problem Description

There is an ongoing demand for increased single thread performance in high performance and general purpose computing. One way to achieve this is the utilization of reconfigurable hardware like FPGAs. Due to limited hardware resources or a large engineering effort it is often not desirable to execute the entire application on reconfigurable hardware. Therefore reconfigurable hardware is commonly combined with a general purpose processor into a system where the reconfigurable part works on the more compute intense parts of the application and the general purpose processor handles the more control flow oriented parts.

A widely researched way to use FPGAs are autonomous or semi autonomous accelerators, that implement the compute intense kernels of an application in the reconfigurable hardware. Another field of research to increase performance is that of extending instruction sets by workload specific custom instructions. In the embedded systems area, there are projects that work on instruction set extension with reconfigurable hardware, whereas in the high performance area, up to now, new instructions are introduced only as fixed function circuits.

The goal of this research project is to propose and investigate a reconfigurable accelerator, that can operate both as an autonomous accelerator for whole kernels and as functional unit executing custom instructions. The challenges to be tackled are the architectural integrations of this accelerator on the one hand and its programmability for a wide spectrum of applications on the other hand.

Problem Details and Work Done

The project seeks to combine the concepts of custom instructions and autonomous accelerators. Custom instructions are designed to replace a series of instructions from the existing instruction set by one new instruction. This way code size and execution times can be reduced. Custom instructions can make use of instruction level parallelism by executing several independent operations concurrently. They can exploit bit level parallelism which custom circuits are created. Custom instructions require an integration with the CPU that allows for very low latency

communication. Custom instructions typically work on data from the CPUs register file. The control flow is usually handled entirely by the CPU. Custom instructions typically lead to moderate speedups, maybe with the exception of custom datapath instructions using bit level parallelism. On the other hand, some forms of custom instructions can be applied to virtually any application and there are approaches for automated identification and integration of custom instructions.
Autonomous accelerators can vary a lot in degree of autonomy, complexity and architectural coupling. In common (all cases) reconfigurable hardware handles at least a part of the control flow of a program. This starts with simple loop accelerators, where the hardware has to maintain an iteration counter of the loop or check for termination criterion. Computes a stride of memory locations and leads up to designs where the accelerator handles very complex tasks and refers to the CPU for example only for operating system services. Depending an application granularity, perfermed partitioning and a involved datasets, the requirements on latency and bandwidth requirements for the interconnect between the two components vary. For a good flexibility of the reconfigurable hardware, it is desirable that it can be integrated to the CPUs address space, work on the same physical memory and possibly share a part of the cache hierarchy with the CPU.

We have developed a first specification of an interface between CPU and accelerator. The requirements of low latency communication for the custom instruction mode and access to the memory hierarchy for the autonomous accelerator mode can be specified. The CPU sends instructions to the RPU through a FIFO and when the FIFO is full. Along with instructions it can send physical memory addresses, when the RPU needs them to perform operations in memory. This way the RPU doesn't need its own memory management unit. Data transfer from and to the CPU's register file is performed through a shared register file that is also used for synchronization. (Figure 1)
We have qualitatively evaluated different use cases with this interface and implemented parts of it in a detailed simulator based on a PowerPC core in the simulation framework Unisim.

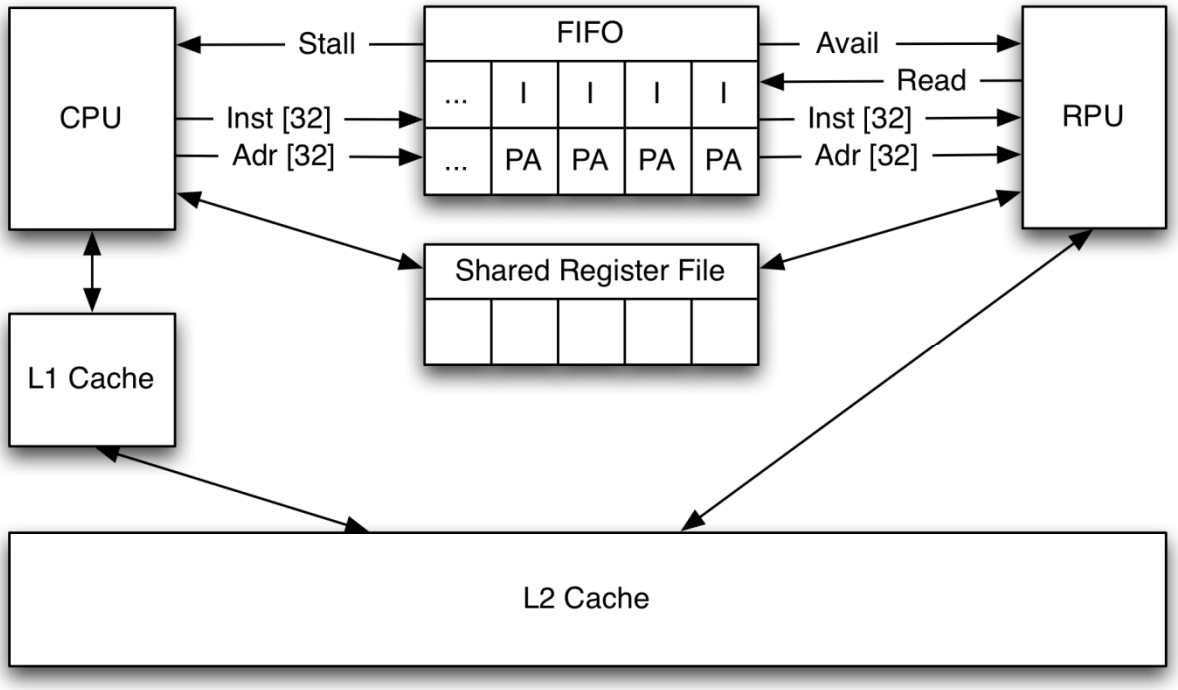


Figure 2: Interface between CPU and RPU

Ongoing work is done on an estimation framework that provides code and runtime analysis based on the LLVM infrastructure. The gathered data will be used for a partitioning of the code blocks between CPU and RPU based on an estimation model. This framework serves three major purposes. First of all it will enable a rough quantitative analysis, how the proposed usage modes perform with the interface. Secondly it is going to give indications about the required internal capabilities of the RPU. Finally it provides a starting point for a tool flow that can identify which code blocks are to be mapped to the RPU and generate custom code for this purpose.

5.1.3 Multi-objective Intrinsic Evolution of Embedded Systems

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Paul Kaufmann, University of Paderborn
Supported by:	DFG, priority program 1183, “Organic Computing”

General Problem Description

This project aims at the investigation and development of intrinsically evolvable embedded systems. Simulated evolution will provide such systems with a means to react properly to unforeseen changes in the environment and the system resources. In an intrinsically evolved system the evolutionary process runs together with the function under evolution on the same target platform. This is a necessary precondition for autonomous operation. While evolutionary techniques have already been applied to the design of software and hardware, intrinsic evolution as an adaptation method is a novel approach. We view intrinsic evolution as a promising mechanism to provide autonomous embedded systems with self-adaptive and self-optimization capabilities. We achieve our goals by combining research in bio-inspired computing with modern embedded system architectures. The vision behind this project is that novel bio-inspired algorithms paired with modern system-on-chip architectures will allow us to construct future embedded systems that exhibit intelligent behavior.

Problem Details and Work Done

To investigate intrinsic digital logic design and optimization methods we have implemented a generic modular framework for evolutionary computations. It is capable of visualizing the optimization and adaptation process and creating statistics, and is able to help users to find the right parameter settings for an experiment (see Figure 1).

Figure 1 Graphical user interface of the MOVES-Framework

Due to framework's modular structure, experiments for a specific application using one of the implemented evolutionary algorithms, representation models and operators can be easily set up and executed. The average and asymptotic behavior of a benchmark can be quickly investigated by the framework's interface to the grid software **Condor** that allows running a large number of experiments on a compute cluster. Within the framework we have implemented several hardware representation models, including the classical FPGA structure oriented Cartesian Genetic Programming Model and embedded CGP, an extension to automatically defined functions. Beside the single-objective classical genetic algorithm, the multi-objective algorithms SPEA2, NSGAII, µGA(2) and IBEA allow to optimize circuits not only regarding functional quality but also for small size and delay. The performance comparison of optimization methods and representation models for digital logic design is often done by evolving arithmetic functions. This class of functions is widely used to benchmark new approaches and algorithms. However, such functions are not considered as the primary application scenario for an autonomous embedded system. Here, we are interested in functions that depend on the distribution of the input data. In such cases, the optimal solution is often unknown or would overextend the computational resources of the embedded system. Signal classification is a typical target application domain. To verify our methods we have set up a system for gathering and classifying muscle signals. The goals for an evolvable classifier are to adapt continuously and autonomously to varying sensor positions and skin conductance, to compensate noise and cross-talk effects from adjacent muscles and to have a considerable recognition rate even after long unmaintained periods. Another application area for testing evolvable hardware principles is the evolution of adaptable cache controllers. Cache memories are

important and well-investigated elements of any modern processor's memory hierarchy. While carefully designed and balanced cache hierarchies greatly improve processor performance, they also require substantial amounts of energy. The key idea of the **EvoCache** approach is presented in Figure 2. A very small reconfigurable logic fabric implements a hashing function that maps a part of a memory address to a cache line index. Our architecture provides additionally a memory mapping function that can store several configurations for the reconfigurable logic fabric, which allows for quickly switching to different memory-to-cache address mappings. We evaluate the use of EvoCache in an embedded processor for two specific applications (JPEG and BZIP2 compression) with respect to execution time, cache miss rate and energy consumption. The evolvable hardware approach for optimizing the cache functions not only significantly improve the cache performance for the training data used during optimization, but also generalize very well for test data. Compared to conventional cache architecture, EvoCache applied to test data achieves a reduction in execution time of up to 14.31% for JPEG (10.98% for BZIP2), and in energy consumption by 16.43% for JPEG (10.70% for BZIP2).

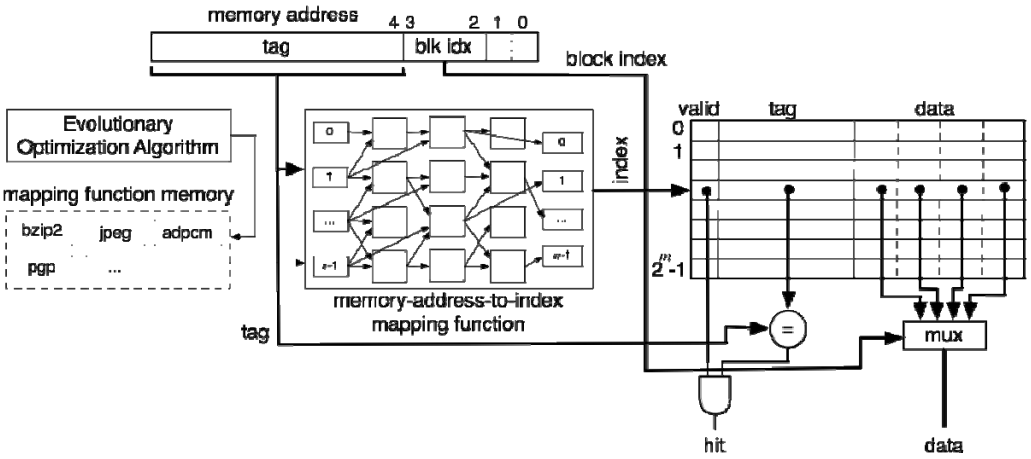


Figure 2 The evolvable cache (EvoCache) architecture provides a configurable mapping from CPU memory addresses to cache indices. The optimization process reconfigures node functions and the wiring between the nodes.

Resource Usage

For the EvoCache experiments we exhaustively used the Arminius cluster as a computing farm for system simulation in a cycle-accurate manner. To this, we employed SimpleScalar system simulator and a parallelized version of our MOVES optimization toolbox.

References

[1] Kaufmann, P.; Plessl, C. and Marco Platzner. EvoCaches: Application-specific Adaptation of Cache Mappings. In: *Proceedings of the NASA/ESA Conference on Adaptive Hardware and Systems (AHS)*, San Francisco, CA, USA, June 2009.

[2] Knieper, T.; Defo, B.; Kaufmann, P. and Platzner, M.: On Robust Evolution of Digital Hardware. In *Proceedings of the 2nd IFIP Conference on Biologically Inspired Collaborative Computing (BICC)*, Milan, Italy, September 2008. Springer.

[3] Kaufmann, P. and Platzner, M.: Advanced Techniques for the Creation and Propagation of Modules in Cartesian Genetic Programming. In *Proceedings of the Genetic and Evolutionary Computation Conference (GECCO)*, Atlanta, Georgia, USA, July 2008. ACM.

[4] Kaufmann, P. and Platzner, M.: MOVES: A Modular Framework for Hardware Evolution. In *Proc. of the 2nd NASA/ESA Conference on Adaptive Hardware and Systems (AHS)*, pp.447-454, Aug. 2007. Received the Best Paper Award in the Evolvable Hardware Category.

[5] Kaufmann, P. and Platzner, M.: Toward Self-adaptive Embedded Systems: Multiobjective Hardware Evolution. *In Proc. Int'l Conf. on Architecture of Computing Systems (ARCS)*, March 2007. Springer, LNCS 4415.

[6] Kaufmann, P. and Platzner, M.: Multi-objective Intrinsic Hardware Evolution. In *Proc. of the MAPLD Int'l Conference*, Sept. 2006.

5.1.4 Operating Systems for Reconfigurable Hardware (ReconOS)

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Enno Lübbers, PC², University of Paderborn
Supported by:	DFG SPP 1148 “Rekonfigurierbare Rechensysteme”

General Problem Description

The project ReconOS aims at the investigation and development of a programming and execution model for dynamically reconfigurable hardware devices. These devices, such as Field-Programmable Gate Arrays (FPGAs), are being used more and more in embedded systems but also as accelerators in general purpose computing. Being a rather new technology, dynamically reconfigurable systems are not sufficiently supported by current design methodologies and tools. Especially the unique feature of partial reconfiguration is still difficult to exploit except for hand-crafted designs.

Extending the established programming model of existing real-time operating systems to the hardware domain would greatly simplify module reusability and design-space exploration for hybrid hardware/software systems. At the same time, it would provide designers with a well-known model for specifying thread synchronization and communication that can be transparently used for hardware and software design.

The main challenges in adapting this programming model to the hardware domain lie in identifying

- which operating system objects’ semantics can be extended to hardware threads
- how these objects and their underlying mechanisms have to be modified to support both hard- and software
- how the decomposition into threads can be used to exploit the partial reconfiguration features of the targeted FPGAs

Problem Details and Work Done

We have extended the popular real-time operating systems eCos and Linux with support for hardware threads running on reconfigurable devices, such as FPGAs. eCos is highly configurable and provides a flexible basis for customizing our operating system to application requirements, while Linux enjoys widespread

popularity and support for wide range of applications. Building on the existing POSIX API allows us to seamlessly extend the programming model used for traditional software-based embedded systems to the hardware domain. We provide transparent mechanisms that permit hardware and software threads to use the same OS services for communication and synchronization. Two communicating threads use only operating system objects and thus do not need to know the execution environment (hard- or software) of their communication partners. This greatly simplifies design space exploration and thread reusability for hybrid hardware/software systems.

A ReconOS hardware thread is usually written in a hardware description language like VHDL and consists of at least two parallel processes, an OS synchronization state machine and one or more user processes. Figure 1 shows the basic structure of a hardware thread. The OS synchronization state machine specifies the OS interactions of the thread and serializes accesses to the operating system. It can be blocked by the OS, thus implementing the semantics of blocking function calls for hardware threads. Any user processes, however, can continue running in parallel. These processes implement the thread's actual functionality and interact with the synchronization state machine through user-defined signals.

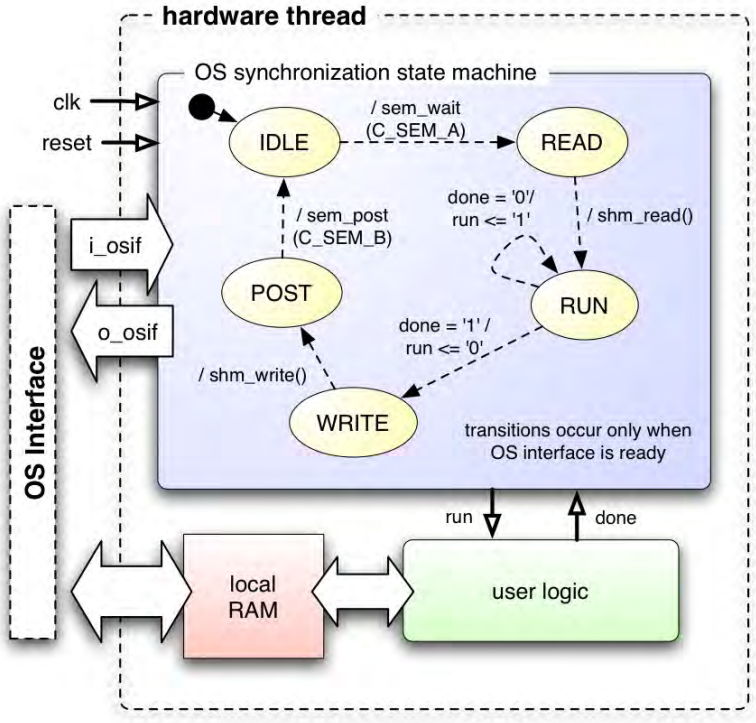


Figure 1: Hardware thread structure

The ReconOS execution model is based on a CoreConnect bus topology implemented in Xilinx FPGAs, an example of which is depicted in Figure 2. The kernel of the operating system and all software threads run on the CPU. Hardware

threads are implemented in the FPGA fabric and are connected to an OS interface (OSIF) block, which is connected to the system bus and provides direct access to the entire system memory space as well as communication registers accessible for OS interaction. Whenever a hardware thread issues a request for an operating system service, its OSIF either executes it directly (if it is implemented in hardware, such as memory accesses) or raises an interrupt to relay the call to the CPU, where the request is executed as a regular software API function call.

An intriguing feature of modern FPGAs is the ability to dynamically reconfigure parts of the device while the remaining portions of the system keep operating. ReconOS exploits this feature to enable multithreading of hardware threads, similar to how multithreading is done on the CPU for software threads. This technique can raise the utilization of the reconfigurable logic area, since inactive hardware threads are dynamically replaced by active ones using partial reconfiguration. This technique involves dedicated logic resources for supporting dynamic reconfiguration, a custom tool chain for specifying hardware thread layout and scheduling parameters, mechanisms for saving and restoring thread state. We have also developed a novel cooperative scheduling technique that differs from established scheduling algorithms for single- or multiprocessor systems and takes the characteristic features of hardware threads into account to minimize logic overhead.

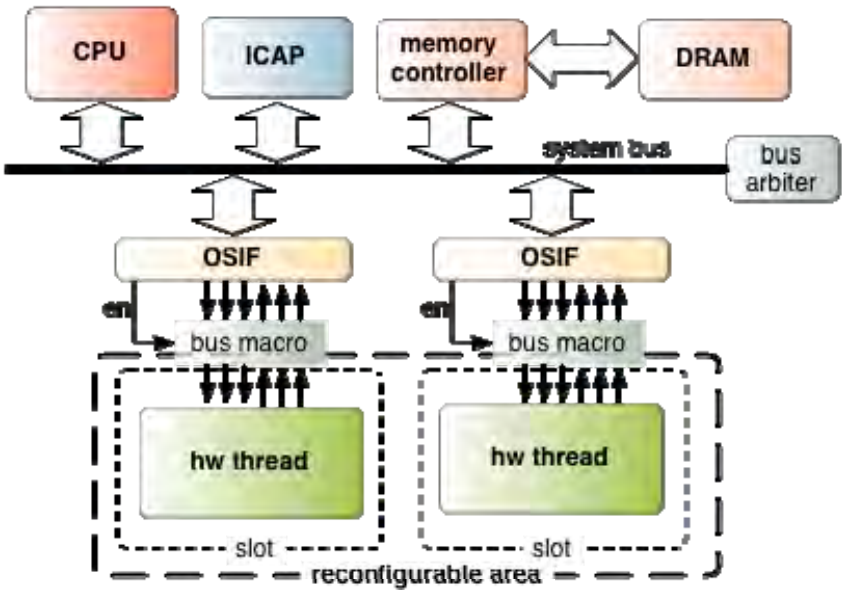


Figure 2: ReconOS run-time system architecture

References

[1] Lübbers, E. and Platzner, M.: „ReconOS: A RTOS Supporting Hard- and Software Threads“, In *Proceedings of 2007 IEEE International Conference on Field Programmable Logic and Applications (FPL'07)*, Amsterdam, August 27-29, 2007.

[2] Lübbers, E. and Platzner, M.: „Communication and Synchronization in Multithreaded Reconfigurable Computing Systems“, In *Proceedings of the 8th International Conference on Engineering of Reconfigurable Systems and Algorithms (ERSA)*, Las Vegas, Nevada, USA, July 2008.

[3] Lübbers, E. and Platzner, M.: „A Portable Abstraction Layer for Hardware Threads“, In *Proceedings of the 18th IEEE International Conference on Field Programmable Logic and Applications (FPL'08)*, Heidelberg, Germany, September 2008.

[4] Happe, M.; Lübbers, E. and Platzner, M.: „A Multithreaded Framework for Sequential Monte Carlo Methods on CPU/FPGA Platforms“, In *Reconfigurable Computing: Architectures, Tools and Applications: 5th International Workshop, ARC 2009, Karlsruhe, Germany, March 2009.*

[5] Lübbers, E. and Platzner, M.: „Cooperative Multithreading in Dynamically Reconfigurable Systems“, In *Proceedings of the 19th IEEE International Conference on Field Programmable Logic and Applications (FPL'09)*, Prague, Czech Republic, August 2009.

[6] Lübbers, E. and Platzner, M.: „ReconOS: Multithreaded Programming for Reconfigurable Computers“, *ACM Transactions on Embedded Computing Systems (TECS)*, Volume 9, Issue 1, October 2009.

[7] Happe, M.; Lübbers, E. and Platzner, M.: „An Adaptive Sequential Monte Carlo Framework with Runtime HW/SW Repartitioning“, In *Proceedings of the 2009 International Conference on Field-Programmable Technology (FPT'09)*, Sydney, Australia, December 2009. To appear.

[8] Lübbers, E. and Platzner, M.: „ReconOS: An Operating System for Dynamically Reconfigurable Hardware“, In *Dynamically Reconfigurable Systems - Architectures, Design Methods and Applications*, Springer, 2010, ISBN 978-90-481-3484-7. To appear.

5.1.5 Instruction Set Customization for High-Performance Reconfigurable Computing

Project coordinator	Dr. Christian Plessl, PC², University of Paderborn
Project members	Mariusz Grad, PC², University of Paderborn

General Problem Description

In this project we investigate and develop hardware architectures and software tool flows for high-performance custom computing. Our objective is to automatically transfer computationally intensive kernels of applications to a dedicated hardware accelerator implemented with Field Programmable Gate Arrays (FPGAs) instead of executing them on the host CPU. It has been demonstrated for hand crafted FPGA accelerators that improvements in execution speed and energy efficiency of several orders of magnitude over conventional CPUs can be achieved for many important applications.

However, this promising new technology is not yet sufficiently supported by current design methodologies and tools, in particular, the challenge to automatically create efficient hardware accelerators is still open. Our long-term research goal is to develop new algorithms and design methods for automated and autonomous hardware accelerator generation from software descriptions, which will significantly simplify the accelerator implementation process and hence promote the use of reconfigurable hardware accelerators.

The main challenges in this area are:

- Designing new computer architectures that allow for accelerating applications with reconfigurable hardware accelerators that are generated and configured during runtime.
- Finding new profiling techniques for analyzing the execution characteristics of applications during runtime and developing performance models for estimating the performance of the accelerated application in order to guide the hardware/software partitioning process.
- Developing new methods and compilation tool flows for automatically translating software functions to hardware accelerators.

Problem Details and Work Done

In our current work, we have developed a new processor architecture named "Woolcano" which allows for customizing the instruction set with user-defined custom instructions. The custom instructions are implemented in reconfigurable logic, which allows to augment the processor's basic instruction set with additional application-specific operations, for example instructions that fuse frequent instruction sequences into a single instruction or with instructions that implement non-standard arithmetic operations.

For evaluating the Woolcano reconfigurable processor architecture we have implemented an FPGA-based hardware prototype. A schematic overview of the Woolcano architecture is presented in Figure 1. The architecture leverages the Xilinx Virtex-4FX FPGA architecture that integrates a dedicated PowerPC CPU core with reconfigurable logic. The Woolcano architecture uses the PowerPC core as the base processor with a fixed instruction set and uses the programmable logic for implementing eight instruction slots that accommodate the user-programmable custom instructions. In contrast to application-specific instruction set processors (ASIPs) which use static custom instructions, our architecture allows to change the custom instructions.

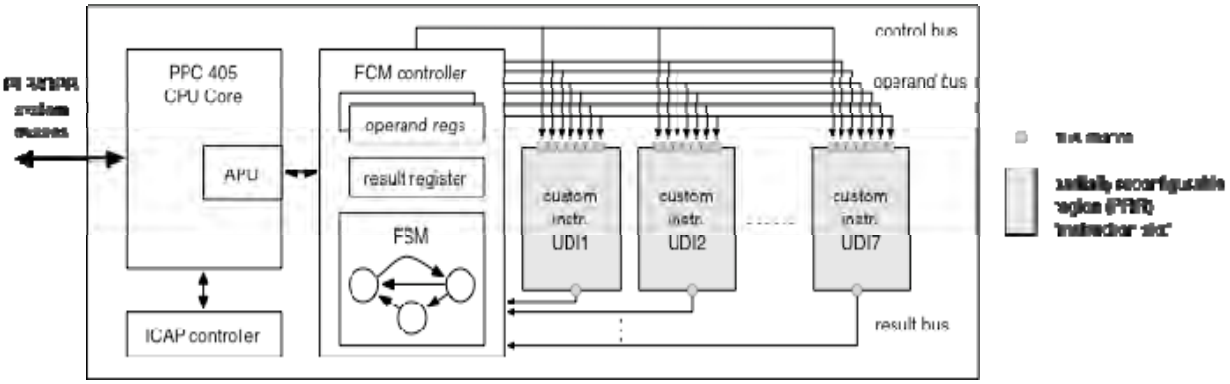


Figure 1 A schematic representation of Woolcano - a reconfigurable processor architecture

For making our architecture easily accessible we have worked on an integrated software and hardware tool flow. This tool flow allows developers to automatically translate software functions into hardware accelerators and to create software binaries using these accelerators.

Figure 2 presents a schematic overview of our tool flow. The tool flow builds on the open-source Low Level Virtual Machine (LLVM) compiler infrastructure. We start from an application in C code which is translated to LLVM Intermediate Representation using the llvm-gcc front end. Using profiling we identify the runtime

intensive parts of the application and select the most promising hotspots. These hotspots are extracted from the code and are translated to a specification in a hardware description language, which is synthesized into configurations for the instruction slots.

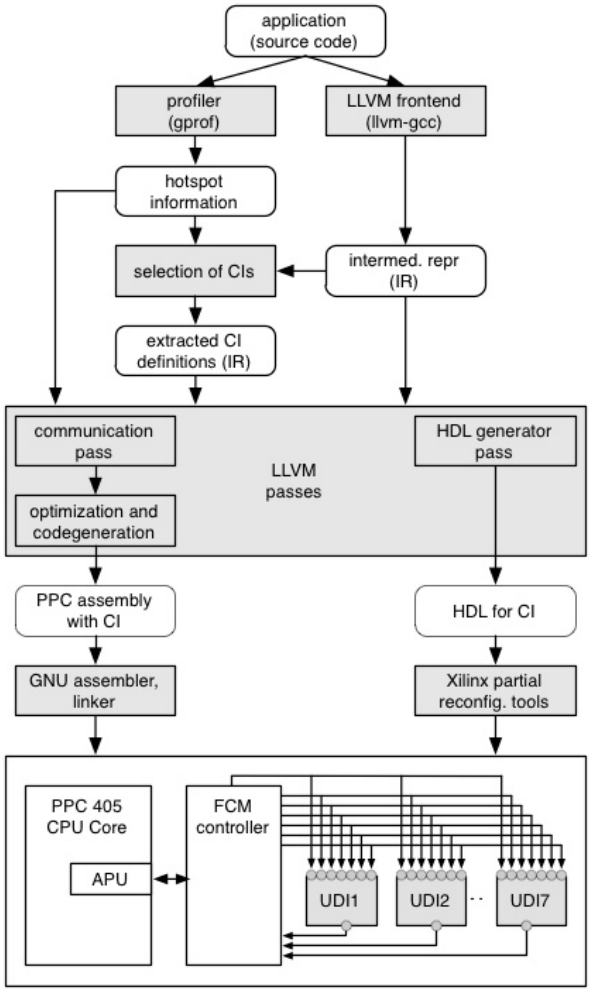


Figure 2 Software and hardware tool flow

In our current research, we are exploring the intriguing feature of modern FPGAs to modify parts of the configuration during execution, while the other parts the system keep operating. This capability opens the possibility to dynamically replace or adapt the custom instructions during runtime. Hence, instead of creating static custom instructions at compilation time, we are studying approaches to defer the identification and synthesis of custom instructions to the runtime. This will enable us to build adaptive computer architectures that use self-optimization to adapt

themselves to the current workload, which is a completely novel and promising research area.

References

[1] Grad, M. and Plessl, C.: “Poster abstract: Woolcano – an architecture and tool flow for dynamic instruction set extension on Xilinx Virtex-4 FX,” in Proc. IEEE Symp. on Field-Programmable Custom Computing Machines (FCCM). IEEE Computer Society, April 2009.

[2] Grad, M. and Plessl, C.: “ Woolcano – an architecture and tool flow for dynamic instruction set extension on Xilinx Virtex-4 FX,” in Proc. of International Conference on Engineering of Reconfigurable Systems and Algorithms (ERSA), July 2009

5.1.6 IMORC: Application Mapping, Monitoring and Optimization for High-Performance Reconfigurable Computing

Project coordinator	Prof. Dr. Marco Platzner, PC², University of Paderborn Dr. Christian Plessl, PC², University of Paderborn
Project members	Tobias Schumacher, PC², University of Paderborn
Supported by:	XtremeData Inc.

General Problem Description

While research has demonstrated the potential of FPGAs as acceleration technology for decades, the creation of accelerators for realistic workloads has been hindered, at least partially, by the lack of commercially available systems. In the last years, however, computing system vendors began to offer machines that combine microprocessors with FPGAs. More recently, FPGA modules that fit into processor sockets have been introduced and provide a fairly standardized way of integrating hardware accelerators into mainstream computing systems.

Developing and optimizing accelerators for such machines is a challenge. Even if FPGA cores for important algorithmic kernels become more and more available, combining them into an overall accelerator remains tricky. Generally, the cores will show data-dependent runtimes and compete for shared resources such as external memory or the host interface, which makes it difficult to decide on a proper number of cores, their topology, the degree of core-level parallelism, data partitioning, etc.

To address these challenges, we have developed IMORC. IMORC is actually two things, an architectural template for creating core-based FPGA accelerators and an on-chip interconnect. The architectural template assists the designer in combining cores to an overall accelerator and greatly facilitates design space exploration, core reuse and portability. The IMORC interconnect relies on a flexible multi- bus structure with slave-side arbitration and offers FIFOs, bitwidth conversion and performance monitoring. Especially performance monitoring is indispensable for debugging and optimizing FPGA accelerators.

Problem Details and Work Done

IMORC assumes applications to be decomposed into a set of communicating cores, which encapsulate computations and access to memory and external communication interfaces.

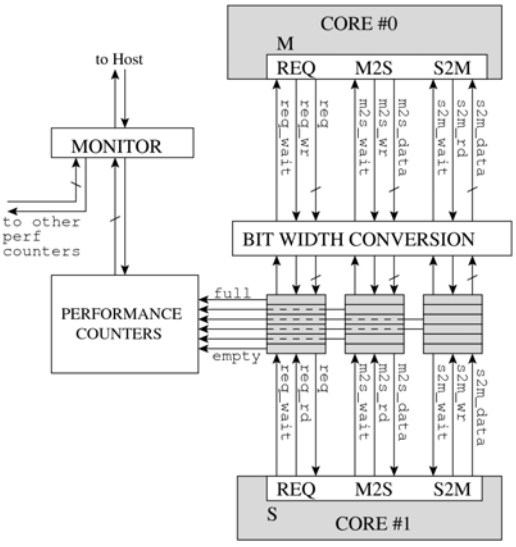


Figure 3: Diagram of an IMORC link

A key element of IMORC is its on-chip interconnect for connecting such cores. Cores in IMORC are connected using links, which are composed of three channels:

REQ request channel with three fields: one field indicating if the transfer is a read or write, a destination address field and a size field

M2S data transfers from master to slave

S2M data transfers from slave to master

Each of the three channels connect master and slave cores using asynchronous FIFOs, enabling both cores to operate in their own clock domains. Additionally, bitwidth conversion modules can be inserted enabling master cores to access slaves at their native data width. Performance counters are inserted, counting the number of times the different FIFOs run full or empty. These values can be monitored in the running system for gathering real performance values with realistic workload.

Additionally to the 1:1 connections presented, IMORC also supports N:1 and N:M connections. For N:1 connections, multiple masters are to be connected to one slave core, which is performed using the IMORC slave arbiters. The slave arbiter monitors the different REQ channels for valid requests and selects an appropriate port, usually in round robin manner. The request is forwarded to the slave core and the corresponding port number together with the request size is forwarded to the read or write datapath, respectively. Here, the appropriate amount of data is transferred from the data channel corresponding to the request.

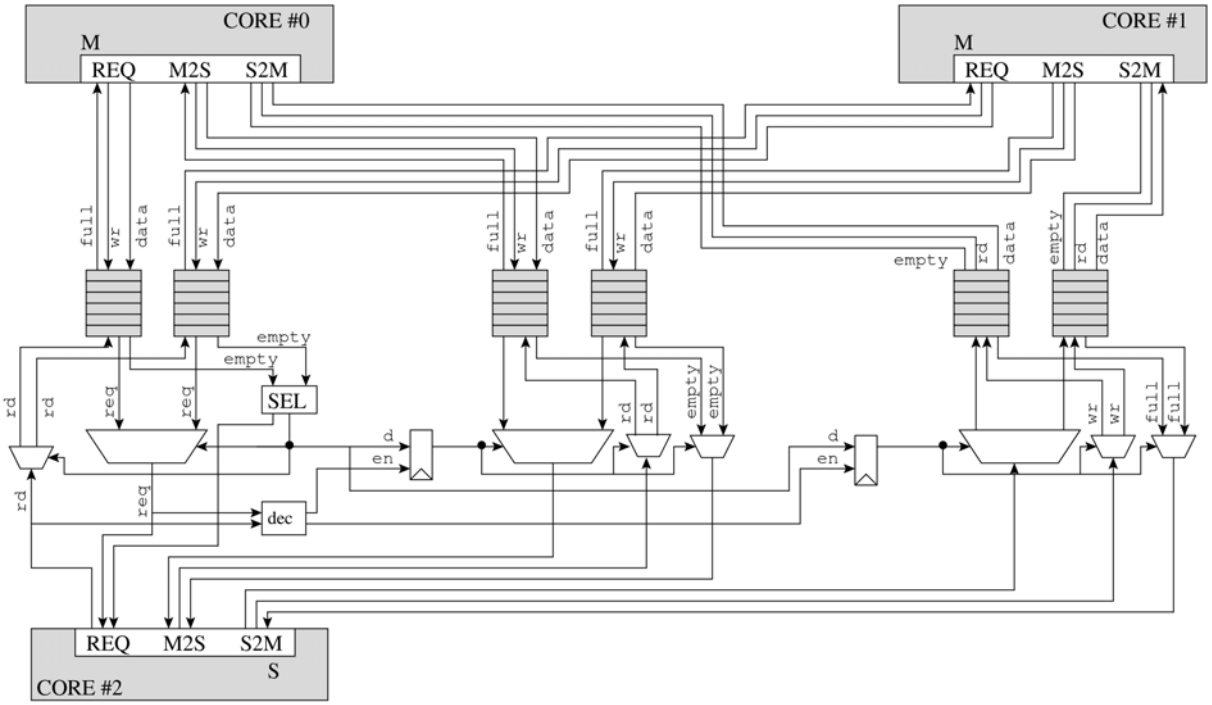


Figure 4: Diagram of an IMORC slave arbiter

1:N connections are supported by using a bus for the FIFOs' wr/rd/wait signals.

This communication scheme provides several benefits to the designer:

- The FIFOs in the links and the separate request and data channels allow designers to decouple the request task from the datapath. The request task can continuously send read/write requests to the slave core, the datapath independently starts operations when data becomes available.
- There is no shared bus forming a central bottleneck.
- High-bandwidth slaves can fulfill the bandwidth requirements of multiple lower-bandwidth master cores, since data is buffered in FIFOs that provide the same bandwidth as the slave's link.
- Cores can transparently access different kinds of memory at their native data width. The bitwidth conversion modules enable cores to access memory of arbitrary width without any information of the concrete memory's layout.

In Addition to the communication infrastructure, IMORC provides a set of utility cores that facilitate the accelerator design:

- **IMORC2REG core:** implements a register block, which is accessible through an IMORC slave interface on the one side and through a native interface on the other side. This interface core can be used for receiving job parameters and presenting them to a core.
- **REGS2IMORC core:** again implements a block of registers, accessible through a native interface. Instead of being accessible through an IMORC

slave interface, it forms an IMORC master and can be used for sending job parameters to other cores.

- **Farming cores:** the IMORC2REGS and REGS2IMORC interface cores form methods for generating jobs to be executed. Often, it is desirable to use multiple instances of a core for executing similar tasks in parallel. The farming cores can take job messages as generated by the REGS2IMORC interface cores and distribute them among multiple IMORC2REGS interface cores for balancing the load between multiple instances of a compute core.
- **Request generator cores:** Many applications need to access data using a predefined or configurable scheme. The request generator cores implement the request path of such cores. The simple form can post a sequence of successive read or write requests with a configurable request size, each. Optionally, using a step parameter the destination address can be incremented further each request, for example for accessing the diagonal elements of a matrix. Additionally, arbitrary sequences of read and write requests can be generated.

These utility cores provide a straight-forward way of generating the request task of accelerator cores, allowing designers to concentrate on the implementation of an optimized datapath. The load sensors which are automatically inserted into the communication infrastructure additionally help in optimizing such accelerators using realistic input data.

Evaluation of the IMORC architectural template was performed on the XtremeData XD1000 reconfigurable platform. The machine provides a dual socket AMD Opteron workstation, where one socket is equipped with an 2.2GHz AMD Opteron processor and the other one with an Altera Stratix II EP2S180 FPGA. Processor and FPGA communicate using a 16bit HyperTransport link running at 800MT/s. 4GB of DDR SDRAM are attached to each the processor and the FPGA. The IMORC support package for this workstation consists of a HT2IMORC interface, which translates HT packets into IMORC packets for CPU initiated communication and additionally allows IMORC to access the CPU's memory using the HyperTransport link. Additionally, an interface to the DDR SDRAM is provided which is based on the Altera DDR SDRAM controller.

In [1], [2] and [3], we give a detailed overview of the IMORC architectural template, our modeling approaches and some case studies demonstrating the potential of this approaches. One of the case studies presented in [2] is an accelerator for the k-th nearest neighbor (KNN) thinning problem.

K-th nearest neighbor methods are widely accepted methods for example in the area of statistics, data analysis and for solving classification problems. The algorithm variant we studied in our work is used for reducing a set of n vectors in a multi-dimensional space to the k vectors that represent the original vectors best. For this purpose, the algorithm starts calculating the distances between all vectors and sorts

these distance values in ascending order.The vector with the unique minimum distance to another vector is discarded and the algorithm starts at the beginning until only k vectors remain.

For the implementation of the IMORC based accelerator, we decomposed the original algorithm into three tasks (distance calculation, sorting, search & discard) and implemented each of these tasks as an IMORC core. The control units of these cores could be implemented nearly completely using the IMORC utility cores, with only a some glue logic and hardly any additional custom control logic. Most of the design time was spent for implementing the datapath.
The design presented in [2] was able to use multiple distance calculator cores and sorter cores, job distribution was performed using the IMORC farming cores. The search & discard core was not parallelized. Figure 3 shows the speedups generated by this accelerator over the original algorithm running on the Opteron CPU of the XD1000 for different configurations (***axb*** means that ***a*** distance calculator and ***b*** sorter cores have been instantiated). The FPGA accelerators were able to achieve a maximum speedup of a factor of 74 over the Opteron host processor.

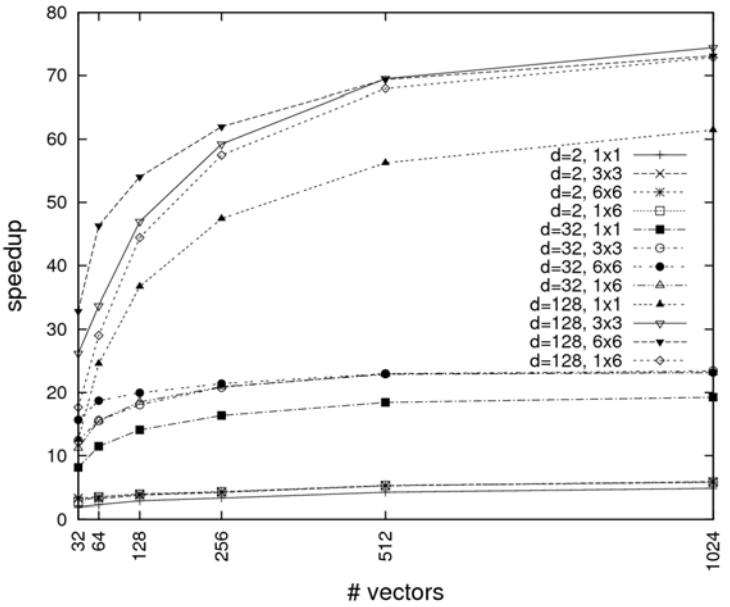


Figure 5: Speedups of the KNN accelerator over the Opteron CPU

Using the IMORC load sensors we also got an insight into the concrete runtime of the different cores. We could see, that for large numbers of vectors the search & discard module took most of the time. This information lately lead to the development of a different search & discard module which is able to be parallelized.

Resource Usage

Development, simulation and synthesis was mainly performed on several fast server systems. For generating different configurations of an accelerator, the Arminius cluster and the Windows HPC cluster was used occasionally. Evaluation of the architectural template was performed on the XtremeData XD1000 reconfigurable workstation.

References

[1] Schumacher, T.; Plessl, C. and Platzner, M.: “IMORC: Application Mapping, Monitoring and Optimization for High-Performance Reconfigurable Computing,” in Proc. IEEE Symp. on Field-Programmable Custom Computing Machines (FCCM ’09). IEEE, 2009.

[2] Schumacher, T.; Plessl, C. and Platzner, M.: “An Accelerator for k-th Nearest Neighbor Thinning based on the IMORC Infrastructure”, in *Proceedings of the 19th International Conference on Field Programmable Logic and Applications (FPL)*, Prague, Czech Republic, August/September 2009. IEEE

[3] Schumacher, T.; Süß, T.; Plessl, C. and Platzner, M.: “Communication Performance Characterization for Reconfigurable Accelerator Design on the XD1000 ”, in Proc. Int. Conf. on ReConFigurable Computing and FPGAs (RECONFIG '09)

5.2 Grid Technologies

5.2.1 Gaussian-as-a-Service

Project coordinator	Jun. Prof. Dr. André Brinkmann, PC², University of Paderborn
Project members	Matthias Keller, PC², University of Paderborn
	Dirk Meister, PC², University of Paderborn
	Dr. Sonja Herres-Pawlis, TU Dortmund
Supported by:	Forschungspreis der Universität Paderborn 2008

General Problem Description

The PC^2 is a service provider for high performance computing infrastructure. Despite the easy access to use the provided infrastructure, users need some degree of technical knowledge about the underlying software-system. Such a degree of technical understanding has to be learned previously. Especially for (external) non-computer-scientist this is a first serious barrier on the way to access the provided computing power. Minimizing that barrier, simplifying the first steps and the whole workflow, will increase the quality of the provided service. With such an elimination of technical knowledge needed, the number of potential users, particularly non-computer-scientists, will increase. Within this project a prototype web service is been developed in cooperation with external non-computer-scientists for an iterative refinement of the software to comprehend requirements in depth, to solve emerging issues, and finally to elevate the overall quality of the service.

Beside well known middleware systems for Grid Computing like Unicore, Globus Toolkit, or gLite, another middleware system is chosen relating to Cloud Computing [1], a commercially driven alternative approach for utilizing compute resources. While Cloud Computing currently gains more and more importance and influence in the industry, it's lakes of standardizations and in depth academic exploration and research. Except for the similarity of utilizing hardware resources with Grid Computing, Cloud Computing has four major differences in the context of this project: service, access, virtualization and scale. The first two differences are emphasized by the service-oriented perspective, which insinuates a high-level abstraction or interface (generally a http-request), which provides an easy and ready-to-use access to the provided services of the cloud.

Those services are often called X-as-a-Service, like Infrastructure-, Platform-, or Software-as-a-Service, which are not invented by Cloud Computing but mostly used in it's context.

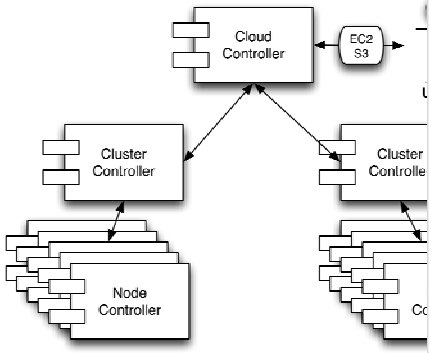


Figure 1: shows the 3-tiered architecture of eucalyptus**.**

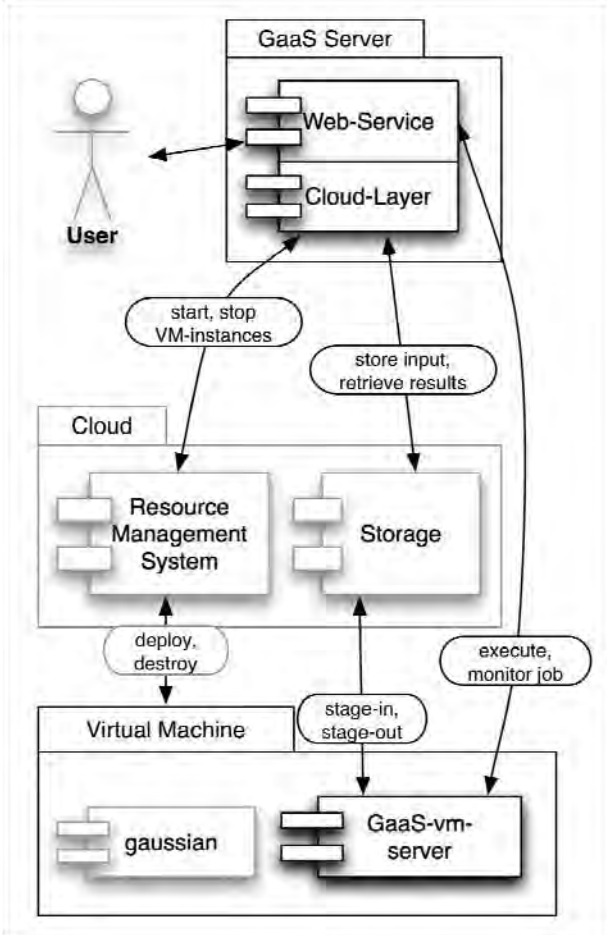


Figure 2: depicts the software architecture of Gaussian as a service. Bold components are part of the prototype.

Because of the unique use case of high performance computing, a High-Performance-Computing-as-a-Service is imaginable as proposed by the Steinbuch Centre for Computing [2]. Acquire the privileges to accessing the service is usually done by creating a web account and therefore substantially easier than applying for Grid Credentials through a personalized administrative process. Another inherent concept of Cloud Computing is virtualization. Besides some efforts of the Grid Computing community to only extend a grid with virtualization capability, Cloud Computing takes the opposite approach where only virtual machines exists and applications or computations run within them. Another difference is the vision of the enormous scale of a cloud, deducing on the one hand the demand for a very scalable architecture and on the other hand a cost efficient management of that resources by e.g. choosing a low maintenance cost place or automation of the administration.

Problem Details and Work Done

The main goal is lowering the technical barrier in aspects of performing a job-workflow and receiving privileges. In particular for the first aspect, the developed software needs to be specialized for this type of job, for the used application, or for a set of similar applications. To reduce the development time for a first prototype, the project focuses on Gaussian. Gaussian [3] supports distributed computing for electronic structure model of molecules. Chemical scientists like Dr. Herres-Pawlis from the technical university of Dortmund and our university currently use this software running on the PC^2 hardware for their research interests.

To utilize hardware resources an open source cloud middleware system called Eucalyptus [4] is appointed. This enables full control over the software to alter it to fit the needs of research, which has already been utilized. Another advantage of Eucalyptus is the three-tiered architecture shown in Figure 1, so that at the top tier resources of multiple side clusters are consolidated. This enables the integration of other clusters in one system, fostering cooperation with other companies or institutes. It also enables the provision of different types of resources. This fact is especially interesting in the field of high throughput computing like an InfiniBand interconnected cluster.

The Eucalyptus Cloud includes a resource management system, which schedules, deploys and starts Virtual Machines (VM) on computing nodes. Therefore a specialized Image-Bundle is provided to start Gaussian computations inside a Virtual Machine. By throwing all together the software architecture depicted in Figure 2 was created.

The following paragraph will shortly outline how the whole job-workflow from a user perspective is been automated by the prototype. The four major actors are the user, the Gaussian Server, the Cloud and the Virtual Machine. The user interacts with a website by e.g. starting, monitoring a job. This website is provided by a web service component of the Gaussian-as-a-Service (GaaS) Server, which is part of the developed prototype. That server stores job input data inside the cloud-infrastructure through a Simple Storage Service (S3) provided by Eucalyptus and starts or stops instances as needed for the job computation inside the cloud through the Elastic Compute Cloud (EC2) service of Eucalyptus. Any Cloud interaction is wrapped through a Cloud-Layer, which supports using another Cloud like the Amazon Cloud or facilitates the adaption to another resource utilization middleware like Globus Toolkit. The Cloud manages the underlying hardware resources and starts the virtual machines using the specialized image-bundle. Inside such a virtual machine another server is running, which implements the stage-in and -out process – preparing and copying input data and saving results – and starts the computation with Gaussian.

The GaaS-Server monitors the job-state through the VM-Server. After a job is finished and the stage-out process is completed, the GaaS-Server stops the job related instances in the cloud. The user can receive the results via the Website.

After three month of analysis and development, currently a stable alpha version is running. Next the first iteration of refinement will start introducing the beta version and a tight cooperation with our chemistry users. A knowledge transfer and comparison to virtualization efforts in the field of Grid Computing is aspired. As future efforts the security aspects of the cloud could be evaluated, e.g. the concept of right-delegation known form the Grid is unsupported but useful for higher-level service like Software-as-a-Service. Further architectural modularization may support arbitrary high performance computing software or resource utilization middleware systems.

References

[1] Mc Evoy, G. V. and Schulze, B.: "Using clouds to address grid limitations," in *MGC'08: Proceedings of the 6th international workshop on Middleware for grid computing*. New York, NY, USA: ACM, 2008, pp. 1-6. [Online]. Available: http://dx.doi.org/10.1145/1462704.1462715

[2] Steinbuch Centre for Computing. Karlsruher Institute of Technology. About High Performance Computing as a Service. [Online]. Available: http://www.scc.kit.edu/forschung/4942.php

[3] Gaussian Website, http://www.gaussian.com/g_prod/g09.htm

[4] Nurmi, D., Wolski, R.; Grzegorczyk, C.; Obertelli, G.; Soman, S.; Youseff, L. and Zagorodnov, D.: "The eucalyptus open-source cloud-computing system," in *Proceedings of 9th IEEE International Symposium on Cluster Computing and the Grid, 2009*. [Online]. Available: http://open.eucalyptus.com/documents/ccgrid2009.pdf

5.2.2 HYDRA – Network embedded system middleware for heterogeneous physical devices in a distributed architecture

Project coordinator	Jun. Prof. Dr. André Brinkmann, PC², University of Paderborn
Project members	Sascha Effert, PC², University of Paderborn Dirk Meister, PC², University of Paderborn Dr. Sonja Herres-Pawlis, TU Dortmund
Supported by:	European Commission (IST-2005-034891)

General Problem Description

Information technologies are nowadays spread in almost every area of modern life. Not only the desktop pc or notebook is part of this movement, but also more and more embedded systems, integrated in house automation, cars or even clothes. To improve the value of such embedded devices Hydra aims to build up on these devices an “Internet of Things”.

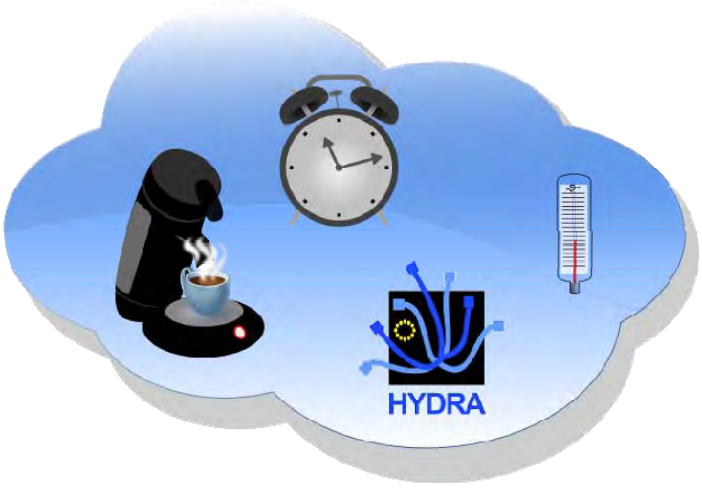


Figure 1: Hydra connecting home devices

“Internet of Things” means that devices are reachable in an easy way over a network by remote applications. Manufacturers designing a hydra enabled device have to care about adding the device to the network. For small devices, like sensors, this can be realized using a Hydra proxy. Gateways are responsible to build a connected network even over different physical network types like Ethernet, Bluetooth or Zigbee.

The Hydra project aims to build a middleware to support this kind of Peer-to-Peer network. It delivers technologies to build virtual devices upon physical hardware description, to develop applications being able to find devices and to communicate with them in a network independent and secure way.

The example described in Figure 1 shows how the Hydra middleware can improve the value of common devices. In most modern homes there are a couple of independent devices, e.g. a coffee maker, an alarm clock and temperature sensors for the heater. Connecting these devices the alarm clock would be able to ring earlier in the winter when the streets are frozen by connecting the temperature sensor. More over it could tell the coffee maker to brew up fresh coffee. But Hydra is not only focused on the home sector but also on the other ones like healthcare and agriculture.

The PC^2 is working in the area of storage in this highly dynamic P2P network. The demands in storage are very special in this area. Devices join and leave the network dynamically, often even without disconnecting. Nevertheless data should be reachable in the network. Sometimes it is also important to keep data locally on devices available. This means applications need to be location aware in the place data is stored. Therefore, if an application needs more storage than the local device has, it can access storage on other devices, e.g. a mobile can store downloaded pictures directly on a camera.

Data should also be stored in a robust way, so that no data loss will happen because some devices fail or are no longer reachable. Therefore sophisticated replication and synchronization algorithms are required, that are able to discover and repair failures fast.

The area of security is also very important in Hydra. Data sent over the network has to be protected, so that other members of the network cannot change or view the data. But it is also necessary to store the data on the devices in a secure way, so that only privileged users are able to read it. This way a user can use non-trusted devices to store even sensible data without having to bother that the device´s owner could access his data.

Problem Details and Work Done

As shown in Figure 2 a number of devices were developed to realize the key functionalities of the Hydra middleware. One of the most important managers is the Network Manager, which is responsible for building a network aware way for communication between devices and applications. Therefore the Network Manager builds virtual representations of managers or devices (entities) on a local device. These entities can be reached over web services using SOAP. The calls to the local representations are tunneled over the physical network to the Network Manager running on the target device, which delegates the call to the real entity.

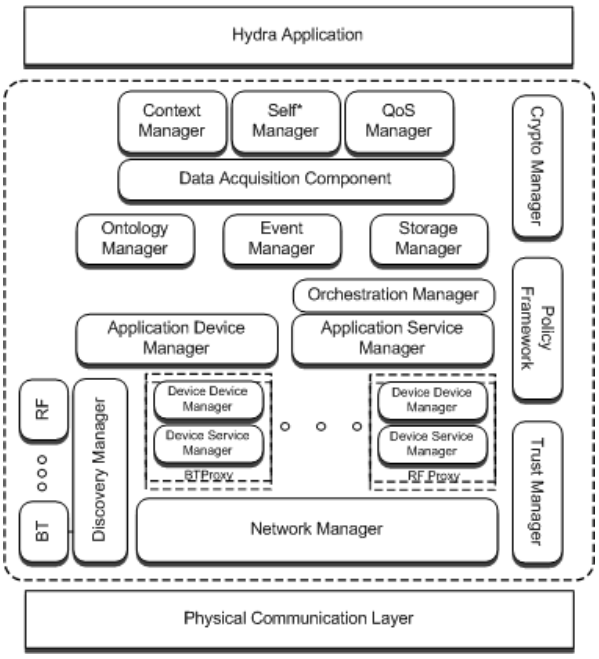


Figure 2: Hydra Managers

For communication each entity in the network aquires a number of Hydra IDs (HIDs). Each HID points to exactly one entity, and therefore the Network Manager can route data to the right target. Entities can have several HIDs for different users or contexts. Hydra enabled UPnP devices can get these HIDs by the Discovery Manager, which can find the devices in the local network and register them in the middleware.

The Crypto Manager allows building up a declarative security layer. Together with the Trust Manager and the Policy Frameworks it can protect the whole communication in Hydra. These Managers can also be used to build security in devices, as will be shown later for the storage area.

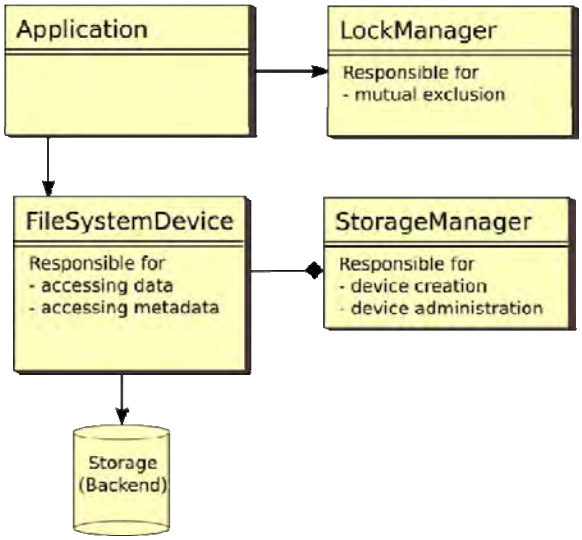


Figure 3: Hydra Storage Architecture

Storage is served in Hydra using the Hydra Storage Architecture described in Figure 3. Each device serving storage to the middleware has a Storage Manager running. This manager is responsible for administration of storage on the local device. The storage itself can be brought to the middleware as some kind of virtual device. As an example we implemented the File System Device. This allows to access data in files and structured in directories. At the moment we implemented three kinds of File System Devices:

- Local File System Device: This device is developed to build a lightweight component to bring local storage into the Hydra middleware. Therefore it delegates the functions of a File System Device to a directory in a local file system.
- Striped File System Device: This device distributes its data over some backend devices without redundancy. Therefore it is something like a RAID 0 implementation.
- Replicated File System Device: This device stores its data on each of its backend devices. Therefore it is some kind of RAID 1 implementation.

The Striped and the Replicated File System Device are designed to exist in parallel on a number of physical devices. The File System Devices can be stacked to improve the value of the storage. Figure 4 shows a combination of Local, Striped and Replicated File System Devices.

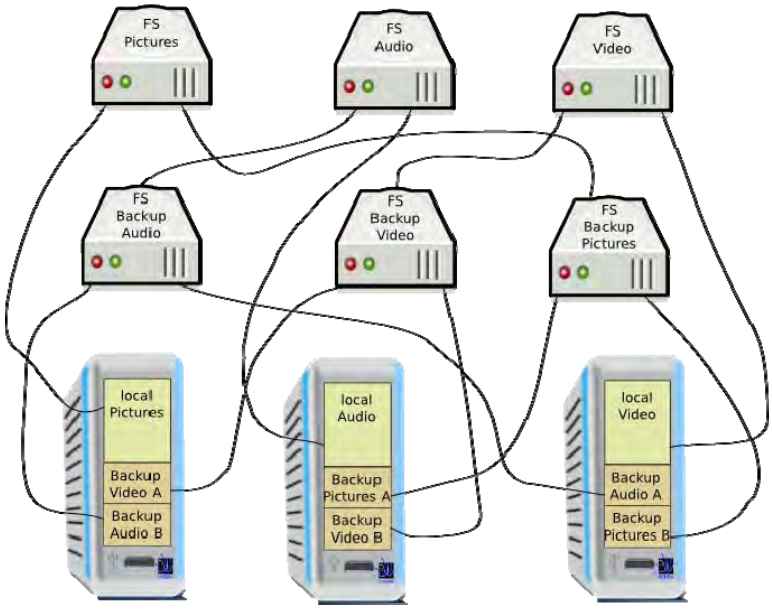


Figure 4: Example of combined File System Devices

In this example we have three Hydra enabled hard disks. Each disk holds an area of storage to hold local data and an area to keep backup data for the other two volumes. Holding the Striped File System Devices (FS Backup Audio, Video and Pictures) and the Replicated File System Devices (FS Audio, Video and Pictures) on each physical device it is possible to access the whole data even if one device is taken away. On a single device it is also possible to access the local stored data using the Replicated File System Device. On reconnection the Replicated File System Devices can synchronize each other.

Security in the Hydra Storage Architecture is realized using the Security Architecture. The Crypto Manager together with the Trust Manager and the Policy Framework allow a secure communication over the underlying network. These Managers can also be used to encrypt data on local storage in a way, that only authorized users can access it. This can be realized independent of the File System Devices. Figure 5 shows an example of a protocol storing information in such a secure way, that even an administrator on all physical devices cannot read the data.

To realize this level of security the user creates a symmetric key for his data and stores it encrypted by his public key on the device. If other users shall also access the data, the key is also stored encrypted with their public key. All data is then stored using the symmetric key. To access the data it is now necessary to hold the symmetric key the data is encrypted with. This key can only be decrypted having the private key of an authorized user. To protect the data against changes it is possible to store a signature for the data on the device.

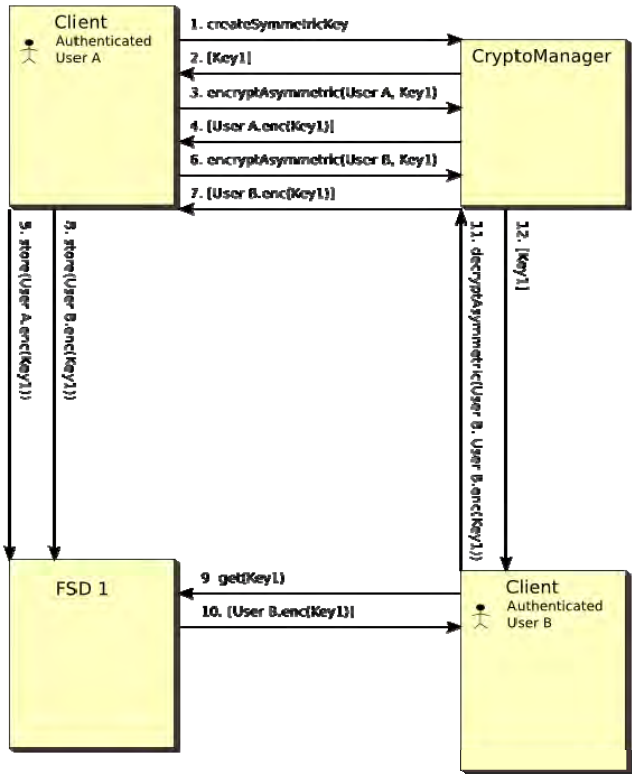


Figure 5: Data Encryption in Hydra Storage Architecture

The Lock Manager has a special role in the Hydra Storage Architecture. It can be used to synchronize access to File System Devices. It is planned to give applications the ability to lock files and directories, so that an atomic access can be realized. The devices itself do not care about locking, this is lead to the application developer. This area will be the most important of the future work of the PC² in the Hydra project.

References

[1] Brinkmann, A; Effert, S. and Gao, Y.: D3.12 Updated Grid Architecture Report, Hydra EU Deliverable, Germany, 2009

5.2.3 MoSGrid - Molecular Simulation Grid

Project coordinator	Ulrich Lang, University of Cologne Lars Packschies, University of Cologne Dirk Blunk, University of Cologne Sebastian Breuers, University of Cologne
Project members	Jun.-Prof. Dr. André Brinkmann, PC², University of Paderborn Georg Birkenheuer, PC², University of Paderborn Sandra Gesing, Eberhard-Karls- University of Tübingen Prof. Dr. Gregor Fels, University of Paderborn Jens Krüger, University of Paderborn Dr. Sonja Herres-Pawlis, University of Paderborn Dr. Alexander Reinefeld, Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB) Ralph Müller-Pfefferkorn, Technische Universität Dresden Richard Grunzke, Technische Universität Dresden Bayer Technology Services GmbH, Leverkusen Origines GmbH, Martinsried GETLIG&TAR, Falkensee BioSolveIT, Sankt Augustin COSMOlogic GmbH&Co.KG, Leverkusen
Supported by:	Bundesministerium für Bildung und Forschung BMBF under project grant **01IG09006**European Commission (IST-2005-034891)

General Problem Description

The chemical industry is one of the most research-intensive sectors of the German economy. The high levels of innovative dynamism foster close cooperation between industry and scientific institutions. The MoSGrid (Molecular Simulation Grid) should generate competitive advantages for this sector of industry and science through the grid. In MoSGrid, the key focus is on setting up and providing grid services for performing molecular simulations. MoSGrid makes the D-Grid infrastructure available for high-performance computing in the area of molecular simulations, including the annotation of metadata results and its provision for data mining and knowledge generation. The scope of MoSGrid is to support the user in all stages of

the simulation process. A portal provides access to data repositories that store information about calculated molecular properties as well as ‘recipies’ – standard methods for the provided applications. With the aid of these recipes, application-specific input files and computing requests can be generated automatically that are subsequently submitted into the Grid (pre-processing and job submission). Furthermore, users will be supported by an evaluation of the calculation results. This facilitates the preparation and processing of data for further calculations and analyses that derive from it. Additional knowledge will be attained by cross-referencing different result data files. Furthermore, the data repository allows external referencing of simulation results.
The D-Grid initiative is already enabling the supported communities to gain simple access to shared computing resources. Based on this technology and tools, MoSGrid will integrate the special requirements of chemically-oriented scientists into the D-Grid infrastructure. The high complexity of this discipline’s software (e.g. quantum mechanics or molecular dynamics) often makes accessing this technology difficult for non-specialist scientists. This difficulty is compounded by the fact that user interfaces, such as graphic accessibility functions, are often not available or are inadequate. The user’s experience is greatly assisted by a clear method selection and simple importing of molecular data, as well as the automatic set-up of a program-specific input data. Consequently, MoSGrid will offer a web-based, graphic user interface, which will enable the transparent use of the installed applications. Therefore, high-quality standard techniques will be suggested on request, e.g. for basic structure optimisation with quantum chemical methods or standard workflows for molecular dynamic research, which scientists can modify based on their own requirements. From the information received, the input data can be automatically generated for the actual simulation calculation, supported by the so-called ‘adapters’. Based on well-known and established methods, jobs are submitted into the grid and supervised. The adapters will be created, maintained and expanded by the consortium and the users. Simulation results will be extracted automatically after the calculations are complete, assisted by a suitable parser adapted to the special output formats of the different programs, and checked for elementary plausibility (post-processing). At the user’s request, these results will be transferred to collaborative data repositories of molecular properties.

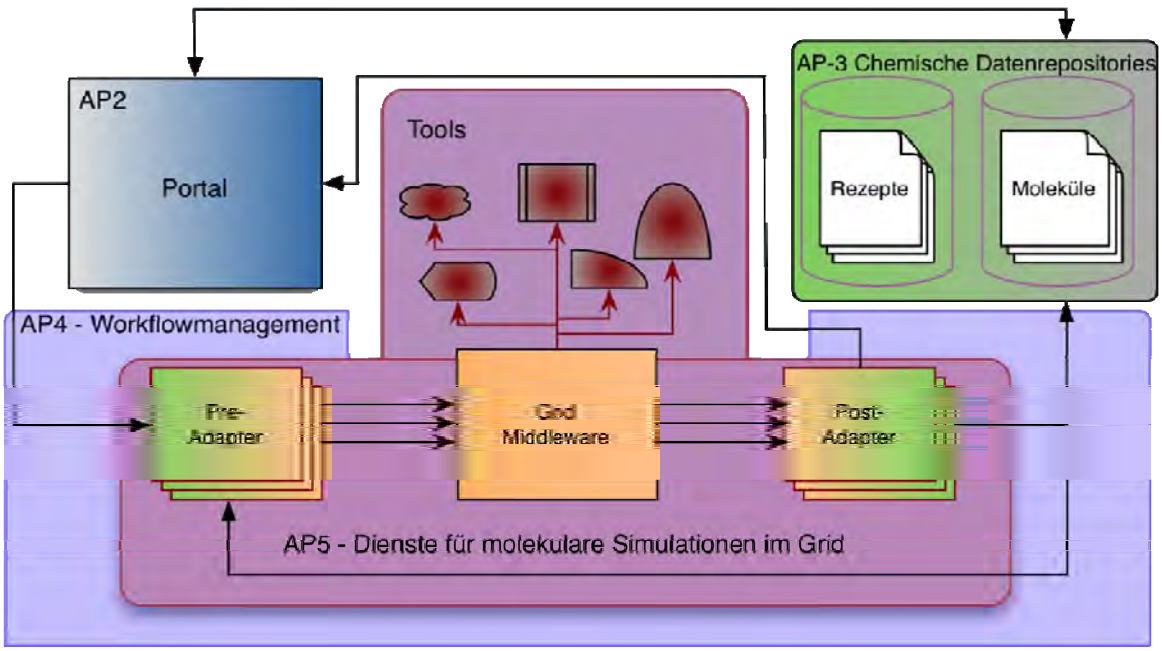
Simple access to shared data is, along with the common use of computing capacity, a fundamental basis for the acceptance of grids in business and science. MoSGrid sets up the technological basis in order to provide results of extensive molecular simulations, that can subsequently be used for example for data mining processes. Parsers aid the generation of these result data sets. In addition, data repositories are being planned, developed and operated, that support scientists through coordinated access to simulation data and the information derived from it to find solutions to complex questions. As a consequence, the generation of metadata is an important

goal for MoSGrid in applying simulation results to complex searches and logical operations. For this, well-known ontolgies will be used, to which it will be possible to add specific requirements through MoSGrid.

Validated workflows and simulation instructions will play a key role, so that the data produced for common datarooms meets certain quality standards. The planned data repositories are of practical importance, according to the expertise of those producing data for a wider circle of data users within and outside of MoSGrid. Topic-specific data can be derived from molecular simulations for the identification of relationships between structural properties. In terms of content, topics such as:

- Fundamental research, such as investigating experimental reaction phenomena;
- Applied research, such as optimisation of materials; and
- Product-related development, such as classification of potentially bioactive agents will be covered.

These broad topics are also documented through the participation of notable business partners in MoSGrid.



The value of the MoSGrid project for business and science relies on the quality, attractive content and sufficiently broad coverage of data, which are only financially possible through the high throughput of computing scenarios in the Grid. The

breadth of expert knowledge is available to the MoSGrid thanks to the participating partners from both the business and scientific communities.

MoSGrid started in September 2009 and has a duration of 36 Month. From the University of Paderborn the PC^2 as well as the chemical AG Fels and AG Pawlis are part of the project.

Problem Details and Work Done

The cooperation between the PC^2 and the Department Chemie of the University of Paderborn in scope of Grid computing was based on a work in on a UNICORE6 GridBean for Gaussian, which later was extended to a complete Grid project for the support of chemistry application and resulted in the Forschungspreis der University of Paderborn in 2008. This was also the starting point for the idea to have a D-Grid chemistry community project which resulted in MoSGrid.

The WP1 from MoSGrid, the Projekt- und Communitymanagement, is lead by the Department Chemie from the University of Paderborn. The PC^2 supports the department in computer science questions and tasks. In Task1-2, the Communitymanagement, a Survey was developed and distributed to a large group of chemists to get knowledge about the requirements of the chemistry community to MoSGrid. In addition to that, the PC^2 tried to get information about the resource requirements of the applications used by the community [1].

In WP2 Portal the main work was done in Task 2-2 , Anforderungsanalyse und Auswahl geeigneter Portaltechnologie. Here the PC^2 supports the University of Tübingen, which is the WP leader in the review of Portal solutions. The evaluated solutions are Liferay [2], GridSphere [3] and P-Grade [4].

In WP4, the Workflow Management, the PC^2 is the WP leader. Until the end of the period under review the workflow analysis was the scope in this WP. The questions where the PC^2 worked on, were to find out which kind of workflows do chemists usually needed. The kind of workflows ranges from very simple ones that are simple applications on one hardware resource to very complex workflows with result dependent sub-jobs that can be MPI distributed application running on many nodes in parallel. A result of the analysis was that even the simple computations will, in MoSGrid, be covered by several workflow steps.

Thus, an example workflow for a simple computation consists of four steps,

1. input of a user,
2. similarity check which ensures with a test on the set of the by now published results that the computation is not previously done,
3. the Meta molecule description that is adapted to the input format needed by the application itself, then the execution of the application, and
4. extraction of the important parts of the result and their display to the user.

Complex workflows can contain many dependent simulation steps as shown before containing similarity checks and pre and post-processing.
From the workflow requirements the PC^2 extracts in cooperation with the University of Cologne the needed workflow constructs, which lead to the required impressiveness of the workflow-language. This will be used in the further part of the project. The PC^2 will continue this work with check of abilities on UNICORE6 and BEPL workflows constructs to MoSGrids requirements and select best matching language and workflow engine.

For this early stage the setup of a combined UNICORE6 infrastructure between Paderborn and Köln was created to allow chemists in MoSGrid the use of Grid infrastructures from the beginning of the project.

References

[1] Niehörster, O.; Birkenheuer, G.; Brinkmann, A.; Elsässer, B.; Herres-Pawlis, S.; Krüger, J.; Niehörster J. and Packschies, L.: Providing Scientific Software as a Service in Consideration of Service Level Agreements, Cracow Grid Workshop (CGW09), Krakau, Polen, 2009.
[2] Liferay, http://www.liferay.com/web/guest/partners/sun.
[3] GridSphere, http://www.gridsphere.org/gridsphere/gridsphere.
[4] P-Grade, http://portal.p-grade.hu/.

5.2.4 DGSI – D-GRID Scheduler Interoperability

Project coordinator	Bernhard Schott, Platform Computing GmbH, Ratingen
Project members	Jun.-Prof. Dr. André Brinkmann, PC², University of Paderborn Georg Birkenheuer, PC², University of Paderborn Axel Keller, PC², University of Paderborn Martin Hofmann-Apitius, Bonn-Aachen International Center for Information Technology (BIT) Wolfgang Ziegler, Oliver Wäldrich, Andreas Hoheisel, Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V. - Institut für Algorithmen und Wissenschaftliches Rechnen (SCAI) - Institut für Rechnerarchitektue und Softwaretechnik (FIRST) Ulrich Schwardmann, Tim Ehlers, Dietmar Sommerfeld, Gesellschaft für wissenschaftliche Datenverarbeitung (GWDG), Göttingen Dr. Alexander Reinefeld, Mikael Högqvist, Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB) Uwe Schwiegelshohn, Alexander Fölling, Alexander Papaspyrou, Technische Universität Dortmund (TUDO) Institut für Roboterforschung, Abteilung Informationstechnik Rainer Spurzem, Klaus Rieger, Ruprecht-Karls-Universität Heidelberg, Helmut Heller, Arthur Carlson, Bayerische Akademie der Wissenschaften, Leibniz-Rechenzentrum (LRZ) Wolfgang E. Nagel, Technische Universität Dresden (TUDR)
Supported by	Bundesministerium für Bildung und Forschung BMBF under project grant **01IG09009**

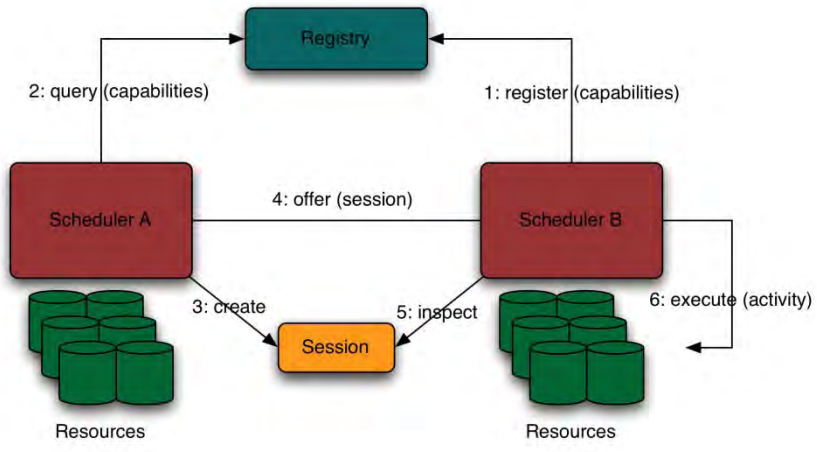
General Problem Description

Most Service Grids share the ability to efficiently distribute user workload to the resources available. This issue, usually generalized under the term *Grid Scheduling* or *Meta Scheduling*, is already very diverse within a community: both submitted jobs

and available resources differ considerably, to the extent that coordination has to handle specialized knowledge about usage scenarios and infrastructure. This leads to very different, community-specific approaches for the development of Grid scheduling services. The resulting incompatibility on the meta-scheduling level, however, proved to be a major hurdle for the coordinated cooperation of different Service Grids especially when focusing on the overall goal of better resource utilization. Moreover, cooperation on a scientific, cross-disciplinary level, is impaired as well. As such, two major use cases for temporarily including alien resources into the own community arise: first, the need to cover peak demand, and second, the usage of specialized resources.

The **D-Grid Scheduler Interoperability (DGSI)** is targeting these use cases with the conception and development of a standards-based interoperability layer for Grid level scheduling in service Grids. By allowing the users of a community to distribute the workload among resources within the management domain of another community while keeping the individual, specialized scheduling solutions being run by the communities, it offers new perspectives for community collaboration, resource sharing, and efficient utilization. For sharing the resources between different communities we follow two different approaches: Activity delegation and resource delegation.

In activity delegation, a Grid scheduler hands over an activity and the management of its execution to the domain of the scheduler of another community. In this way, an incompatibility of the basis middleware of two communities can be bridged orthogonally to the first approach introduced. This approach also requires negotiation between both Grid scheduling services.

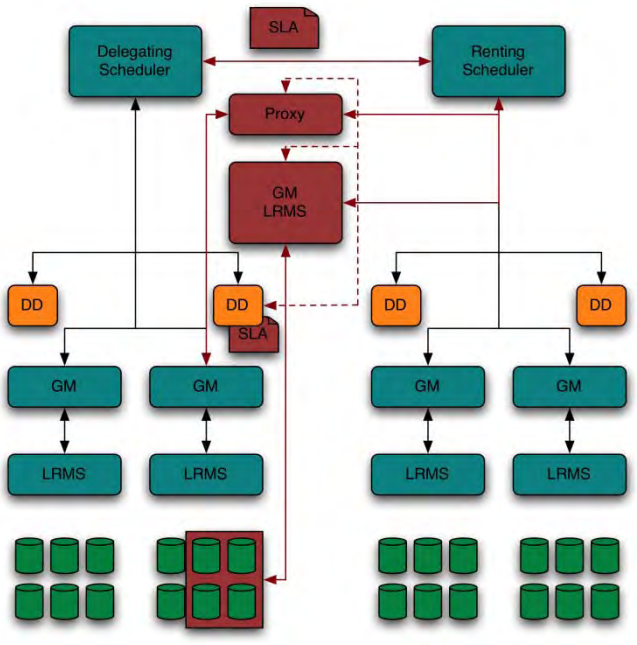


Resource delegation has become an interesting alternative to the activity delegation due to its advantages like support for local requirements, e.g. special workflow scheduling tools or better control over the delegated resources. At the same time, business models for resource delegation have been evolving, and providing Cloud

resources to customers is based on similar delegation mechanisms like those envisioned to use in the proxy-approach.
During the definition phase of the DGSI project two alternative technologies for resource delegation have been identified. Both will be developed and implemented in DGSI.
The first approach focuses on the management of delegated resources and is exclusively realised on top of the base middleware. The result of a negotiation between two community schedulers is a proxy of the middleware interface to the resources with the following tasks:

1. Encapsulation of the delegated resources
2. Monitoring of the agreed terms of usage
3. Hiding of the security-relevant adaptation and of the delegation of rights

The second approach primarily considers the configuration of the resources to be delegated. Besides the base middleware layer it includes also activities on the layer of the local RMS systems. Here, the resources become available only after the requested middleware has been deployed for these resources, which might include a lightweight local RMS. No modifications are required for the existing middleware systems. The approach is flexible since the resources can be prepared virtually for every middleware. Access rights for the resources can be configured as part of the deployment.



Both approaches have an initial resource discovery phase followed by a negotiation phase where the community scheduler initiating the delegation negotiates with other community schedulers, which represent the access points to the detected resources. For the negotiation and the agreement on the terms of the resource delegation WS-

Agreement [1] has been selected as protocol and language for creating Service Level Agreements. WS-Agreement is a specification of the Open Grid Forum (OGF) developed and maintained by the Grid Resource Allocation Protocol Working Group (GRAAP-WG) [2].

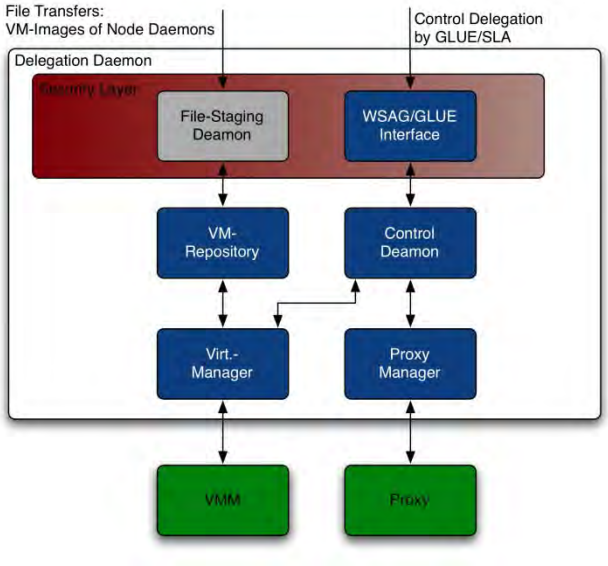
DGSI started in June 2009 and has a duration of 36 Month.

Problem Details and Work Done

The main work of the PC^2 was done in AP3 „Delegation von Ressourcen“ where the PC^2 is the workpackage leader.

In focus on the tasks T3-1 “Evaluation existierender Grid-Systeme” the PC^2 worked in the evaluation of OGSA-BES and GLUE. The task was to check for their ability to be used for resource delegation. The results were documented in Deliverable D3-1. The Open Grid Forum (OGF) defined the OGSA – Basic Execution Service (OGSA – BES) specification, to standardize a Web-Service interface. Grid clients can send a request to the interface that is accessed using WS-Addressing Endpoint References (EPR). The BES activities are described using the Job Submission Description Language (JSDL). OGSA-BES includes an extensible resource and state model for activities. The GLUE specification is an information model for Grid entities. It describes resources using natural language as well as UML class diagrams and it is designed to be independent from concrete data models. A binding from GLUE to concrete data models is available for XML Schema, LDAP Schema and SQL.

Aim of task3-2, “Definition der administrativen Voraussetzungen“, is the specification of the architecture of the software used to manage the resource delegation and definition of the administrative requirements first. The PC^2 is the Task leader. The delegation daemon (DD) is running on the distinct grid clusters systems. The Meta scheduler uses the DD for managing the confirmed delegation. The PC^2 does the work on the architecture and functionality definition for the Delegation Daemon.



Due to security reasons the DD needs an own account. This account is used to start Proxies or VMs. The account has to be available on the cluster nodes and needs sudo rights for the switch user command since the account will start the LRMS daemons on the nodes. The WSAG or Glue based Interface provides the methods that are used by the local grid Meta scheduler to control and manage a resource delegation. The control daemon is responsible for the management of the DD and the setup of general system components. Task of the proxy manager is the setup, start, controlling and destroying of the proxy processes. Task of the virtualization manager is starting, monitoring and stopping the virtual frontends. It is possible to use libvirt for the steering of the VMM. The VM repository is the repository where images of virtual machines can be stored. This allows that a scheduler, who frequently uses delegated resources, does not necessarily need to transfer a virtual machine image for every delegation every time. The VM repository will also contain standard GM installation like Globus 4.0.x or Globus 4.2.x for a scheduler. The file staging daemon allows the foreign Grid Meta scheduler to transfer and store the VM images in the repository. It might be sufficient to support gridFTP for this purpose.

In task 6.1, led by ZIB, the information Systems were defined, the PC^2 supported this work by filling in a survey on needs about an information system in scope on the resource delegation.
The first ides of the project were presented at CGW09[3].

References

[1] WS-Agreement specification: http://www.ogf.org/documents/GFD.107.pdf
[2] GRAAP-WG: http://www.ogf.org/gf/group_info/view.php?group=graap-wg
[3] Birkenheuer, G.; Carlson, A.; Fölling, A.; Högqvist, M.; Hoheisel, A.; Papaspyrou, A.; Rieger, K.; Schott, B. and Ziegler, W.: Connecting Communities on the Meta-Scheduling Level: The DGSI Approach! Cracow Grid Workshop (CGW09), Krakau, Polen, 2009.

5.2.5 AssessGrid – Advanced Risk Assessment and Management for Trustable Grids

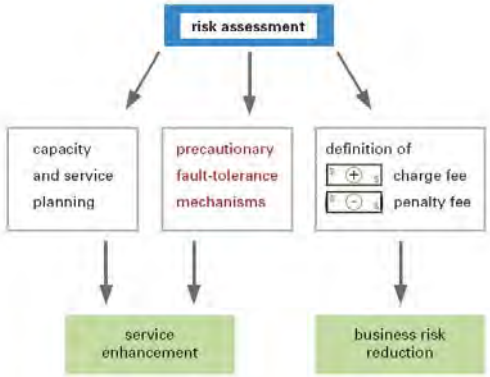
Project coordinator	Prof. Dr. Odej Kao, TU Berlin
Project members	Dr. Kerstin Voß PC², University of Paderborn Georg Birkenheuer, PC², University of Paderborn Dr. Dominic Battré, TU Berlin Christer Carlsson, Abo Akademi Finland Franck Tetard, Abo Akademi Finland Irina Georgescu, Abo Akademi Finland Melanie Biette, Atos Origin Spain Josep Martrat, Atos Origin Spain Igor Rosenberg, Atos Origin Spain Manuel Quijada, Atos Origin Spain Simon Alexandre, CETIC Belgium Stephane Mouton, CETIC Belgium Christoph Ponsard, CETIC Belgium Karim Djemame, School of Computing, University of Leeds United Kingdom Iain Gourlay, School of Computing, University of Leeds, United Kingdom Jamed Padgett, School of Computing, University of Leeds, United Kingdom Matthias Hajari, Wincor Nixdorf, Germany Jörg Stümke, Wincor Nixdorf, Germany Oliver Weissmann, TÜV Rheinland Help AG [Germany] Jörg Stümke, TÜV Rheinland Help AG [Germany]
Supported by	European Commission (IST – 031772)

General Problem Description

In our everyday life we book various services and benefit from a broad public and commercial infrastructure making our life more convenient. Usually there are several providers offering identical or similar services and products. The selection of an appropriate service is based on various parameters: price and availability are major criteria, but the reputation and thus the assumed quality of service also play a major role. The reputation expresses a long-term tradition and customer trustworthiness. New companies without this type of reputation publish test and evaluation reports to prove their quality and to attract customers. Similar mechanisms exist in other fields, e.g. hotel guests study the number of stars, put these in relation to the national

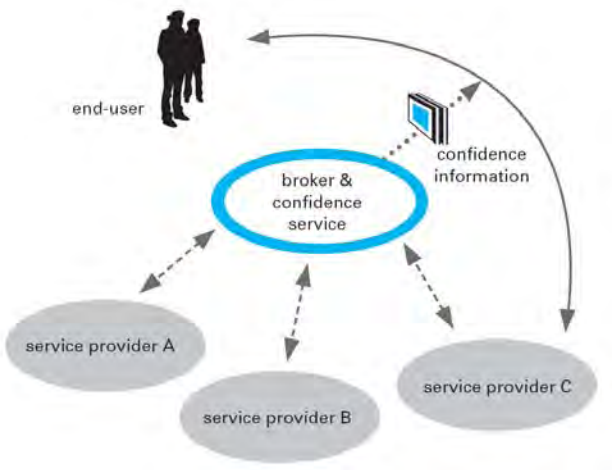
standard and try to get as much quality of service (QoS) as possible within their budget. Furthermore, they visit web sites where former guests comment their stay and give their subjective impression in different categories. Auction buyers for instance take a close look at the past evaluation of the seller and have a preference for well-ranked persons following the locality principle: A good performance in the past is an indicator for a good performance in the near future. We send our children to schools with an excellent reputation, give money to research institutions with outstanding records and hope, the job/product/service will be delivered with the highest possible quality.

In case of Grids a significant need for information on reputation exists. Should Grid users send a job/mission into a cloud of resources and should not care, who is going to execute the work? In particular should they do it if holding deadlines is crucial for their project progress or research work? The complete virtualization of resources is a powerful technological development, but Grid services are only used in the academic environment. Customers need some information about the provider reputation and quality on one hand and a legal agreement (implicit or explicit) on the other hand, before they are ready to assign a mission to a certain provider. While the Grid community undertook significant efforts by developing Service Level Agreements (SLAs), the need for reputation for gaining trustworthiness in the Grid technology is uncovered. This is one reason, why adopters underline - despite the high level of Grid technology development - core shortcomings related to security, trustworthiness, and dependability of the Grid for commercial applications and services. Since the SLA concept is a risk for both sides, a commercial SLA provisioning and usage is not available. Users want to be sure that their job will be treated according to the SLA. But providers are cautious on adoption, as agreeing on SLAs including penalty fees is a business risk: system failure, operator unavailability etc. can lead to an SLA violation. Providers need risk assessment methods as decision support for accepting/rejecting SLAs, for price/penalty negotiation, for activating fault-tolerance actions, and for capacity and service planning. Customers need the estimation and aggregated confidence information for provider selection and fault-tolerance/penalty negotiations.



AssessGrid addresses the issues of reputation and trustworthiness for all groups of Grid participants and provides methods and tools to assess and to manage a possible probability of failure in all Grid layers. The investigated risk management scenarios reflect the perspective of Grid end-users, brokers, and providers. The results will support all Grid actors by increasing the transparency, reliability, and trustworthiness as well as providing an objective foundation for planning and management of Grid activities. End-users will have a connection to a confidence service and thus access to reputation indicators suitable for the specific job. The providers will receive objective indicators about the quality of their own infrastructure, methods for risk estimation for different situations (low/high loaded resources, vacation time, overloaded network, etc.), and a decision-support for system development, management, and planning in order to detect and remove bottlenecks. Self-organizing fault tolerance mechanisms use risk indicators as thresholds to increase the reliability. In case of failures and thus risk above the threshold, the business policy will be adapted, e.g. longer slack-times will be negotiated, the penalty fee will be reduced or even SLAs will be rejected. Furthermore, spare resources or a redundant processing will be activated. Providers will also need a platform for an objective comparison and competition, which is likely to be located at the Grid broker. They have a large number of submitted jobs, so over time they can learn a lot about the quality of a certain provider and thus create and publish reputation indicators. These indicators express the risk of failure or the risk of job execution with lower quality and offer a platform for provider rankings and competition.

The demonstration of the development will be based on three sample scenarios, related to the three different groups of Grid participants – end-users, broker, and providers.



AssessGrid is funded by the European Commission as a STREP in the scope of the FP6 Specific Programme for “integrating and strengthening the European Research Area” (SP1). After a first negotiation meeting, the project started in April 2006 and ended after 36 months in March 2009.
The TÜV RHEINLAND HELP AG joined the project in 2008 to work on the Business perspective of risk assessment and management.

Problem Details and Work Done
Main issue of the year 2008 was to finish Workpackage 3 and start working in Workpackage 4. Workpackage 3 had the main goal to implement the broker scenario. The work was distributed among seven tasks coordinated by University of Leeds. Task 3.1, Dynamic Data Provision, and 3.2, Dynamic Consultant/Confidence Service, were completed in January 2008.

Task 3.3, the Dynamic Risk Assessment, applied risk management tools to use probabilistic risk. Task 3.3 was completed in June 2008 and improved the prototype by considering dynamic risk assessment. ÅBO AKADEMI developed a risk assessment method based on the Wiener process. With that the second prototype carried out a risk assessment for the Probability of Failure (PoF) for any job of any duration requiring any number of nodes in a cluster. The PC² was strongly involved here by the development of the Consultant Service, which collected monitoring information and build statistics that were used by the dynamic risk assessment. This has turned out to be a challenge during work with the second prototype as Grid and cluster operators are not routinely collecting statistics of node and job failures, the reasons for the failures, the duration of crashes, and the repair times for failing nodes. Task 3.4 was to enhance broker’s scheduling algorithm to handle Grid workflows and was completed in May 2008. The Broker Service prototype is a Globus 4.0 service using a WS-Agreement [1] interface for SLA negotiation and the Broker can act as a virtual provider (contractor). For the external workflow representation, it was decided that the workflow would be represented within the SLA request using a construct within the WS-Agreement specification. For the internal workflow representation, Directed Acyclic Graphs (DAGs) were used. Finally, the work carried out that the deployment of a Workflow Assessor could obtain a risk assessment for workflow mapping onto one or many providers. Task 3.5, the Enhanced Provider Service Quality, was completed in May 2008. In order to support SLA aware scheduling, TU Berlin implemented a scheduler for OpenCCS [2] that respects constraints of earliest start and latest finish time of jobs. The PC^2 extended this scheduler for possible decisions when jobs shall be migrated to different providers for better risk management. Further, for an improved communication between the Negotiation Manager and OpenCCS, the PC^2 extended

the protocol proxy (PP) and the TU Berlin incorporated this into the Negotiation Manager. The new PP allows OpenCCS now to request a job migration. OpenCCS creates a checkpoint file of the running application and delegates the responsibility to the Negotiation Manager. The Negotiation Manager was extended to locate suitable free resources, create an SLA with the RMS on the remote, and monitors the execution. On the remote site, a Negotiation Manager instance takes care of copying the checkpoint files using GridFTP (Stage-In), triggering the execution with OpenCCS, and copying back the result. The negotiation manager was extended to allow multi-node MPI jobs. In this task the TU Berlin and the PC^2 integrated the results of the EC-funded HPC4U [3] project in the AssessGrid software stack and added the methods to plan appropriate Fault Tolerance (FT) mechanisms the negotiation process. The risk management behaviour of the AssessGrid software stack was designed and implemented by the PC^2. Checkpointing is automatically enabled for all SLA jobs, in order to reduce the overall risk. For the Risk assessment and management a pool of spare resources was implemented into OpenCCS. These resources will not be used during negotiating SLA jobs; instead they will remain idle or be occupied by best effort jobs. Thus these resources are usable as FT resources for risk management activities. In case of a node outage of resources where an SLA job is running, they can be used by as displacement for crashed resources and thus can prevent SLA violations. In case of a node outage the dynamic risk management tries to reschedule the jobs with the last checkpoint and place it on the spare resources if possible. If no free resources are available to hold all SLA jobs, the risk management tries to negotiate for external execution of the endangered jobs. In case of failing to negotiate a profitable migration and fulfil the SLAs, it is checked based on the penalty and chance of failure, which SLA should be dropped and violated in order to save the biggest possible profit with the remaining SLA jobs [4]. Task 3.6, End-user Workflow Definition, was completed in July 2008. The task considers the End-user Workflow Definition, and was extended to allow users to create the workflows and submit them. The workflow visual rendering had to be implemented by ATOS Origin based on its core aspect, a Directed Acyclic Graph (DAG). The system integration and validation, was completed in July 2008.

Deliverables were the Consultant Service and Dynamic Risk Assessment submitted in Mach 2008 as software and report, and in August 2008the Risk-enhanced Broker Service as software as well as the Verification And Validation Report.

WP4 – Provider Scenario

Workpackage 4 has the main goal to implement the provider scenario. The work is distributed among five tasks, which were coordinated by the TU Berlin. WP 4 was completed in March 2009.

The work in task 4.1, the Advanced Risk Assessment, was coordinated by ÅBO Akademi. The work carried out is focused on a final development of the Risk Assessment (RA) theory, models and methods for Grid computing. The work in task 4.2, Provider Outsourcing and Topology Analysis, focuses on the development of a simulation environment that allows testing the strategies developed in the previous workpackages and to analyze strategic choices and their effect in terms of risk management. Extensions to the simulation environment includes metrics published by the provider, the implementation of a cheap cancellation policy to enhance the negotiation, and a new risk assessment approach developed in cooperation with PC^2, TÜV Rheinland Help AG, ÅBO Akademi, and the TU Berlin [5]. Within this work the PC^2 implemented several technical modifications of the module responsibilities and job management in the OpenCCS resource management system. At the beginning of the project the assumption was made that different compute nodes within the same cluster might have different probabilities of failures. As a consequence, the interaction with the Risk Assessor was integrated in the Machine Manager module of OpenCCS that is responsible for an explicit job-node-mapping. The research results in AssessGrid show that similar compute nodes assigned to the same compute cluster are similar stable and no explicit differentiation during the scheduling is necessary from a risk perspective. As a consequence to improve the usability, the PC^2 simplified the organization of risk - awareness by integrating all risk related functions into one single module – the Planning Manager [6]. This modification has no impact for other AssessGrid modules; however, it supports the usage and enhancement of the AssessGrid OpenCCS version since arbitrary scheduling strategies can be now used in the Machine Manager module. The second major modification in OpenCCS implemented by the PC^2 and the TU Berlin is the extension of the job duration. Since OpenCCS is planning-based, the scheduler assigns resources to jobs for a priori specified duration. To increase the probability of successfully providing SLAs, providers initiate checkpointing as default. Generating such a checkpoint costs time – if the resource reservation duration without the time needed for generating checkpoints is shorter than the execution time specified by the end-user, the SLA is violated. Consequently, the provider has to internally extend the duration for generating checkpoints. Furthermore the extension should consider that after a resource outage a specific timeslot is needed to resume the job execution from the latest checkpoint as well as repeating the lost computation steps. Such an extension is for parallel executing jobs of major importance since the computation on all resources involved has to resume from the latest checkpoint and dynamically extending the job duration is often not possible in systems with a high workload. In order to integrate the job duration extension, first of all an estimation of the time needed to generate a checkpoint is required. An appropriate monitoring is integrated into OpenCCS and the Consultant Service. The Risk Assessor is responsible for determining the extension of the duration that is then considered in the complete scheduling process in OpenCCS. Finally, the

modules for simulation and analysis of bottlenecks extend OpenCCS. A simulation environment developed by the TU Berlin reduced the necessary simulation time from several hours to few minutes, so now different provider strategies can be evaluated in order to select the strategy maximizing the benefit and minimizing the risk of failures and penalties [6,7,8]. In scope of the task 4.3, Advanced Confidence Service, the University of Leeds established an AssessGrid broker reputation system [9]. The designed algorithm to rank providers is based on provider information, past performance, and user feedback. Within this work the PC^2 finalized the consultant service and integrated it into OpenCCS. The monitoring services are used to get relevant data and to estimate the time needed for a checkpoint. For the End-user Support for Confidence Service, the portal was re-implemented by ATOS with a new design and look and feel. The System integration and validation was completed in February 2009.

Deliverables were the Advanced Risk Assessment report delivered in Oktober 2008, the Vertically Integrated Risk Management as software in January 2009, the Verification And Validation Report also in January 2009, and an Update Verification and Validation Report in May 2009.

Cooperation with other projects

AssessGrid intensified the contact with selected EC-funded projects such projects GridTrust, GridEcon, BEinGRID, HPC4U, SORMA, VIntEL, SLA@SOI, Phosphorus, and the BMBF funded project SLA4D-Grid. These projects have a similar focus: GridTrust helps the consortium to collect and verify requirements, BEinGrid provides a platform for Grid technologies applicable for the Grid commercialization like the self-organizing fault tolerance mechanisms developed in scope of HPC4U.

SORMA deals with the development of methods and tools for an efficient market-based allocation of resources, through a self-organizing resource management system, using market-driven models supported by extensions for Grid infrastructures. The VIntEL project deals with distributed simulations in a military context, based on services. The vision of SLA@SOI is the ability to flexibly trade IT-based services as economic goods, i.e. under well-defined and dependable conditions, with automated negotiation and self-management, and with clearly associated costs. The Phosoporus project deals with on-demand and end-to-end resource provisioning for guaranteeing QoS. The SLA4D-Grid project is currently in negotiation phase. Goal of this project is the establishment of SLA mechanisms in the German D-Grid infrastructure.

References

[1] Battré, D.; Kao, O. and Voss, K.: Implementing WS-Agreement in a Globus Toolkit 4.0 Environment, In Usage of Service Level Agreements in Grids Workshop in conjunction with The 8th IEEE International Conference on Grid Computing (Grid 2007), September 2007.

[2] Open Computing Center Software (OpenCCS), https://www.openccs.eu/core/

[3] Highly Predictable Cluster for Internet-Grids (HPC4U), EU-funded project IST-511531. http://www.hpc4u.org.

[4] Battré, D.; Hovestadt, M.; Kao, O.; Keller, A. and Voss, K.: Enhancing SLA Provisioning by Utilizing Profit-Oriented Fault Tolerance, *Proceedings of the 20th IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS) 2008, Orlando, Florida, USA, November 2008.*

[5] Battré, D.; Birkenheuer, G.; Hovestadt, M.; Kao, O. and Voss, K.: Applying Risk Management to Support SLA Provisioning, Proceedings of the Cracow Grid Workshop 2008.

[6] Battré, D.; Hovestadt, M.; Kao, O.; Keller, A. and Voss, K.: Quality Assurance of Grid Service Provisioning by Risk Aware Managing of Resource Failures, *CRiSIS 2008: Third International Conference on Risks and Security of Internet and Systems, 28 - 30 October 2008.*

[7] Battré, D.; Hovestadt, M.; Kao, O.; Keller, A. and Voss, K.: Implementation of Virtual Execution Environments for improving SLA-compliant Job Migration in Grids, *Proceedings of the IEEE International Conference on Services Computing (SCC 2008), p.47-52, IEEE Computer Society, 2008.*

[8] Battré, D.; Hovestadt, M.; Keller, A.; Kao, O. and Voss, K.: Virtual Execution Environments and the Negotiation of Service Level Agreements in Grid Systems. *SVM 2008: 2nd International DMTF Academic Alliance Workshop on Systems and Virtualization Management: Standards and New Technologies, 21-22 October 2008.*

[9] Gourlay, I.; Djemame, K. and Padgett, J.: Evaluating Provider Reliability in Grid Resource Brokering to appear in Proceedings of the 11th IEEE International Conference on High Performance Computing and Communications (HPCC'2009), Seoul, Korea, June 2009.

5.3 Distributed and parallel applications

5.3.1 Electromyography-based Movement Classification

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Mariusz Grad, PC², University of Paderborn
	Dr. Christian Plessl, PC², University of Paderborn
Supported by:	AiF, “Neuartige Prothesenschäfte mit adaptiver Formsteuerung”, “Neuartige adaptive Gelenke für Knie- und Fußprothesen”

General Problem Description

One of the fastest runners on earth has no legs - the South African Oscar Pistorius took gold medals for sprinting at the 2008 Summer Paralympics and even applied for the regular 2008 Summer Olympic Games. Pistorius' success was possible by employing carbon fiber; a modern material to create the prostheses springs. In our project we, together with a further research organization and two industrial partners working towards materials with active behavior combining carbon fiber with Piezo electric elements. Employing these adaptable materials as prostheses' springs and sockets improves prosthesis comfort and allow the amputee a more natural way of using it.

Materials with complex and alterable properties need intelligent control to unveil their potential. In the area of prostheses control for lower limb amputees conventional sensor set up would not gain enough information for robust steering of a complex prosthesis. Here, the evaluation of muscular activity provides prosthesis control information about the intended leg movement and the leg's current state.

In our group, we investigate pattern-matching algorithms for classification of Electromyography Signals (EMG). Along with conventional classification approaches as the k-th Nearest Neighbor (kNN), Support Vector Machines (SVM) and Artificial Neuronal Networks (ANN), we explore hardware based classification architectures, as they are natively power-efficient and incrementally re-learnable, matching the embedded systems context of an adaptable prostheses controller closely.

Problem Details and Work Done

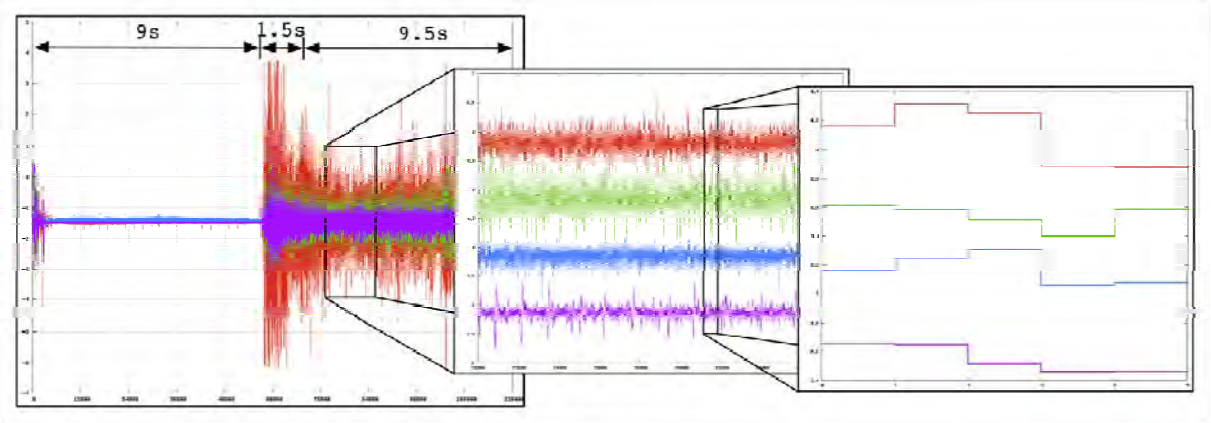


Figure 1 EMG signal recorded by four pairs of skin-attached electrodes.

We use electromyography-based movement classification for two distinct goals: first, the control of a prosthesis socket that can change it's shape to fit amputees stump and muscle tension contours during regular walking or stairs climbing, and second, the control of knee and foot prostheses joints, connected by materials with alterable mechanical properties as e.g. the spring stiffness. To do this, we model the desired controller behavior in the time domain, partition it into phases and assign for every phase classification goals covering the detection of the phase itself, amputees movement selection and emergency situations. In our the current work we concentrate on a robust classification of EMG signals. Our signal processing chain essentially consists of two algorithmic steps: signal's data reduction by extraction of the signal's specific attributes, also called features, and the recognition of signal's features by means of a pattern matching algorithm.

Figure 1 shows a typical shape for muscular activity recorded by four pairs of skin-attached electrodes on a forearm. In the first step the preprocessing algorithms remove the DC offset and rectify the signal. In the second step the feature extraction is done by calculating multiple moving averages for about 300 milliseconds on the data. This is depicted in Figure 2.

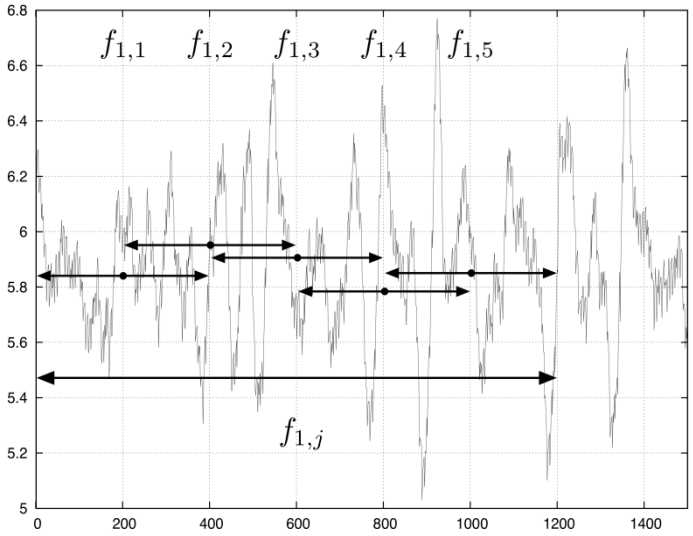


Figure 2 Feature extraction: Moving average filters reduce the amount of data.

The feature extraction is repeated up to 100 times per seconds on updated signal's data for continuous prosthesis control. With this the signal preprocessing is finished and a subsequent pattern-matching algorithm decides to which movement a feature correspond.

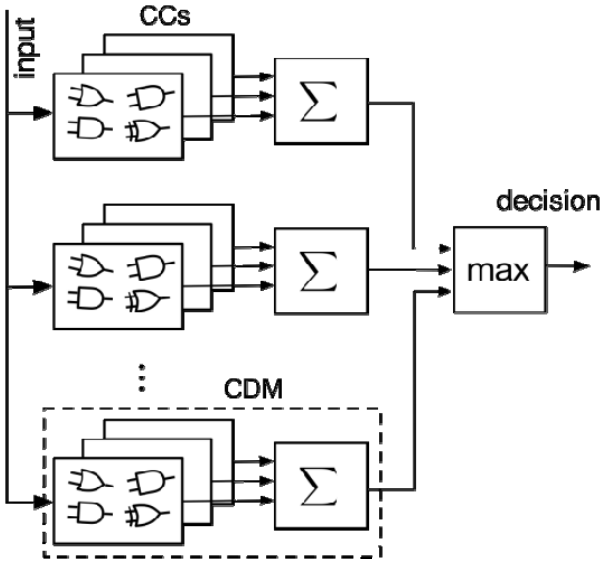


Figure 3 Hardware-based pattern matching architecture. Each Category Detection Module (CDM) contains multiple category classifiers (CC). A CC decides to which category the input data corresponds. Category with the most activated CCs defines the pattern matcher output.

We have developed a pattern matching architecture based on reconfigurable hardware targeting low-power operation mode and adaptability. The structure is presented in Figure 3. Multiple category detectors are combined in a single Category Detection Module (CDM). The goal of a category detector is to decide whether the input data correspond to its category. All CDMs sum positive responses, and the category with the most activated category detectors define the classifier's decision.

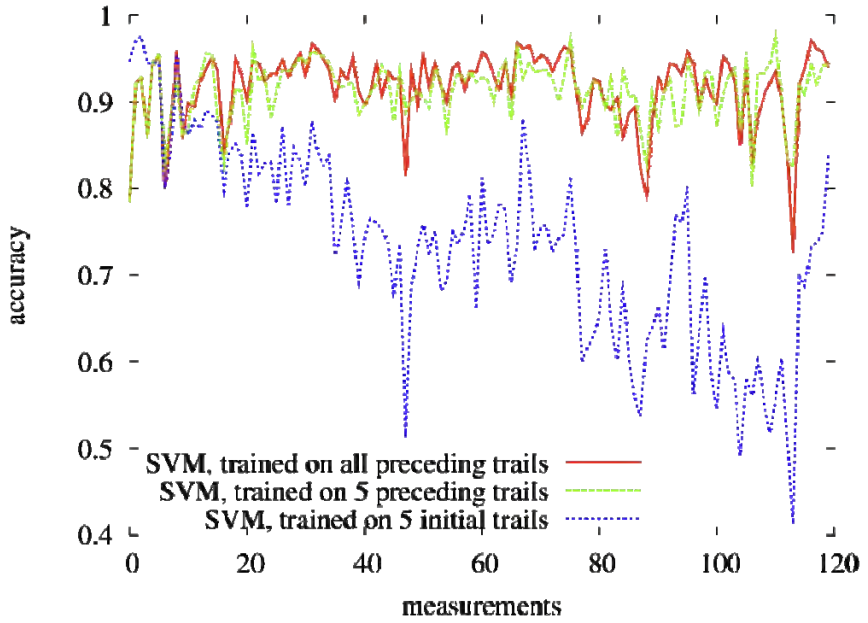


Figure 4 Classification accuracy degrades when a pattern-matching algorithm is not retrained. During a single day five to six trials were recorded. A classification algorithm was trained with the data from the i) first five trials, ii) last five trials, and iii) all preceding trials. Te accuracy for the latter two cases differs insignificantly. Support vector machines were used to perform the experiment.

Classifier adaptability is essential to the area of EMG classification as the classification accuracy degrades over time. Figure 4 shows the behavior for a SVM classifier trained initially on the data of the first day and verified with the data on the remaining 20 day, trained with data from day 1...i and verified with data of day i+1 and trained with data of the previous day and verified with data of the following day. Without continuously retraining, the classification performance drops significantly. Thus, to maintain precise classification, the EMG classifier has to be retrained periodically.

References

[1] Boschmann, A.; Kaufmann, P.; Platzner, M. and Winkler, M.: Towards Multi-movement Hand Prostheses: Combining Adaptive Classification with High Precision Sockets. In *Proceedings of the 2nd Technically Assisted Rehabilitation (TAR'09)*, Berlin, Germany, 2009.

[2] Glette, K.; Torresen, J.; Kaufmann, P. and Platzner, M.: A Comparison of Evolvable Hardware Architectures for Classification Tasks. In *Proceedings of the 8th International Conference on Evolvable Systems: From Biology to Hardware (ICES)*, LNCS. Springer, September 2008.

[3] Glette, K.; Torresen, J.; Gruber, T., Sick, B.; Kaufmann, P. and Platzner, M.: Comparing Evolvable Hardware to Conventional Classifiers for Electromyographic Prosthetic Hand Control. In *Proceedings of the NASA/ESA Conference on Adaptive Hardware and Systems (AHS)*, Noordwijk, The Netherlands, June 2008. Won Best Paper Award in the 'Evolvable Hardware' Category

5.3.2 Medical Image Reconstruction

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Tobias Beisel, PC², University of Paderborn
	Dr. Stefan Lietsch, PC², University of Paderborn

General Problem Description

Current internal medicine uses to a great extend non-invasive methods to examine, classify and treat disease patterns before applying surgical procedures. One major area of application is computed tomography with its different modalities. Computed Tomography (CT) and Positron Emission Tomography (PET) are important instances of the used techniques. Figure 1 shows examples of CT and PET scanners. PET scanners are much bigger, more expensive and the technology used is also more sophisticated compared to the 3-dimensional X-ray technology of the CT scanner.

(a) (b)

Figure 1: A PET (a) and a CT (b) scanner

Image reconstruction uses the information from a series of 2D images measured by the scanners and the geometry of those, to reconstruct 3D images displaying the measured area of interest of the patient by using complex statistical methods.

These algorithms suffer from a long runtime based on enormous amounts of data and mostly complex algorithms to be applied on the data. The resulting time

expense is not only burdening for the patient, but also comes with a reduced cost efficiency for the medical institute. The PC² aims on finding customized solutions to accelerate the algorithms without reducing the quality of their results. The main approach followed is to parallelize the algorithms using different current and new parallelization techniques on diverse modern hardware. The hardware used for this purpose is aimed to be optimally suited to the problem domain. Thus, different parallel architectures are incorporated for speeding up the reconstruction. These architectures especially include current Many-Core architectures, a cluster system and modern Graphic Processor Units (GPUs).

Problem Details and Work Done

To approach the problem of image reconstruction one has to understand the fundamentals of the underlying technology and the algorithms used. While the measurement technologies and the algorithms of the different modalities differ in detail, the principle problem domain is the same.

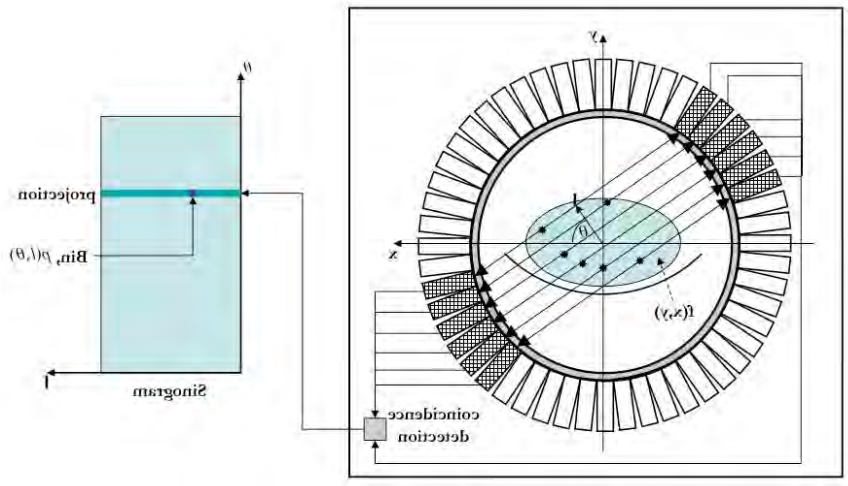


Figure 2: Schematic setup of a PET measurement

Figure 2 shows the schematic setup of a PET scanner and the measurement process. A tracer is used to produce chemical reactions at tumor-infected cells of the patient. In case of such an event, an annihilation of two photons occurs, where the photons veer away from each other in about 180°. These are measured by the detector ring at the edge of the scanner and combined to coincidences. The line between the detectors of a coincidence, called Line-of-Response (LOR), gives the only information about where the event has originally occurred. Thus, the exact place is unknown. The events are counted in sinograms, where each entry (called Bin) represents the count of events on a specific LOR. Each sinogram again

represents one slice of the measured region. The combination of those 2-dimensional (2D) slices finally represents the complete measurements of the 3-dimensional (3D) body.

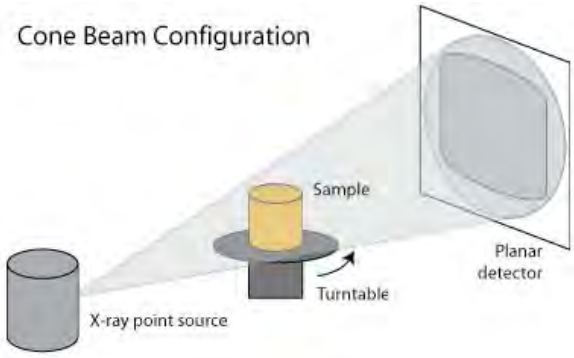


Figure 3: Schematic setup of a Cone-Beam CT measurement

Cone Beam CT (CBCT) is an enhancement of the conventional medical CT. Figure 3 shows a schematic image of its general functioning. Instead of a set of x-ray measurements from different angles, one beam in shape of a cone is made, such that a larger part of the body can be measured with pulsed beams. That way the exposure by gammarays can be reduced up to 90%. Instead of single detectors, a sensitive planar detector absorbing the beams is used for the measurement. The measurement as well as the reconstruction is faster using this method. The mathematical model is slightly different, as a deformation is inserted by the point-source measurement.

In both PET and the CT the measured body is transformed from an n-dimensional measurement space to a series of (n-1)-dimensional measurements by projections of the scanner. These so-called forward-projections have to be inverted to calculate the original 3D representation of the body. Two classes of algorithms solve this problem: analytic and algebraic reconstruction methods.

Analytic Reconstruction Methods

Analytic methods solve the problem by doing a single back-projection by inverting the forward-projection. The best-known algorithm is the Inverse Radon Transformation and its various modifications. They all use line integrals to calculate the original image from the measured projections. To reduce noise and correct distortions a filter step is succeeded. The so-called Filtered Back Projection (FBP) is the standard implementation of this approach and still often used in clinical environment. While it is fast, it leads to artifacts in the resulting image using PET.

Algebraic Reconstruction Methods

Algebraic methods in contrast deliver far better image quality as they are insensitive to noise, but suffer from a long runtime. This is based on the iterative approach, which uses a series of forward- and back-projections to incrementally update and improve the image estimates. Starting with an initial estimate, a forward projection of this image is compared to the real measurements and a back-projection step is incorporating the found differences afterwards to achieve a better estimate. This is repeated until the updates are insignificantly small or the algorithm exceeds a certain number of iterations. These methods are based on statistical methods using the Expectation Maximization - Maximum Likelihood (EM-ML) method, which result in complex computations in each iteration.

Both methods have to handle big amounts of data and thus need a lot of memory during the calculation. In addition it demands a considerable time to complete the reconstruction, which can need up to hours.

Speeding up the Image Reconstruction

Parallel implementations of both the PET reconstruction and the Cone-Beam CT reconstruction were approached from existing sequential algorithms. For PET the STIR [1] package was used, which is well known in the PET community. It includes as well a FBP and an EM-ML based algorithm called OSMAPOSL. The FPB was parallelized using the OpenMP API for multi-core platforms. Despite the already very fast algorithm, a speedup of up to 2.4 was achieved on an 8-Core system.

The OSMAPOSL algorithm was parallelized using MPI, so it was capable to be used on cluster systems. Depending on the amount of data, a speedup of about 8 was achieved on up to 20 cluster nodes.

Considering the acquisition costs for a medical institution, an affordable system was aspired and tested using an 8-Core Intel Clovertown system. The same implementation was tested on this system and achieved Speedups of up to 3.3. Although these are less compared to the cluster, the overall runtime much shorter, i.e. by a factor of 10. [2]

For Cone-Beam CT the implementation was based on the “Image Reconstruction Toolkit”, a set of MATLAB algorithms provided by J. A. Fessler of the University of Michigan [3]. The toolkit, amongst other algorithms, implements the OS-SPS (Ordered Subsets – Separable Paraboloidal Surrogate) algorithm, which is a new approach of making the iterative reconstruction more accessible for parallel execution by resolving dependencies among the image pixels given in the original EM-ML approach.

In a first step of accelerating this algorithm, the implementation was ported to a NVIDIA GPU using the CUDA Framework [4] and MEX-files [5], which provide functions to interface C, C++ or Fortran functions to MATLAB. This connects the simple algorithm design of MATLAB with the computational power of parallel

architectures. CUDA was chosen to utilize the SIMD model of the GPUs, which maps very well to the data-intensive computations of medical algorithms. First results show a speedup, which is superior to a provided Pthreads implementation [6]. The results are subject to verification.
Generally these results are limited by the iterative approach of the algorithms and the big amount of data communicated between the processing units, such that reasonable handling of data is very important.

Resource Usage

This project uses resources of the Arminius cluster system and the Clovertown test systems for MPI and thread/OpenMP based parallelization of medical image reconstruction. In addition an Intel Workstation was equipped with the most current NVIDIA Geforce GTX 295 GPU as a test system for the CT image reconstruction.

References

[1] Thielemans, K.: et. al., STIR: Software for Tomographic Image Reconstruction Release 2 Proc. IEEE Medical Imaging Conference 2006, San Diego, CA.
[2] Beisel, T.; Lietsch, S.; Thielemans, K.: A method for OSEM PET reconstruction on parallel architectures using STIR, Medical Imaging Conf., 2008
[3] Ahn, S.; Fessler, J.A.: Globally convergent image reconstruction for emission tomography using relaxed ordered subsets algorithms, IEEE Trans. Med. Imag., vol. 22, no. 5, pp. 616619, May 2003
[4] NVIDIA CUDA - Compute Unified Device Architecture, Website: http://www.nvidia.com/object/cuda_home.html#
[5] The MathWorks – MEX-files Guide, Websitehttp://www.mathworks.com/support/tech-notes/1600/1605.html?BB=1
[6] Groppe, D.: GPU-basierte Beschleunigung neuer Bildrekonstruktions-algorithmen in der Tomographie aus MATLAB, Master Thesis, PC², 2009

5.3.3 Medical Image Processing

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Tobias Beisel, PC², University of Paderborn
Supported by:	Zentrales Innovationsprogramm Mittelstand (ZIM)

General Problem Description

Magnet Resonance Imaging (MRI) is an important part of current internal medicine, allowing non-invasive examinations to diagnose and treat medical conditions. It is especially used to identify and classify cancer and tumors before applying surgical procedures.

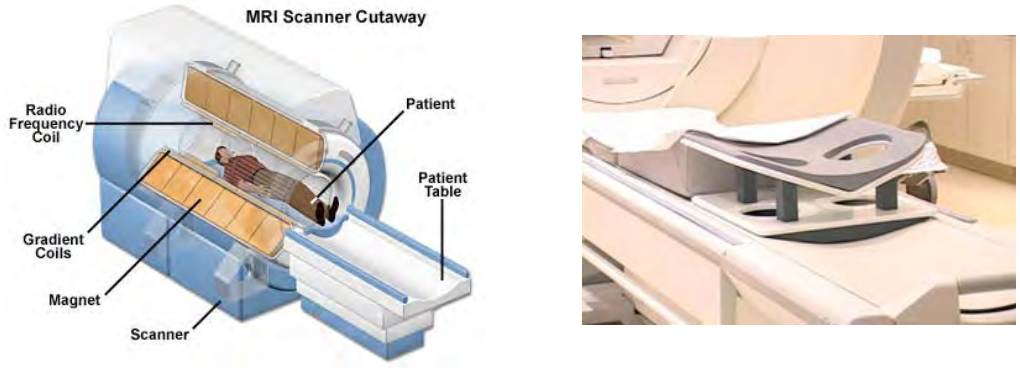


Figure 1: Setup of a MRI system, breast MRI attachment

MRI uses a powerful magnetic field and radio frequency during the measurement and a computer to reconstruct detailed images of bones, soft tissues and organs from the measurements. Figure 1 shows the general setup of an MRI scanner.

Passing an electric current through the wire loops surrounding the patient creates a strong magnetic field. In the meantime, the radio frequency coils in the magnet send and receive radio waves. This triggers protons in the body to align themselves. Once aligned, radio waves are absorbed by the protons, which stimulate spinning. Energy is released after exciting the molecules, which then emit energy signals that are picked up by the coil. This information is sent to a computer processing all the signals and generating an image. The final product is a 3-dimensional image representation of the area being examined. Unlike Computed Tomography (CT) scanning or general x-ray studies, no ionizing radiation is involved with an MRI.

One major field of application is the breast cancer and tumor detection using an attachment to the scanner as shown in Figure 1. An example outcome can be seen in Figure 2, where a cancer can be seen in the upper half of the right breast (white area).

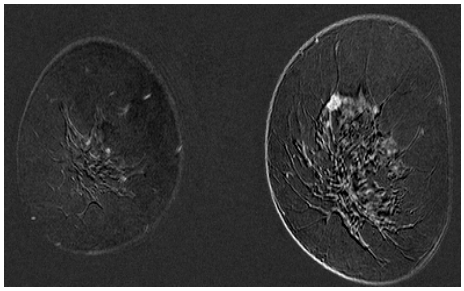


Figure 2: Resulting image of a breast MRI examination

Subsequent to the measurement a tool-flow of different image processing algorithms is used to support the radiologists identifying and rating tumor and cancer cells. These include image registration, image segmentation and different methods of feature extraction and classification. The registration aims on matching a series of 3D images measured over time into each other, such that they can be used as a single image for diagnosis purposes. The segmentation additionally extracts special regions of interest from the images, such that irrelevant information is deleted. This e.g. might emphasize the tumor regions or the organs affected. Classification then finally uses feature extraction algorithms to analyze the images based on special medical knowledge about how tumor or cancer regions are natured.

All of these algorithms work on large amounts of data and experience a long runtime based on complex algorithms. The time waiting on the results is burdening for the patient and comes with a reduced cost efficiency for the medical institute. The CADMEI GmbH [1] and the PC² aim on developing new algorithms and finding customized solutions to accelerate the application. The main approach followed is to parallelize the algorithms using different current and new parallelization techniques on diverse parallel hardware. The hardware used for this purpose is aimed to be suited best possible to the set of algorithms. Thus, a combination of different parallel architectures is incorporated for speeding up the complete toolflow. These architectures especially include current Many-Core architectures and Graphic Processor Units (GPUs), but also more specialized and less common hardware like Field Programmable Gate Arrays (FPGAs) and other co-processors like ClearSpeed accelerators.

Problem Details and Work Done

The aforementioned algorithms are designed, developed and accelerated in a ZIM [2] funded cooperation between the PC² and the CADMEI GmbH. The project is funded for 2 years and started in July 2009. The goal of the project is to develop a fast and fully automatic diagnosis tool for female breast cancer detection using MRI. The system shall implement the complete tool-flow needed to evaluate already reconstructed images for a fully qualified diagnosis. Systems exist, which demand a high level of interaction with the radiologist and deliver only low-level computer aided detection methods. Possibly replacing a second radiologist demands high quality of results. The system approached in this project will have algorithms of high-level knowledge representation like automatic segmentation and thus will enable automatic morphological rating of tracer accumulations. The fundamentals of an existing prototype are described in [3].

In addition it is in the interest of the patient and the medic to have the examination findings available as soon as possible. Thus acceleration using parallel architectures is aspired. While the CADMEI GmbH is involved in algorithm and framework development of the diagnosis system based on medical knowledge, the role of the PC² is to consult the CADMEI GmbH during the algorithm development by the design of data structures, which map very well on parallel architectures. Moreover, the PC² will accelerate the developed algorithms on appropriate architectures and design a hardware product setup, which will be optimized in terms of cost-benefit ratio.

Image Registration

In most cases an MRI examination delivers a series of images over time. To use the overall information of these images, they have to be combined to a single image, before further analysis can be done. Different so-called registration algorithms solve this requirement, but only very few solutions are available which support 3-dimensional registration. We aim on developing a 3D registration algorithm that shall be capable of being extended for the use of multi-modal registration. The intended algorithm used is a 3D extended version of the KLT Feature Tracker [4].

Feature Tracking is one of the fundamental operations in image processing. Tracking algorithms were originally developed to track features in movie sequences. Features are recognizable characteristics of the images, typically corner-like structures. Surveys have been made about what features are used best [5]. As movie sequences at bottom are a series of images, this technique can be transferred to the medical image registration. Extracting and tracking features from a series MRI images gives sufficient information about how subsequent images are situated to each other, such that they can be morphed into each other by translation vectors. Figure 3 shows an example of a tracking algorithm applied to ultrasound images.

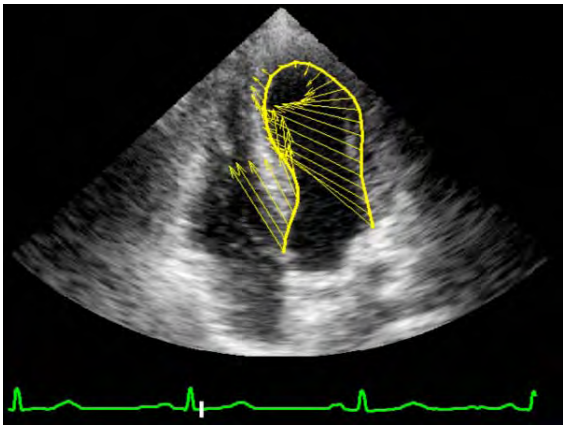


Figure 3: Vector-based result of a feature tracking algorithm (ultrasound)

Parallelization is possible on different levels of abstraction. The Feature Extraction is done on a pixel-basis and thus may be done independently for each of the pixels. Each feature afterwards could be tracked in parallel and also the morphing of the images can be done in parallel. The algorithms used have to be well thought-out, as the images used are very large and need to be shared among all parallel processes. Special memory management and data structures are needed for this purpose. The algorithm is currently ported to GPUs and Multi-Core architectures.

Image Segmentation

Using the registered images, the segmentation detects the regions of which are most probably cancer or tumor regions. Those regions are detected by the color value of each voxels. The voxels with highest values are presumed to be situated in malicious regions. The most common segmentation algorithms use these voxels are starting points for region growing methods. These let the detected regions grow until the voxel values fall below a certain threshold. Choosing this threshold carefully is essential for good results. This is trained by learning algorithms using examples with well-known results. Figure 4 gives an example of segmented regions in the brain of the patient.

In this part of the project a new algorithm shall be developed which is based on complex mathematical calculations.[1] This new approach requires new techniques of acceleration and is intended to be implemented on a FPGA.

[1] The approach is subject to non-disclosure-agreements and can not be described in detail

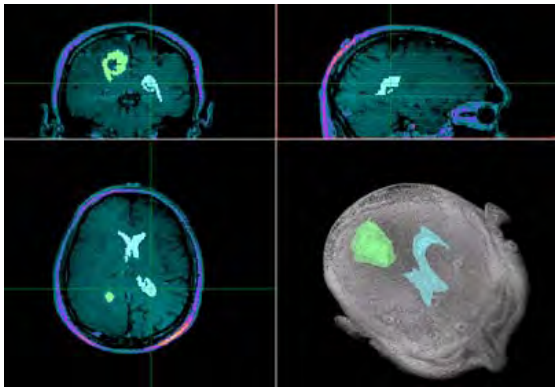


Figure 4: Segmented brain tumor regions

Feature Extraction and Classification

Classification algorithms predict the dignity of the segmented objects, rating if they are good-natured or malicious. Also, false-positive extracted objects have to be eliminated. The algorithms used are standard algorithms, which do not have to be accelerated.

Feature extraction algorithms play a major role preparing the classification, delivering a characterization of segmented objects that allow a rating of suspicious regions. Feature extraction is based on a list of feature descriptions, which can be extracted by image processing algorithms independent of the image quality. The descriptions specify well-known medical characteristics of malicious cells. The runtime of this step is depending on the number of segmented objects and the length of the feature list. The better the intended result, the longer is the list of features and the longer is the needed runtime. Thus, a parallel processing of the completely independent segmented objects can result in a great benefit regarding the total runtime.

As the same extraction algorithms have to be applied independently to different parts of the images, the algorithm is perfectly suited for a GPU implementation using a fallback Multi-Core approach if only few suspicious regions have to be examined.

Resource Usage

Within this project a set of different current accelerator technologies is used. A current NVIDIA GeForce GTX 295 GPU and a ClearSpeed e710 board are combined in an 8-core Workstation.

References

[1] CADMEI – Software für Medizinsysteme GmbH, Website: www.cadmei.com
[2] Zentrales Innovationsprogramm Mittelstand, Website: http://www.zim-bmwi.de
[3] Vomweg, T.W., Mayer, D.; Maciak, A.; Rösler, T. and Mattiuzzi, M.: CADMRM A full automatic Breast Cancer Diagnosis Tool in CE MRM and Image Processing, Framework for Construction of CAD System, in ECR, 2008
[4] Tomasi, C. and Kanade, T.: Detection and Tracking of Point Features, in CMU Techreport, 1991
[5] Shi, J. and Tomasi, C.: Good features to track, in Proceedings of Computer Vision and Pattern Recognition, IEEE, 1994

5.3.4 Hardware Accelerated Monte-Carlo Game Tree Search

Project coordinator	Prof. Dr. Marco Platzner, University of Paderborn
Project members	Dr. habil. Ulf Lorenz, University of Darmstadt
	Lars Schäfers, PC², University of Paderborn
Supported by:	Microsoft Research, Cambridge

General Problem Description

As the world's best chess players are computers since some years ago, computer scientists are now faced with the next challenge which is the ancient asian board game called Go (chin.: wéiqí, kor.: baduk) [1]. Computing the best, or at least a good move to a given board position for the game of Go is in the focus of researchers working on artificial intelligence since many years. While applying the same algorithms and ideas that were used for the chess game showed only little success, a monte-carlo based approach brought great improvements in the past few years [2]. The best computer-go programs have recently reached a good amateur playing strength.

In the game of Go the number of possible moves a player can select from is very large compared to the playable moves in the chess game. Furthermore there are no good policies known to diminish the number of moves in a save way by classifying for example senseless or clearly bad moves. As a result of this we need to explore a very large game tree to compute a good follow up move to a given game situation. In a monte-carlo based approach only single paths of the whole tree get explored and statistics about the outcomes are collected at tree nodes close to the root. We call this exploration of a single path from the root node to a leaf node of the game tree a monte-carlo sample. The accuracy of the statistics and so the accuracy of the whole procedure increases with the number of samples collected.

Problem Details and Work Done

In the “Gomputer” project we aim to use special purpose hardware as FPGAs (Field Programmable Gate Arrays) and GPGPUs (General Purpose Graphic Processing Unit) to accelerate the monte-carlo sample computation, thus exploit fine grained parallelism. On a higher level we intend to use multi-core systems in a compute cluster to distribute the whole search. As increasing the number of monte carlo samples is one hand, investigations concerning the sample quality need to be made

on the other hand. Therefore the analysis and development of machine learning algorithms to extract game specific knowledge from professional game records that can be used during the sample generation thereafter becomes an important task.

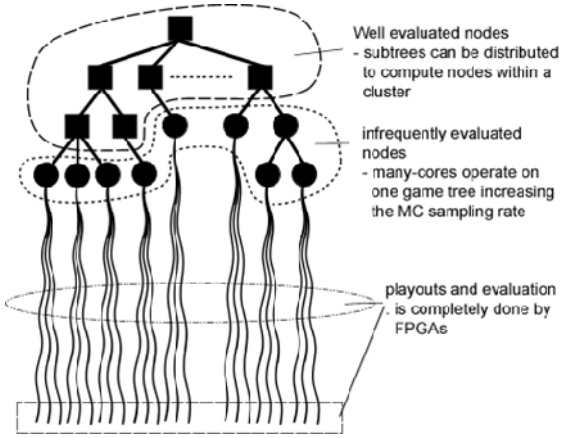


Figure 1: A possible monte-carlo game tree representation

Based on experiences collected during a project group and a master thesis[3] at PC², a Go playing program was implemented that can make use of a multi-core system. Furthermore first attempts were made to compute monte-carlo samples on a FPGA and a GPGPU. The program is able to extract several kinds of Go knowledge from a set of game records. Altogether it is able to compete with the currently top rated Go programs on small board size (i.e. 9x9).

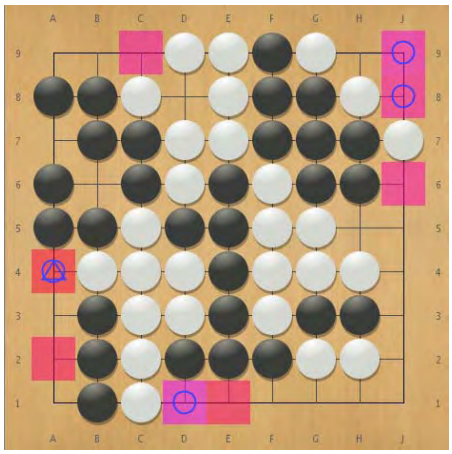


Figure 2: Screenshot showing a Go board with score estimates (in form of colors) for some possible follow-up moves computed by our Go program.

Resource Usage

The monte-carlo tree search algorithm itself, but also the incorporation of automatically learned knowledge has several parameters that need to be tuned. As it is difficult to derive parameter settings solely through theoretical assumptions, a huge number of games were run to determine good parameter values empirically. To overcome the computational needs we used nodes of the ARMINIUS cluster [4] to run the games. No communication between the nodes was necessary for this task.

Currently research is done concerning the parallelization of the tree search on shared memory systems. The SMP Compute Server [5] located at the PC² is ideally suited for this task and therefore used to carry out performance experiments.

References

[1] see http://www.intergofed.org/ (website of The International Go Federation)
[2] "Modification of UCT with Patterns in Monte-Carlo Go", S. Gelly et al., Technical Report 6062, INRIA, 2006.
[3] Schäfers, L.: “Analyse neuer Spielbaumsuchverfahren, wie sie im Computer Go angewendet werden”, Master Thesis at University of Paderborn, 2008
[4] The ARMINIUS Cluster at PC²: http://pc2.uni-paderborn.de/hpc-systems-services/available-systems/arminius-cluster/
[5] The SMP Server at PC²: http://pc2.uni-paderborn.de/hpc-systems-services/available-systems/smp-server/

5.4 Testbeds and Benchmarking

5.4.1 System Evaluation, Benchmarking and Operation of Experimental Cluster Systems

Project coordinator	Dr. Jens Simon, PC², University of Paderborn
Project members	Axel Keller, PC², University of Paderborn
	Andreas Krawinkel, PC², University of Paderborn
	Holger Nitsche, PC², University of Paderborn
Supported by:	Fujitsu Technology Solutions
	ict AG

General Problem Description

In the year 2009, the PC² has installed an InfiniBand connected cluster system for the research groups of the theoretical physics of the University of Paderborn. The system consists of 57 compute nodes with 456 processor cores and 1560 GByte of main memory. A Network Attached Storage (NAS) system is connected with 1-Gigabit-Ethernet to all nodes of the cluster. The capacity of harddisks of the NAS is 48 TByte. Emerging technologies, computer systems, interconnects, and software systems have been evaluated by the PC² in the selection phase of the cluster system and further evaluations are done for the next generation systems. Besides system evaluation and benchmarking of new cluster technologies, different experimental or special purpose cluster systems are operated for research groups of the University of Paderborn.

Problem Details and Work Done

Different computer systems and cluster technologies have been evaluated. The tested systems are up-to date two sockets Intel Xeon systems with dual- and quad-core processors, two and four sockets AMD Opteron with dual- and quad-, and hexa-core processors, and some special purpose computer systems with reconfigurable hardware. These systems were equipped with different configurations of high-speed interconnects (InfiniBand single, double, and quad data rate, MyriNet 10G, and Gigabit Ethernet) and different operating systems of Linux and the Microsoft operating system Windows HPC Server 2008. All benchmarking results are published on the web sides of the Paderborn Benchmarking Center (1).

Co-Operations: The PC² benchmarking center is also doing system evaluation and benchmarking for external companies and organizations. The PC² has a long-term co-operation with Fujitsu-Siemens Computers where Paderborn acts as a Competence Center for High Performance Computing. System benchmarking is also done for the companies ict AG and christmann informationstechnik + medien.

Company	Provided Equipment
ict AG	Loan equipment 4 two sockets quad-core Xeon systems 7/09 - 9/09
BlueArc	NAS Titan T2200, 30TByte 08/09 – 09/09
NetApp	NAS FAS 3170, 8TByte 08/09 – 09/09
Isilon	NAS IQ 9000, 27 TByte 08/09 – 10/09

References

[1] Simon, J.: PC² Benchmarking Center, http://wwwcs.uni-paderborn.de/pc2/about-us/staff/jens-simons-pages/benchmarkingcenter.html

5.4.2 Onelab2: OneLab Extensions Towards Routing-in-a-Slice

Project coordinator	Prof. Dr. Holger Karl, PC², University of Paderborn
Project members	Jens Lischka, PC², University of Paderborn
Supported by:	7th Framework of the European Commission

General Problem Description

Alongside networking research, experimentally-driven research is key to success in exploring the possible futures of the Internet. In PlanetLab Europe, the OneLab project provides an open, general-purpose, and shared experimental facility, both large-scale and sustainable, which will allow European industry and academia to innovate today and assess the performance of their solutions.

The second phase of the OneLab project, OneLab2, builds on the original OneLab project's foundations, continuing work on the PlanetLab Europe testbed, increasing its international visibility and extending it in both functionality and scale.

PlanetLab was originally built to develop new technologies for distributed storage, network mapping, peer-to-peer systems, distributed hash tables, and query processing. To do so researchers built their own overlay network topologies in user space. There was no need for direct Layer2 access or for the creation of Layer2 topologies. As a consequence the evaluation and testing of new, IP-independent routing protocols (e.g. data centric networking, pub/sub systems) on PlanetLab nodes is a problem, as it is not possible for a process running in PlanetLab to distinguish between different incoming interfaces or to determine which outgoing interface to use -- the very core function of a router cannot be emulated. The cause of this problem is PlanetLab's network virtualization design.
Routing-in-a-slice (RiaS) tries to overcome this problem by the application of new network virtualisation techniques on the PlanetLab Europe infrastructure. The objective is to offer researchers a convenient tool for building their own, custom, virtual Layer2 topologies on PlanetLab Europe, upon which it becomes meaningful to execute lower-level routing and forwarding experiments.

Problem Details and Work Done

Layer2 topology creation on PlanetLab nodes has to deal with three main issues:

1. Network Virtualisation,
2. Virtual Network Mapping (VNM), and
3. Monitoring.

Network virtualisation is necessary to realize to run many virtual networks with different topologies, each of them running its own protocol, routing software etc., upon the same network infrastructure simultaneously without affecting each other. Currently it is impossible to create topologies that behave as if they were actual Layer2 topologies on the current PlanetLab platform.

Another aspect of virtual topology creation is the Virtual Network Mapping problem. Once a researcher has defined his custom virtual network topology in a *Network Topology Description File*, the components (virtual nodes and links) have to be mapped onto the physical nodes and links (or possibly even paths) of the underlying infrastructure. This task is called *virtual network mapping (VNM)* or Resource Mapping. This job is done by the *VN Mapper*.

In contrast to existing Resource Allocation approaches like SWORD [1] or NetFinder [2] our RiaS system not only chooses a set of appropriate nodes that satisfy the researchers needs but is also able to create the desired topology.

Finally, monitoring is needed to feed the VN Mapper with a proper description of the available resources (e.g. CPU for nodes and data rate for links) of the physical network. This information can be collected inside a central database; in a later implementation, it need not be centralized but can also be distributed.

RiaS Architecture

Figure 1 depicts how the components of our RiaS system work together. A central database holds information about the available resources of the PlanetLab Europe network and creates the physical network topology description. This physical network information is accessible to the VN Mapper, either upon request or by periodic updates.

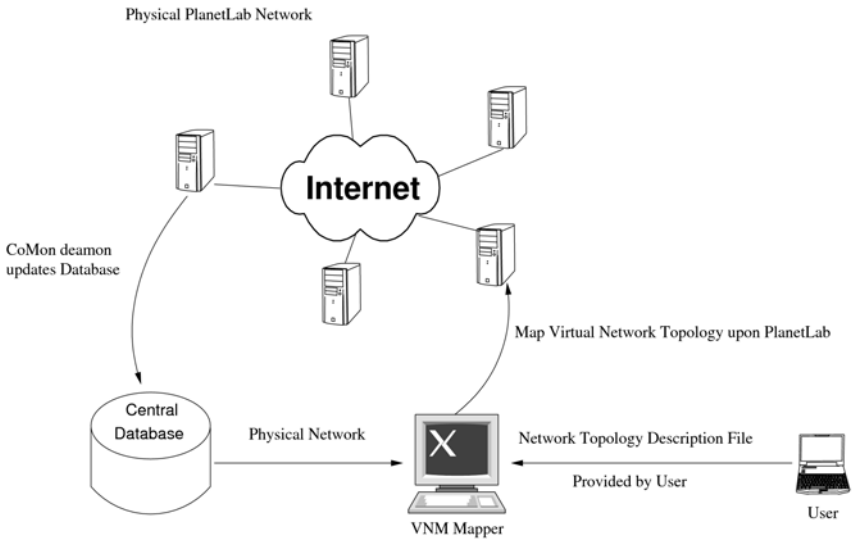


Figure 1 RiaS Architecture

A researcher who wants to reserve a slice to run a network experiment sends a description of his custom network topology, a so called *virtual network requests (VNR)*, to the VN Mapper. The VN Mapper then tries to allocate the necessary PlanetLab resources and configures the topology. Finally, the researcher is informed when and where his slice is available and can login to the nodes of the requested topology to run his tests.

Extension Requirements

Our objective is to enable PlanetLab to be used as evaluation and test platform for new routing protocols that do not rely on IP. In addition researchers should be able to run their existing routing software and protocols on PlanetLab without the need to modify them. To achieve this routing functionality we must be able to create and configure multiple network interfaces inside PlanetLab slices.

In the following section we provide answers to the questions how the network virtualisation on PlanetLab currently works, what kind of problems arise related to routing-in-a-slice, and how we can fix this.

Network Virtualisation

PlanetLab uses the Linux VServer technology [3] for host virtualization. Linux VServer is a container-based virtualization approach which allows several virtual Linux hosts to run simultaneously on a single, shared kernel; no virtual host has direct access to the hardware. A set of such virtual hosts working together forms a PlanetLab slice. This concept allows to share the hardware resources of PlanetLab nodes among a large number of PlanetLab slices simultaneously in a very efficient way.

This container-based virtualisation design has also a disadvantage. All VServer virtual hosts share the same kernel and also share the same network stack. The issue is that routing experiments have to manipulate the central routing table and that such a routing table manipulation would affect all other experiments running on this PlanetLab node since they all share the same kernel and in particular the same network stack.
Suppose one Planetlab slice wants to change his default route in the routing table. This would change the default route for all remaining PlanetLab slices on this particular node since they all use the same routing table, leading to great chaos. As another example, suppose a user wants to add a virtual network interface. This interface would be visible and configurable by all other slices on this PlanetLab node since it is added to the shared stack which is accessible by all slices.
PlanetLab solves this problem by a very restrictive VServer network configuration setting. The VServers on PlanetLab nodes are configured in such a manner that the user owns no rights to change/add routing table entries or to configure/add new NICs or tunnels. This makes it hard for researchers to build their own topologies on PlanetLab. In particular it is impossible to build Layer2 topologies.
Currently the network virtualisation on PlanetLab is done by *PlanetLab Virtualised Network Access (VNET) [4]*. VNET relies on *Connection Tracking* which is part of Linux's *Netfilter* system [5]. VNET associates every inbound packet with a connection structure which ensures that slices send and receive only packets associated with connections that they own. A connection structure mainly consists of source and destination IP address, source and destination port number, and an exchange ID (XID). Each time a connection is established such a structure is inserted into a connection table. The kernel now knows the connections of a particular slice and drops packets from other slices. Note that the distinction between connections on a PlanetLab node is actually done by port numbers and XID since all slices on a PlanetLab node share the same IP address. One major drawback with respect to our objectives is that VNET can only support the IP protocols TCP, UDP, ICMP, GRE and PPTP.
Although there exists a possibility to create packet sockets in VNET, called *Safe Raw Sockets*, their protocol family attribute must be set to PF-INET and thus their use is restricted to the IP protocol family and so there is no Layer2 access possible. This is a major problem for testing new IP-independent routing protocols or software on PlanetLab.
Thus, to create Layer2 topologies we have to make some changes to the virtualisation techniques that are currently in use. To overcome the problem RiaS makes use of container-based virtualisation approach extended by *Network Namespaces (NetNS) [6].* Network namespaces allow to assign a private set of network resources to one or several processes. These have their own set of network devices, IP addresses, routes, sockets, and so on. Other processes outside the namespace cannot access these network resources.

Using network namespaces on PlanetLab would require some changes to the PlanetLab kernel to integrate the NetNS patch set and run each VServer with its own network namespace, but it would not conflict with PlanetLab's container-based design philosophy and is therefore much better to migrate to PlanetLab compared to full virtualisation.

Virtual Network Mapping

A researcher should be able to associate the resources (nodes and links) of his virtual network topology with various capacity requirements (e.g. CPU, data rate, or delay) which must be satisfied by the underlying physical infrastructure.
Efficiently assigning virtual network resources to physical resources (Virtual Network Mapping) satisfying a previously defined set of capacity constraints is no trivial task and can be shown to be NP-complete. In addition to efficiency, a network mapping algorithm has to meet the following requirements:

- Make efficient use of the underlying physical resources such that a large number of virtual networks can be mapped onto the physical resources at the same time.
- Mapping virtual networks of reasonable size (100 - 200 nodes) should not take more than a few seconds.
- Handle dynamically arriving virtual network requests that stay in the network for an arbitrary time before departing.
- Handle admission control. Since the physical resources are limited, some virtual network requests have to be rejected or postponed to avoid violation of resource guarantees for existing virtual networks.

An existing approach that meets nearly all requirements is described in [7], but our evaluations showed that the algorithm is inefficient for larger network requests (virtual networks with more than 20 nodes). Therefore, we implemented our own virtual network mapping algorithm based on subgraph isomorphism detection which we presented at the VISA 09 workshop in August 2009 [8].

Monitoring

Monitoring the PlanetLab nodes is necessary to provide the VN Mapper with informations about the current resource consumption on the physical network. Currently we obtain node usage informations by periodically polling the *CoMon* [9] daemon on each PlanetLab node.
To measure the data rate, bandwidth and delay between PlanetLab nodes we use the results of the Scalable Sensing Service S^3 project [10] which is already deployed on PlanetLab. S^3 provides web-services based access to data-rate- and latency informations between all pairs of PlanetLab nodes.

References

[1] Oppenheimer, D.; Albrecht, J.; Patterson, D. and Vahdat, A.: Distributed Resource Discovery on PlanetLab with SWORD, In WORLDS, 2004
[2] Zhu, Z. and Ammar, M.: Overlay network assignment in PlanetLab with NetFinder, Technical Report GT-CSS-06-11, 2006
[3] Linux-VServer, http://linux-vserver.org
[4] Huang, M.: VNET: PlanetLab Virtualized Network Access, 2005
[5] Linux Netfilter, http://www.netfilter.org
[6] NetNS, http://lxc.sourceforge.net/network.php
[7] Yu, M.; Yi, Y.; Rexford, J. and Chiang, M.: Rethinking Virtual Network Embedding: Substrate Support for Path Splitting and Migration, SIGCOMM Comput. Commun. Rev., 2008
[8] Lischka, J. and Karl, H.: A virtual network mapping algorithm based on subgraph isomorphism detection, VISA '09: Proceedings of the 1st ACM workshop on Virtualized infrastructure systems and architectures, 2009
[9] Park, K. and Pai, V.: CoMon: a mostly-scalable monitoring system for PlanetLab, SIGOPS Oper. Syst. Rev., 2006
[10] Yalagandula, P.; Sharma, P.; Banerjee, S.; Basu, S. and Lee, S.J.: S3: A scalable Sensing Service for Monitoring Large Networked Systems, INM '06: Proceedings of the 2006 SIGCOMM workshop on Internet network management, 2006

6 User Projects

6.1 Simulation of Iron-Sulfur Proteins

Project coordinator	Prof. Dr. Dominik Marx, Ruhr-University of Bochum
Project members	Dr. N. Nair, Ruhr-University of Bochum
	Dr. E. Schreiner, Ruhr-University of Bochum
Supported by:	DFG (DFG MA 1547/7)

General Problem Description

Proteins containing iron-sulfur prosthetic groups serve a variety of biological roles including catalysis, regulation and electron transfer in photosynthetic and respiratory electron transport chains over the full range of living organisms, encompassing aerobic, anaerobic and photosynthetic bacteria, plants, fungi and animals [1-3]. Most common Fe--S proteins include [2Fe--2S], [3Fe--4S], and [4Fe-4S] centers. Rubredoxin is an exception, since it has only one single iron center which is tetrahedrally coordinated by cysteine residues. Typically, the iron ions are tetrahedrally coordinated by protein cysteinyl side groups with additional coordination to each iron provided by “inorganic” sulfides. But there are also several examples of non-cysteinyl ligands to Fe-S clusters, including histidine ligation to the Fe_2S_2 core (Rieske proteins), coordination by oxygen of serine and aspartate residues or even by a water molecule [1-3].

One of the largest classes of mobile electron carriers in biology is represented by ferredoxins (Fds). In plants, algae or photosynthetic bacteria [2Fe--2S] Fds mediate the transfer of two electrons, in two successive one electron steps, from photosystem I to Ferredoxin-$NADP^+$ oxidoreductase (FNR), which reduces $NADP^+$ to NADPH [4]. For the Fd from the cyanobacterium *Anabaena* PCC7119 the protein structure was obtained in crystal with a resolution of 1.3 and 1.17 for the oxidized and the reduced form, respectively [5]. In the same work the authors found, that depending on the oxidation state two alternative conformations of Cys46 exist, “CO-in” and “CO-out”.

The ability to delocalize electron density over the entire prosthetic group makes Fe-S clusters ideally suited for their primary role in mediating biological electron transport. To understand the physical nature of such clusters, quantum chemical calculations

have been performed to estimate redox potentials, inner-sphere reorganization energies, the influence of valence electron delocalization on the exchange coupling [6] and the correlation of g-tensors with structural parameters [7]. Recently, studies were carried out to account for the influence of the protein environment on the magnetic properties of iron-sulfur clusters, their redox potentials [8] and even possible electron transfer pathways [9]. Most of these investigations were limited to an idealized picture concerning the structure of the iron-sulfur clusters as well as the surrounding protein. However, it has been shown most recently for rubredoxin (Rd) that a molecular description of environmental effects, in particular polarization and fluctuations, is crucial [10]; note that Rd features only a single Fe center and thus no magnetic interactions.

Commonly found [2Fe-2S] clusters in proteins are having antiferromagnetically spin coupled iron-centers. It is therefore a multiconfigurational problem to treat the low-spin state in quantum chemical calculations because many determinants are necessary to represent the low-spin state wavefunction. Though sophisticated quantum-chemical methods can be used to describe the coupled state which, however, suffer from having to take into account both “static” and “dynamic” electron correlation. Computationally this raise a big challenge in terms of system size and in particular for performing molecular dynamics. During the first periods of our project, we have developed a technique, which we call extended broken symmetry (EBS) scheme, in which a two determinant approach is used to estimate the forces and energies of the magnetically coupled in their low-spin (LS) ground state. This new approach employs a projection on estimating the forces and energies by which it is not necessary to access the wavefunction of the LS state; see Refs: [11,12]. In the last year of our project, we have extended this method to study proteins and applied to study the magnetostructural dynamics of [2Fe-2S] anabaena ferredoxin.

Problem Details and Work Done

With a protein structure of very high resolution and a method allowing for molecular dynamics simulation in the antiferromagnetically coupled electronic ground state of binuclear homovalent transition metal clusters it becomes possible to study the behavior of iron-sulfur clusters embedded in a protein matrix. This magnetostructural dynamics was studied by QM/MM MD simulations of *Anabaena* PCC7119 Fd in two different conformations, namely the “CO-in” and the “CO-out” conformations, using the new extended BS approach.

During the initial period of this project a general formula for describing the energy of the low-spin ground state was derived. This is based on the projection of energies of high-spin state and a broken symmetry state. Based on this, the forces on the nuclei

at the projected low-spin state can be easily obtained, thus enabling the dynamics/geometry optimization at the LS ground state, without accessing the complicated wavefunction [11,12]. This method is called extended broken symmetry (EBS).

In the first year of the project, the EBS scheme we have developed, allowed the propagation of an isolated [2Fe-2S] cluster, thus calling for a coupling to force fields to take the protein environment into account. The coupling approach used here is based on the CPMD/Gromos QM/MM interface [13]. Since the LS charge density is not known, it is crucial to obtain all contributions to hierarchical electrostatics consistently with the chosen projection scheme.

We have implemented these procedures in the CPMD/Gromos code and detailed testing has been performed [14]. To use the CPMD/Gromos QMMM code efficiently for transition metal systems, we have also enabled the electrostatic interaction calculation for the Vanderbilt ultra-soft psuedopotentials. The protein model we used for research is based on the oxidized *Anabaena* PCC7119 Fd [5] (pdb: 1qt9, chain B) assuming standard protonation states and solvation with 13265 TIP3P water molecules while retaining the water molecules from the crystal structure and adding 23 Na^+ and 5 Cl^- to establish a neutral system. Protein interactions are described using AMBER94 and the partial charges of the [2Fe-2S] core were determined by Bader analysis of the BS density of $[Fe_2S_2(SH)_4]^{2-}$ in vacuo. The hybrid QM/MM simulations [13] were carried out using the CPMD/Gromos interface within the CPMD program package [13,15], both extended by the EBS scheme. The QM fragment consisted of the [2Fe-2S] cluster core supplemented by the Sγ, Cβ and Hβ atoms of the four cysteinyl ligands; the dangling bonds at Cβ were saturated using capping H atoms constrained to the Cα-Cβ connecting line. The QM fragment was described within spin-unrestricted Kohn-Sham DFT in its plane wave/ pseudopotential formulation [13].

The PBE functional was chosen and the core electrons were taken into account by ultrasoft pseudopotentials at a cutoff of 30 Ry containing additional d-projectors in case of S as well as scalar relativistic corrections and semicore states for Fe [13]. Finite cluster boundary conditions [13] were imposed on a large cubic simulation box of 40 a.u. with a total charge of -2e. Car-Parrinello propagation [13] was performed with a time step of 4 a.u. (≈ 0.12 fs) using a fictitious orbital mass parameter of 500 a.u. and substituting the H masses by D. Separate Nosé--Hoover chain thermostats [13] at 300 K were coupled to the nuclei and atoms in the QM and MM systems, respectively, in addition to thermostatting separately the set of HS and BS orbitals. After equilibration of 3 ps trajectories of nearly 16 and 12~ps were collected for the CO-in and CO-out conformations, respectively.

The average structure of the [2Fe-2S] moiety is fairly symmetric and planar in vacuo whereas it is best described as a nonplanar and distorted lozenge within the biomolecular environment. Our simulations also showed how intimately the structure of such iron-sulfur cofactors is coupled to the particular hydrogen bond pattern spanned by the protein; more details are in Ref. [11].

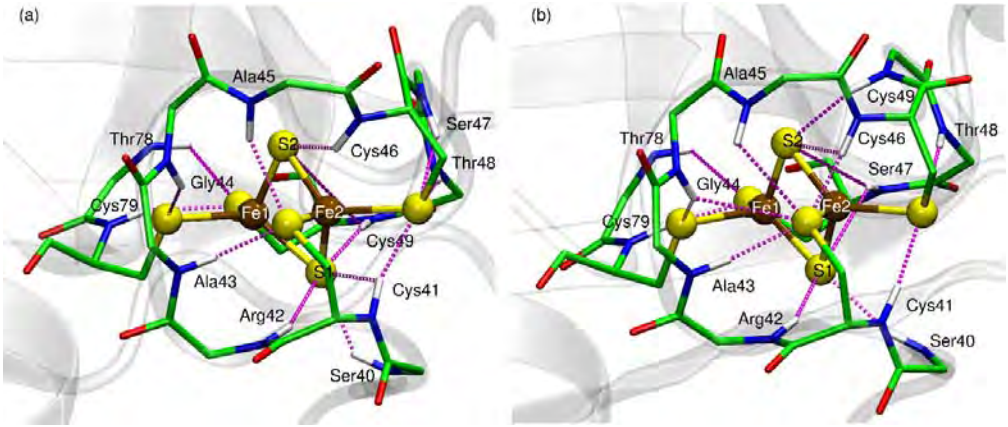


Figure 1: Local environment of the iron-sulfur cluster in Anabaena Fd (a) CO-in and (b) CO-out conformer. The oxygen atoms are shown in red, nitrogen blue, carbon green and hydrogen atoms are white. The yellow and brown spheres represent sulfur and iron atoms, respectively. Hydrogen bonds are indicated by dotted purple lines.

Furthermore, we have seen that the cluster is less compact in Fd and that the average absolute value of J is decreased therein (-403 cm^{-1} in vacuo and -386 cm^{-1} for CO-in conformation), thus showing a direct influence of the protein environment. At the same time, the difference in the average value of J for the CO-in (J=-386 cm^{-1}) and CO-out (J=-360 cm^{-1}) conformations reveals the influence of different protein environments. It is also interesting to observe that the amplitude of J fluctuations is larger in the CO-out conformation compared to CO-in (see Figure 2).

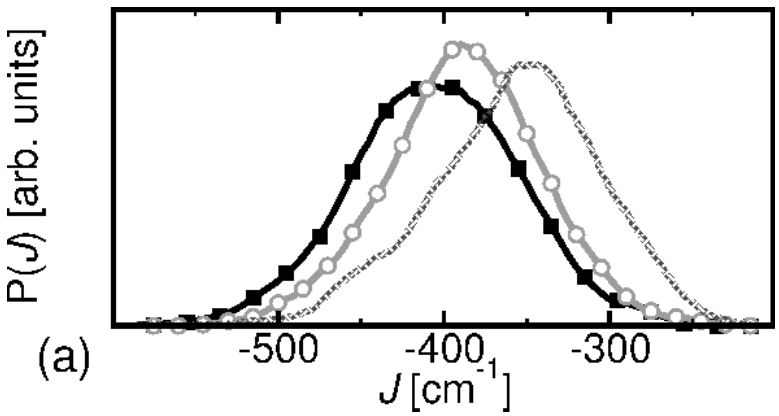


Figure 2: Comparison of the probability distribution of J obtained from EBS simulations for the iron-sulfur cluster in vacuo (filled squares) to that in solvated Fd in its CO-in (open circles) and CO-out (patterned line) conformations.

A true magnetodynamical quantity, which is accessible due to our novel technique, is the power spectrum *J(ω)* in Figure 3 as obtained for the iron-sulfur cluster in vacuo as well as for the CO-in and CO-out conformers of Fd. Power spectra of vibrations and *J(ω)* were computed from Fourier transforms of velocity and *J* time-autocorrelation functions, respectively. Cross correlations to the D_{2h} normal modes provides information on the vibrational motion of the cluster responsible for peaks in *J(ω)* spectrum, or in other words dynamic mangnetostructural relations. Major features of the *J(ω)* spectrum are assigned to the two totally symmetric modes which describe the inner core vibrations in terms of angles ($A_{g,A}$) and distances ($A_{g,D}$) are sufficient to explain the dynamics of *J*. However, there is conformation-specific fine structure: within the CO-in conformation in Fd the B_{2u} symmetric mode also directly affects *J* and, in addition, the two B_{1g} modes modulate *J(t)* by coupling to the A_g modes, which is in contrast to the CO-out conformer. Furthermore, there is a high-frequency component of *J(ω)* around 3300 cm^{-1} in the protein that can be traced back to very specific hydrogen bonds, namely Cys46-S1 and Cys49-S2 in the CO-in conformer and Ser40-S1 and Ser47-S2 in the CO-out Fd. Many other interesting aspects about the relationship of the magnetic coupling constants to the structural dynamics and protein environment are present in our publication Ref. [11] and in the Ph.D. thesis Ref. [14], and therefore not described here in detail.

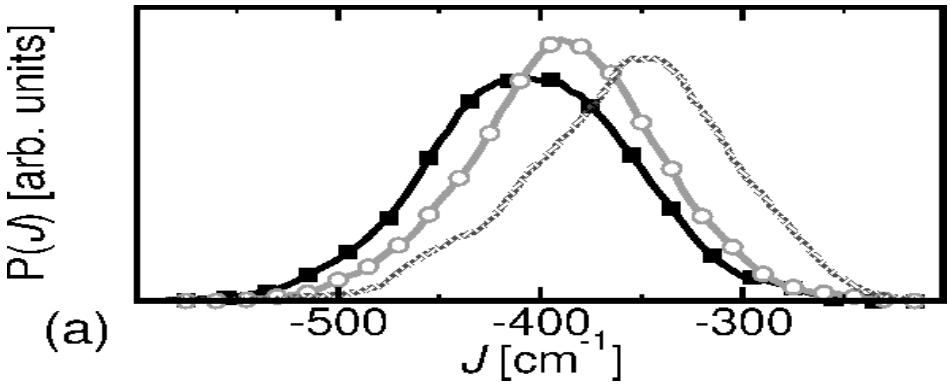


Figure 3: Magnetostructural dynamics of the oxidized binuclear iron-sulfur cluster. (a) Power spectra J(w) for the cluster obtained in vacuo (filled squares) and within Fd in its CO-in (open circles) and CO-out conformation (patterned solid line). In the inset, which shows the spectra in the range 3200 to 3400 cm-1. Power spectra of J together with the frequency dependent correlations of J and the motion along relevant modes of the [2Fe--2S] subsystem in vacuo (b) and within Fd in its CO-in (c) and CO-out conformation (d).

Experimental values of *J* for Anabaena Fd are not available, but similar proteins like spinach Fd yield values nearly -183 cm^{-1} [16]. Our estimate of J is about 3-4 times larger than the experimental value. Overestimation of the absolute value of J by about a factor of two is a well-known problem in DFT when using generalized gradient approximations. It is a direct result of the self-interaction error leading to artificially delocalized magnetic orbitals. Hybrid functionals can cure this problem to an extent but due to the computational complexity we haven't followed this route. In future, we will be combining our EBS technique with self-interaction correction based on a recently developed self-consistent linear response DFT+U approach [17].

Resource Usage

We have used the ARMINUS Xeon cluster for the computations. Jobs were submitted using the batch system, using a maximum of 41 processors at a time. The interconnect was infiniband. The program CPMD [6,7] used for these calculations is very well parallelized using MPI. During the production runs, the cluster was used on a daily basis.

References

[1] Hall D.O.; Cammack R. and Rao K.K.: (1971) Nature 233:136-138.
[2] Rees D.C.; Howard J.B.: (2003) Science 300:929-931.
[3] Johnson D.C.; Dean D.R.; Smith A.D. and Johnson M.K.: (2005) Annu. Rev. Biochem. 74: 247-281.
[4] Shin M. and Arnon D.I.: (1965) J. Biol. Chem. 240: 1405-1411.
[5] Morales R.; Chron M.H.; Hudry-Clergeon G.; Petíllot Y.; Norager S.; Medina M. and Frey M.: (1999) Biochemistry 38: 15764-15773.
[6] Noodleman L.; Peng C.Y.; Case D.A. and Mouesca, J.M.: (1995) Coord. Chem. Rev. 144: 199-244.
[7] Gambarelli S. and Mouesca J.M.: Inorg. Chem. 43: 1441-1451.
[8] Li J.; Nelson M.R.; Peng C.Y.; Bashford D. and Noodleman L.: (1998) J. Phys. Chem. A 102: 6311-6324.
[9] Morales R.; Frey M. and Mouesca J.M.: (2002) J. Am. Chem. Soc. 124: 6714-6722.
[10] Sulpizi M.; Raugei S.; VandeVondele J.; Carloni P. and Sprik M.: (2007) J. Phys. Chem. B 111: 3969-3976.
[11] Schreiner E.; Nair N.N.; Pollet R.; Staemmler V. and Marx D.: (2007) Proc. Nat. Acad. Sci. 104: 20725.
[12] Nair N.N.; Schreiner E.; Pollet R.; Staemmler V. and Marx D.: (2008) J. Chem. Theory Comput. 4: 1174.
[13] Marx D. and Hutter J.: (2009) Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods (Cambridge University Press, Cambridge).
[14] Schreiner, E.: Biochemical Aspects of Iron-Sulfur Systems: Magnetostructural Properties of Ferredoxins and Prebiotic Peptide Synthesis Involving Pyrite (PhD Thesis, Lehrstuhl für Theoretische Chemie, Ruhr--Universität Bochum, Germany, 2007).
[15] Hutter et al J CPMD, IBM Corp 1990-2007, MPI fuer Festkoerperforschung Stuttgart 1997-2001, see also http://www.cpmd.org.
[16] Palmer G.; Dunham W.R.; Fee J.A.; Sands R.H.; Lizuka T. and Yonetani T.: (1971) Biochim Biophys Acta 408: 306-318.
[17] Kulik H.J.; Cococcioni M.; Scherlis D.A. and Marzari N.: (2006) Phys. Rev. Lett. 97:103001

6.2 Mechanochemistry of Thiolates on Gold Surface

Project coordinator	Prof. Dr. Dominik Marx, Ruhr-University of Bochum
Project members	Dr. Jordi Ribas-Arino, Ruhr-University of Bochum
	Dr. E. Schreiner, Ruhr-University of Bochum
Supported by:	Alexander von Humboldt Foundation / Catalan Government (Beatriu de Pinos Fellowship to Jordi Ribas-Arino) / Deutsche Forschungsgemeinsschaft (Reinhart Koselleck Grant to Dominik Marx)

General Problem Description

Most chemical reactions must be activated by some form of energy. The oldest approach is to use fire, that is, thermal energy leading to thermochemistry, but other "chemistries" are activated by light or electricity, that is, photochemistry or electrochemistry. Most recently, however, the capability to manipulate molecules on the atomic scale by Atomic Force Microscopy techniques has opened the door to induce and control chemical reactions and to construct new nanoscale architectures by applying external mechanical forces.[1] In the current project we are investigating by means of first principles calculations which chemical phenomena and which nanostructures can be generated when complex thiolates are pulled off a gold surface. We have chosen these particular molecule-metal junctions because they are well accessible to experiments and because previous theoretical work has shown that it is possible to draw gold nanowires when alkylic thiolates are pulled off a stepped gold surface or off small gold clusters.[2]

Our simulations have revealed for the first time that the mechanochemical behavior of aromatic and alkylic thiolates can be different, the reason being a weakening of the sulfur-gold bond in going from the alkylic thiolate to the aromatic one. The mechanochemistry of bidentate thiolates on gold surfaces is also being explored. The results obtained so far indicate that this kind of thiolates distort quite dramatically the gold surface when they are pulled off it but that at the end they are not able to detach any gold atom off the surface because a sulfur-sulfur bond is formed instead. Finally, our simulations have also revealed that upon pulling tridentate thiolates off gold surfaces, gold clusters can be formed and that carbon-carbon bonds can be activated, depending on the organic skeleton of the organic ligand. Overall, our simulations have implications for the stability and degradation of

molecule/metal junctions as used, for instance, in coatings and molecular electronics.

Problem Details and Work Done

COMPUTATIONAL DETAILS

In this project we have considered the Au (111) surface as a representative of extended gold systems. Periodically repeated slabs of four or five layers of gold atoms have been employed to model the surface. The four-layer and five-layer slabs consist of thirty and sixteen gold atoms per layer, respectively. We have used either one surface or the other depending on the size of the thiolate adsorbed onto it. Previous tests carried out with slabs containing twelve gold atoms per layer showed that such size of slab was not sufficient to produce results that are not biased by the periodic boundary conditions imposed in our calculations. Some of our simulations have been carried out with completely flat surfaces and some of them with surfaces including a vacancy on the first layer, since it is well known that the Au(111) surface are usually characterized by a large atomic roughness with both adatoms and vacancies.[3]

To mimic a typical mechanical pulling experiment involving a thiolate attached to a gold surface the coordinates of the gold atoms of the bottom layers of the slab are frozen and the top methyl group of the thiolate is constrained to move in a plane parallel to the bottom layers of the slab. Stepwise static pulling in small increments (0.2 Angstroms) is first applied and then the system is optimized with the mentioned constraints. These static calculations have been performed with the CPMD code[4] and the *Quantum ESPRESSO* package[5], which are plane wave/pseudopotential implementations of Density Functional Theory.[6] The PBE functional[7] together with ultrasoft pseudopotentials[8] with a cutoff of 25 Ry have been used.

RESULTS

The simulations performed so far with the alkylic and aromatic thiolates have uncovered that the mechanochemical behavior of these two species can be different in certain cases, as opposed to what is usually assumed. As can be seen in Fig. 1, when an alkylic thiolate is pulled off a flat gold surface, a gold-gold bond is eventually broken, i.e., the alkylic thiolate is able to detach a gold atom off the surface. On the contrary, when an aromatic thiolate is pulled off the flat surface, the sulfur-gold bond is the bond which breaks upon mechanical stress. The aromatic thiolate (see Figure 1) is able to lift a gold atom of the first layer of the surface but not to detach any gold atom off the surface. It is noted in passing that Figure 1 clearly discloses that the mechanical detachment pathways of the aromatic and alkylic thiolates differ from the very first steps of the computational experiment.

Electronic structure calculations have allowed us to rationalize such different mechanochemical behavior, the reason being a weakening of the sulfur-gold bond in going from the alkylic thiolate to the aromatic one. It is worth mentioning that such difference in mechanochemical behavior between different types of monodentate thiolates has not been observed when such thiolates are pulled off a gold surface with one vacancy. In this particular case, the mechanical stress results eventually into the rupture of a gold-gold bond in both systems.

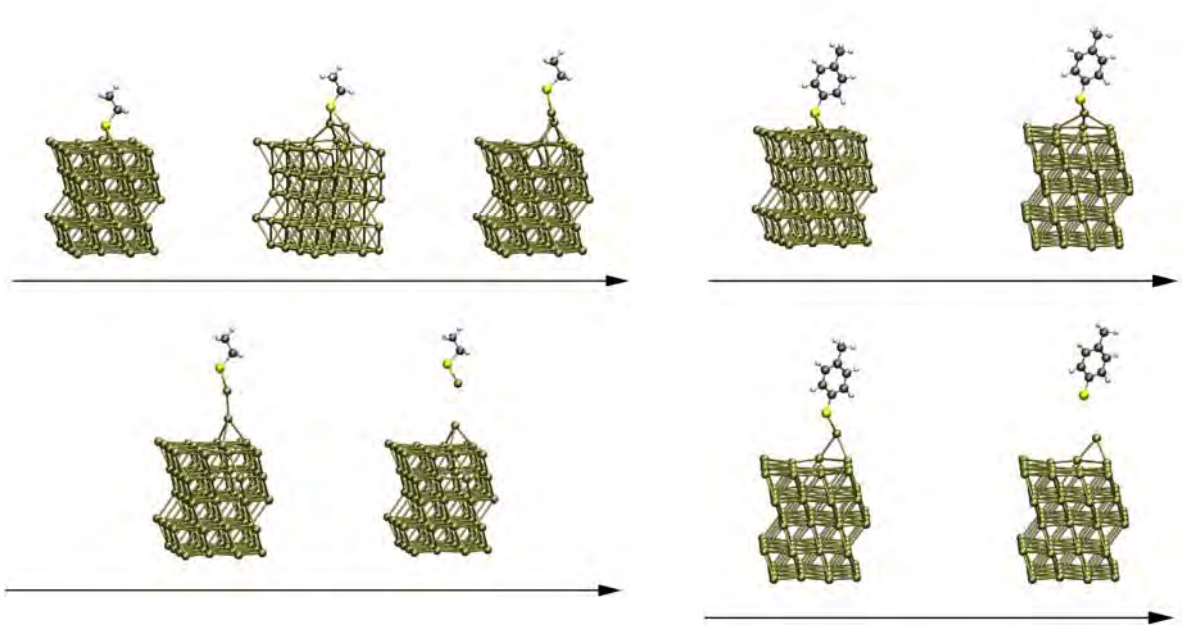


Figure 1: Nanostructures obtained in the static pulling simulations of an alkylic thiolate (left) and an aromatic thiolate (right)

Regarding the static pulling simulations of bidentate thiolates, the results obtained so far with several of them reveal a similar pattern, which is schematized in Figure 2.

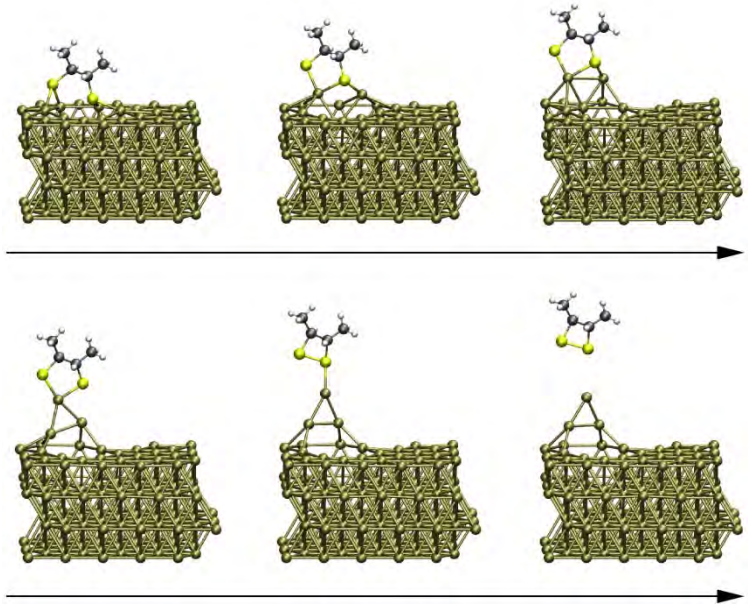


Figure 2: Nanostructures obtained in the static pulling simulations of a bidentate thiolate

The bidentate thiolates induce a notable distortion of the underlying gold surface upon pulling; indeed, they are able to lift three gold atoms. Nevertheless, they are not able to detach any gold atom off the surface because a sulfur-sulfur bond is formed instead.

Finally, the mechanochemistry of tridentate thiolates is even more complex than the so-far considered cases. Let us consider the tridentate thiolates depicted in Figurs 3 and 4. Both thiolates are adsorbed on a gold surface with one vacancy. Both thiolates differ in their organic skeleton. Specifically, the thiolate of Figure 4 is much more rigid than the one in Figure 3 because it has a triple carbon-carbon bond. The thiolate of Figure 3 is able to lift four gold atoms of the first layer of the surface in the initial steps of the pulling experiment. After this, however, the mechanical stress does not result in any rupture of Au-Au or Au-S bonds, but in the rupture of a carbon-carbon bond! It is worth mentioning that we have obtained the same result when the thiolate employed has a larger terminal alkylic chain (with four methylene units instead of one).

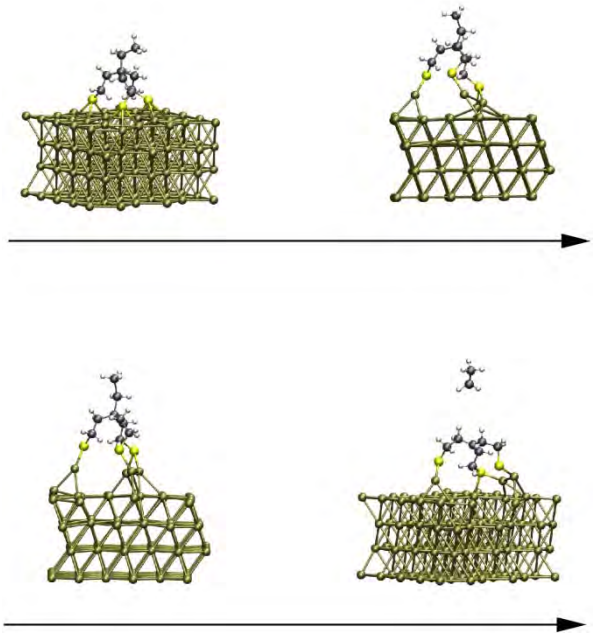


Figure 3: Nanostructures obtained in the static pulling simulations of a tridentate thiolate

As for the rigid tridentate ligand (the one with a triple C-C bond), Figure 4 illustrates which nanostructures can be generated when it is pulled off a gold surface with one vacant. In this particular case, the thiolate is able to extract a whole gold cluster containing four gold atoms with tetrahedral shape. This unprecedented result shows that thiolates are not only able to extract gold nanowires off a gold surface[2a] but that they are also able to extract whole clusters.

All the results obtained in our systematic study of mechanochemistry of thiolates on gold surfaces will be sent for publication in short. On the other hand, these results were partially presented in the Bunsentagung 2008 (1st-3rd May), in Saarbruecken.

CURRENT AND FUTURE WORK

Concerning the mechanochemistry of aromatic thiolates, we are currently investigating which is the effect of adding substituents to the aromatic ring. In particular, we want to test if it is possible to weaken or strengthen the sulfur-gold bond by tuning the electronic structure of the aromatic ring. Preliminary calculations suggest that amino and nitro substituent groups might be suitable for that purpose.

With reference to the mechanochemistry of tridentate ligands, we are now exploring which mechanochemistry can be triggered by the same thiolates previously used when pulled off flat gold surfaces. Intermediate results suggest that dramatic

distortions of the surface take place in these cases and that flat gold clusters can be lifted.

Finally, motivated by the differences between mechanochemical dissociation pathways and thermal dissociation pathways found in the system consisting of thiolates adsorbed on copper surfaces[9], we aim at exploring by means of *ab initio* molecular dynamics simulations[6] the thermal dissociation pathways of the thiolates that have been considered so far.

Overall, we want to explore to what extent it is possible to generate and manipulate nanostructures at will in thiolate-gold systems and which is the role played by the temperature and the subsequent dynamical effects.

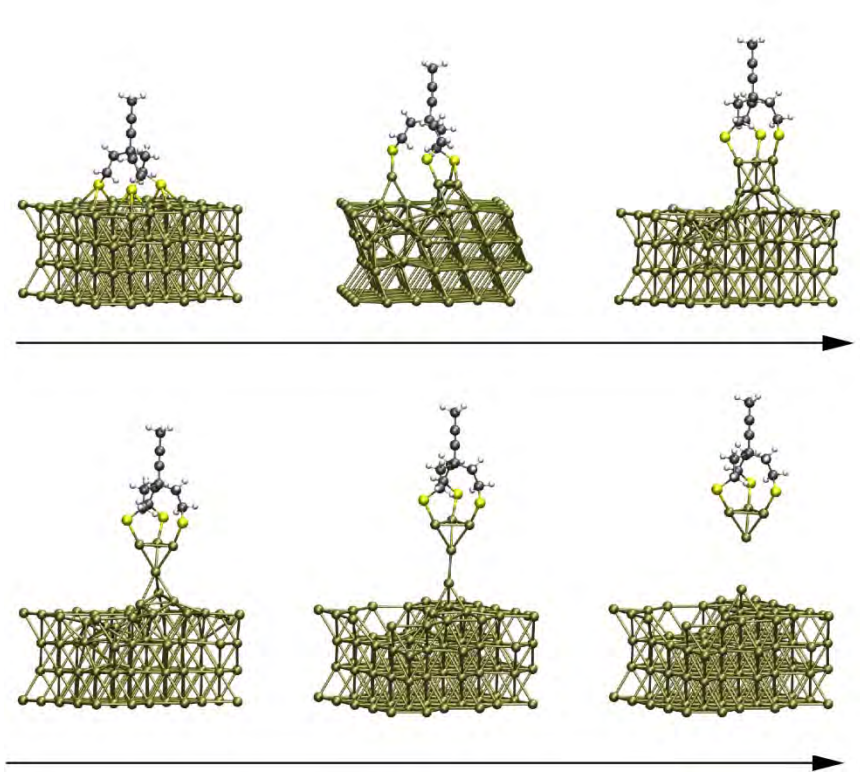


Figure 4: Nanostructures obtained in the static pulling simulations of a tridentate thiolate

Resource Usage

The simulations of this project are run on the processors of the ARMINIUS cluster (400 processors 64-bit INTEL Xeon with Infiniband communication). Both packages we are using (CPMD and Quantum-Espresso) are truly parallel and efficiently use the Infiniband interconnect. We usually run jobs with 16-24 processors running in parallel on a daily basis, but the codes easily scale up to much larger processor numbers if available for true throughput/capacity simulations. We are using the

resources of the ARMINIUS cluster because of the compute power of the nodes in conjunction with the fast Infiniband interconnect.

References

[1] Beyer, M.K. and Clausen-Schaumann, H.: Chem. Rev. 2005, 105, 2921
[2] (a) Krüger, D.; Fuchs, H.; Rousseau, R.; Marx, D.and Parrinello, M.: Phys. Rev. Lett. 2002, 89, 186402; (b) D. Krüger, R. Rousseau, H. Fuchs, D. Marx Angew. Chem. Int. Ed. 2003, 42, 2251.
[3] Mazzarello, R.; Cossaro, A.; Verdini, A.; Rousseau, R.; Casalis, L.; Danisman, M.F.; Floreano, L.; Scandolo, S.; Morgante, A. and Scoles, G.: Phys. Rev. Lett. 2007, 98, 016102.
[4] Hutter, J.: et al. CPMD V3.12; Copyright IBM Corp 1990-2001, Copyright MPI für Feskörperforschung Stuttgart 1997-2001. see www.cpmd.org
[5] www.quantum-espresso.org
[6] Marx, D. and Hutter, J.: Ab initio Molecular Dynamics: Basic Theory and Advanced Methods; Cambridge University Press: Cambridge, 2009.
[7] Perdew, J. P.; Burke, K. and Ernzerhof, M.: Phys. Rev. Lett. 1996, 77, 3865.
[8] Vanderbilt, D.: Phys. Rev. B (Rapid Communications), 1990, 41, 7892.
[9] Konopka, M.; Turansky, R.; Reichert, J.; Fuchs, H.; Marx, D.and Stich, I.: Phys. Rev. Lett. 2008, 100, 115503.

6.3 Lipid-Protein Interactions in Lipid Membranes

Project coordinator	Prof. Dr. Friederike Schmid, University of Bielefeld
Project members	Dipl.-Phys. Beate West, University of Bielefeld
Supported by:	DFG (Sonderforschungsbereich 613)

General Problem Description

Biomembranes play a central role in both the structure and function of all biological cells. The biomembrane consists of a liquid-like bilayer of amphiphile lipids, into which membrane proteins and other macromolecules are inserted or attached. The major role of the lipids is to form a stable bilayer matrix with which the proteins interact. The lipids are also responsible for the physicochemical characteristics of the membrane. The proteins, e.g. receptors, enzymes and ion channels are the biochemical active components.

The interaction between proteins inserted into the lipid bilayer is of great importance for the functionality of the membrane. On the one hand there are the direct protein-protein interactions, for example van der Waals forces and electrostatic forces for charged inclusions. The electrostatic interactions in biologically relevant constellations are predominantly shielded by the aqueous environment of the membrane [2,13]. On the other hand the perturbation of the lipid bilayer by the proteins can induce indirect lipid-mediated interactions. These indirect interactions contribute significantly to the entire interaction between proteins [3,5,6,9,10]. Different effects can induce indirect interactions [5]:

1. Hydrophobic mismatch will occur if the length of the hydrophobic section of the protein is much smaller or much larger than the hydrophobic thickness of the lipid bilayer.
2. The proteins affect the lateral structure of the lipid bilayer: The number of possible conformations of the lipids is reduced in the vicinity of the proteins, in addition proteins can induce a tilt of the lipid molecules.
3. Proteins can induce a strong membrane curvature.

We investigate the influence of transmembrane proteins on the lipids on the one hand and the membrane-mediated interactions between proteins inserted into the lipid bilayer on the other hand.

Problem Details and Work Done

For our simulations we use a coarse-grained membrane model [4]. The bilayer model consists of a self-assembled bilayer of lipids in a solvent environment. Each lipid is represented by six tail beads and one slightly larger head bead. The adjacent beads of the lipid chain are bound to each other by a finite extensible nonlinear elastic potential (FENE potential). Beads not connected with each other interact via a truncated and lifted Lennard-Jones potential. Head-head and head-tail interactions are purely repulsive and tail-tail interactions also have an attractive component. The solvent environment is represented by explicit solvent beads [7,8]. They behave like unbound head beads, except for not interacting with each other.

The proteins are modeled as rigid cylinders whose diameters correspond to simple beta-helices. They are free to move in all three directions of the lipid bilayer. The proteins interact with each other and the lipids in the xy-plane via a Lennard-Jones kind of potential. The interaction between tail beads and proteins is repulsive and attractive. All other interactions are purely repulsive.

The system is simulated using Monte Carlo methods at constant pressure, temperature and particle number with periodic boundary conditions in a simulation box of variable size and shape. The program is parallelized using a geometrical decomposition scheme [11,12].

We have studied the elastic properties of lipid bilayers in different phases [16] and under tension [17]. Then we simulated a lipid bilayer with one and two proteins in the lipid phase [15]. Two parameters are changed:

1. The hydrophobic length L of the proteins. The values of the hydrophobic length are chosen such that we have one case of negative ($L = 4\sigma_t$), no ($L = 6\sigma_t$), and positive ($L = 8\sigma_t$), hydrophobic mismatch.
2. The hydrophobicity parameter (protein-tail interaction strength) e_{pt} is varied between 1.0 and 6.0, whereas a hydrophobicity of 1.0 is sufficient to trap the center of the protein inside the lipid bilayer.

In order to investigate the deformation of a bilayer by a single protein we measure the bilayer thickness as a function of the distance from the protein (illustration 1).

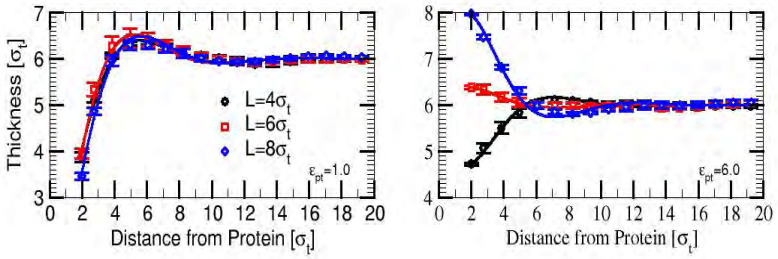


Illustration 1: Radial membrane thickness in the vicinity of one protein in the fluid phase.

The hydrophobicity parameter must exceed a certain parameter in order to produce classical hydrophobic matching. When the hydrophobicity is too small the protein repels the lipids independent of the value of L. The bilayer surfaces get pinned by the protein for values of the hydrophobicity parameter larger than e_{pt} = 4.0. The thickness profiles are not strictly monotonic but rather show a characteristic over- or undershooting. The solid lines in illustration 1 are the fit to an elastic theory [14], which describes the thickness profiles very well.

In order to calculate the effective pair potential w(r) between two proteins we have to determine the radial distribution function g(r) as a function of the protein-protein distance r:

$$w(r) = -k_B T \ln g(r)$$

k_B is the Boltzmann constant and T is the temperature.

The radial distribution function is obtained by an umbrella sampling procedure. Illustraion 2 shows the effective pair potential for different values of the hydrophobic length L and for different hydrophobicity parameters e_{pt}.

Except for a hydrophobicity parameters e_{pt} = 1.0, where the interaction is too weak, the curves show an oscillatory behaviour. The oscillations have a period of approximately $1\sigma_t$ indicating that they are caused by packing effects of the lipid chains.

The effective pair potential shows a minimum at close distances followed by a shallow maximum. Apart from the first minimum the minima become more shallow with increasing distance and/or decreasing hydrophobicity parameter e_{pt}. With increasing e_{pt} the layering effect becomes more pronounced. The lipids pack more tightly, if they are closer to the protein surface. This is a result of the strong Lennard-Jones potential we use as interaction potential.

The first minimum disappears for high hydrophobicity parameters and deepens with decreasing e_{pt}. It is a result of different effects: First, there is the direct protein-

protein interaction and the solvent-induced interaction between the hydrophilic protein section located outside of the lipid bilayer. Second, we have the depletion-type interaction induced by the lipids.

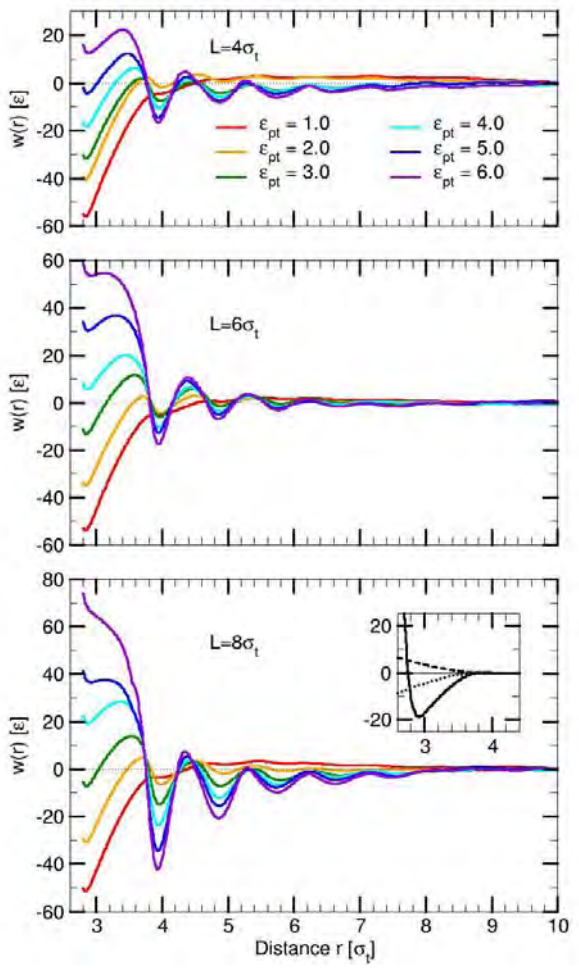


Illustration 2: Effective pair potential between two proteins in the fluid phase.

Resource Usage

Our simulations run on the cluster ARMINIUS. Our program is parallelized with MPI. Depending on the system size we want to investigate we need between 2 and 4 nodes.

References

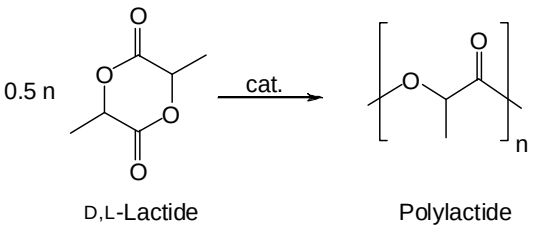
[1] Aranda-Espinoza, H.; Berman, A.; Dan, N.; Pincus, P. and Safran, S.: Interaction between Inclusions Embedded in Membranes, Biophysical Journal 71, 648, 1996
[2] Ben-Tal, N. and Honig, B.: Helix-helix interactions in lipid bilayers, Biophysical Journal 71, 3046, 1996
[3] Bloom, M.; Evans, E. and Mouritsen, O.G.: Physical properties of the fluid lipid-bilayer component of cell membranes: a perspective, Quart. Rev. Biophys. 24, 293, 1991
[4] Düchs, D. and Schmid, F.: Phase behavior of amphiphilic monolayers: Theory and simulations, J. Phys: Cond. Matt. 13, 4853, 2001
[5] Gil, T.; Ipsen, J.H.; Mouritsen, O.G.; Sabra,V.C.; Speretto, M. and Zuckermann, M.J.: Theoretical analysis of protein organization in lipid membranes, Biochimica and Biophysica Acta 1376, 245, 1998
[6] Lague, P.; Zuckermann, M.M. and Roux, B.: Protein inclusion in lipid membranes: A theory based on the hypernetted chain integral equation, Faraday Disc. 111, 165, 1998
[7] Lenz, O. and Schmid, F.: Structure of Symmetric and Asymmetric Ripple Phases in Lipid Bilayers, Phys. Rev. Lett. 98, 058104, 2007
[8] Lenz, O. and Schmid, F.: A simple computer model for liquid lipid bilayers, J. Mol. Liquids 117(1-3), 147, 2005
[9] May, S.: Theories on structural perturbations of lipid bilayers, Curr. Opn. Coll. Interf. Sci. 5, 244, 2000
[10] Mouritsen, O.G. and Bloom, M.: Models of lipid-protein interactions in membranes, Quarterly Reviews of Biophysics: Biomol. Struct. 22, 145, 1993
[11] Schmid, F.; Düchs, D.; Lenz, O. and West, B.: A generic model for lipid monolayers, bilayers, and membranes, Computer Physics Communications 177(1-2), 168, 2007
[12] Uhlherr, A.; Leak, S.J.; Adam, N.E.; Nyberg, P.E.; Doxastakis, M.; Mavrantzas, V.G. and Theodorou, D.N.: Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors, Computer Physics Communications 144(1), 1, 2002
[13] Walther, D.; Kuzmin, P. and Donath, E.: Brownian dynamics simulation of the lateral distribution of charged membrane components, Eur. Biophys. J. 24, 125, 1996
[14] Brannigan, G. and Brown, F.L.H.: Contributions of the Gaussian curvature and nonconstant lipid volume to protein deformation of lipid bilayers, Biophysical Journal 92, 864, 2007
[15] West, B.; Brown, F.L.H. and Schmid, F.: Membrane-Protein Interactions in a Generic Coarse-Grained Model for Lipid Bilayers, Biophysical Journal 96, 101, 2009
[16] West, B. and Schmid, F.: Properties of Lipid Membranes in the Fluid and the Gel State: A Coarse-Grained Monte-Carlo Study, Soft Matter, submitted
[17] Neder, J.; West, B.; Nielaba, P. and Schmid, F.: Coarse-Grained Simulations of Membranes under Tension, The Journal of Chemical Physics, submitted

6.4 Density Functional Methods using Gaussian03 in the Development of Catalysts for the Ring-Opening Polymerisation of Lactide

Project coordinator	Dr. Sonja Herres-Pawlis, University of Paderborn
Project members	Dr. Sonja Herres-Pawlis, University of Paderborn
Supported by:	University of Paderborn

General Problem Description

Over the past decades biodegradable polymers have raised increasing interest in fundamental research and also in the chemical industry. Polylactides (PLA) have proven to be the most attractive and useful class of biodegradable polyesters among the numerous polyesters studied so far. Due to their favourable and sustainable material properties as well as their broad range of application reaching from packaging (bottles, films), fibres for tissue and clothes, to use in medical and pharmaceutical fields (retarding drugs, biodegradable screws and sutures) and the fact that they can be produced from inexpensive renewable raw materials like corn, sugar beets or even agricultural waste, PLAs are qualified to be a viable alternative to petrochemical-based plastics. To achieve high molecular weight, PLAs are obtained by metal catalysed ring-opening polymerisation (ROP) of lactide, the cyclic diester of lactic acid (Scheme 1).[1-10]



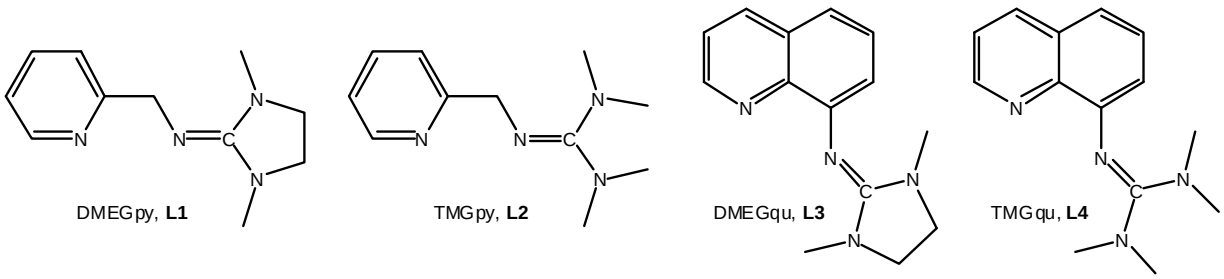
Scheme 1. ROP of d,l-lactide.

Today, PLA is produced by more than 10 chemical companies worldwide and has already left the niche of exotic polymers. For the technical production the most widely used initiator is Sn(II)-ethylhexanoate ($SnOct_2$). But the fact that all tin compounds are cytotoxic[1,11] forces the development of alternative initiators, especially when PLAs should be used for pharmaceutical, medical or food applications. An auspicious non-toxic option are zinc salts or complexes.[1] Because they are mostly colourless, inexpensive and non-toxic[2,3] zinc complexes with N-

donor-functionalised ligands for instance β-diketiminates[12,13] and Schiff bases[14] were introduced as active catalysts for the ROP of lactide in order to enhance the polymerisation process and to replace the common Sn-based catalysts. Besides the cationic portion, the importance of the anionic component has to be highlighted as well.[15] In spite of great efforts in this field, there is still great demand for highly active, non-toxic and stable complexes, which can be easily handled.[16]

As we reported recently,[17] zinc guanidine complexes show a high potential as active catalysts in the ring-opening polymerisation of D,L-lactide combined with an acceptable stability. Several examples of (guanidine)zinc complexes have already been reported,[18] whereof some complexes possess catalytic activity in selected processes, which makes guanidines a very promising ligand class leading to catalytically active zinc complexes.[19] The anionic guanidinate ligands have already been shown to stabilise lactide-polymerising complexes but they are sensitive to moisture and air.[20,21]A related ligand class is represented by the 2-iminoimidazolines[22] which offer great donor properties and stabilise catalytic active complexes as well.[23]

In order to improve the activity of guanidine based zinc complexes we modified the ligand system by substituting one guanidine function by an amine group. This substitution changes the electronic environment by replacing one “hard” guanidine function by a “soft” pyridine donor and simultaneously the accessibility to the zinc centre by substituting one bulky guanidine by a non-bulky pyridine unit. This guanidine-amine hybridligands combine the excellent donor properties of guanidines with additional coordination space for the pre-coordination of substrates and they also exhibit an modular synthesis protocol, which combines different spacer and guanidine groups and thus admits a flexible ligand design.[24,25-30] The use of pyridyl and quinolyl units leads to the guanidine-pyridine hybridligands N-(1,3-Dimethylimidazolidin-2-yliden)pyridin-8-amine (DMEGpy, **L1**), 1,1,3,3-Tetramethyl-2-((pyridin-2-yl)methyl)guanidine (TMGpy, **L2**), N-(1,3-Dimethylimidazolidin-2-yliden)quinolin-8-amine (DMEGqu, **L3**) and 1,1,3,3-Tetramethyl-2-(quinolin-8-yl)guanidine (TMGqu, **L4**) which are depicted in Scheme 2.[26-29]



Scheme 2. Guanidine-pyridine hybridligands.[26-29]

We were able to synthesise and characterise of the first zinc complexes including the guanidine-pyridine hybridligands DMEGpy (**L1**), TMGpy (**L2**), DMEGqu (**L3**) and TMGqu (**L4**). These zinc complexes were screened towards their catalytic activities in the polymerisation of lactide. The actual study extensively correlates experimental results to DFT calculations to rationalize the reactivity. Furthermore, it is highlighted that the classical controversy between stability and activity can be compensated by an integrated approach.

Problem Details and Work Done

The following complexes were synthesised and then theoretically modelled (Table 1, Figure 1).

Figure 1. Overview of the modelled zinc complexes

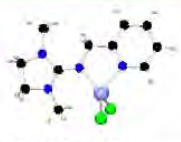
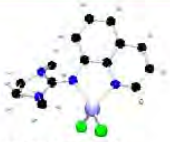
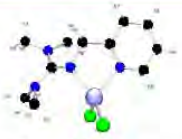
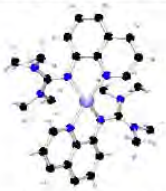
	DMEGpy	DMEGqu	TMGpy	TMGqu
$ZnCl_2$	 [Zn(DMEGpy)Cl_2]	 [Zn(DMEGqu)Cl_2]	 [Zn(TMGpy)Cl_2]	 [Zn(TMGqu)Cl_2]
$ZnAc_2$	 [Zn(DMEGpy)$(CH3COO)_2$]	 [Zn(DMEGqu)$(CH_3COO)_2$]	 [Zn(TMGpy)$(CH_3COO)_2$]	 [Zn(TMGqu)$(CH_3COO)_2$]
$ZnTf_2$		 [Zn(DMEGqu)$_2$][CF_3SO_3]$_2$		 [Zn(TMGqu)$_2$][CF_3SO_3]$_2$

Table 1. Overview of the synthesised guanidine-pyridine hybridligand stabilised zinc complexes.

	$ZnCl_2$	**$Zn(CH_3COO)_2$**	**$Zn(CF_3SO_3)_2$**
DMEGpy L1	$[Zn(DMEGpy)Cl_2]$ **C1**	$[Zn(DMEGpy)(CH_3COO)_2]$ **C5**	- [a]
TMGpy L2	$[Zn(TMGpy)Cl_2]$ **C2**	$[Zn(TMGpy)(CH_3COO)_2]$ **C6**	- [a]
DMEGqu L3	$[Zn(DMEGqu)Cl_2]$ **C3**	$[Zn(DMEGqu)(CH_3COO)_2]$ **C7**	$[Zn(DMEGqu)_2][CF_3SO_3]_2$ **C9**
TMGqu L4	$[Zn(TMGqu)Cl_2]$ **C4**	$[Zn(TMGqu)(CH_3COO)_2]$ **C8**	$[Zn(TMGqu)_2][CF_3SO_3]_2$ **C10**

[a] This complex could not be structurally characterised.

Theoretical description of the zinc complexes

The structural trends described above are discussed under consideration of gas phase DFT calculations. The electronic structures of the zinc complexes C1-C10 have been examined using the B3LYP density functional theory and the 6-31G(d) and 6-31G+(d) basis sets, implemented by the Gaussian 03 suite of programs.[31] Geometry optimisations were performed using the coordinates from X-ray data as starting point in case of C1-C10.

For the 6-31G(d) basis set, the computed complex structures are in good agreement with their solid state structures whereas the 6-31G+(d) basis sets generally yield too long bond lengths. The soft donating character of the pyridine and of the guanidine is significantly overestimated by this diffuse basis set which has been observed in several cases.[32] For the most complexes, the Zn-N distances are predicted about 0.03 Å too long which is a known tendency for such systems.[32,33] Hence, the ligands L1-L4 and the model ligand HGqu have been examined using the B3LYP density functional theory and only the 6-31G(d) basis set (Figure 2).

The tetrahedral coordination environments in C1-C8 are correctly described by both basis sets. Special emphasis is laid on the angles between the ZnN_2 and the ZnX_2 planes which are in good accordance with the angles found in the solid state. The coordination of the acetate ions in the complexes C5-C8 is in good agreement as well. Interestingly for the acetate complexes, contacts of the benzyl or quinoline spacer hydrogen atoms to the acetate oxygen atoms are found which were confirmed by DPFGSE-NOE NMR measurements in solution. For the acetate complex C5, two conformers were found in the solid state. Their differences regarding the $Zn\text{-}N_{py}$ and $Zn\text{-}N_{gua}$ bond length is displayed qualitatively in the DFT, too. Their energy difference has been calculated to 1.4 kcal/mol which explains the coexistence within one single crystal.

The bis(chelate) complexes C9 and C10 are correctly described as well: the trigonal bipyramidal coordination situation is well reflected in the N_{py}-Zn-N_{py} angles (169.5 for C9 and 167.8° for C10) which are depicting the apical sites. Moreover, the h^2-binding mode of the triflate and the Zn-O bond lengths are in good agreement to the X-ray structures. In comparison with the solid state structures, the calculated C=N guanidine "double" bond lengths are extremely close to the X-ray data. Especially the differences between the four coordinating ligands are well reflected: for TMGqu and DMEGqu complexes this bond is generally about 1.335 Å, for TMGpy and DMEGpy complexes this bond is shortened to the range of about 1.317 Å. Concomitantly, the tendency for the structural parameter s is correctly predicted: the quinoline containing systems exhibit a slightly higher s (0.98-0.99) than the pyridine systems (0.94-0.96) which is in good accordance to the solid state structures.

Moreover, particularly the effect that the guanidine units twist against the chelate plane in dependence of the ligand in the complexes C1-C8 could be reproduced by DFT. The following trend could be deduced: in quinoline systems, the guanidine exhibits a contact between the guanidine substituents and the ortho-position. In order to avoid the steric hindrance, the whole guanidine unit twists enclosing an angle of 45° with the chelate plane. Simultaneously, the levelling within the guanidine unit increases up to s = 1 because the guanidine leaves the conjugation with the aromatic system. In the pyridine systems, the spacer is more flexible and allows other ways of avoiding the steric hindrance between guanidine substituents and the rest of the ligand molecule which results in a smaller twist angle accompanied by a smaller s value. As the same trend was found experimentally, it can not be related to packing effects but intrinsic forces within the complexes.

The DFT analysis of the ligands and a model ligand without substituents (HGqu) shows that the focus on the steric interactions is only a partial aspect of this twist effect (Figure 2). Even without substituents, the twist amounts up to 50°. The aromatic influence is crucial for the guandine system: the analysis of the Mulliken charges of the ligands (Table 5) reveals that the guanidine N imine atom is significantly more negative in quinoline ligands and complexes than in pyridine ones. Furthermore, the guanidine double bonds in the quinoline ligands are calculated to a mean value of 1.287 Å (pyridine-guanidine ligands: 1.283 Å) which is longer than the values for reported aliphatic guanidines (1.277 Å)[34] but in the range of aromatic guanidines (1.282 Å)[35]. In aromatic guanidines, the rotation around the C=N bonds is facilitated by the interaction with the aromatic system which manifests in coalescence behaviour for the corresponding guanidine substituents.[25] Thus, it is understandable that the C=N bonds are longer and the C-N bonds shorter as in the pyridine systems where the guanidine moiety is bound to the benzyl group and not directly to the aromatic ring. Hence, in the quinoline systems the s value must be higher than for the pyridine systems due to electronic reasons.

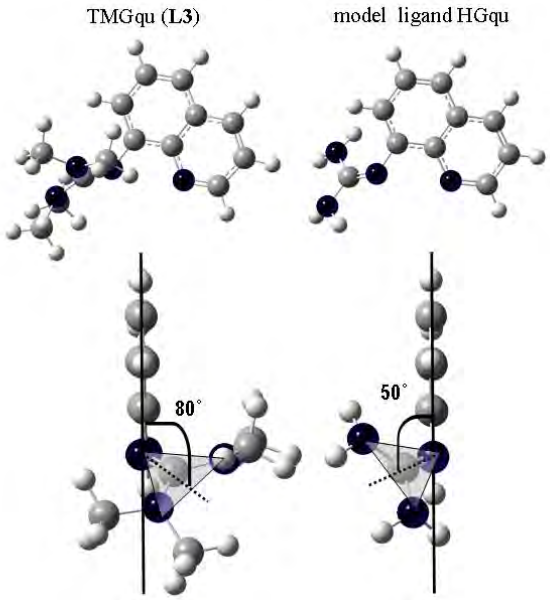


Figure 2. Comparison of the calculated structure of TMGqu (**L3**) with the model ligand HGqu (rb3lyp(6-31G(d)))

For a more detailed analysis of the electronic structure the Mulliken charges have been determined. The resulting charges for the ligands and their complexes are summarised in the Tables 2-5. These charges do not represent absolute charges but the trends among the complexes give an impression of electronic effects. A pronounced effect is the difference between the DMEG and TMG groups. As the geometry optimisations predict, the intra-guanidine twist is significantly smaller in the DMEG groups (12°) because of the ethylene backbone which restricts the intra-guanidine torsion geometrically. In all analysed complexes, the imine N atom in DMEG groups is around 0.05 more negative than that in TMG groups. At the same time, the corresponding amine N atoms in the DMEG containing systems are slightly more negative and the central guanidine C atoms are considerably more positive than those in the TMG containing systems. This result is in good accordance with the theoretical calculations on TMG and DMEG containing ligands performed by Tamm et al.[23a]

An important result of this analysis is the remarkable positive charge on the zinc atom in the bis(chelate) complexes of 1.004 (C9) and 0.994 (C10) in comparison to the other complexes with zinc charges around 0.68 for the chloride complexes and zinc charges around 0.87 for the acetate complexes. This finding documents the higher Lewis-acidity of the zinc atom in C9 and C10 compared to the C1- C8.

Table 2. Mulliken charges in electron units (charge of electron is equal to -1) of **C1**, **C2**, **C5** and **C6** (rblyp, 6-31G(d)).

	[Zn(DMEGpy)Cl$_2$]	[Zn(TMGpy)Cl$_2$]	[Zn(DMEGpy)(CH$_3$COO)$_2$]		[Zn(TMGpy)(CH$_3$COO)$_2$]
	C1	**C2**	**C5a**	**C5b**	**C6**
Zn	0.682	0.667	0.860	0.872	0.862
N_{py}	-0.571	-0.566	-0.579	-0.598	-0.580
N_{gua}	-0.675	-0.622	-0.659	-0.673	-0.615
C_{gua}	0.823	0.696	0.796	0.811	0.680
N_{amine}	-0.458	-0.404	-0.449	-0.449	-0.422
	-0.475	-0.423	-0.469	-0.478	-0.405
X=Cl, OAc	-0.516	-0.494	-0.600	-0.608	-0.618
	-0.518	-0.530	-0.618	-0.612	-0.597

Table 3. Mulliken charges in electron units (charge of electron is equal to -1) of **C3**, **C4**, **C7** and **C8** (rblyp, 6-31G(d)).

	[Zn(DMEGqu)Cl$_2$]	[Zn(TMGqu)Cl$_2$]	[Zn(DMEGqu)(CH$_3$COO)$_2$]	[Zn(TMGqu)(CH$_3$COO)$_2$]
	C3	**C4**	**C7**	**C8**
Zn	0.692	0.697	0.881	0.886
N_{py}	-0.644	-0.641	-0.657	-0.650
N_{gua}	-0.781	-0.745	-0.788	-0.755
C_{gua}	0.806	0.684	0.812	0.706
N_{amine}	-0.451	-0.403	-0.434	-0.411
	-0.458	-0.409	-0.454	-0.392
X=Cl, OAc	-0.502	-0.501	-0.610	-0.606
	-0.536	-0.530	-0.602	-0.606

Table 4. Mulliken charges in electron units (charge of electron is equal to -1) of **C9** and **C10** (rblyp, 6-31G(d)).

	$[Zn(DMEGqu)_2][CF_3SO_3]_2$	$[Zn(TMGqu)_2][CF_3SO_3]_2$
	C9	**C10**
Zn	1.004	0.994
N_{py}	-0.638, -0.641	-0.655, -0.619
N_{gua}	-0.811, -0.792	-0.736, -0.771
C_{gua}	0.800, 0.757	0.648, 0.645
N_{amine}	-0.447, -0.448	-0.399, -0.399
	-0.443, -0.448	-0.395, -0.392
O	-0.617	-0.601
	-0.621	-0.668

Table 5. Mulliken charges of ligands **L1**-**L4** (rblyp, 6-31G(d)).

	DMEGpy	TMGpy	DMEGqu	TMGqu
	L1	**L2**	**L3**	**L4**
N_{py}	-0.473	-0.460	-0.501	-0.490
N_{gua}	-0.544	-0.469	-0.598	-0.525
C_{gua}	0.722	0.606	0.756	0.613
N_{amine}	-0.478	-0.417	-0.455	-0.419
	-0.454	-0.424	-0.461	-0.421

These zinc complexes were proven to be active initiators in the ring-opening polymerisation of D,L-lactide with only few exceptions. PLAs with molecular weights (M_w) of up to 176000 g/mol could be obtained. This value represents a significant augmentation towards bisguanidine zinc complexes. These results corroborate our strategy of building up N donor ligands with different donor strengths and substituents with varied steric demands. In complexes with the same ligand the activity of the initiator depends on the anionic component of the zinc salt. We found that the zinc triflate complexes are excellent catalysts for application in the ROP of lactide. A possible explanation is the flexible coordination of one triflate to the zinc centre leading to a facilitated pre-coordination of the lactide molecule and the distinct positive charge at the zinc in comparison with the tetrahedral complexes which offers a higher Lewis-acidity for the activation of the lactide. In addition, we could confirm the effect observed for bisguanidine zinc complexes that lower temperatures allow side reactions to be avoided during the polymerisation and thus give higher molecular masses. Regarding the aspect of sustainability, the guanidine-pyridine hybridligand zinc complexes possess an advantageous combination of properties: they are non-toxic, can be stored on air without loss of activity and give PLAs with high M_w values at industrially attractive conditions. This bundle of properties makes the guanidine zinc systems an excellent and use-oriented class of catalysts for the ring-opening polymerisation of lactide. Further investigations will focus on the kinetics of the polymerisation process and a mechanism of the d,l-lactide activation and polymerisation.

Resource Usage

The calculations were executed at the ARMINIUS cluster at the PC^2. DFT calculations using Gaussian03 can only use up to 8 nodes parallely. Due to the high number of calculations which have to be accomplished, several calculations were done at the same time separately each with 4 double-core nodes using the Ethernet interconnect of the cluster. In this context, the ARMINIUS cluster provides outstanding computational power. Furthermore, the PC^2 facility gives us the possibility to use Gaussian03 as parallel version.

Geometry optimisations, energy calculations and frequency calculations were run as parallel processes on 4 nodes at the same time. The calculations were set up on a daily basis. Geometry optimisations including the energy calculation have an averaged duration of some days up to 3 weeks depending on the size of the molecule and the chosen basis sets. Normally, the calculations were set up for 6 days and then restarted if required. Frequency and time-dependent density functional calculations can not be restarted, such that the calculations have to be set up for 6 -12 days by experience. Usually, we use between 12 and 40 nodes at the same time.

References

[1] a) Kricheldorf, H.R.: Chemosphere 2001, 43, 49; b) Kricheldorf, H. R.; Bornhorst, K. and Hachmann-Thiessen, H.: Macromolecules 2005, 38, 5017; c) Kricheldorf, H.R. and Rost, S.: Polymer 2005, 46, 3248; d) Kricheldorf, H.R.; Hachmann-Thiessen, H. and Schwarz, G.: Biomacromolecules 2004, 5, 492.

[2] Wu, J.; Yu, T.-L.; Chen, C.-T. and Lin, C.-C.:Coord. Chem. Rev. 2006, 250, 602.

[3] O'Kneefe, B. J.; Hillmyer, M. A. and Tolman, W.B.: Dalton Trans. 2001, 2215.

[4] Drumwright, R.W.; Gruber, P.R. and Henton, D.E.: Adv. Mat. 2000, 12, 1841.

[5] Mehta, R.; Kumar, V.; Bhunia, H.; Upadhyay, N.S. and Macromol, J.: Sci., Part C: Polym. Rev. 2005, 45, 325.

[6] Dechy-Carbaret, O.; Martin-Vaca, B. and Bourissou, D.: Chem. Rev. 2004, 104, 6147.

[7] Garlotta, D. and Polym, J.: Environ. 2001, 9, 63.

[8] Nakano, K; Kosaka, N.; Hiyama, T. and Nozaki, K.: Dalton Trans. 2003, 4039.

[9] Okada, M.: Prog. Polym. Sci. 2002, 27, 87.

[10] Jacobson, S.; Degée, Ph.; Fritz, H.G.; Dubois, Ph. And Jérôme, R.: Polym. Eng. Sci. 1999, 39, 1311.

[11] Mazarro, R.; de Lucas, A., Gracia, I.; Rodríguez, J.F.and Biomed, J.: Mat. Res. Part B: Appl. Biomat. 2007, 85, 196.

[12] Cheng, M.; Attygalle, A.B., Lobkovsky, E.B.; Coates, G.W. and Am, J.; Chem. Soc. 1999, 121, 11583.

[13] Chamberlain, B.M.; Cheng, M.; Moore, D.R.; Ovitt, T.M., Lobkovsky, E.B., Coates, G.W. and Am, J.: Chem. Soc. 2001, 123, 3229.

[14] Chisholm, M.H.; Gallucci, J.C.and Zhen, H.S.: Inorg. Chem. 2001, 40, 5051.

[15] Cole, S.C.; Coles, M.P. and Hitchcock, P.B.: Organometallics 2004, 23, 5159.

[16] Gupta, A.P. and Kumar, V.: Eur. Polymer J. 2007, 43, 4053.

[17] Börner, J.; Herres-Pawlis, S.; Flörke, U.; Huber, K. and Eur. J.: Inorg. Chem. 2007, 5645.

[18] a) Wittmann, H.; Schorm, A., Sundermeyer, J.: Z. Anorg. Allg. Chem. 2000, 626, 1583; b) Oakley, S. H.; Soria, D. B.; Coles, M. P. and Hitchcock, P. B.: Polyhedron 2006, 25, 1247; c) Wittmann, H.; Raab, V., Schorm, A.; Plackmeyer, J. and Sundermeyer, J.: Eur. J. Inorg. Chem. 2001, 1937; d) Aoki, S., Iwaida, K.; Hanamoto, N.; Shiro, M. and Kimura, E.: J. Am. Chem. Soc. 2002, 124, 5256; e) Ishikawa, T. and Kawahata, M.: EP 1752451A1, 2007.

[19] a) Köhn, U.; Schulz, M.; Görls, H. and Anders, E.: Tetrahedron: Asymmetry 2005, 16, 2125; b) Walter, M.; Wermann, K.; Lutsche, M.; Günther, W.; Görls, H. and Anders, E.: J. Org. Chem. 2006, 71, 1399.

[20] Coles, M. and Hitchcock, P.: Eur. J. Inorg. Chem. 2004, 2662.

[21] Ajellal, N.; Lyubov, D.M.; Sinenkov, M.A.; Fukin, G.K., Cherkasov, G.V.; Thomas, C.M.; Carpentier, C.F. and Trifonov, A.A.: Chem. Eur. J. 2008, 14, 5440.

[22] Kuhn, N.; Grathwohl, M.; Steinmann, M. and Henkel, G.: Z. Naturforsch. 1998, 53b, 997.

[23] a) Tamm, M.; Petrovic, D.; Randoll, S.; Beer, S., Bannenberg, T.; Jones, P.G. and Grunenberg, J.: Org. Biomol. Chem. 2007, 5, 523; b) Petrovic, D.; Hill, L.M.R.; Jones, P.G.; Tolman, W.B. and Tamm, M.: Dalton Trans. 2008, 887; c) Panda, T. K.; Hrib, C.G.; Jones, P.G.; Jenter, J.; Roesky, P.W. and Tamm, M.: Eur. J. Inorg. 2008, 4270.

[24] Herres-Pawlis, S.; Flörke, U. and Henkel, G.: Eur. J. Inorg. Chem. 2005, 3815.
[25] Herres-Pawlis, S.; Neuba, A., Seewald, O.; Seshadri, T.; Egold, H.; Flörke, U. and Henkel, G.: Eur. J. Org. Chem. 2005, 4879.
[26] Hoffmann, A.; Börner, J.; Flörke, U. and Herres-Pawlis, S.: Inorg. Chim. Acta, 2008, DOI: 10.1016/j.ica.2008.06.002
[27] Börner, J.; Flörke, U.; Döring, A.; Kuckling, D.; Jones, M.D. and Herres-Pawlis, S.: Sustainability 2009, in print.
[28] Börner, J.; Flörke, U.; Döring, A.; Kuckling, D. and Herres-Pawlis, S.: Macromol. Symp. 2009, submitted.
[29] Wortmann, R.; Herres-Pawlis, S., Flörke, U. and Henkel, G.: Manuscript in preparation.
[30] a) Neuba, A.; Haase, R.; Bernard, M.; Flörke, U. and Herres-Pawlis, S.: Z. Anorg. Allg. Chem., accepted; b) Raab, V.: Ph.D. Thesis, University of Marburg, 2001; c) Herres-Pawlis, S.: Ph.D. Thesis, University of Paderborn, 2005.
[31] Gaussian 03, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Jr., Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H., Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J.E.; Hratchian, H.P.; Cross, J.B., Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C., Ochterski, J.W.; Ayala, P.Y.; Morokuma, K.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Zakrzewski, V.G.; Dapprich, S., Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Kaghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S., Cioslowski, S.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M.A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, A.; Gill, P. M. W.; Johnson, B.; Chen, W., Wong, M.W.; Gonzalez, C. and Pople, J.A.: Gaussian, Inc., Wallingford CT, 2004.
[32] Frison, G.; Ohanessian, G. and Comput, J.: Chem. 2007, 29, 416.
[33] Wörl, S.; Hellwinkel, D., Pritzkow, H.; Hofmann, M. and Krämer, R.: Dalton Trans., 2004, 2750.
[34] Herres, S.; Flörke, U. and Henkel, G.: Acta Crystallogr., 2004, C60, o358 – o360.
[35] Raab, V., Kipke, J.; Gschwind, R.M. and Sundermeyer, J.: Chem. Eur. J., 2002, 1682.

6.5 Multiobjective Optimization for Transistor Sizing of CMOS Logic Standard Cells Using Set-Oriented Numerical Techniques

Project coordinator (Supervisor)	Prof. Dr. Ulrich Rückert, System and Circuit Technology, University of Paderborn, Prof. Dr. Dellnitz, Applied Mathematics, University of Paderborn
Project members (Scientists)	Dipl.-Math. Matthias Blesken, System and Circuit Technology, University of Paderborn Dipl.-Inf. Dominik Steenken, Applied Mathematics, University of Paderborn Dipl.-Math. Katrin Witting, Applied Mathematics, University of Paderborn

General Problem Description

The design of resource efficient integrated circuits (IC) requires solving a minimization problem of more than one objective given as measures of available resources. This multiobjective optimization problem (MOP) is formulated for the smallest unit, the standard cells, and by its solution the performance of the entire IC can be improved. The traditional way of sizing the transistors of a standard logic cell does not focus on the resources directly. In our work transistor sizing is approached via an MOP and solved by set-oriented numerical techniques. A comparison of the computed Pareto optimal designs to elements of a commercial standard cell library indicates that for some gates the performance can even be significantly improved.

Our techniques can be used not only to improve given standard cell libraries but they can also be used to develop new ones. Ongoing work includes the design of a sub-threshold standard cell library in a 65nm technology. Transistor sizing of sub-threshold standard cells for digital ultra-low power systems is a very challenging task because robustness has to be considered as an important design objective in addition to the conflicting resources power consumption and propagation delay. We regard this task as an MOP and show that the support of numerical algorithms for multiobjective optimization is necessary and beneficial in the design process of CMOS logic standard cells.

Problem Details and Work Done

First results and a description of the optimization algorithms used are published in [1]: To compute the Pareto set set-oriented numerical algorithms implemented in the software tool GAIO (Global Analysis of Invariant Objects, see www.math.upb.de/~agdellnitz) are applied. The exploration of the search space is done by iteratively dividing it. The new approach provides the designer with all possible sizings for a resource efficient CMOS logic gate. Our results particularly indicate that commercial logic gates can be improved.

For the computations we make use of two different types of set-oriented algorithms for the numerical approximation of the Pareto set. The subdivision algorithm quickly provides a general idea of the shape of the Pareto set. A subsequent run of the recovering algorithm is performed to further refine the approximation to a given accuracy.

1. The subdivision algorithm (cf. [2,3]): The principal approach of the subdivision algorithm we use for the computations can be characterized as follows: Based on a covering of the feasible parameter space (a box), the Pareto set is approximated numerically by a successive refinement and selection of boxes in parameter space. In each step, all boxes are bisected and test points are generated in each of these boxes. A non-dominance test is applied to the test points and dominated points are deleted. Afterwards empty boxes are deleted (see Figure 1).

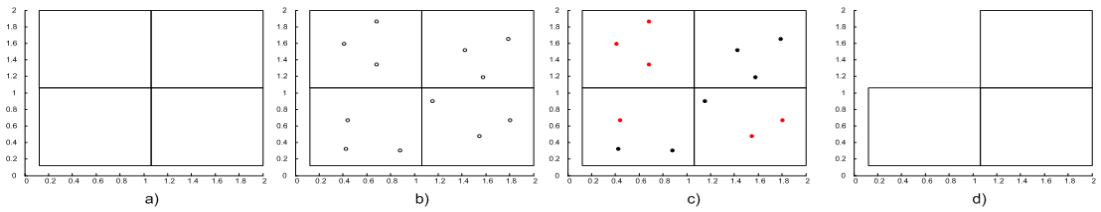


Figure 1 Steps of the subdivision algorithm

2. The recovering algorithm (cf. [2,3]): If one or a few Pareto points are already known, the recovering techniques allow the computation of those entire, connected components of the Pareto set that contain these points. For this, small boxes around the known points are defined, and other Pareto optimal points are generated by studying neighboring boxes. Here, again test points (in our case just one point at the center) are generated within a box of the desired size and its neighboring boxes. Boxes that contain non-dominated points are added to the box collection. This procedure is then repeated for

these new boxes. In case of a compact search space the algorithm terminates when no more boxes can be added. In Figure 2 the recovering process is illustrated.

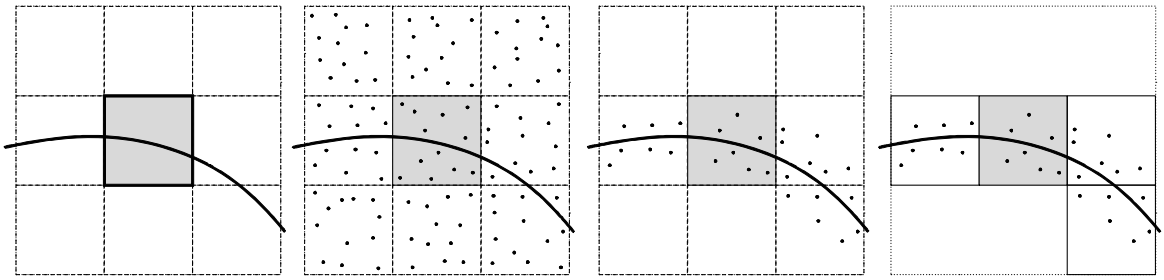


Figure 2 Steps of the recovering algorithm

We present results of inverters, NAND and NOR gates and compare them to gates in a commercial 65nm and in a 90nm CMOS technology standard cell library. The objective functions are given by the noise margin NM, the propagation delay t_{pd}, and the dynamic energy consumption $E_{in} + E_{dyn}$ induced by the input capacitance and current from supply voltage to ground. Computations have been run in two different setups. At first all widths of the nMOSFET W_n and pMOSFET W_p are set equal. Secondly, with respect to the bulk effect the width of the transistors connected in series are independent of each other. Thus, the search space expands to a third dimension. In the following, whenever reference cells will be compared to computed Pareto points, the Pareto points will be chosen to meet the same delay, meaning that they will have the same driving strength.

1. Two-dimensional search: The Pareto set and front of the 65nm CMOS inverter is shown in Figure 3. All four reference points from the commercial standard cell library can be improved since they lie outside the Pareto set. The distance to the Pareto front means that there are resource efficient inverters that will at the same time posess a higher noise margin, less delay time and less energy dissipation than the reference points. The Pareto set of the 90nm inverter looks similar. The advantages in noise margin NM and energy dissipation $E_{in}+E_{dyn}$ are up to 4%. Similar results were achieved for the 90nm inverter and the 65nm NOR gate. Points from the Pareto set could e.g. be chosen to be maximal in one objective while still maintaining optimal compromises in the others. Analogous computations for NAND cells and 90nm NOR cells show that the reference points of the chosen commercial library cannot be improved significantly. It turns out that almost all reference points lie on the Pareto set. However, our approach gives a global picture of all possible Pareto optimal solutions.

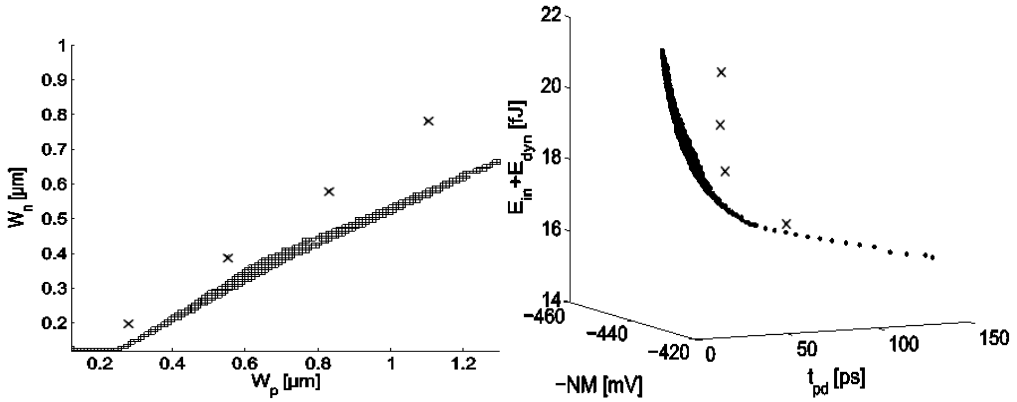


Figure 3 Pareto set and front of the 65nm NOR gate with reference points

2. Three-dimensional search: The multiobjective approach allows to add new search parameters without restating the design problem using the same GAIO algorithms. Therefore, the widths of transistors connected in series do not need to be equal. In fact, taking the bulk effect into account results in better performance. In Figure 4 we show how the Pareto front of the 65nm NOR gate improves from the setup with $W_{p1} = W_{p2}$ to W_{p1} independent of W_{p2}. Gates with equal driving strength reach a 7.8% higher noise margin and up to 4.4% lower energy dissipation.

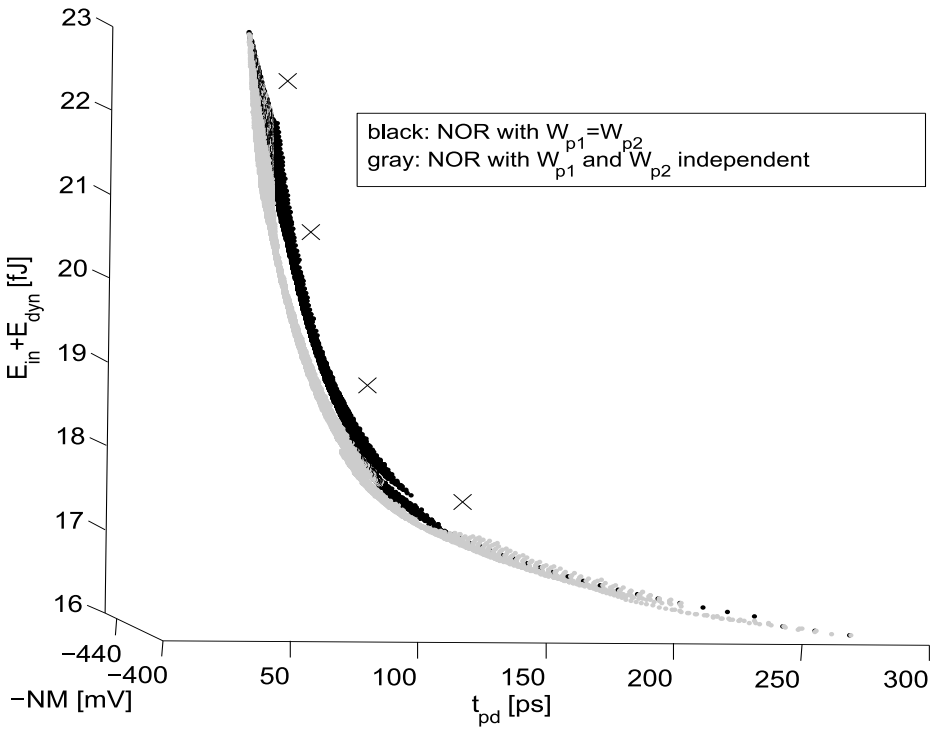


Figure 4 Pareto fronts of the 65nm CMOS NOR gate

A multiobjective approach has been used to improve the performance of simple logic cells with respect to noise margin, propagation delay and dynamic energy consumption. For the computation of the Pareto set set-oriented numerical techniques from the software tool GAIO have been used. A parallelized version of a subdivision and a recovering algorithm has been developed motivated by time consuming function evaluations. This parallelization made it possible to obtain good approximations of the Pareto set within adequate computational time. The results of the multiobjective optimization have been compared to elements of a commercial standard cell library. Even though the commercial cells have been designed with the know-how of decades, improvements in all considered objectives can be obtained for inverters and 65nm NOR gates. The approximation of Pareto sets for NAND and 90nm NOR gates has shown that almost all reference points of the standard cell library are Pareto optimal and thus cannot be improved further. However, our approach allows to provide a global picture of all Pareto optimal solutions. The GAIO algorithms can therefore be added to the design process of an IC as a valuable tool that provides a better view on the design space and more freedom to choose a solution with the desired performance. The multiobjective approach also is more flexible than the classic one. The number of free parameters and objectives can easily be increased. As we have seen in this work, a three-dimensional search improves the results of the two-dimensional search even further. Therefore, applications to more complex cells with more design parameters can be expected to have an even higher gain in their resource efficiency. Our techniques can be used not only to improve given standard cell libraries but they can also be used to develop new ones. Ongoing work includes the design of a sub-threshold standard cell library in a 65nm technology.

Resource Usage

In order to speed up the algorithms w.r.t. the time consuming function evaluation (1-3 seconds per simulated circuit), a parallelization infrastructure that allows to evaluate an arbitrary number of points simultaneously was implemented (cf. [4]). This infrastructure features a client interface within GAIO and a Compute Server which distributes work among a set of computation clients as indicated in Figure 5.

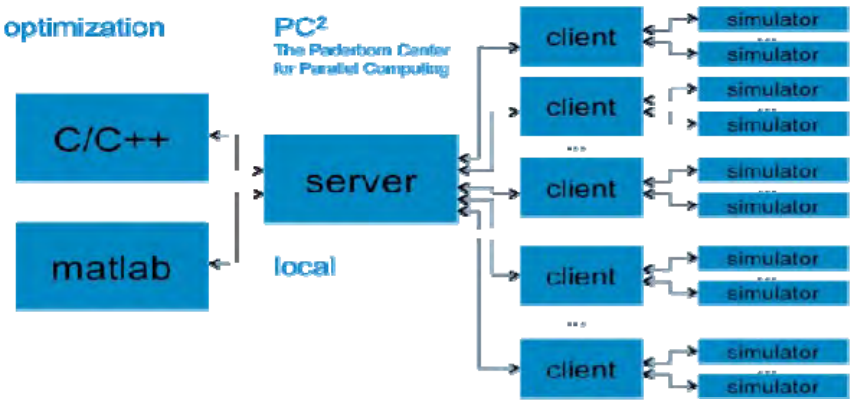


Figure 5 Distribution of circuit simulations

The clients then perform the actual simulations. The algorithms themselves were restructured to maximize the number of points that can be evaluated simultaneously. Due to the large time share of circuit simulations the speedup is almost linear with respect to the number of computation clients.

We use the arminus cluster of the PC^2 frequently on an almost daily basis. The computation time of the clients can be split into very small time intervals such that the clients can always be placed on at least a few available nodes in the ccs system. Due to the limited number of software licenses for the simulator the number of clients is bounded to 25.

References

[1] Blesken, M.; Rückert, U.; Steenken, D., Witting, K. and Dellnitz, M.: “Multiobjective Optimization for Transistor Sizing of CMOS Logic Standard Cells Using Set-Oriented Numerical Techniques,” NORCHIP Conference, 2009. 27th, 2009

[2] Dellnitz, M.; Schütze, O. and Hestermeyer, T.: Covering Pareto Sets by Multilevel Subdivision Techniques, Journal of Optimization, Theory and Applications, 124(1), pp. 113-136, 2005.

[3] Schütze, O.: Set Oriented Methods for Global Optimization, PhD thesis, University of Paderborn, Germany, 2004.

[4] Steenken, D.: Multiobjective Optimization and Sensitivity Evaluation of IC Standard Cells Using Set-oriented Numerical Methods, Diploma thesis, University of Paderborn, 2009.

6.6 Investigations towards the proton shuttle mechanism of the enzymatic phosphodiester cleavage of human RNase H

Project coordinator	Prof. Dr. Gregor Fels, University of Paderborn,
Project members	Dr. Brigitta Elsässer, University of Paderborn

General Problem Description

The genetic information of living cells is encoded in the DNA and is translated into proteins via messenger RNA-molecules (mRNA) that are copied from the DNA during transcription. Both, mRNAs as well as non-coding RNAs are degraded by Ribonuclease enzymes (RNase) as part of their life cycles, therefore these enzymes play a key role in the maturation and metabolism of all RNA molecules. RNase H belongs to the nucleotidyl-transferase (NT) superfamily and catalyses the cleavage of phosphodiester linkages of the RNA strand in the DNA:RNA hybrid duplex at its minor groove and specifically hydrolysis the P–O3' bond of the RNA chain behind each nucleoside. This process requires divalent metal ions, preferably Mg^{2+}.

In retroviruses, RNase H activity is encoded as a part of the reverse transcriptase (RT) that converts a retroviral single strained RNA genome into double strained DNA. Due to the RNase H activity in HIV reverse transcriptase (HIV-RT), it represents a promising target for anti-HIV drug design. In our study we focused on a computational investigation of the hydrolytic mechanism of *human* RNase HI (PDB Code 2QKK) as an essential step in RNA cleavage using a comprehensive QM/MM theoretical method that is based on high level DFT calculation of the interactions in the QM region and the inclusion of the interactions of the surrounding protein and solvent water in the MM region. Starting from the X-ray structure of the mutated enzyme-substrate complex we changed the enzyme into the active form to reach the reactant state. Using a series of constrained and relaxation steps we could model the product state and intermediate states. Finally we performed transition state search and energy barrier calculations over the rate limiting step of the reaction. Docking experiments supported the structure of the reactant state complex and verified the interactions between the enzyme and its substrate.

As an important biological molecule RNase H represent a key pharmaceutical targets and the understanding on a molecular basis is, therefore a keystone in the development of corresponding inhibitory drugs against disease like AIDS.

Problem Details and Work Done

Among the various known RNases H, *E. coli* RNase HI has been most extensively studied for structure-function relationships by X-ray analysis[1,2,3] site-directed mutagenesis,[4] and NMR studies[5]. Therefore, originally it has been the object of our studies. The crystal structures of *E. coli* RNase H were first determined in 1990 and revealed a novel *a b* fold containing a carboxylate triad in the catalytic center.[1,2] A similar fold and related active sites have can be found in other RNase enzymes[6-8,9] DNA transposases, and retroviral integrases.[10]

However, recently the first crystal structures of the catalytic domain mutant *human* RNase H[7] (Figure 1) and *Bacillus halodurans* RNase H[6] complexed with an RNA:DNA hybrid substrate was reported. The active site of *human* RNase H consists of the amino acids Asp145, Glu186, Asp210 and Asp274. These four carboxylate residues are highly conserved in the amino acid sequences of other RNase H proteins and are essential for the required activity.[1,7,9,11-13] Nowotny et al. have shown that the RNA strand of the hybrid duplex is recognized by the protein through its interaction with the 2'-OH groups, and catalytic action occurs via a two-metal ion mechanism[6,7,12,14] as proposed by Steitz.[15] The RNA-binding domain of human RNase H is responsible for the cleavage of the hetero duplex substrate between 7 and 12 nucleotides from the 3´-DNA/5´-RNA terminus.[16] However, the amino acids of the catalytic site are not involved in the substrate binding interaction.[17] An RNase H domain is also present at the C-terminus of retroviral reverse transcriptase and plays an essential role in converting a single-stranded retroviral genomic RNA into a double-stranded DNA for integration into host chromosomes.[18] In vivo studies demonstrated that inactivation of RNase H results in non-infectious virus particles.[19,20] Inhibitors of this enzyme could therefore provide new drugs against diseases like HIV. Their design necessitates a detailed understanding of the underlying enzymatic mechanism.

Although RNase H enzymes play an important role in a wide range of cellular and retroviral functions and in gene therapy, the mechanism of the metal-dependent catalysis pathway still remains in question. It has been proposed that RNase H requires two Mg^{2+} ions for the catalytic activity from which the first Mg positions the attacking water, and the second Mg^{2+} destabilizes the substrate, while the two ions together stabilize the intermediate structure and the transition states.[4,21-23] However, there is not much of computational evidence on this topic.

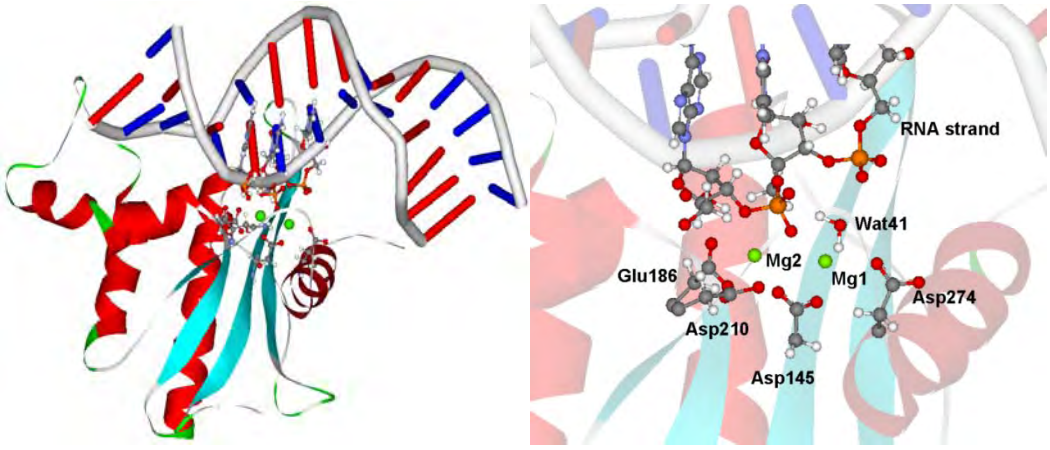
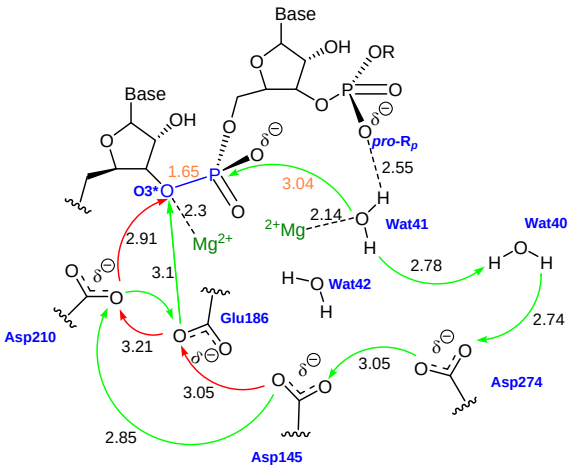


Figure 1. Structure of *human* RNase H. (Left) Cartoon of the RNase H (cartoon) RNA:DNA hydride complex (tubes with ladder) and the active site residues, Mg^{2+} (green), water and RNA are represented by balls and sticks. (Right) Close up of the catalytic pocket showing the conserved key carboxylate residues, and the magnesium ion (green), which participate in the catalytic action.

We employed a DFT/B3LYP quantum mechanical/molecular mechanics (QM/MM) approach using the extensive functionality provided by the recently developed QM/MM[24,25] modules in the NWChem[26] software package to simulate the attack of the nucleophil on the scissile phosphate and the proton transfer from the attacking water molecule to the 3'-oxygen of the released ribose. In order to explore the reaction mechanism in atomistic details we treated the protein and nucleotide groups that are candidates for participating in the chemical reaction quantum chemically and the surrounding protein with the solvent environment was described by the methods of molecular mechanics. To transfer the proton according to Scheme 1 the so called "spring method" was applied. In this method one or more harmonic restraints between the affected atoms were imposed to drive the system over several intermediates and reaction barriers to the intermediate and product state while at the same time allowing the MM system (initially equilibrated to the reactant structure) to adjust to the changes. In the simplest case, when only one spring was applied we set a constraint for the desired P–O or O–H distance. In further experiments we used a new feature of NWChem[26] to set more springs at the same time. In this second method the desired P–O or O–H distance is not a fixed value but an interval in which the system is allowed to find a local minimum. When a reasonable estimate of each constrained stage is obtained, the constraints will be lifted, and the system is going to be optimized using a sequence of optimizations and dynamical relaxation steps

RNase H cleaves the phosphodiester linkages between any two nucleotides specifically in the RNA strand of the RNA:DNA hybrid duplex. The catalytic process is initiated by a nucleophilic attack on the phosphorous, where the nucleophilic species could be either a water molecule (Wat41) or a hydroxide ion generated by the dissociation of a solvent water molecule from the vicinity. A possible catalytic

mechanism for the hydrolysis proceeds via nucleophilic attack of an OH^- group on the scissile phosphorous accompanied by a proton hopping mechanism that shuttles the proton from the water molecule to the O3e catalytic process is initiated by a nucleophilic attack on the phosphorous,$^{2+}$ ions present in the active site support the formation of a stable associated in-line S_N2-type phosphorane intermediate as well as each of the proton hopping stage (see scheme 1).



Scheme 1. Reactant state active site of the RNase H RNA:DNA hybride and the possible proton hopping pathways for the O3′−P cleavage: Pathway A follows the green arrows, pathway B deviates at Asp145 via the red arrows and proceeds from there via Glu186 and Asp210 towards O3′. In both cases Wat41 delivers the attacking nucleophile and the proton. Black and orange numbers are distances between the heavy atoms.

Since the existence of a free OH^- in a biological system is not very likely, therefore we suggest that water rather than a hydroxide ion is the nucleophile that attacks the phosphorous and the nucleophilic water is likely to deprotonate in the course of the attack. We have, therefore, looked for a pathway the proton could take from the water molecule to the O3′ oxygen, and – at least at that time – we have found the proton hopping mechanism as the only plausible way to shuttle the proton over quite some distance as summarized in Scheme 1. To explore the mechanism of the proton transfer first we applied a series of constraint between the migrating hydrogen atom and the oxygen of the given amino acid residue or the cleaved nucleotide. In a subsequent calculation the spring was eliminated and system was optimized to generate a stabile intermediate along the reaction coordinates.

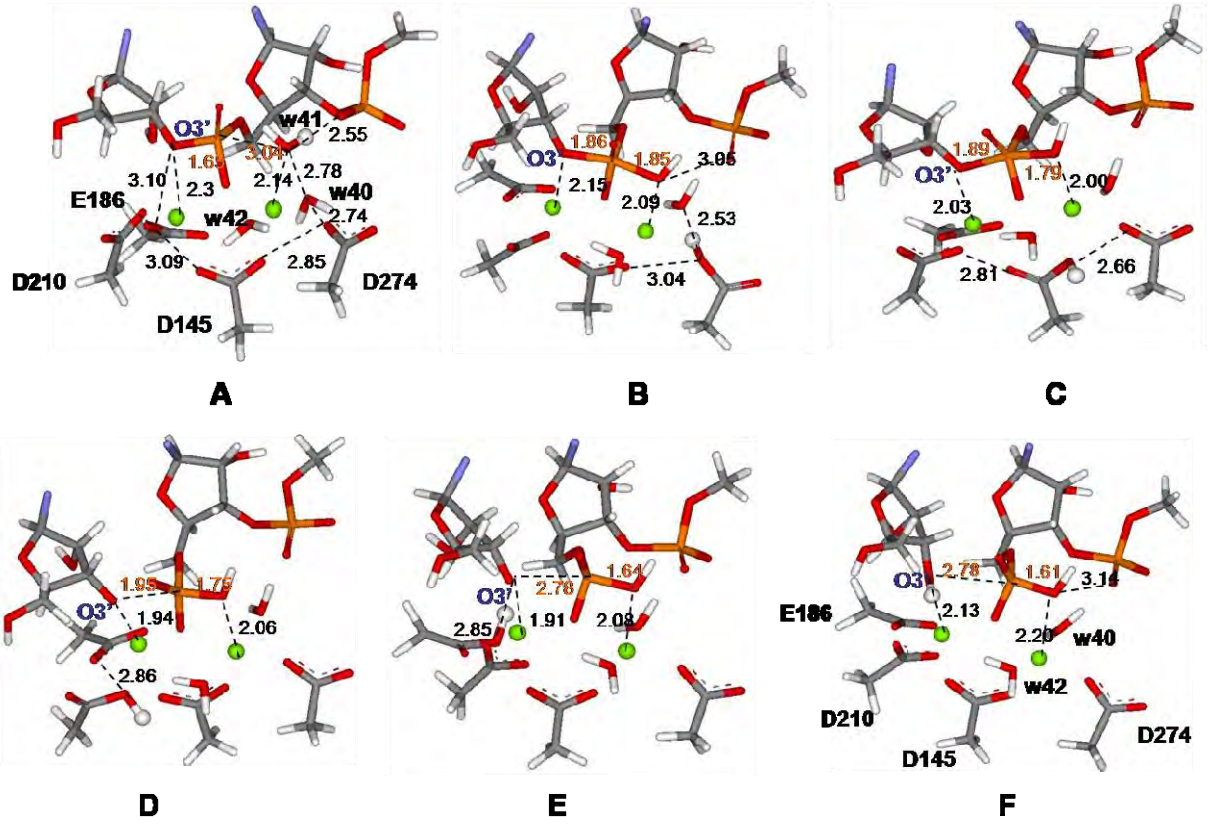


Figure 2. Energy optimized structures of reactant state (**A**), reaction intermediates (**B-E**) and product state (**F**) for the O3'−P cleavage. Black numbers depict H-bond distances; orange numbers are P−O bond lengths. The structures of A-F correspond to the QM region in each calculation. The bonds between the QM and MM region are capped with H-atoms.

In our simulations the proton from Wat41 was shuttled to the O3'-oxygen by a cascade of proton hopping steps that proceeds from Wat40 via Asp274, Asp145, Asp210 and Glu186 to its final destination at O3' (Figure 2, **A-F**). We could identify three stable intermediate structures along the reaction coordinate and we suppose that the rate-limiting highest energy barrier is the initial step of the catalytic cascade, i.e. the formation of the nucleophil and the first proton transfer. At point **F** the reaction is completed and the residues returned back almost exactly to their original positions as in the reaction state (for the corresponding RMSD values see Figure 3) while the two divalent metal ions shifted away from the O3' and O3P atoms. Therefore, after the cleaved nucleotide is displaced from the active site a new nucleotide can approach and the catalytic cascade can start all over.

Figure 3 shows the QM/MM energy profile for the hydrolysis reaction of RNase H as described above. After each proton hopping step we performed free energy calculations in order to estimate the total QM/MM energy levels corresponding to reaction states **A-F** of the proposed mechanism. Although we did find stable intermediates for each single step described in the scheme (Scheme 1 and Figure 2) and distances that very well match all requirements of the proton

hopping mechanism, the corresponding energy landscape as derived from free energy calculation yielded a rather high energy difference between the initial structure (**A**) and the first stable (and highest energy) intermediate (**B**) of about 30 kcal/mol with a barrier height of 40 kcal/mol. There is no experimental data for the exact energetics of each RNase H activity, therefore the comparison of the calculated reaction free energy is very limited. Shaw-Reid et al.[27] studied the *in vitro* RNase H cleavage rates of HIV-1 Reverse-Transcriptase enzyme using fluorescent resonance energy transfer method by examining the effects of different RNA:DNA substrate sequence and length. Although our calculated values are in the range of metal complexed hydrolysis reactions (~34-42 kcal/mol)[28-30] these are significantly higher than experimental estimates for the analogous hydrolysis by RNase H of *Bacillus halodurans*.[31]

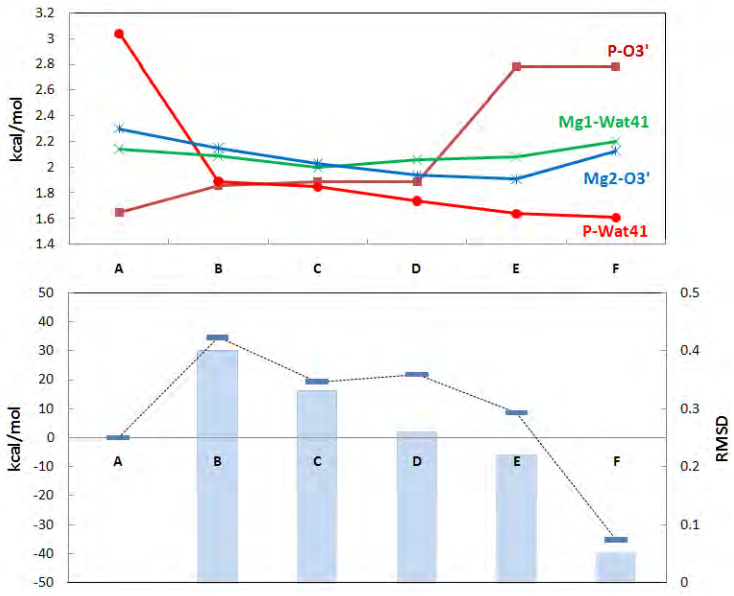


Figure 3. Top: P−O and Mg−O distances of the most relevant bonds along the reaction coordinate. Bottom: Energy level diagram for the proton transfer steps, and RMSD values (for all atoms) of the QM region amino acid residues, in comparison with the reactant stage structure. Note that the residues return to their original places after the reaction is completed. The structures of **A-F** correspond to the intermediate structure (see the attached manuscript)

Resource Usage

For our calculations the highly parallel software package of NWChem[26] was used installed on the Arminius cluster at the Paderborn Centre for parallel computing (PC²) (hpcLine, Xeon EM64T 3.2 GHz, 2.6 TFlop Fujitsu Siemens Cluster with 400 processors). The resources were used daily.

References

[1] Katayanagi, K.; Miyagawa, M.; Matsushima, M.; Ishikawa, M.; Kanaya, S.; Ikehara, M.; Matsuzaki, T. and Morikawa, K.: Nature 1990, 347, 306-309.
[2] Yang, W.; Hendrickson, W. A.; Crouch, R. J. and Satow, Y.: Science 1990, 249, 1398-1405
[3] Katayanagi, K.; Miyagawa, M.; Matsushima, M.; Ishikawa, M.; Kanaya, S.; Nakamura, H.; Ikehara, M.; Matsuzaki, T. and Morikawa, K.: Journal of Molecular Biology 1992, 223, 1029-1052
[4] Kanaya, S.; Kohara, A.; Miura, Y.; Sekiguchi, A.; Iwai, S.; Inoue, H.; Ohtsuka, E. and Ikehara, M. Journal of Biological Chemistry 1990, 265, 4615-4621.
[5] Oda, Y.; Iwai, S.; Ohtsuka, E.; Ishikawa, M.; Ikehara, M. and Nakamura, H.: Nucleic Acids Research 1993, 21, 4690-4695.
[6] Nowotny, M.; Gaidamakov, S. A.; Crouch, R. J.; Yang, W. Cell 2005, 121, 1005-1016.
[7] Nowotny, M.; Gaidamakov, S. A.; Ghirlando, R.; Cerritelli, S. M.; Crouch, R. J.; Yang, W. Molecular Cell 2007, 28, 513-513.
[8] Lai, L.H.; Yokota, H.; Hung, L.W.; Kim, R.and Kim, S.H.: Structure with Folding & Design 2000, 8, 897-904
[9] Ishikawa, K.; Okumura, M.; Katayanagi, K.; Kimura, S.; Kanaya, S.; Nakamura, H. and Morikawa, K.: Journal of Molecular Biology 1993, 230, 529-542.
[10] Lai, L. H.; Yokota, H.; Hung, L. W.; Kim, R. and Kim, S. H. Structure with Folding & Design 2000, 8, 897-904.
[11] Rice, P. A. and Baker, T. A.: Nature Structural Biology 2001, 8, 302-307.
[12] Hostomska, Z.; Matthews, D. and Hostomsky, Z.: Journal of Acquired Immune Deficiency Syndromes and Human Retrovirology 1993, 6, 673-673.
[13] Nowotny, M. and Yang, W. Embo Journal 2006, 25, 1924-1933.
[14] Pari, K.; Mueller, G. A.; DeRose, E. F.; Kirby, T. W. and London, R. E.: Biochemistry 2003, 42, 639-650.
[15] Yang, W.; Lee, J. Y. and Nowotny, M.: Molecular Cell 2006, 22, 5-13.
[16] Steitz, T. A. and Steitz, J. A. Proceedings of the National Academy of Sciences of the United States of America 1993, 90, 6498-6502.
[17] Yang, W.; Lee, J. Y. and Nowotny, M.: Molecular Cell 2006, 22, 5-13.
[18] Steitz, T. A. and Steitz, J. A.: Proceedings of the National Academy of Sciences of the United States of America 1993, 90, 6498-6502.
[19] Wu, H. J.; Lima, W. F. and Crooke, S. T.: Journal of Biological Chemistry 2001, 276, 23547-23553.
[20] Katayanagi, K.; Okumura, M. and Morikawa, K.: Proteins-Structure Function and Genetics 1993, 17, 337-346.
[21] Hughes, S. H.; Arnold, E.; Hostomska, Z. In Ribonuclease H; Crouch, R. J. and Toulme, J. J.: Eds.; INSERM: Paris, 1998, p 195-224.
[22] Schatz, O.; Cromme, F. V.; Gruningerleitch, F. and Legrice, S. F.: J. Febs Letters 1989, 257, 311-314.
[23] Tanese, N. and Goff, S. P.: Proceedings of the National Academy of Sciences of the United States of America 1988, 85, 1777-1781.
[24] Nakamura, H.; Oda, Y.; Iwai, S.; Inoue, H.; Ohtsuka, E.; Kanaya, S.; Kimura, S.; Katsuda, C.; Katayanagi, K.; Morikawa, K.; Miyashiro, H. and Ikehara, M.: Proceedings of the National Academy of Sciences of the United States of America 1991, 88, 11535-11539.
[25] Oda, Y.; Yoshida, M. and Kanaya, S. Journal of Biological Chemistry 1993, 268, 88-92.

[26] Hughes, S. H.; Arnold, E. and Hostomska, Z.: In Ribonuclease H; Crouch, R. J., Toulme, J. J., Eds.; INSERM: Paris, 1998, p 195-224.
[27] Schatz, O.; Cromme, F. V.; Gruningerleitch, F. and Legrice, S. F.: J. Febs Letters 1989, 257, 311-314.
[28] Tanese, N. and Goff, S. P.: Proceedings of the National Academy of Sciences of the United States of America 1988, 85, 1777-1781.
[29] Nakamura, H.; Oda, Y.; Iwai, S.; Inoue, H.; Ohtsuka, E.; Kanaya, S.; Kimura, S.; Katsuda, C.; Katayanagi, K.; Morikawa, K.; Miyashiro, H. and Ikehara, M.: Proceedings of the National Academy of Sciences of the United States of America 1991, 88, 11535-11539.
[30] Oda, Y.; Yoshida, M. and Kanaya, S.: Journal of Biological Chemistry 1993, 268, 88-92.
[31] Uchiyama, Y.; Miura, Y.; Inoue, H.; Ohtsuka, E.; Ueno, Y.; Ikehara, M. and Iwai, S.: Journal of Molecular Biology 1994, 243, 782-791.
[32] Valiev, M.; Garrett, B. C.; Tsai, M. K.; Kowalski, K.; Kathmann, S. M.; Schenter, G. K. and Dupuis, M.: Journal of Chemical Physics 2007, 127, -.
[33] Valiev, M.; Kawai, R.; Adams, J. A. and Weare, J. H.: Journal of the American Chemical Society 2003, 125, 9926-9927.
[34] Bylaska, E. J. d. J., W.; Aprà, E.; Windus, T.L.; Straatsma, T.P.; Hirata, S.; Valiev, M.; Hackler, M.; Pollack, L.; Kowalski, K.; Harrison, R.; Dupuis, M.; Smith, D.M.A; Nieplocha, J.; Tipparaju V.; Krishnan, M.; Auer, A.A.; Brown, E.; Cisneros, G.; Fann, G.; Fruchtl, H.; Garza, J.; Hirao, K.; Kendall, R.; Nichols, J.; Tsemekhman, K.; Wolinski, K.; Anchell, J.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsel, H.; Deegan, M.; Dyall, K.; Elwood, D.; Glendening, E.; Gutowski, M.; Hess, A.; Jaffe, J.; Johnson, B.; Ju, J.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nakajima, T.; Niu, S.; Rosing, M.; Sandrone, G.; Stave, M.; Taylor, H.; Thomas, G.; van Lenthe, J.; Wong, A. and Zhang, Z.: Version 5.1 ed.; Pacific Northwest National Laboratory: Richland, Washington 99352-0999, USA, 2007
[35] Shaw-Reid, C.A.; Munshi, V., Graham, P., Wolfe, A., Witmer, m.; Danzeisen, R., Olsen, D.B.; Carroll, S.S.; Embrey, M.; Wai, J.S.; Miller, M.D.; Cole, J.L. and Hazuda, D.J.: Journal of Biological Chemistry 2003, 278, 2777-2780.
[36] Akola, J. and Jones, R. O.: Journal of Physical Chemistry B 2003, 107, 11774-11783.
[37] Amano, T.; Ochi, N.; Sato, H.; Sakaki, S. Journal of the American Chemical Society 2007, 129, 8131-8138.
[38] Lia, R.Z.; Yu, J.G.; Raushel, F.M.; Himo, F.: Chemistry-a European Journal 2008, 14, 4287-4292.
[39] Lima, W. F.; Wu, H. J.; Nichols, J. G.; Prakash, T. P.; Ravikumar, V. and Crooke, S. T.: Journal of Biological Chemistry 2003, 278, 49860-49867.

6.7 Investigating issues of tautomerism and isomerism by quantum chemistry

Project coordinator	Prof. Dr. Gütschow, Pharm. Inst., University of Bonn
Project members	Dr. Paul W. Elsinghorst, Pharm. Inst., University of Bonn

General Problem Description

The project addresses issues of tautomerism and isomerism and their contribution to small molecule-protein interactions. While tautomerism reflects the possibility of one molecule to exist in more than one constitution with respect to where hydrogen atoms are present within their structure, isomerism gives rise to more than one spatial structure of a molecule that may or may not be interconvertible at ambient temperature. The interaction of small molecules, *e.g.* endogenous substances, pharmaceuticals or toxins, with their target proteins, *e.g.* enzymes or receptors, is – from a chemical point of view – basically the result of an energetically favorable complex of the two. Their interaction is driven by a complex interplay related to hydrophobic, electrostatic, or dipole-dipole attractions and hydrogen bonds.

During the last two decades medicinal chemistry has developed sophisticated *in silico* techniques to explore small molecule-protein interactions from a theoretical point of view. What is nowadays referred to as molecular docking or molecular dynamics plays a key role in modern drug development. The software tools available basically take the three-dimensional structure of a small molecule and a protein and search for a favorable complex by twisting/bending their structures according to chemical and/or physical laws. The results accuracy depends very much on the quality of the input structures.

With respect to tautomerism some of the software tools available can generate possible tautomers of one structure, but usually do not consider their energetic likeliness. Thus, comparing theoretically possible tautomers regarding to their intrinsic energy states and interconvertability at room temperature, will probably rule out some of them. Isomerism can also be temperature-dependent. Bonds within a molecular structure may cause rotational barriers, *i.e.* the parts of both ends of a bond may not rotate freely around their connecting bond because of spatial clashes between them. Rotational barriers may be overcome by twisting/bending the molecular structure at a certain energy cost. If room temperature can not afford this energy cost, the resulting two structures are referred to as atropisomers and need to be considered separately.

Quantum chemical software packages include suitable techniques to assess the energetic state associated with possible tautomers/isomers of small molecules. Their high demand of computational resources limits the use on standalone PC's and makes them predestined to HPC systems. Two well established software packages (GAUSSIAN03, ORCA) were used in this project to address two real-world problems in combination with other *in silico* methods and experimental data.

Problem Details and Work Done

A. (see also ref. 1)

2-(Benzoylimino)-3-(*o*-cyanoaryl)thiazolidin-4-ones **4** were obtained when reacting *N*-benzoyl-*N'*-(*o*-cyanoaryl)thioureas with ethyl bromoacetate under alkaline conditions (Figure 1). Atropisomerism in the 3-(*o*-cyanoaryl)thiazolidin-4-ones **4a**,**b**,**g** was influenced by the size of the *o*-cyanoaryl ring, and was investigated by means of NMR measurements and theoretical calculations.

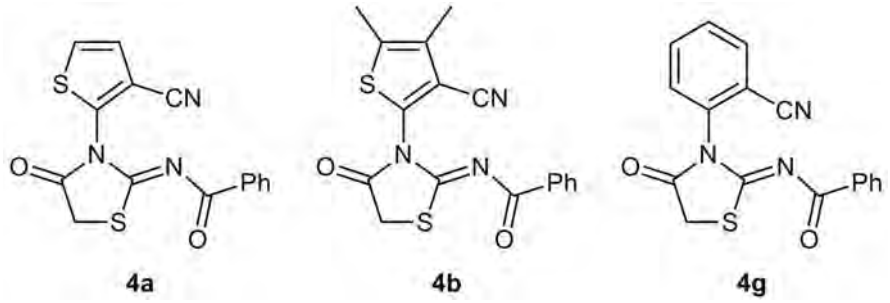


Figure 1 *Three* N-*benzoyl*-N'-*(*o*-cyanoaryl)thioureas, **4a**,**b**,**g** were chosen to investigate their rotational barriers around the ring connecting bond.*

DFT calculations were carried out using GAUSSIAN03 to affirm the NMR based hypothesis, that an internal rotational barrier between the nitrile group and the carbonyl and acylimino function of the thiazolidin-4-one lead to atropisomers. On the basis of their crystal structures, *Z*-configured **4a**,**b**,**g** were used for a relaxed potential energy surface (PES) scan at BP86/LANL2DZ level, where a 5° stepwise complete rotation of the dihedral angle φ regarding the C–N bond connecting the cyanoarene and the thiazolidin-4-one was applied (Figure 2).

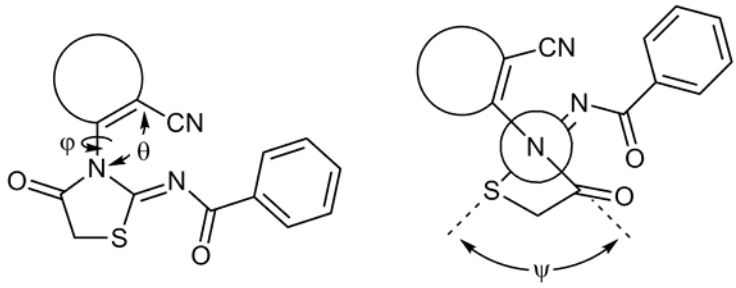


Figure 2 Thiazolidin-4-ones 4a, 4b, and 4g with the rotation angle φ. The compounds differ with respect to the angle θ defining how close the nitrile is bent towards the thiazolidin-4-one and with respect to ψ. The dihedral angle ψ is defined by the bond vectors connecting the four atoms C(=O)–N–C(=N)–S of the thiazolidin-4-one moiety.

Rotamers close to the transition state were identified from PES scans and subsequently subjected to transition state optimization at the B3LYP/6-311G** level of theory or additional PES scans at the B3LYP/6-311G** level, if no transition state was reached. Frequency calculations were then carried out for transition states and B3LYP/6- 311G** optimized maxima as well as minima to provide free energy values for the rotational barriers. Minima obtained by DFT optimization closely resembled the crystal structures with RMSD values lower than 1 Å (Table 1).

Compound	RMSD (Å)	Bond angles (°)		Internal rotational barriers (°, kJ/mol)			
		θ	ψ	$\varphi_{carbonyl}$	$\Delta G^{‡}_{rot,\ carbonyl}$	φ_{imine}	$\Delta G^{‡}_{rot,\ imine}$
4a	0.512	125.9	2.7	198	64	350	59
4b	0.459	124.2	6.0	199	66	350	67
4g	0.438	120.1	1.4	187	87	348	95

Table 1 RMSD values of optimized minima and crystal structures, as well as relevant bond angles, internal rotational barriers and corresponding energies of compounds **4a**, **4b** and **4g**.

Two rotational barriers were observed, at φ ~ 190° and φ ~ 350°, corresponding to the steric proximity of the cyano and carbonyl group and a clash between the cyano and imine group, respectively. A minor shift of the rotational barriers was observed when **4a**, **4b**, and **4g** were compared. This might be attributed to a slight tilt of the thiazolidin-4-one ring, defined by the dihedral angle ψ. The combination of the three angles φ, θ, and ψ describes the vicinity of the cyano and carbonyl/imine moieties,

and thus serves as a measure of how close the functional groups are to each other (Figure 2).

Compared to **4a** and **4b**, the corresponding $\Delta G^{\ddagger}_{rot}$ values of compound **4g** increased significantly (64/59 and 66/67 versus 87/95 kJ/mol). This was mainly attributed to the decreased θ value for **4g** (124.2 and 125.9 versus 120.1°), thus resulting in hindered rotation of **4g**. The calculations for **4a**, **4b**, and **4g** were consistent with the spectroscopic data of the thiazolidin-4-ones. On the one hand, the five-membered cyanothienyl derivatives **4a**,**b** did not form stable atropisomers at room temperature, since the larger angle θ allowed the substituents to pass each other. On the other hand, the six-membered cyanophenyl derivative **4g** with a smaller θ value had sufficient steric repulsion for hindered rotation and was a axially chiral racemate. Accordingly, **4g** showed diastereotopic methylene protons in its ^{1}H-NMR spectrum. Additionally, NMR experiments showed that rotation in **4a** could not be restricted at lower temperature down to -40 °C, nor that rotation was allowed in **4g** at higher temperature up to 70 °C.

B. (see also ref. 2)

Cholinesterases are involved in the pathological formation of β-amyloid plaques. To investigate this pathohistological hallmark of Alzheimer's disease we prepared a high-affinity, fluorescent cholinesterase inhibitor. Its fluorescence intensity was significantly enhanced upon binding to cholinesterases. Using this probe, brain samples from mice and humans affected by Alzheimer's disease were successfully analyzed for β-amyloid plaques. Unexpectedly, it was discovered, by competition experiments, that the compound binds to amyloid structures, rather than to cholinesterases inside of the plaques.

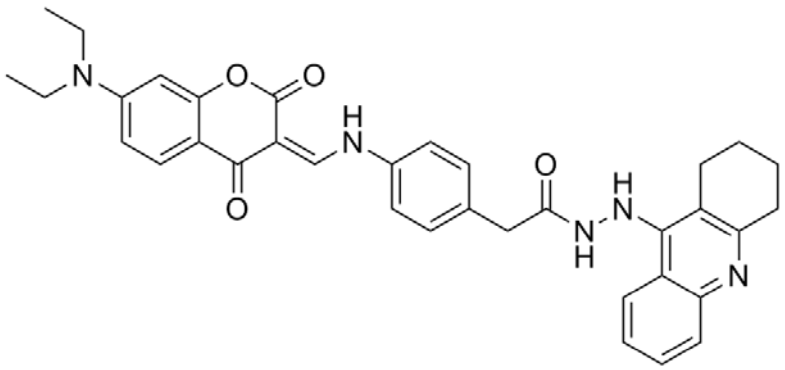
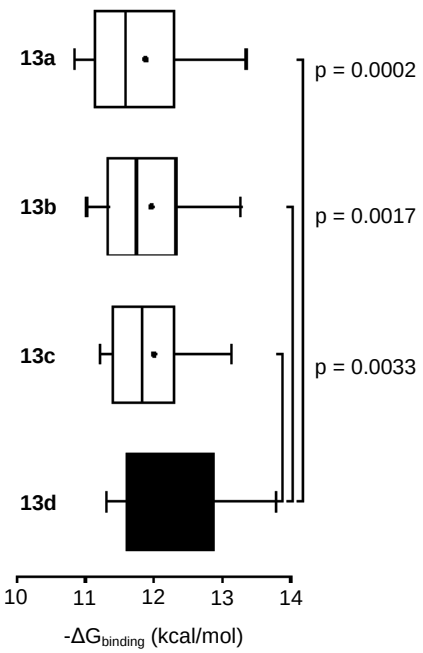
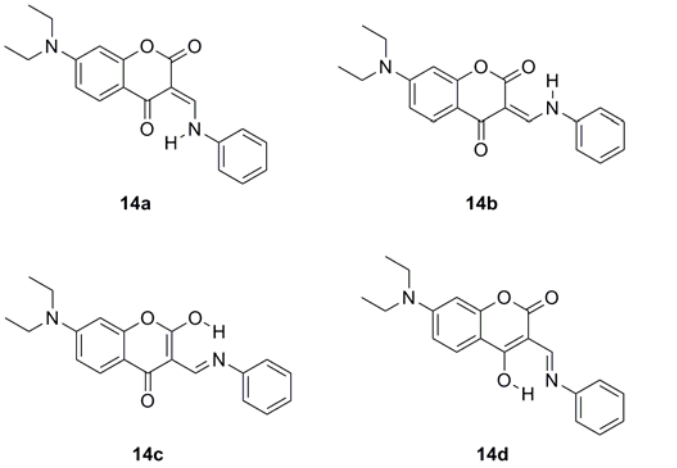


Figure 3 Structure of 13, a heterodimeric, fluorescent AChE inhibitor developed to investigate brain samples with respect to the distribution of β-amyloid plaques in vivo.

To affirm the anticipated dual binding mode of 13 with respect to the two binding sites offered by AChE, a molecular docking approach was undertaken. Special attention was paid to possible tauto-mers of the β,β-diacyl enamine moiety that renders 13 a versatile hydrogen bonding partner at the PAS. These structures exist with respect to E/Z-isomerism at the enamine bond and also with regard to keto–enol tautomerism of the 4-hydroxycoumarin moiety.





Hybrid Function	Energy difference **14** (kcal/mol)		
	a *vs.* **d**	**b** *vs.* **d**	**c** *vs.* **d**
B3LYP/6-311++G**	+ 5.7897	+ 4.8543	– 7.1837
B3PW91/6-311++G**	+ 5.1596	+ 4.1606	+ 4.1915

Table 2 All tautomers **13a-d** (structures analog to **14a-d**) were docked into AChE. Statistical analysis of the upper quartile was applied to select the most appropriate tautomer for detailed investigation (shaded boxplot; one-way ANOVA p = 0.0004, unpaired t-test results inside the Figure). Energy differences between tautomers **14a-d** were calculated by DFT.

All tautomers **13a-d** were docked to acetylcholinesterase in a primary study to compare the results by statistical means. The 4-hydroxycoumarin tautomer **13d** was ranked significantly higher as measured by the total estimated energy freed upon binding (Table 2). To verify that this ranking was not because of intramolecular energy consumption, but due to favorable protein-directed hydrogen bonding, the intramolecular energy differences were also estimated by quantum chemistry. The energy differences calculated from a set of simplified tautomers **14** representing the β,β-diacyl enamine moiety of **13** are listed in Table 2. At B3LYP/6-311++G** and B3PW91/6-311++G** level of theory, all energy differences were found within a range of 7 kcal/mol, *i.e.* below the estimated total energies of approximately 12 kcal/mol freed upon binding and structure **13d** might be adopted as a result of hydrogen bonding. Subsequently, an in-depth investigation of the binding of **13d** to AChE was carried out. The results of which are reported elsewhere.

C. (see also ref. 3)

Both, taxifolin and alphitonin appear as native constituents of plants and were previously described as quercetin metabolites of intestinal bacteria. Taxifolins refer to the trans-configured diastereomers of dihydroquercetin, whereas the cis-configured ones are called epitaxifolins. A complex interplay of racemization and epimerization connects all diastereomers **1**-**4** through at least one intermediate **5** of so far unknown structure. In addition, taxifolin may undergo a ring contraction to produce alphitonin **6**, a benzofuranone. This reaction can either be achieved at elevated temperature or by action of a partially purified enzyme preparation from Eubacterium ramulus.

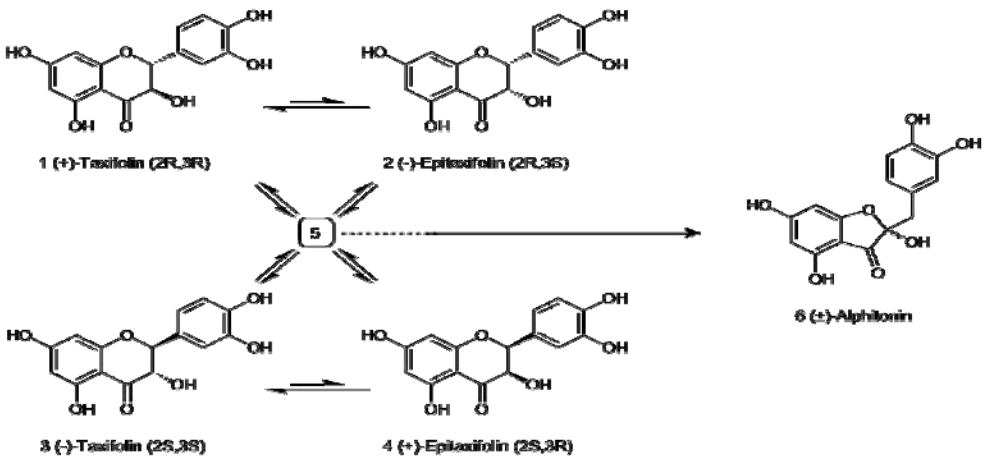


Figure 5 All calculations were carried out using ORCA applying a COSMO environment to simulate a methanolic solution. Briefly, PES scans were carried out at BP86/SVP level of theory. Energy minima were selected by visual inspection and subjected to further refinement at B3LYP/TZVP level of theory. CD spectra were obtained from these structures using a TDDFT/B3LYP/TZVP approach and were weighted according to their RI-SCS-MP2/TZVP energies.

To elucidate the conversion of taxifolin to alphitonin on a molecular basis we established a chiral HPLC system capable of separating all taxifolin diastereomers. Theoretically predicted CD spectra were acquired to assign each structure to the CD recording from the HPLC. Therefore, minimum energy conformers were obtained from PES scans simulating a full rotation of the B–C ring connecting bond (Figure 5, left). Corresponding CD spectra were weighted by Boltzmann statistics and compared to literature assignments (Figure 5, right).

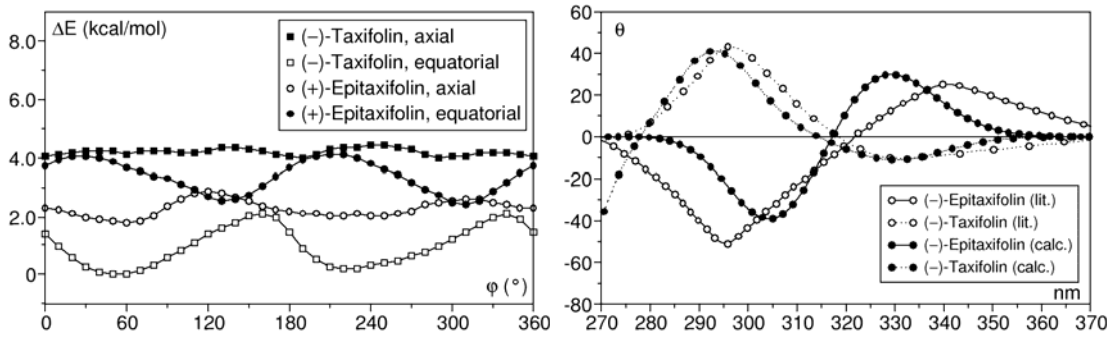


Figure 5 All calculations were carried out using ORCA applying a COSMO environment to simulate a methanolic solution. Briefly, PES scans were carried out at BP86/SVP level of theory. Energy minima were selected by visual inspection and subjected to further refinement at B3LYP/TZVP level of theory. CD spectra were obtained from these structures using a TDDFT/B3LYP/TZVP approach and were weighted according to their RI-SCS-MP2/TZVP energies.

Resource User

cluster: Arminius, software: Gaussian, Orca

References

[1] Häcker, H.-G.; Elsinghorst, P.W.; Michels, S.; Daniels, J.; Schnakenburg, G. and Gütschow. M.: 2-(Benzoylimino)thiazolidin-4-ones: formation by an alternative ring closure and analysis of rotational barriers. Synthesis 2009, 1195–1203.

[2] Elsinghorst, P.W.; Härtig, W.; Goldhammer, S.; Grosche, J. and Gütschow, M.: A gorge-spanning, high-affinity cholinesterase inhibitor to explore β-amyloid plaques. Org. Biomol. Chem. 2009, 7, 3940–3946.

[3] Elsinghorst, P.W.; Cavler, T.; Müller, A.; Blaut, M.; Braune, A. and Gütschow, M.: The rearrangement of taxifolin to alphitonin: chiral investigations. Lebensmittelchemikertag, 2009, poster AT48.

6.8 Two-Dimensional Fourier-Transform Spectroscopy of Semiconductor Quantum Wells

Project coordinator	Jens Förstner, Department Physik, University of Paderborn Torsten Meier, Department Physik, University of Paderborn
Project members	Irina Kuznetsova, Department Physik, University of Paderborn
Supported by:	DFG through the Emmy-Noether junior research group “Computational Nanophotonics” of Jens Förstner (FO 637/1-1) and the research training group GRK 1461 “Micro- and Nanostructures in Optoelectronics and Photonics

Introduction

Since a few decades, physicists, chemists, biologists, and engineers strive for an understanding of material properties on the basis of their atomic or molecular structure. The mechanical, electrical, optical and further properties of material systems are determined by the arrangements of constituents on the nanoscale and their dynamical interactions. Nanostructures can be made artificially by modern growth techniques, e.g., epitaxy or self-organization. To understand and compute the properties of matter and their interaction with electric and magnetic fields on the nanoscale it is essential to use quantum mechanics, i.e., to describe the involved particles by waves that may interfere. Such computations typically lead to large sets of coupled partial differential equations that need to be evaluated on large computer clusters.

In the project presented here, we compute and discuss nonlinear optical properties of two-dimensional semiconductor quantum wells. Generally, semiconductor nanostructures such as quantum wells, wires, and dots are widely used, e.g., in light-emitting diodes, photodetectors, and solid-state lasers. Semiconductor nanostructures consist of two or more semiconductor material and the interfaces between these materials are typically not perfectly smooth on a microscopical scale but contain a certain degree of disorder. This often unavoidable disorder may strongly affect the electronic and optical response of the system. In the following, we show how certain aspects of the disorder can be investigated using nonlinear optical spectroscopy.

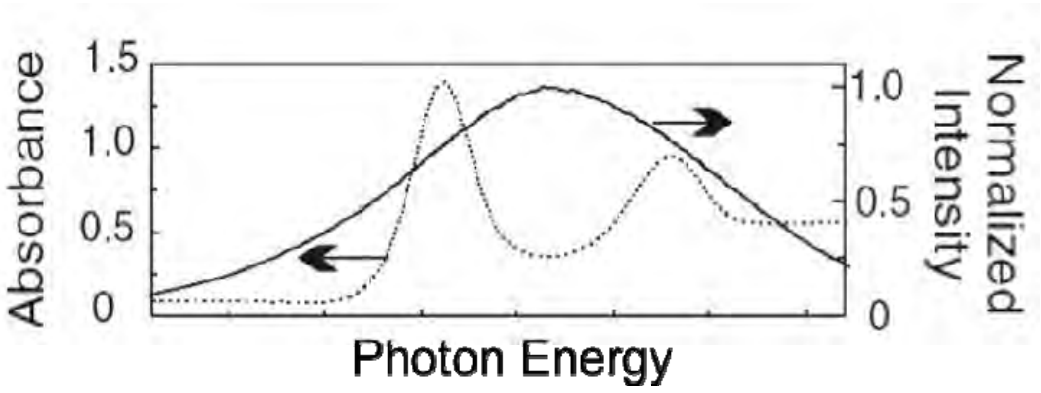


Figure 1: Absorption spectrum of GaAs-quantum well (dotted line) and excitation field spectrum (solid line) taken from Ref. [2]. Dotted line has two peaks, which correspond to different kinds of excitons. The second (on the right) exciton "sits" on the top of the continuum of the first exciton (on the left), which is at higher energy.

We study disordered semiconductor nanostructures on a microscopic level using a sequence of ultrashort (femtosecond) weak external light pulses and evaluate a 2-dimensional Fourier-Transform spectrogram (2DFTS) [1]. Sending an optical field to a semiconductor quantum well we create excitons. An exciton is a bound state of an electron (negatively charged) and the inverse particle, which presents a missing electron, the so-called "*hole*" (positively charged). The absorption spectrum of a semiconductor quantum well contains discrete bound excitonic lines and continua, see Figure 1. The spectral position of the excitonic line is related to the binding energy of the electron-hole pair, i.e. the exciton. The absorption spectra of these excitonic excitations have a certain width that can be used to assess the quality of the nanostructure. However, the width of an excitonic spectral line can have more than one contribution. In a perfectly ordered semiconductor the line is called homogeneously broadened. This broadening reflects the loss of phase information, which was introduced into the material system by the external light field. Dephasing processes include interaction with lattice vibrations and radiative decay of the excitonic excitation. In disordered nanostructures there is in addition a so-called inhomogeneous contribution due to spatially varying resonance frequencies in the disordered sample. The main question addressed by our investigations is: How does disorder affect the excitonic line width?

Numerical Results and Discussion

In order to answer the question about the influence of the disorder on the excitonic line width, a very useful method is to apply **nonlinear** optical spectroscopy [3]. Why is the (much simpler to calculate) *linear* absorption spectrum not a proper method for solving this problem? The main disadvantage of using the absorption spectrum is that the excitonic line contains two kinds of contributions. The main contribution is

given by the dephasing time, i.e., the homogeneous line width. An additional contribution to the width of the excitonic line due to disorder is inhomogeneous line width. Finally, the excitonic line width was considered as the sum of homogenous and inhomogeneous contributions to the excitonic line width. As an additional complication, disorder not only contributes to the inhomogeneous width, as was generally believed, but also to the homogeneous width. Evidence for this has been pointed out by Weiser et al. [4]. However, it was not possible to numerically simulate the influence of disorder in sufficient detail because of limited computer resources. Our present research, thanks to improved computer facilities, yields deeper inside into the action of disorder on optical properties of semiconductor nanostructures. Homogeneous and inhomogeneous contributions can be separately identified by applying nonlinear ultrafast optical measurements to a nanostructure [5].

Differently to absorption spectra shown in Figure 1 and Figure 2 (top), in the nonlinear optics we can display excitonic line as a two-dimensional peak (Figure 2 (c)). This so called 2DFTS technique allows one to investigate semiconductor nanostructures more deeply. The power of this technique relies on variety of information: amplitude, real- and imaginary part 2DFT-spectra, and on more detailed spectral information. In order to interpret these experimental results, a theoretical study is necessary that shows to what extent the disorder influences both the homogeneous and inhomogeneous contribution to the linewidth. This study is based on the semiconductor-Bloch-Equations that also contain biexcitonic many-particle correlations. These equations represent a large set of differential equations that have to be solved numerically. Only in the last few years it has become possible to calculate nonlinear optical response for disordered semiconductors in schematic models.

The amplitude spectra in Figure 2 (c) and (d) demonstrate the influence of disorder. Comparing ordered (c) and disordered case (d), we obtained, due disorder, a broadening of the peak along and perpendicular to the diagonal as well. These directions are specific, along the diagonal the line width is the same as taken from the absorption spectrum. The line width which is perpendicular to the diagonal provides the homogeneous line width which is modified due to disorder. Since the homogenous line width was an input parameter, we can extract the pure contribution of the disorder. For precise determination of contribution of disorder to the homogeneous line width we use the imaginary-part 2DFTS (Figure 2 (a) and (b)). Comparing these contributions taken from ordered (a) and disordered case (b) we find an increase by about 0.22 meV due to disorder [6]. We found that the coupling of neighboring localized exciton, due to disorder, to the continuum of neighboring localized excitons is the physical process which leads to this increase. However our model studies show that for certain material parameters of the semiconductor model an additional process of averaging can take place. As a consequence of the

averaging process we can also obtain the decrease of the disorder-induced homogeneous line width. Using variations of 2DFTS we can also determine the inhomogeneous line width separately.

Additionally, we compare our theoretical results with measured 2DFTS [6] and demonstrate that our theory can qualitatively reproduce the experimental data. In particular, the so-called butterfly form of the imaginary-part 2DFT-spectra (see also Figure 2 (b)) agrees with the measurements [6]. This form can be simulated only using microscopic implementation of disorder in the semiconductor model.
Finally, we have determined the disorder contribution to the homogeneous line width for both excitonic lines shown in Figure 1. (dotted), which for the high energy peak quite demanding task due to the continuum present there. In our paper [6] we demonstrate spectral dependence of the homogeneous line width induced by disorder. This broadening increases for higher energy (see the black arrows on Figure 2 (b)). The reason for that is additional coupling of the localized exciton to the continua of the neighboring excitons.

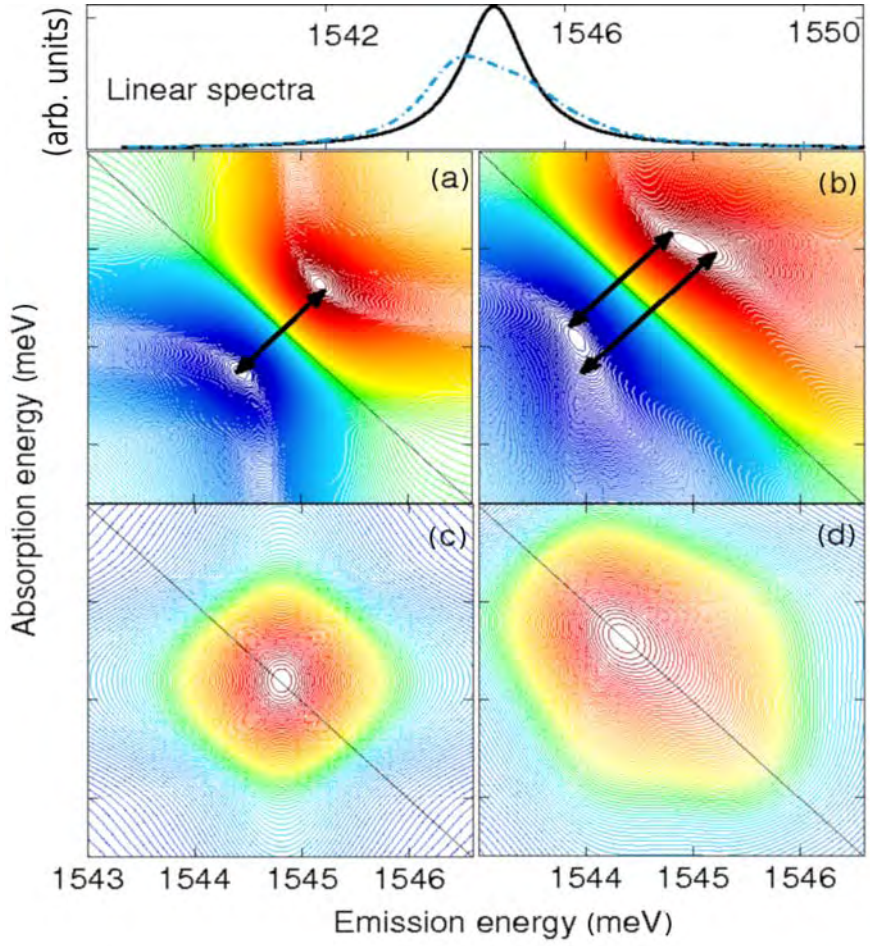


Figure 2: Top: Linear spectra of ordered (solid line) and disordered (dotted line) semiconductors. Normalized imaginary-part 2DFTS for the ordered (a) and disordered (b) semiconductors. Normalized amplitude 2DFTS for the ordered (c) and disordered (d) semiconductors. Figure was taken from [6].

Resource Usage

The calculations required the solution of the large number of coupled differential equations for matrix-valued quantities as given by the semiconductor Bloch-equations including many-body correlations. The performance of our calculations is strongly dependent on the size of the modeled system. Since disorder has been introduced into the model, the translational symmetry, which would reduce the number of differential equations, could not be used. A high number of realizations of disorder is furthermore important to yield smoothed spectra. Thanks the immense computing power of the cluster the mentioned challenges could be met (case a)).

Our runs have been performed sequentially on the Arminius cluster. Each sequence of runs takes about 44 hours (for the given size of the system), and has been submitted in the loop. One run contains about 100 sequences. In average we have carried out about 1 run per week, i.e. 100 nodes weekly in the period from April to July 2009. The amount of runs corresponds to the number of realizations, i.e. the bigger number of realizations the more real is our system. Finally the big size and number of realizations that are required in order to describe a real semiconductor nanostructure, need enormous computing power. The work has been performed using the available hardware at the PC². Additionally, also ongoing grant for supercomputer time at the John-von-Neuman Institut für Computing, Forschungszentrum Jülich, have been used.

References

[1] Kuznetsova, I.; Thomas, P.; Meier, T., Zhang, T.; Li, X.; Mirin, R.P. and Cundff, S.T.: Sol. State Comm. 142, 154 (2007).
[2] Li, X., Zhang, T.; Borca, C.N. and Cundiff, S.T.: Phys. Rev. Lett. 96, 057406 (2006).
[3] Meier, T.; Thomas, P. and Koch, S.W.: Coherent Semiconductor Optics - From Basic Concepts to Nanostructure Applications, Springer, Berlin, 2007.
[4] Weiser, S.; Meier, T.; Möbius, J.; Euteneuer, A.; Mayer, E.J., Stolz, W.; Hofmann, M.; Rühle, W.W.; Thomas, P. and Koch, S.W.: Phys. Rev. B 61, 13088 (2000).
[5] Kuznetsova, I.; Meier, T.; Thomas, P. and Cundiff, S.T.: Phys. Rev. B 76, 153301 (2007).
[6] Kuznetsova, I.; Gogh, N.; Förstner, J.; Meier, T.; Cundiff, S:T.; Varga, I. and Thomas, P.. Submitted to Phys. Rev. B

6.9 Novel Simulation Methods for Electro-Hydrodynamics

Project coordinator	Professor Dr. Friederike Schmid, Universität Bielefeld
Project members	Dr. Jens Smiatek, Universität Bielefeld
Supported by:	Volkswagen Stiftung

General Problem Description

We present mesoscopic simulations of the counterion-induced electroosmotic flow in different electrostatic coupling regimes. Two simulation methods are compared, Dissipative Particle Dynamics (DPD) [1,2] and coupled Lattice-Boltzmann/Molecular Dynamics (LB/MD) [3,4,5]. For the weak-coupling regime, analytic expressions for the flow profiles in the presence of partial-slip as well as no-slip boundary conditions can be derived from the Poisson-Boltzmann and Stokes equations, which are in good agreement with the numerical results. The influence of electrofriction and partial slip on the flow profiles is investigated in detail.

Microfluidic devices like bio-MEMS (micro-electronical-mechanical-systems) and bio-NEMS (nano-electronical-mechanical-systems) have attracted broad interest over the last years due to their huge potential in biotechnology.

The flow profiles in such micro- or nanosized devices are strongly influenced by the properties of the boundaries due to the large surface-to-volume ratio in these systems. Surface characteristics like the wetting behavior and/or slippage have a dramatic effect on the microscopic flow, leading to sometimes unexpected behavior.

One particularly important mechanism is electroosmotic transport: in contact with a liquid, many materials commonly used in nanotechnology (polydimethylsiloxane (PDMS)) become charged due to ionizations of surface groups. As a consequence, surfaces are often covered by a compensating counterion layer. In an external electric field, the ions are driven in one direction, dragging the surrounding solvent with them.

As a result, a flow is induced in the fluid, the electroosmotic flow (EOF) [6]. This electrokinetic effect has numerous consequences. For example, it alters drastically the migration dynamics of mesoscopic objects like polyelectrolytes or colloids. In microchannels, the EOF generated at the channel walls results in a total net flow, which is technologically attractive because it can be controlled and manipulated more easily on the submicrometer scale than pressure- or shear-driven flow.

As analytical predictions for flow in such complex systems are often hard to derive, numerical simulations are used to investigate it in detail. The requirements on computer simulations are high: They must include the full hydrodynamics of the fluid while guaranteeing, at the same time, optimal computational efficiency. This has led

to the development of a number of coarse-grained mesoscopic simulation schemes. Several methods like Lattice Gas Automata, the Lattice-Boltzmann Method (LB), Dissipative Particle Dynamics (DPD) and Multi-Particle Collision Dynamics (MPC) are nowadays used to model liquids at a coarse-grained level.
Compared to atomistic Molecular Dynamics simulations, these approaches give access to much longer time- and length scales and are therefore suited to study the long-time behavior of soft matter systems and transport phenomena.
Although the theoretical background of these methods is well understood, their lattice/off-lattice and thermal/athermal character impedes a straightforward mapping between them.
Comparative studies of specific soft matter problems with different simulation methods are therefore scarce.
We present the results of DPD- and coupled Lattice-Boltzmann/Molecular Dynamics (LB/MD) simulations for the counterion-induced EOF without salt ions in a slit pore.
Although this geometry does not allow to test the full coupling between ions and solvent, it has the advantage of possessing an analytical solution, which allows a precise test of the accuracy of the methods.
As mentioned earlier, flow profiles depend heavily on the boundary conditions at the surfaces. We derive an analytic equation for the counterion-induced EOF in the presence of no-slip as well as partial-slip boundaries for the regime of ``weak electrostatic coupling'', the regime where the Poisson-Boltzmann theory is valid, and compare it to our simulation results. Furthermore, we also study the influence of the discrete character of wall charges, compared to perfectly homogeneous walls.
In this report we focus on the numerical results. Details of the analytical calculation and a complete description of the simulation methods as well as further results can be found in [7,8].

Problem details and work done

In the following we focus on the comparison between the DPD- and the coupled LB/MD scheme and the corresponding EOF profiles. Comparing different simulation methods mean to match basic fluid parameters like the solvent density and the solvent viscosity.
For a comparison we therefore have to match the main solvent properties and single particle properties like the self diffusion coefficient. The mean square displacement of a tracer particle gives an estimate for the diffusion coefficient whereas the solvent viscosity can be measured in terms of the velocity autocorrelation function.

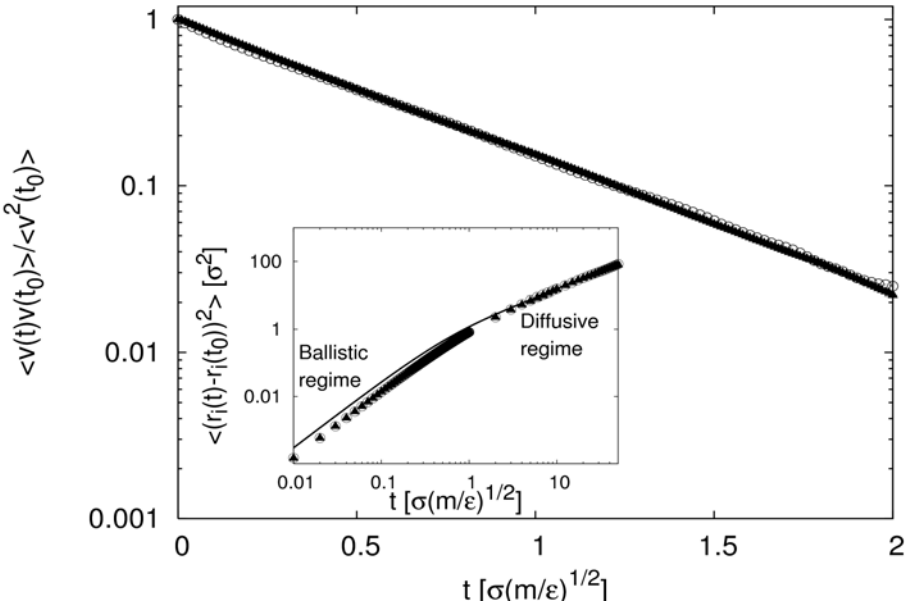


Figure 1: Main: Velocity autocorrelation for a tracer particle in the DPD method (circles) and in the coupled LB/MD scheme (triangles). Small: Mean square displacement of a tracer particle in both methods for short times. The transition between the ballistic and the diffusive regime occurs at identical times for both methods. The black line in the inset corresponds to analytical results.

Figure 1 shows the results of the velocity autocorrelation and the mean square displacement of tracer particles in both methods for short times. As it can be seen by a systematic comparison, both methods can be tuned easily to achieve the same results which gives the possibility to match the flow profiles of the electroosmotic flow in both methods.

Fig. 2 indicates that for the same parameter sets both flow profiles are in agreement for no slip boundary conditions. No slip means that the fluid velocity at the hydrodynamic boundary positions vanishes. Thus it is possible to effectively simulate a specific problem with different simulation methods to derive identical numerical results.

The influence of slippage, which is a more realistic situation has been incorporated into the DPD method by a recently developed method [2]. Slippage occurs if the solvent velocity at the hydrodynamic boundary positions does not vanish which can be described by a slip length larger than zero. Applying this method further allows to systematically tune the slip length to cover the whole range between full slip and no slip.

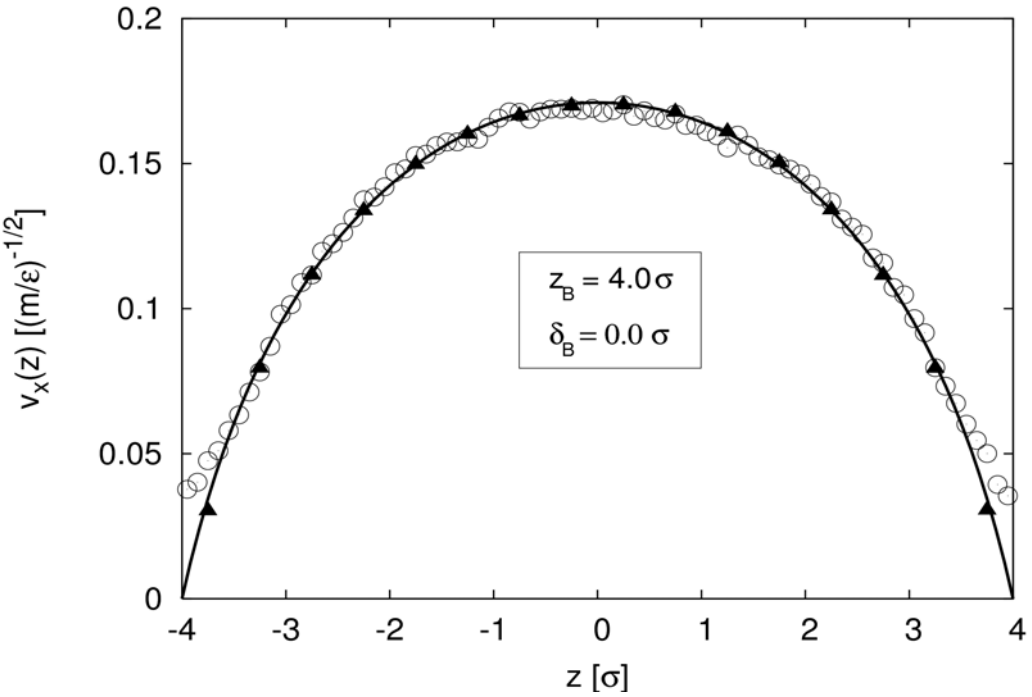


Figure 2: Flow profiles for the DPD- (circles) and the coupled LB/MD scheme (triangles). The black line corresponds to the analytical theory.

Further attention has to be spent on the characteristics of the electrostatic configuration. It is a well known fact that stronger coupled electrostatic systems exert an electrostatic friction on the solvent ions.

We simulated the influence of electrofriction in the weak-coupling situation via taking into account inhomogeneously and homogeneously charged walls.

Fig. 3 presents the results for the different environment conditions. Large slip lengths indicate a slip behaviour whereas small slip lengths are nearly identical to no slip boundary conditions. It is obvious that the flow profiles are drastically enhanced by larger slip length meaning less friction at the hydrodynamic boundaries. As Fig. 3 further indicates, the influence of electrofriction is negligible for these weakly coupled systems due to identical flow profiles for homo- and inhomogeneously charged walls. Even the ion distribution is not significantly varying due to the presence of inhomogeneously charged walls.

Future work includes the consideration of systems in the presence of salt. We plan to investigate the influence of slippage and electrostatic screening lengths on the migration behaviour of polyelectrolytes in microchannels.

We have to thank Dr. Marcello Sega, Prof. Dr. Christian Holm and Dr. Ulf D. Schiller for supporting our DPD data with the results of the coupled LB/MD simulations.

All simulations have been carried out with the freely available software package ESPResSo [9,10].

Resource Usage

We run our simulations on the Fujitsu-Siemens Computers hpcLine-Cluster "ARMINIUS" at the PC² with the open source software package "ESPResSo" (An Extensible Simulation Package for Research on Soft Matter) which is fully parallelized. The parallelization is MPI-based and we use the cluster daily due to the immense accelaration of computing time by running the simulations in parallel.

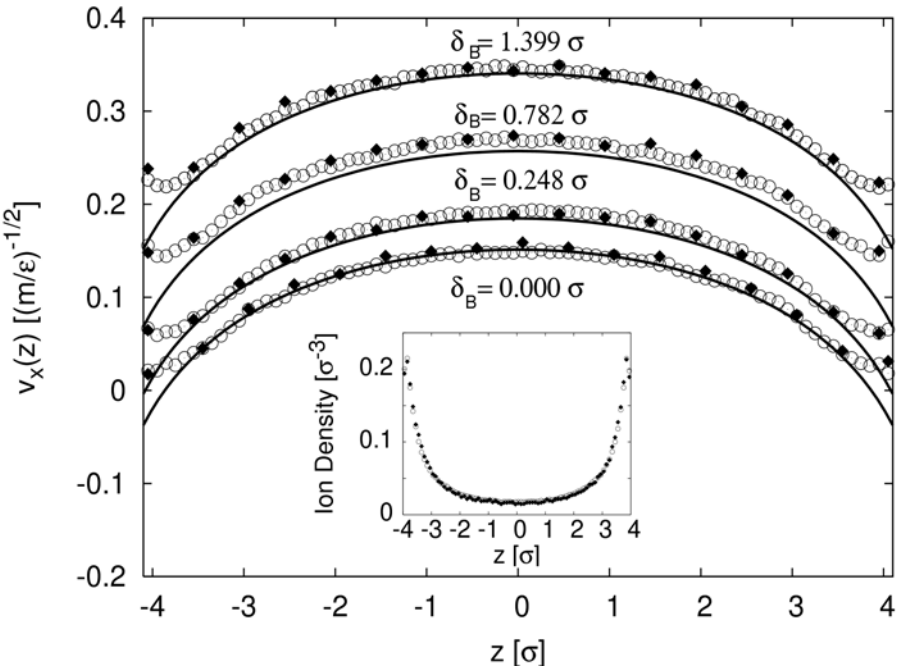


Figure 3: Main: Flow profiles for different boundary conditions in the DPD method. Circles correspond to homogeneously charged walls whereas triangles represent inhomogeneously charged walls. Slippage effects drastically enhance the flow profiles with the presented values of the slip length. Small: Ion distribution for homogeneously and inhomogeneously charged walls. The charge distribution has no significant influence on the ion distribution in the weak coupling regime.

References

[1] Hoogerbrugge, P.J. and Koelman, J.M.: Europhys. Lett. 19, 155 (1992)
[2] Espanol, P. and Warren, P.B.: Europhys. Lett. 30, 191 (1995)
[3] McNamara G.R. and Zanetti, G.: Phys. Rev. Lett. 61, 2332 (1988)
[4] Benzi, R.; Succi, S. and Vergassola, M.: Phys. Rep. 22, 145 (1992)
[5] Ahlrichs, P. and Dünweg, B.: Chem. J., Phys. 111, 8225 (1999)
[6] Hunter, R.J.: "Foundations of Colloid Science", Clarendon Press, Oxford (1987)
[7] Smiatek, J.; Allen, M.P. and Schmid, F.: Europ. Phys. J. E 26, 115 (2008)
[8] Smiatek, J.; Sega, M.; Schiller, U.D., Holm, C. and Schmid, F.: J. Chem. Phys. 130, 44702 (2009)
[9] ESPResSo- Homepage: http://www.espresso.mpg.de (2002-2009)
[10] Limbach, H.J.; Arnold, A.; Mann, B.A. and Holm, C.: Comp. Phys. Comm. 174, 704 (2006)

6.10 VOF-Simulation of Oil Drops Rising in Water

Project coordinator	Professor Dr. Dieter Bothe, CSI, TU-Darmstadt Prof. Dr.-Ing. H.-J. Warnecke, University of Paderborn
Project members	Dr. Martin Schmidtke, Forschungszentrum Dresden-Rossendorf

General Problem Description

Two-phase flows with oil and water play an important role in oil production as well as in oil processing. On the other hand, oil in water can be used as model for liquid carbon dioxide in the deep sea. One idea to reduce the contamination of the atmosphere with carbon dioxide from exhaust fumes is to deposit CO_2 in the deep see. This is the background for experiments on the rising behavior of oil drops in water [1].

As a complement to experiments, numerical simulations offer a unique and cost-efficient chance for a detailed investigation of two-phase flows. Additionally, all relevant quantities such as velocity or pressure are completely accessible within the computational domain.

Numerical simulations of hydrodynamics are carried out with an extended version of the highly parallelized code FS3D (in cooperation with the ITLR Stuttgart), which employs an advanced Volume of Fluid (VOF) method [2]. The high degree of parallelization of the code allows high resolution of the computational domain, such that the relevant length scales inside the liquid phase are resolved during the simulations. In previous works FS3D was used to simulate the free rise of bubbles in liquid flow [3-6]. Opposite to bubbles, oil drops have similar density as water and a viscosity several times higher than the viscosity of water. Due to the high viscosity of oil the internal flow inside oil drops driven by the external water flow is very damped in contrast to air bubbles.

However, some similarities of rising oil drops with air bubbles can be observed: Small drops tend to rise on rectilinear trajectories (with little or no lateral motion), whereas large drops tend to show up oscillating lateral motions (e.g. zigzagging) due to vortex shedding behind the drops.

Problem Details and Work Done

The code FS3D used in this work was originally developed for gas-liquid flows. The application to oil drops in water proved to be challenging, because typical oil viscosities exceed the viscosity of water by far (see table 1). High fluid viscosities cause a fast diffusion of momentum and therefore require small time steps in our simulations. In first simulations too large time steps were chosen. This caused an unphysical distortion of the oil drops leading to a breakup into two parts. By reducing the time step this can be overcome, resulting in a high demand of computational power.

Fluid	*Water*	*Corn Oil*	*Castor oil*
Density	1000 kg/m^3	915 kg/m^3	957 kg/m^3
Viscosity	1 mPa s	45 mPa s	900 mPa s

Tab. 1: Density and Viscosity of water and two different oils

Both corn oil and castor oil drop behaviour in water have been investigated comprehensively by Haljasmaa [1]. Since castor oil is even twenty times more viscous than corn oil, most simulations were performed for corn oil. In Figure 1, the terminal velocities (i.e. the final velocity after an acceleration time) of corn oil drops rising in water are shown in dependency of the drop size. The drop size is given as equivalent diameter, which is the diameter of a sphere with the same volume as the drop. In the experiment, the terminal velocity increases with the drop diameter in the range d<11mm. These drops rise either on a straight line directly upwards or show only little lateral motion. Drops in the range d>11mm rise with a significant lateral oscillation, i.e. they rise on a zigzagging trajectory. This goes along with a lower terminal velocity which is significantly lower than for drops in the range 8mm < d < 11mm.

In the simulations a significant lateral oscillation is already observed for drops at d=9mm. The terminal velocity of this drop is underestimated, whereas the agreement of the terminal velocities in experiment and simulation are satisfying for larger and smaller drop diameters.

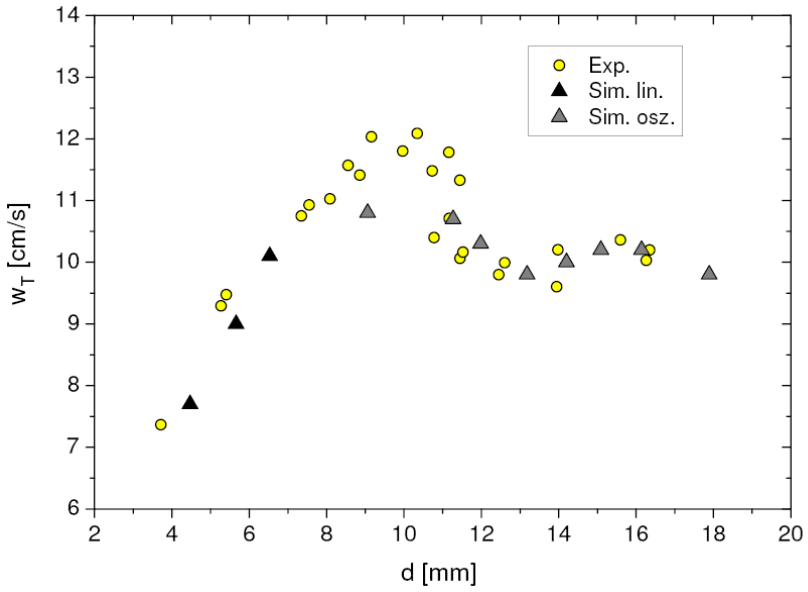


Fig 1: *Terminal velocity of corn oil drops rising in water in dependency of drop equivalent diameter. Circles: Experiment [1], triangles: Simulation*

In the following the process of the lateral drop oscillation is investigated more detailed. In Figure 2 the velocity fields around a large drop (d=14mm) are shown for three different subsequent moments. One can see easily that vortices appear behind the drop and are washed away. This phenomenon is called vortex shedding. In the left frame a vortex is formed behind the left side of the drop, whereas in the right frame a vortex can be seen behind the right edge of the drop. The side of the vortex shedding is alternating regularly between left and right similar to the well-known von Karman vortex street behind rigid bodies. During the vortex shedding the drop center oscillates sideward and the drop shape also oscillates. The drop in the middle frame shows smaller lateral extension than the other ones. Note that we consider here only the plane defined by the zigzagging trajectory. Furthermore the velocity fields shown in Figure 2 represent only a cut out of the large computational domain.

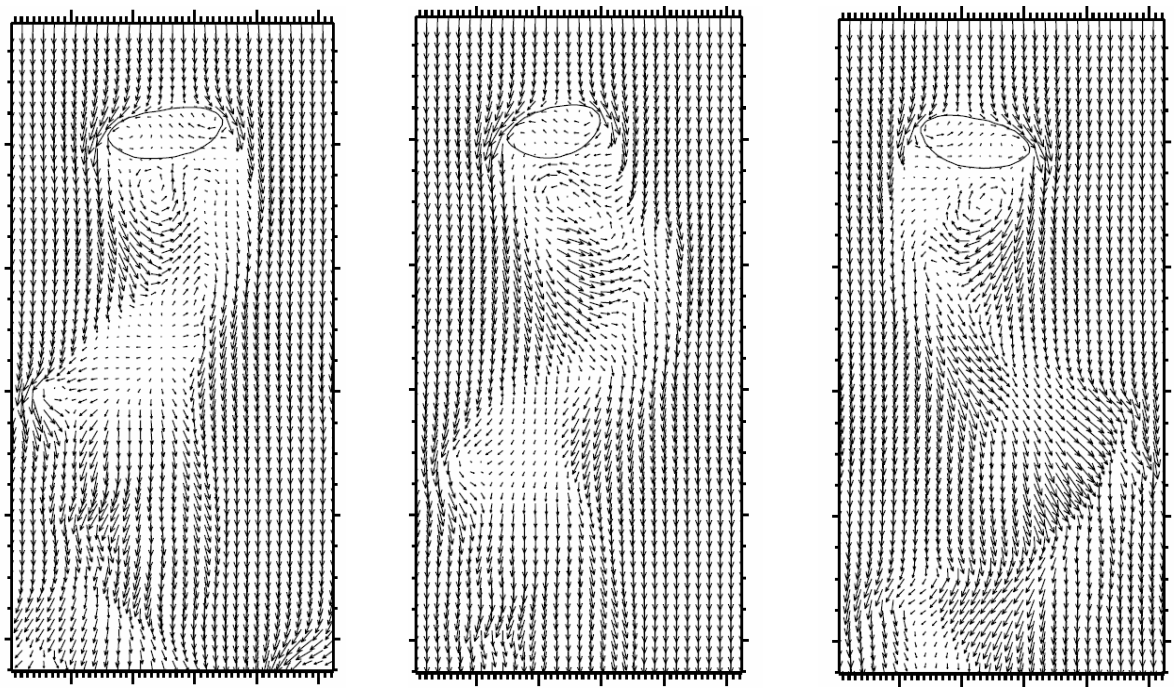


Fig.2. : Velocity fields around a large corn oil drop (d=14mm) at different instances

Let x be the upward direction (gravity in the direction of –x) and y be the direction of the lateral oscillation. The frames in Figure 2 show x-y planes. Then z is the direction perpendicular to this plane. Figure 3a shows the vertical and the horizontal velocity during the drop oscillation. The vertical drop velocity v_x oscillates around a mean value of 10 cm/s. The frequency of this oscillation velocity is four times higher than the frequency of the lateral velocity v_y. Simultaneously the drop shapes oscillate (Fig. 3b). The frequency of these oscillations is twice as high as the frequency of the lateral velocity.

Figure 3b reveals that a contraction of the drop in y-direction (decrease of Δy) goes along with an expansion of Δz. The lateral drop extensions oscillate with a frequency twice as high as the lateral drop velocity. The oscillation of the vertical drop extension Δz is very weak compared to the horizontal ones, but it has a similar frequency. A Fourier analysis of the signal reveals that oscillation Δz contains the double, the triple and quadruple frequency with respect to the base signal given by v_y

It is planned to investigate the interrelation of drop center oscillation and drop shape oscillation for various drop sizes in detail by applying fast Fourier transformation.

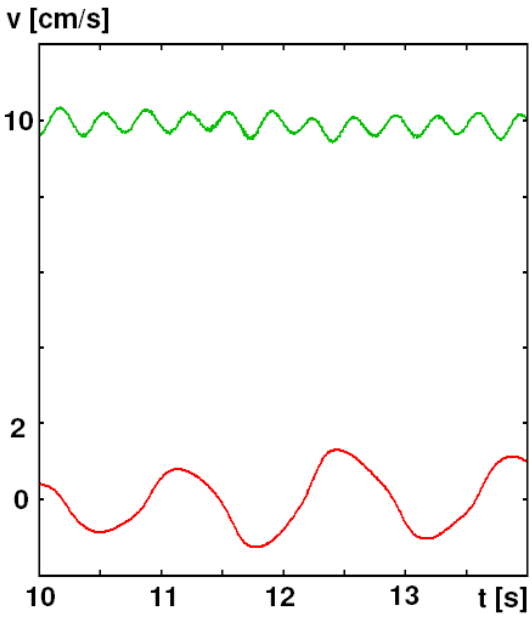


Figure 3a. : Vertical (v_x: green) and lateral (v_y: red) drop velocity.

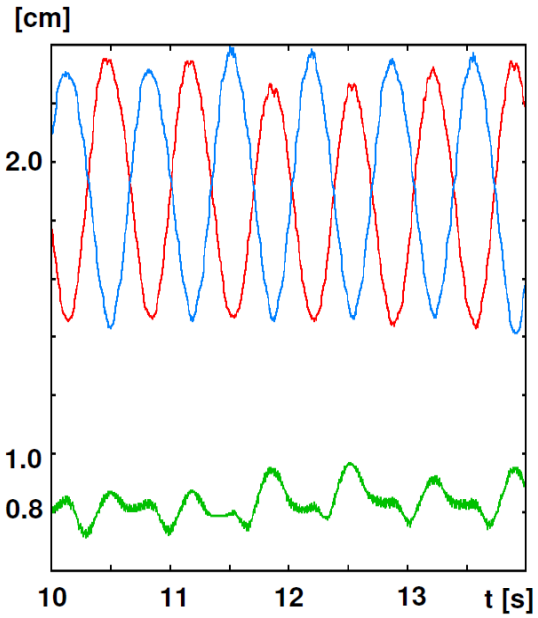


Figure 3b. : Vertical (Δx, green) and lateral drop extensions (Δy , red) and (Δz , blue)

Resource Usage at PC²

The simulations performed required a very high resolution of the computational domain (1-16 million cells). On a single processor, the governing equations can be solved for a maximum number of 250.000 cells. Therefore, parallelization is necessary in order to compute on large domains or to provide high resolution, respectively. The number of required CPUs varies from 2 to 64. The employed Volume of Fluid code FS3D is completely parallelized (based on MPI) and runs on the PSC2 and the ARMINIUS cluster.

References

[1] Haljasmaa, I.: On the Drag of Fluid and Solid Particles freely moving in a Continuous Medium, Dissertation, University of Pittsburgh 2006.

[2] Rieber, M.: Numerische Modellierung der Dynamik freier Grenzflächen in Zweiphasenströmungen, VDI Fortschritt Berichte, Reihe 7, Nr. 459

[3] Koebe, M. Numerische Simulation aufsteigender Blasen mit und ohne Stoffaustausch mittels der Volume of Fluid (VOF) Methode, Dissertation, University of Paderborn, 2004Zweiphasenströmungen, VDI Fortschritt Berichte, Reihe 7, Nr. 459

[4] Bothe, D.; Koebe, M.; Wielage, K.; Prüss, J.; Warnecke, H.-J.: Direct Numerical Simulation of Mass Transfer Between Rising Gas Bubbles and Water. In: Sommerfeld, M. (Ed.): Bubbly Flows - Analysis, Modelling and Calculation, Springer, Berlin, Heidelberg, New York, 2003.

[5] Schmidtke, M.: Untersuchung der Dynamik fluider Partikel auf Basis der Volume of Fluid Methode, Dissertation, Universität Paderborn, 2008
[6] Direct Numerical Computation of the Lift Force acting on Single Bubbles, 6th International Conference on Multiphase Flow, Leipzig, Germany, 2007

6.11 Molecular self-organization and chemical reactions on solid surfaces studied from massive parallel first-principles calculations

Project coordinator	Professor Dr. Wolf Gero Schmidt, University of Paderborn
Project members	Dr. Eva Rauls, University of Paderborn Dr. Uwe Gerstmann, University of Paderborn Dr. Simone Sanna, University of Paderborn Dr. Stephan Blankenburg, University of Paderborn Dr. Stefan Wippermann, University of Paderborn M.Sc. Marc Landmann, University of Paderborn Dipl.-Phys. Andreas Hermann, Massey University, New Zealand Dipl.-Phys. Christian Thierfelder, Massey University, New Zealand Dipl.-Phys. Susan Biering, Masssey University, New Zealand
Supported by	DFG SCHM 1361/8, DFG SCHM 1361/9, DFG SCHM 1361/10, DFG SCHM 1361/11, DFG SCHM 1361/12, Nachwuchsgruppe des NRW-MIWF

General Problem Description

Supramolecular architectures created by self-organisation and self-assembly from surface adsorbed molecules are a field of intense recent research. This interest is driven by the scientific challenge to understand the driving forces for the formation of the often very complex structures as well as the hope to utilize such structures either directly or as starting point for further technological steps, e.g., as templates.

The intermolecular interactions ranging from indirect, substrate mediated and Coulomb interactions to various bonding schemes ranging from weak dispersive interactions and hydrogen bonds to covalent bonds set the stage for a large number of possibilities to form one- and two-dimsional molecular networks of varying robustness. While many potential applications of supramolecular structures will require a thermal and chemical stability that can only be achieved upon covalent bonding, only little is known about the formation of covalent bonds between adsorbates. Certainly it can be expected that the formation of covalent bonds

between surface adsorbed molecules occurs significantly differently when compared to the corresponding reaction in solution or in bulk films.

For a systematic investigation of molecular self-organization, suitable model systems need to be found that allow studying the molecular interactions reproducibly and with high accuracy and, furthermore, with different experimental and theoretical methods. Surface adsorbed molecules are an obvious choice. Like this, the molecules become accessible to sophisticated surface analysis tools such as scanning tunneling microscopy (STM) or atomic force microscopy (AFM) as well as electron diffraction techniques, infrared and other optical spectroscopies.

In computational materials science, we aim at identifying the driving forces that lead to phenomena of molecular self-organization and self-assembly of surface adsorbed molecules. To this end, we perform numerical simulations that describe the competing effects of molecule-molecule and molecule-substrate interaction on a theoretical basis and in close cooperation with the experiment. A large number of degrees of freedom (typical calculations deal with several hundreds of atoms, i.e, thousands of electrons) leads to long and demanding calculations that require both numerically efficient, stable algorithms and powerful parallel computers.

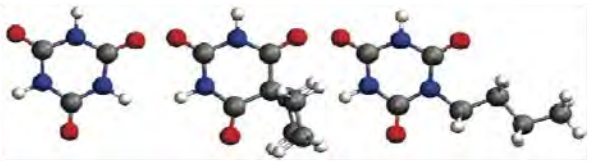


Figure 1: The three molecules CYA, DEB and BuCYA. From Ref. [2].

One example we investigated during the last year is the influence of an exchange of a functional group on the self assembling behavior of a small organic molecule. A suitable molecule for such a systematic study is the cyanuric acid (CYA), see Fig.1. Adding two short alkyl chains leads to the diethylbarbituric (DEB). A third variant occurs if only one alkyl chain is attached to one of the nitrogen atoms, butylcyanuric acid (BuCYA). Like this, the three molecules vary not only in their chemical compositions but also in symmetry, flexibility.

Experimentally, these molecules have been investigated after adsorption on a metal surface, i.e. Au(111), which does not strongly interact with the adsorbate. The molecules can, thus, swim rather freely on the surface and their interaction be studied without perturbations.

All three molecules aggregate on the surface and form hydrogen bonded networks. STM-observations reveal a trigonal network for the CYA, a double row structure for the DEB, and a disordered phase for the BuCYA, though with certain local order patterns.

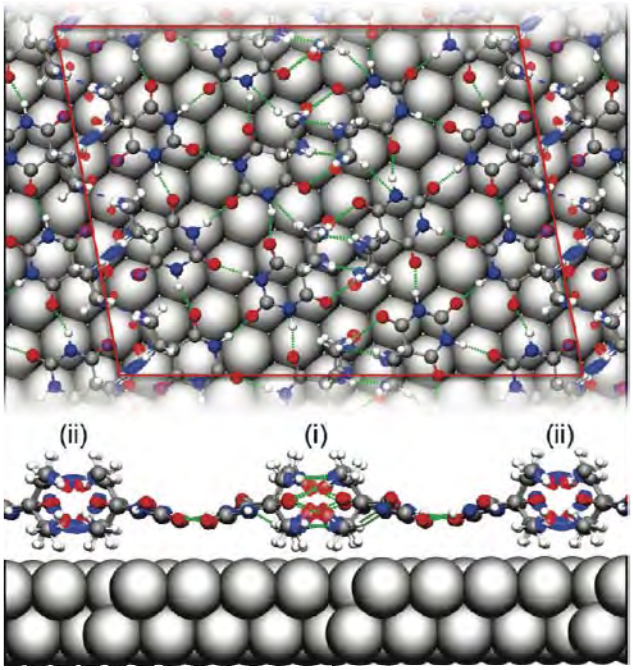


Figure 2: The complicated hydrogen bonded double row pattern exhibited by the DEB-molecules. Selforganisation is not caused by fH-bonding alone, but a new feature, so-called di-hydrogen bonds between the two short alkyl chains were calculated to play a crucial role in the intermolecular interaction. From Ref.[2].

With our calculations, we could interpret these observations and propose structural models which can explain the different behavior of the molecules to aggregate. The functional groups could be shown not only to break the symmetry or work as a spacer between molecular rows but truly take part in the intermolecular interaction. Especially for the functional group of the DEB-molecule, interesting effects were found.

Aggregation in the double row structure depicted in Figure 2 is clearly favored over aggregation in other structures one could imagine, like e.g. hexagons or other row-like patterns. A comparison of the experimental STM-image with an STM-image simulated for our calculated structural model of the adsorbate shows perfect agreement and explains the origin of the observed bright spots, see Figure 3.

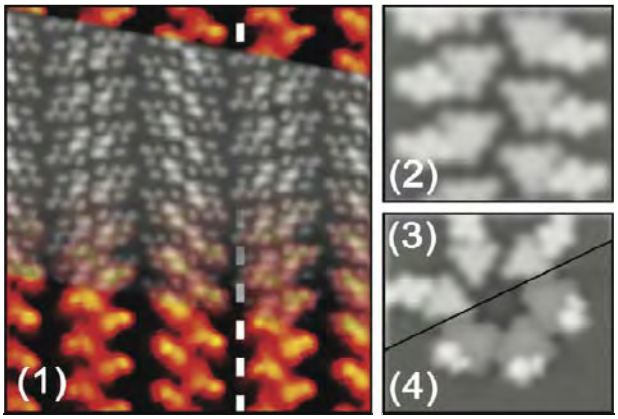


Figure 3: STM simulation and experimental STM-image in superposition for the DEB-molecules (part 1 of the image). The bright spots were calculated to arise from the alkyl chains. From Refs. [2] and [3].

For the BuCYA, calculations show, in contrast to DEB, that there is no clear preference for either row formation or formation of hexagons or pentagons. Both are energetically more or approximately degenerate. Furthermore, the alkyl chain of BuCYA can lie either flat on the surface like in the simulation in Figure 3 (part 2 and 3), or folded back above the ring of the molecule as shown in the STM simulation in Figure 3 (part 4). This explains the coexistence of the different aggregation patterns in an overall disordered adsorbate phase.

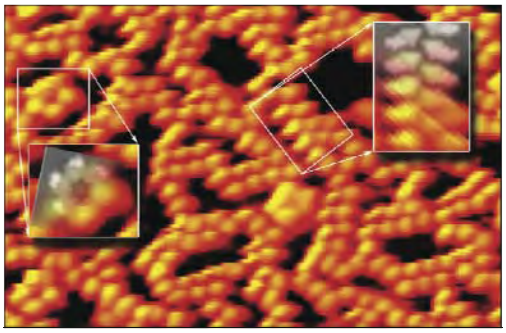


Figure 4: STM simulations and experimental STM-image in superposition for the BuCYA-molecules. Several patterns, as also shown in detail in Figure 3 (part 2-4) are found in the adsorbate. From Refs. [2] and [3].

Another example of our work during the last years deals with chemical reactions and how the presence of a surface can modify it. The two organic molecules 4,4-diamino-p-terphenyl (DATP) and 3,4,9,10-perylenetetracarboxylic-

dianhydride (PTCDA). Experiments show the formation of a variety of hydrogen bonded binary networks of these molecules on a Au(111) surface depending on the preparation conditions and stoichiometry. One of these networks is shown in Figure 5.

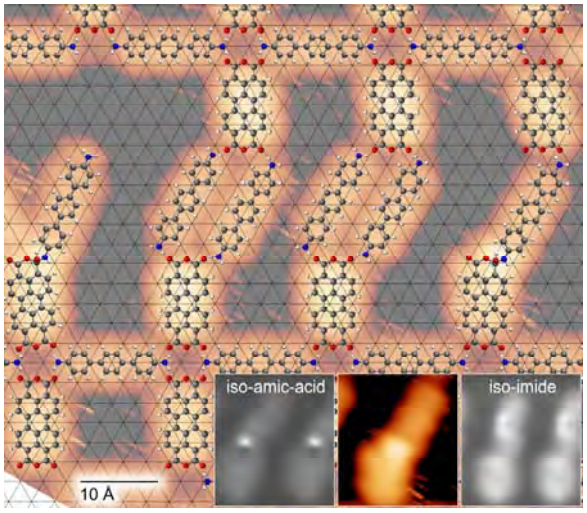


Figure 5: Part of a network of DATP and PTCDA on a Au(111) surface.

In contrast to the example described above, also the formation of covalently bonded molecular chains has been observed. For the design of nanostructures, this is highly important, since it enables us to build molecular structure using the help of a supporting substrate, but then remove the substrate and use the pure, stable molecular nanostructure for further device processing without an unwanted and potentially disturbing substrate.

One promising chemical reaction that leads to such covalently bonded nanostructures, is the peptide bonding mechanism, i.e. an imidization reaction. Two organic molecules with an amine and a carboxyle group, respectively, can be connected by such a reaction upon loss of one H_2O-molecule per newly formed bond.

On a surface with a molecular adsorbate, such a reaction can e.g. be induced by annealing of self-organized network structures. In chemistry, imidization is well known in the gas phase. However, on the surface, a second reaction path opens up. With our calculations of the energetics of the molecules, the intermediate structures, the adsorbates and the reaction products, we could explain these findings. For the first step in the imidization reaction, we have calculated the energy barrier that is linked to the approach of the two molecules on the surface and the hydrogen transfer and bond formation. The complete reaction is shown in Figure 6.

In gas phase, i.e. 3D, the imide is the only stable reaction product. On the surface, in contrast, another reaction product can be formed, the iso-imide. The role of the surface and how the reaction runs in detail, was subject of our calculations.
The surface reduces the mobility and flexibility of the molecules by weakly interacting mainly with the pi-system of the phenyl rings of the molecules. A second effect can be found in the deformation, which can only be mediated by the surface. Like this, the transfer of the hydrogen atom from the NH2-group of DATP to one of the O-atoms of the carboxyle group of the PTCDA is supported and is lowered energetically also for the iso-imide.

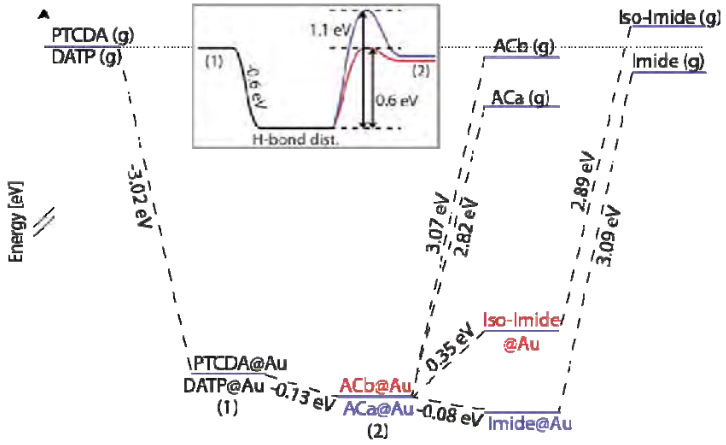


Figure 6: Complete reaction diagram of DATP and PTCDA on a Au(111) surface. From Ref. [4].

The activation energy for the formation of both the imide and the iso-imide lies in a thermodynamically likely range and has even been calculated to be lower for the iso-imide than for the imide. The second step in the imidization is then determined by the intermediate formed in the first step. If ACa is formed (cf. Figure 6), the second step leads most probably to the imide, while ACb would most likely lead to the iso-imide. Both imide-links can be seen in the experimental STM-image in Figure 7: the straight link corresponds to the “usual” imide, while the link in the characteristic angle corresponds to an iso-imide link.

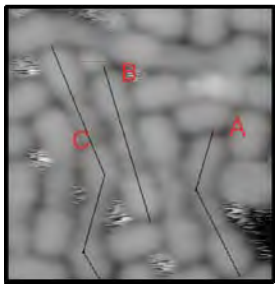


Figure 7: STM-image after high temperature annealing of a H-bonded network of DATP and PTCDA on a Au(111) surface. Covalently bonded molecular chains can be seen, containing both imide- and iso-imide links.

The surface, thus, induces a dimensionality constraint on the system and thereby catalyzes the reaction. In quasi-2D, it has become possible to build nanostructures that cannot be produced in a three-dimensional molecular gas phase or solution.

For these calculations as for many other calculations dealing with molecular adsorbates on surfaces, it turned out that long range dispersive forces play an important role. Since this, in some cases, does not only mean an energy shift, i.e. a quantitative effect, but also a qualitative effect, i.e. a different reaction, our first principles methods have, thus, to be extended. Results for the system described above showed large qualitative differences between a plain DFT calculation and a DFT calculation extended by semi-empirically treated dispersive interactions. First the latter agree with the experimental findings. In general, it is, thus, an important task to rule out the parameter dependence of a semiempirical approach and include these dispersive interactions into a first principles description. Some of our work resources was, therefore, put on such questions.

Resource Usage

The calculations were done using grants of computer time from the Paderborn Center for Parallel Computing PC^2 and the Höchstleistungs-Rechenzentrum Stuttgart (NEC SX-9).

References

[1] Schmidt, W.G.; Seino, K.; Preuss, M.; Hermann, A.; Ortmann, F. and Bechstedt, F.: “Organic molecule adsorption on solid surfaces: chemical bonding, mutual polarisation and dispersion interaction“, Appl. Phys. A **85**, 387 (2006).

[2] Blankenburg, S.; Rauls, E. and Schmidt, W.G.: „The role of dihydrogen bonds for the stabilization of self-assembled molecular nanostructures“, J. Phys. Chem. C 113, 12653 (2009).

[3] Xu, W.; Dong, M.; Gersen, H.; Rauls, E.; Vazquez-Campos, S.; Crego-Calama, M.; Reinhoudth, D.N., Stensgaard, I.; Laegsgaard, E.; Linderoth, T.R. and Besenbacher, F.: ”Influence of Alkyl Side Chains on Hydrogen-Bonded Molecular Surface Nanostructures”, Small 4, 1620 (2008).

[4] Rauls, E., Blankenburg, S. and Schmidt, W.G.: ”Chemical reactivity on surfaces: Modeling the imide synthesis from DATP and PTCDA on Au(111)”, Phys. Rev. B, 81, 125401 (2010).

7 Summary of References (alphabetical order)

[1] Ahlrichs, P. and Dünweg, B.: Chem. J., Phys. 111, 8225 (1999)

[2] Ajellal, N.; Lyubov, D.M.; Sinenkov, M.A.; Fukin, G.K., Cherkasov, G.V.; Thomas, C.M.; Carpentier, C.F. and Trifonov, A.A.: Chem. Eur. J. 2008, 14, 5440.Akola, J. and Jones, R. O.: Journal of Physical Chemistry B 2003, 107, 11774-11783.

[3] Amano, T.; Ochi, N.; Sato, H.; Sakaki, S. Journal of the American Chemical Society 2007, 129, 8131-8138.Ahn, S.; Fessler, J.A.: Globally convergent image reconstruction for emission tomography using relaxed ordered subsets algorithms, IEEE Trans. Med. Imag., vol. 22, no. 5, pp. 616619, May 2003

[4] Aranda-Espinoza, H.; Berman, A.; Dan, N.; Pincus, P. and Safran, S.: Interaction between Inclusions Embedded in Membranes, Biophysical Journal 71, 648, 1996

[5] Battré, D.; Kao, O. and Voss, K.: Implementing WS-Agreement in a Globus Toolkit 4.0 Environment, In Usage of Service Level Agreements in Grids Workshop in conjunction with The 8th IEEE International Conference on Grid Computing (Grid 2007), September 2007.

[6] Battré, D.; Hovestadt, M.; Kao, O.; Keller, A. and Voss, K.: Enhancing SLA Provisioning by Utilizing Profit-Oriented Fault Tolerance, Proceedings of the 20th IASTED International Conference on Parallel and Distributed Computing and Systems (PDCS) 2008, Orlando, Florida, USA, November 2008.

[7] Battré, D.; Birkenheuer, G.; Hovestadt, M.; Kao, O. and Voss, K.: Applying Risk Management to Support SLA Provisioning, Proceedings of the Cracow Grid Workshop 2008.

[8] Battré, D.; Hovestadt, M.; Kao, O.; Keller, A. and Voss, K.: Implementation of Virtual Execution Environments for improving SLA-compliant Job Migration in Grids, Proceedings of the IEEE International Conference on Services Computing (SCC 2008), p.47-52, IEEE Computer Society, 2008.

[9] Battré, D.; Hovestadt, M.; Keller, A.; Kao, O. and Voss, K.: Virtual Execution Environments and the Negotiation of Service Level Agreements in Grid Systems. SVM 2008: 2nd International DMTF Academic Alliance Workshop on Systems and Virtualization Management: Standards and New Technologies, 21-22 October 2008.

[10] Battré, D.; Hovestadt, M.; Kao, O.; Keller, A. and Voss, K.: Quality Assurance of Grid Service Provisioning by Risk Aware Managing of Resource Failures, CRiSIS 2008: Third International Conference on Risks and Security of Internet and Systems, 28 - 30 October 2008.

[11] Beisel, T.; Lietsch, S.; Thielemans, K.: A method for OSEM PET reconstruction on parallel architectures using STIR, Medical Imaging Conf., 2008

[12] Ben-Tal, N. and Honig, B.: Helix-helix interactions in lipid bilayers, Biophysical Journal 71, 3046, 1996

[13] Benzi, R.; Succi, S. and Vergassola, M.: Phys. Rep. 22, 145 (1992)

[14] Beyer, M.K. and Clausen-Schaumann, H.: Chem. Rev. 2005, 105, 2921

[15] Blankenburg, S.; Rauls, E. and Schmidt, W.G.: „The role of dihydrogen bonds for the stabilization of self-assembled molecular nanostructures“, J. Phys. Chem. C 113, 12653 (2009)
[16] Blesken, M.; Rückert, U.; Steenken, D., Witting, K. and Dellnitz, M.: “Multiobjective Optimization for Transistor Sizing of CMOS Logic Standard Cells Using Set-Oriented Numerical Techniques,” NORCHIP Conference, 2009. 27th, 2009
[17] Bloom, M.; Evans, E. and Mouritsen, O.G.: Physical properties of the fluid lipid-bilayer component of cell membranes: a perspective, Quart. Rev. Biophys. 24, 293, 1991
[18] Birkenheuer, G.; Carlson, A.; Fölling, A.; Högqvist, M.; Hoheisel, A.; Papaspyrou, A.; Rieger, K.; Schott, B. and Ziegler, W.: Connecting Communities on the Meta-Scheduling Level: The DGSI Approach! Cracow Grid Workshop (CGW09), Krakau, Polen, 2009.
[19] Börner, J.; Herres-Pawlis, S.; Flörke, U.; Huber, K. and Eur. J.: Inorg. Chem. 2007, 5645.
[20] Börner, J.; Flörke, U.; Döring, A.; Kuckling, D.; Jones, M.D. and Herres-Pawlis, S.: Sustainability 2009, in print.
[21] Börner, J.; Flörke, U.; Döring, A.; Kuckling, D. and Herres-Pawlis, S.: Macromol. Symp. 2009, submitted.
[22] Bothe, D.; Koebe, M.; Wielage, K.; Prüss, J.; Warnecke, H.-J.: Direct Numerical Simulation of Mass Transfer Between Rising Gas Bubbles and Water. In: Sommerfeld, M. (Ed.): Bubbly Flows - Analysis, Modelling and Calculation, Springer, Berlin, Heidelberg, New York, 2003.
[23] Boschmann, A.; Kaufmann, P.; Platzner, M. and Winkler, M.: Towards Multi-movement Hand Prostheses: Combining Adaptive Classification with High Precision Sockets. In Proceedings of the 2nd Technically Assisted Rehabilitation (TAR’09), Berlin, Germany, 2009.
[24] Brannigan, G. and Brown, F.L.H.: Contributions of the Gaussian curvature and nonconstant lipid volume to protein deformation of lipid bilayers, Biophysical Journal 92, 864, 2007
[25] Brinkmann, A; Effert, S. and Gao, Y.: D3.12 Updated Grid Architecture Report, Hydra EU Deliverable, Germany, 2009
[26] Bylaska, E. J. d. J., W.; Aprà, E.; Windus, T.L.; Straatsma, T.P.; Hirata, S.; Valiev, M.; Hackler, M.; Pollack, L.; Kowalski, K.; Harrison, R.; Dupuis, M.; Smith, D.M.A; Nieplocha, J.; Tipparaju V.; Krishnan, M.; Auer, A.A.; Brown, E.; Cisneros, G.; Fann, G.; Fruchtl, H.; Garza, J.; Hirao, K.; Kendall, R.; Nichols, J.; Tsemekhman, K.; Wolinski, K.; Anchell, J.; Bernholdt, D.; Borowski, P.; Clark, T.; Clerc, D.; Dachsel, H.; Deegan, M.; Dyall, K.; Elwood, D.; Glendening, E.; Gutowski, M.; Hess, A.; Jaffe, J.; Johnson, B.; Ju, J.; Kobayashi, R.; Kutteh, R.; Lin, Z.; Littlefield, R.; Long, X.; Meng, B.; Nakajima, T.; Niu, S.; Rosing, M.; Sandrone, G.; Stave, M.; Taylor, H.; Thomas, G.; van Lenthe, J.; Wong, A. and Zhang, Z.: Version 5.1 ed.; Pacific Northwest National Laboratory: Richland, Washington 99352-0999, USA, 2007
[27] CADMEI – Software für Medizinsysteme GmbH, Website: www.cadmei.com Düchs, D. and Schmid, F.: Phase behavior of amphiphilic monolayers: Theory and simulations, J. Phys: Cond. Matt. 13, 4853, 2001
[28] Chamberlain, B.M.; Cheng, M.; Moore, D.R.; Ovitt, T.M., Lobkovsky, E.B., Coates, G.W. and Am, J.: Chem. Soc. 2001, 123, 3229.

[29] Cheng, M.; Attygalle, A.B., Lobkovsky, E.B.; Coates, G.W. and Am, J.; Chem. Soc. 1999, 121, 11583.
[30] Chisholm, M.H.; Gallucci, J.C.and Zhen, H.S.: Inorg. Chem. 2001, 40, 5051.
[31] Cole, S.C.; Coles, M.P. and Hitchcock, P.B.: Organometallics 2004, 23, 5159.
[32] Coles, M. and Hitchcock, P.: Eur. J. Inorg. Chem. 2004, 2662.
[33] Dechy-Carbaret, O.; Martin-Vaca, B. and Bourissou, D.: Chem. Rev. 2004, 104, 6147.
[34] Dellnitz, M.; Schütze, O. and Hestermeyer, T.: Covering Pareto Sets by Multilevel Subdivision Techniques, Journal of Optimization, Theory and Applications, 124(1), pp. 113-136, 2005.
[35] Direct Numerical Computation of the Lift Force acting on Single Bubbles, 6th International Conference on Multiphase Flow, Leipzig, Germany, 2007
[36] Drumwright, R.W.; Gruber, P.R. and Henton, D.E.: Adv. Mat. 2000, 12, 1841.
[37] Elsinghorst, P.W.; Härtig, W.; Goldhammer, S.; Grosche, J. and Gütschow, M.: A gorge-spanning, high-affinity cholinesterase inhibitor to explore β-amyloid plaques. Org. Biomol. Chem. 2009, 7, 3940–3946.
[38] Elsinghorst, P.W.; Cavler, T.; Müller, A.; Blaut, M.; Braune, A. and Gütschow, M.: The rearrangement of taxifolin to alphitonin: chiral investigations.
[39] ESPResSo- Homepage: http://www.espresso.mpg.de (2002-2009)
[40] Espanol, P. and Warren, P.B.: Europhys. Lett. 30, 191 (1995)
[41] Frison, G.; Ohanessian, G. and Comput, J.: Chem. 2007, 29, 416.
[42] Garlotta, D. and Polym, J.: Environ. 2001, 9, 63.
[43] Gaussian Website, http://www.gaussian.com/g_prod/g09.htm
[44] Gaussian 03, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Jr., Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G.A.; Nakatsuji, H., Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J.E.; Hratchian, H.P.; Cross, J.B., Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C., Ochterski, J.W.; Ayala, P.Y.; Morokuma, K.; Voth, G.A.; Salvador, P.; Dannenberg, J.J.; Zakrzewski, V.G.; Dapprich, S., Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Kaghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S., Cioslowski, S.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M.A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, A.; Gill, P. M. W.; Johnson, B.; Chen, W., Wong, M.W.; Gonzalez, C. and Pople, J.A.: Gaussian, Inc., Wallingford CT, 2004.
[45] Gambarelli S. and Mouesca J.M.: Inorg. Chem. 43: 1441-1451.
[46] Gil, T.; Ipsen, J.H.; Mouritsen, O.G.; Sabra,V.C.; Speretto, M. and Zuckermann, M.J.: Theoretical analysis of protein organization in lipid membranes, Biochimica and Biophysica Acta 1376, 245, 1998
[47] Glette, K.; Torresen, J.; Kaufmann, P. and Platzner, M.: A Comparison of Evolvable Hardware Architectures for Classification Tasks. In Proceedings of the 8th International Conference on Evolvable Systems: From Biology to Hardware (ICES), LNCS. Springer, September 2008.
[48] Glette, K.; Torresen, J.; Gruber, T., Sick, B.; Kaufmann, P. and Platzner, M.: Comparing Evolvable Hardware to Conventional Classifiers for Electromyographic Prosthetic Hand Control. In Proceedings of the NASA/ESA

Conference on Adaptive Hardware and Systems (AHS), Noordwijk, The Netherlands, June 2008. Won Best Paper Award in the 'Evolvable Hardware' Category
[49] Grad, M. and Plessl, C.: “Poster abstract: Woolcano – an architecture and tool flow for dynamic instruction set extension on Xilinx Virtex-4 FX,” in Proc. IEEE Symp. on Field-Programmable Custom Computing Machines (FCCM). IEEE Computer Society, April 2009.
[50] Grad, M. and Plessl, C.: “ Woolcano – an architecture and tool flow for dynamic instruction set extension on Xilinx Virtex-4 FX,” in Proc. of International Conference on Engineering of Reconfigurable Systems and Algorithms (ERSA), July 2009
[51] GRAAP-WG: http://www.ogf.org/gf/group_info/view.php?group=graap-wg
[52] Gourlay, I.; Djemame, K. and Padgett, J.: Evaluating Provider Reliability in Grid Resource Brokering to appear in Proceedings of the 11th IEEE International Conference on High Performance Computing and Communications (HPCC'2009), Seoul, Korea, June 2009.
[53] GridSphere, http://www.gridsphere.org/gridsphere/gridsphere.
[54] Groppe, D.: GPU-basierte Beschleunigung neuer Bildrekonstruktions-algorithmen in der Tomographie aus MATLAB, Master Thesis, PC², 2009
[55] Gupta, A.P. and Kumar, V.: Eur. Polymer J. 2007, 43, 4053.
[56] Happe, M.; Lübbers, E. and Platzner, M.: „A Multithreaded Framework for Sequential Monte Carlo Methods on CPU/FPGA Platforms“, In Reconfigurable Computing: Architectures, Tools and Applications: 5th International Workshop, ARC 2009, Karlsruhe, Germany, March 2009.
[57] Happe, M.; Lübbers, E. and Platzner, M.: „An Adaptive Sequential Monte Carlo Framework with Runtime HW/SW Repartitioning“, In Proceedings of the 2009 International Conference on Field-Programmable Technology (FPT’09), Sydney, Australia, December 2009. To appear.
[58] Häcker, H.-G.; Elsinghorst, P.W.; Michels, S.; Daniels, J.; Schnakenburg, G. and Gütschow. M.: 2-(Benzoylimino)thiazolidin-4-ones: formation by an alternative ring closure and analysis of rotational barriers. Synthesis 2009, 1195–1203.
[59] Hall D.O.; Cammack R. and Rao K.K.: (1971) Nature 233:136-138.
[60] Haljasmaa, I.: On the Drag of Fluid and Solid Particles freely moving in a Continuous Medium, Dissertation, University of Pittsburgh 2006.
[61] Herres-Pawlis, S.; Flörke, U. and Henkel, G.: Eur. J. Inorg. Chem. 2005, 3815.
[62] Herres-Pawlis, S.; Neuba, A., Seewald, O.; Seshadri, T.; Egold, H.; Flörke, U. and Henkel, G.: Eur. J. Org. Chem. 2005, 4879.
[63] Herres, S.; Flörke, U. and Henkel, G.: Acta Crystallogr., 2004, C60, o358 – o360.
[64] Highly Predictable Cluster for Internet-Grids (HPC4U), EU-funded project IST-511531. http://www.hpc4u.org
[65] Hoffmann, A.; Börner, J.; Flörke, U. and Herres-Pawlis, S.: Inorg. Chim. Acta, 2008, DOI: 10.1016/j.ica.2008.06.002
[66] Hoogerbrugge, P.J. and Koelman, J.M.: Europhys. Lett. 19, 155 (1992)
[67] Hostomska, Z.; Matthews, D. and Hostomsky, Z.: Journal of Acquired Immune Deficiency Syndromes and Human Retrovirology 1993, 6, 673-673.
[68] http://pc2.uni-paderborn.de/research-projects/projects/pg-vsc
[69] http://www.csipc2.de
[70] Huang, M.: VNET: PlanetLab Virtualized Network Access, 2005

[71] Hughes, S. H.; Arnold, E. and Hostomska, Z.: In Ribonuclease H; Crouch, R. J., Toulme, J. J., Eds.; INSERM: Paris, 1998, p 195-224.
[72] Hughes, S. H.; Arnold, E.; Hostomska, Z. In Ribonuclease H; Crouch, R. J. and Toulme, J. J.: Eds.; INSERM: Paris, 1998, p 195-224
[73] Hunter, R.J.: "Foundations of Colloid Science", Clarendon Press, Oxford (1987)
[74] Hutter et al J CPMD, IBM Corp 1990-2007, MPI fuer Festkoerperforschung Stuttgart 1997-2001, see also http://www.cpmd.org.
[75] Hutter, J.: et al. CPMD V3.12; Copyright IBM Corp 1990-2001, Copyright MPI für Feskörperforschung Stuttgart 1997-2001. see www.cpmd.org
[76] Ishikawa, K.; Okumura, M.; Katayanagi, K.; Kimura, S.; Kanaya, S.; Nakamura, H. and Morikawa, K.: Journal of Molecular Biology 1993, 230, 529-542.
[77] ISC2009, http://www.supercomp.de/isc09/
[78] Jacobson, S.; Degée, Ph.; Fritz, H.G.; Dubois, Ph. And Jérôme, R.: Polym. Eng. Sci. 1999, 39, 1311.
[79] Johnson D.C.; Dean D.R.; Smith A.D. and Johnson M.K.: (2005) Annu. Rev. Biochem. 74: 247-281.
[80] Kaufmann, P.; Plessl, C. and Marco Platzner. EvoCaches: Application-specific Adaptation of Cache Mappings. In: Proceedings of the NASA/ESA Conference on Adaptive Hardware and Systems (AHS), San Francisco, CA, USA, June 2009.
[81] Kaufmann, P. and Platzner, M.: Advanced Techniques for the Creation and Propagation of Modules in Cartesian Genetic Programming. In Proceedings of the Genetic and Evolutionary Computation Conference (GECCO), Atlanta, Georgia, USA, July 2008. ACM.
[82] Kaufmann, P. and Platzner, M.: MOVES: A Modular Framework for Hardware Evolution. In Proc. of the 2nd NASA/ESA Conference on Adaptive Hardware and Systems (AHS), pp.447-454, Aug. 2007. Received the Best Paper Award in the Evolvable Hardware Category.
[83] Kaufmann, P. and Platzner, M.: Toward Self-adaptive Embedded Systems: Multiobjective Hardware Evolution. In Proc. Int'l Conf. on Architecture of Computing Systems (ARCS), March 2007. Springer, LNCS 4415.
[84] Kaufmann, P. and Platzner, M.: Multi-objective Intrinsic Hardware Evolution. In Proc. of the MAPLD Int'l Conference, Sept. 2006
[85] Katayanagi, K.; Miyagawa, M.; Matsushima, M.; Ishikawa, M.; Kanaya, S.; Ikehara, M.; Matsuzaki, T. and Morikawa, K.: Nature 1990, 347, 306-309.
[86] Yang, W.; Hendrickson, W. A.; Crouch, R. J. and Satow, Y.: Science 1990, 249, 1398-1405
[87] Katayanagi, K.; Miyagawa, M.; Matsushima, M.; Ishikawa, M.; Kanaya, S.; Nakamura, H.; Ikehara, M.; Matsuzaki, T. and Morikawa, K.: Journal of Molecular Biology 1992, 223, 1029-1052
[88] Katayanagi, K.; Okumura, M. and Morikawa, K.: Proteins-Structure Function and Genetics 1993, 17, 337-346.
[89] Kanaya, S.; Kohara, A.; Miura, Y.; Sekiguchi, A.; Iwai, S.; Inoue, H.; Ohtsuka, E. and Ikehara, M. Journal of Biological Chemistry 1990, 265, 4615-4621.
[90] Kerrighed, http://www.kerrighed.org
[91] Knieper, T.; Defo, B.; Kaufmann, P. and Platzner, M.: On Robust Evolution of Digital Hardware. In Proceedings of the 2nd IFIP Conference on Biologically Inspired Collaborative Computing (BICC), Milan, Italy, September 2008. Springer.

[92] Koebe, M. Numerische Simulation aufsteigender Blasen mit und ohne Stoffaustausch mittels der Volume of Fluid (VOF) Methode, Dissertation, University of Paderborn, 2004 Zweiphasenströmungen, VDI Fortschritt Berichte, Reihe 7, Nr. 459
[93] Köhn, U.; Schulz, M.; Görls, H. and Anders, E.: Tetrahedron: Asymmetry 2005, 16, 2125; b) Walter, M.; Wermann, K.; Lutsche, M.; Günther, W.; Görls, H. and Anders, E.: J. Org. Chem. 2006, 71, 1399.
[94] Konopka, M.; Turansky, R.; Reichert, J.; Fuchs, H.; Marx, D.and Stich, I.: Phys. Rev. Lett. 2008, 100, 115503.
[95] Kricheldorf, H.R.: Chemosphere 2001, 43, 49; b) Kricheldorf, H. R.; Bornhorst, K. and Hachmann-Thiessen, H.: Macromolecules 2005, 38, 5017; c) Kricheldorf, H.R. and Rost, S.: Polymer 2005, 46, 3248; d) Kricheldorf, H.R.; Hachmann-Thiessen, H. and Schwarz, G.: Biomacromolecules 2004, 5, 492.
[96] Krüger, D.; Fuchs, H.; Rousseau, R.; Marx, D.and Parrinello, M.: Phys. Rev. Lett. 2002, 89, 186402; (b) D. Krüger, R. Rousseau, H. Fuchs, D. Marx Angew. Chem. Int. Ed. 2003, 42, 2251.
[97] Kuhn, N.; Grathwohl, M.; Steinmann, M. and Henkel, G.: Z. Naturforsch. 1998, 53b, 997.
[98] Kulik H.J.; Cococcioni M.; Scherlis D.A. and Marzari N.: (2006) Phys. Rev. Lett. 97:103001
[99] Kuznetsova, I.; Meier, T.; Thomas, P. and Cundiff, S.T.: Phys. Rev. B 76, 153301 (2007).
[100] Kuznetsova, I.; Gogh, N.; Förstner, J.; Meier, T.; Cundiff, S.T.; Varga, I. and Thomas, P.. Submitted to Phys. Rev. B
[101] Kuznetsova, I.; Thomas, P.; Meier, T., Zhang, T.; Li, X.; Mirin, R.P. and Cundff, S.T.: Sol. State Comm. 142, 154 (2007).
[102] Lague, P.; Zuckermann, M.M. and Roux, B.: Protein inclusion in lipid membranes: A theory based on the hypernetted chain integral equation, Faraday Disc. 111, 165, 1998
[103] Lai, L.H.; Yokota, H.; Hung, L.W.; Kim, R.and Kim, S.H.: Structure with Folding & Design 2000, 8, 897-904
[104] Lai, L. H.; Yokota, H.; Hung, L. W.; Kim, R. and Kim, S. H. Structure with Folding & Design 2000, 8, 897-904.
[105] Lebensmittelchemikertag, 2009, poster AT48
[106] Lenz, O. and Schmid, F.: Structure of Symmetric and Asymmetric Ripple Phases in Lipid Bilayers, Phys. Rev. Lett. 98, 058104, 2007
[107] Lenz, O. and Schmid, F.: A simple computer model for liquid lipid bilayers, J. Mol. Liquids 117(1-3), 147, 2005
[108] Li, X., Zhang, T.; Borca, C.N. and Cundiff, S.T.: Phys. Rev. Lett. 96, 057406 (2006).
[109] Li J.; Nelson M.R.; Peng C.Y.; Bashford D. and Noodleman L.: (1998) J. Phys. Chem. A 102: 6311-6324.
[110] Lia, R.Z.; Yu, J.G.; Raushel, F.M.; Himo, F.: Chemistry-a European Journal 2008, 14, 4287-4292.
[111] Liferay, http://www.liferay.com/web/guest/partners/sun.
[112] Lima, W. F.; Wu, H. J.; Nichols, J. G.; Prakash, T. P.; Ravikumar, V. and Crooke, S. T.: Journal of Biological Chemistry 2003, 278, 49860-49867.
[113] Limbach, H.J.; Arnold, A.; Mann, B.A. and Holm, C.: Comp. Phys. Comm. 174, 704 (2006)
[114] Linux-VServer, http://linux-vserver.org

[115] Linux Netfilter, http://www.netfilter.org
[116] Lischka, J. and Karl, H.: A virtual network mapping algorithm based on subgraph isomorphism detection, VISA '09: Proceedings of the 1st ACM workshop on Virtualized infrastructure systems and architectures, 2009
[117] Lübbers, E. and Platzner, M.: „ReconOS: A RTOS Supporting Hard- and Software Threads“, In Proceedings of 2007 IEEE International Conference on Field Programmable Logic and Applications (FPL'07), Amsterdam, August 27-29, 2007.
[118] Lübbers, E. and Platzner, M.: „Communication and Synchronization in Multithreaded Reconfigurable Computing Systems“, In Proceedings of the 8th International Conference on Engineering of Reconfigurable Systems and Algorithms (ERSA), Las Vegas, Nevada, USA, July 2008.
[119] Lübbers, E. and Platzner, M.: „A Portable Abstraction Layer for Hardware Threads“, In Proceedings of the 18th IEEE International Conference on Field Programmable Logic and Applications (FPL'08), Heidelberg, Germany, September 2008.
[120] Lübbers, E. and Platzner, M.: „Cooperative Multithreading in Dynamically Reconfigurable Systems“, In Proceedings of the 19th IEEE International Conference on Field Programmable Logic and Applications (FPL'09), Prague, Czech Republic, August 2009.
[121] Lübbers, E. and Platzner, M.: „ReconOS: Multithreaded Programming for Reconfigurable Computers“, ACM Transactions on Embedded Computing Systems (TECS), Volume 9, Issue 1, October 2009.
[122] Lübbers, E. and Platzner, M.: „ReconOS: An Operating System for Dynamically Reconfigurable Hardware“, In Dynamically Reconfigurable Systems - Architectures, Design Methods and Applications, Springer, 2010, ISBN 978-90-481-3484-7. To appear.
[123] Marx, D. and Hutter, J.: Ab initio Molecular Dynamics: Basic Theory and Advanced Methods; Cambridge University Press: Cambridge, 2009.
[124] Marx D. and Hutter J.: (2009) Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods (Cambridge University Press, Cambridge).
[125] May, S.: Theories on structural perturbations of lipid bilayers, Curr. Opn. Coll. Interf. Sci. 5, 244, 2000
[126] Mazarro, R.; de Lucas, A., Gracia, I.; Rodríguez, J.F.and Biomed, J.: Mat. Res. Part B: Appl. Biomat. 2007, 85, 196.
[127] Mazzarello, R.; Cossaro, A.; Verdini, A.; Rousseau, R.; Casalis, L.; Danisman, M.F.; Floreano, L.; Scandolo, S.; Morgante, A. and Scoles, G.: Phys. Rev. Lett. 2007, 98, 016102.
[128] McNamara G.R. and Zanetti, G.: Phys. Rev. Lett. 61, 2332 (1988)
[129] Mehta, R.; Kumar, V.; Bhunia, H.; Upadhyay, N.S. and Macromol, J.: Sci., Part C: Polym. Rev. 2005, 45, 325.
[130] Meier, T.; Thomas, P. and Koch, S.W.: Coherent Semiconductor Optics - From Basic Concepts to Nanostructure Applications, Springer, Berlin, 2007.
[131] Mc Evoy, G. V. and Schulze, B.: "Using clouds to address grid limitations," in MGC'08: Proceedings of the 6th international workshop on Middleware for grid computing. New York, NY, USA: ACM, 2008, pp. 1-6. [Online]. Available: http://dx.doi.org/10.1145/1462704.1462715
[132] "Modification of UCT with Patterns in Monte-Carlo Go", S. Gelly et al., Technical Report 6062, INRIA, 2006.

[133] Morales R.; Chron M.H.; Hudry-Clergeon G.; Petíllot Y.; Norager S.; Medina M. and Frey M.: (1999) Biochemistry 38: 15764-15773.
[134] Morales R.; Frey M. and Mouesca J.M.: (2002) J. Am. Chem. Soc. 124: 6714-6722.
[135] Mouritsen, O.G. and Bloom, M.: Models of lipid-protein interactions in membranes, Quarterly Reviews of Biophysics: Biomol. Struct. 22, 145, 1993
[136] Nakamura, H.; Oda, Y.; Iwai, S.; Inoue, H.; Ohtsuka, E.; Kanaya, S.; Kimura, S.; Katsuda, C.; Katayanagi, K.; Morikawa, K.; Miyashiro, H. and Ikehara, M.: Proceedings of the National Academy of Sciences of the United States of America 1991, 88, 11535-11539.
[137] Nakamura, H.; Oda, Y.; Iwai, S.; Inoue, H.; Ohtsuka, E.; Kanaya, S.; Kimura, S.; Katsuda, C.; Katayanagi, K.; Morikawa, K.; Miyashiro, H. and Ikehara, M.: Proceedings of the National Academy of Sciences of the United States of America 1991, 88, 11535-11539
[138] Nakano, K; Kosaka, N.; Hiyama, T. and Nozaki, K.: Dalton Trans. 2003, 4039.
[139] Nair N.N.; Schreiner E.; Pollet R.; Staemmler V. and Marx D.: (2008) J. Chem. Theory Comput. 4: 1174
[140] Neder, J.; West, B.; Nielaba, P. and Schmid, F.: Coarse-Grained Simulations of Membranes under Tension, The Journal of Chemical Physics, submitted
[141] NetNS, http://lxc.sourceforge.net/network.php
[142] a) Neuba, A.; Haase, R.; Bernard, M.; Flörke, U. and Herres-Pawlis, S.: Z. Anorg. Allg. Chem., accepted; b) Raab, V.: Ph.D. Thesis, University of Marburg, 2001; c) Herres-Pawlis, S.: Ph.D. Thesis, University of Paderborn, 2005.
[143] Niehörster, O.; Birkenheuer, G.; Brinkmann, A.; Elsässer, B.; Herres-Pawlis, S.; Krüger, J.; Niehörster J. and Packschies, L.: Providing Scientific Software as a Service in Consideration of Service Level Agreements, Cracow Grid Workshop (CGW09), Krakau, Polen, 2009.
[144] Noodleman L.; Peng C.Y.; Case D.A. and Mouesca, J.M.: (1995) Coord. Chem. Rev. 144: 199-244.
[145] Nowotny, M.; Gaidamakov, S. A.; Crouch, R. J.; Yang, W. Cell 2005, 121, 1005-1016.
[146] Nowotny, M.; Gaidamakov, S. A.; Ghirlando, R.; Cerritelli, S. M.; Crouch, R. J.; Yang, W. Molecular Cell 2007, 28, 513-513.
[147] Nowotny, M. and Yang, W. Embo Journal 2006, 25, 1924-1933.
[148] Nurmi, D., Wolski, R.; Grzegorczyk, C.; Obertelli, G.; Soman, S.; Youseff, L. and Zagorodnov, D.: "The eucalyptus open-source cloud-computing system," in Proceedings of 9th IEEE International Symposium on Cluster Computing and the Grid, 2009. [Online]. Available: http://open.eucalyptus.com/documents/ccgrid2009.pdf
[149] NVIDIA CUDA - Compute Unified Device Architecture, Website: http://www.nvidia.com/object/cuda_home.html#
[150] O'Kneefe, B. J.; Hillmyer, M. A. and Tolman, W.B.: Dalton Trans. 2001, 2215
[151] Oda, Y.; Yoshida, M. and Kanaya, S. Journal of Biological Chemistry 1993, 268, 88-92
[152] Oda, Y.; Yoshida, M. and Kanaya, S.: Journal of Biological Chemistry 1993, 268, 88-92
[153] Oda, Y.; Iwai, S.; Ohtsuka, E.; Ishikawa, M.; Ikehara, M. and Nakamura, H.: Nucleic Acids Research 1993, 21, 4690-4695.
[154] Okada, M.: Prog. Polym. Sci. 2002, 27, 87.
[155] OpenCCS, https://www.openccs.eu/

[156] Oppenheimer, D.; Albrecht, J.; Patterson, D. and Vahdat, A.: Distributed Resource Discovery on PlanetLab with SWORD, In WORLDS, 2004
[157] P-Grade, http://portal.p-grade.hu/.
[158] Pari, K.; Mueller, G. A.; DeRose, E. F.; Kirby, T. W. and London, R. E.: Biochemistry 2003, 42, 639-650
[159] Park, K. and Pai, V.: CoMon: a mostly-scalable monitoring system for PlanetLab, SIGOPS Oper. Syst. Rev., 2006
[160] Palmer G.; Dunham W.R.; Fee J.A.; Sands R.H.; Lizuka T. and Yonetani T.: (1971) Biochim Biophys Acta 408: 306-318.
[161] Perdew, J. P.; Burke, K. and Ernzerhof, M.: Phys. Rev. Lett. 1996, 77, 3865.
[162] Raab, V., Kipke, J.; Gschwind, R.M. and Sundermeyer, J.: Chem. Eur. J., 2002, 1682.
[163] Rauls, E., Blankenburg, S. and Schmidt, W.G.: ”Chemical reactivity on surfaces: Modeling the imide synthesis from DATP and PTCDA on Au(111)”, Phys. Rev. B, 81, 125401 (2010).
[164] Ressourcenverbund Nordrhein-Westfalen (in German), http://www.rv-nrw.de
[165] Rees D.C.; Howard J.B.: (2003) Science 300:929-931.
[166] Rice, P. A. and Baker, T. A.: Nature Structural Biology 2001, 8, 302-307.
[167] Rieber, M.: Numerische Modellierung der Dynamik freier Grenzflächen in Zweiphasenströmungen, VDI Fortschritt Berichte, Reihe 7, Nr. 459
[168] Schäfers, L.: “Analyse neuer Spielbaumsuchverfahren, wie sie im Computer Go angewendet werden”, Master Thesis at University of Paderborn, 2008
[169] Schatz, O.; Cromme, F. V.; Gruningerleitch, F. and Legrice, S. F.: J. Febs Letters 1989, 257, 311-314
[170] Schatz, O.; Cromme, F. V.; Gruningerleitch, F. and Legrice, S. F.: J. Febs Letters 1989, 257, 311-314.
[171] Schmid, F.; Düchs, D.; Lenz, O. and West, B.: A generic model for lipid monolayers, bilayers, and membranes, Computer Physics Communications 177(1-2), 168, 2007
[172] Schmidt, W.G.; Seino, K.; Preuss, M.; Hermann, A.; Ortmann, F. and Bechstedt, F.: “Organic molecule adsorption on solid surfaces: chemical bonding, mutual polarisation and dispersion interaction“, Appl. Phys. A **85**, 387 (2006).
[173] Schmidtke, M.: Untersuchung der Dynamik fluider Partikel auf Basis der Volume of Fluid Methode, Dissertation, Universität Paderborn, 2008
[174] Schumacher, T.; Plessl, C. and Platzner, M.: “IMORC: Application Mapping, Monitoring and Optimization for High-Performance Reconfigurable Computing,” in Proc. IEEE Symp. on Field-Programmable Custom Computing Machines (FCCM ’09). IEEE, 2009.
[175] Schumacher, T.; Plessl, C. and Platzner, M.: “An Accelerator for k-th Nearest Neighbor Thinning based on the IMORC Infrastructure”, in Proceedings of the 19th International Conference on Field Programmable Logic and Applications (FPL), Prague, Czech Republic, August/September 2009. IEEE
[176] Schumacher, T.; Süß, T.; Plessl, C. and Platzner, M.: “Communication Performance Characterization for Reconfigurable Accelerator Design on the XD1000 ”, in Proc. Int. Conf. on ReConFigurable Computing and FPGAs (RECONFIG '09)
[177] Schreiner E.; Nair N.N.; Pollet R.; Staemmler V. and Marx D.: (2007) Proc. Nat. Acad. Sci. 104: 20725.

[178] Schreiner, E.: Biochemical Aspects of Iron-Sulfur Systems: Magnetostructural Properties of Ferredoxins and Prebiotic Peptide Synthesis Involving Pyrite (PhD Thesis, Lehrstuhl für Theoretische Chemie, Ruhr--Universität Bochum, Germany, 2007).
[179] Schütze, O.: Set Oriented Methods for Global Optimization, PhD thesis, University of Paderborn, Germany, 2004.
[180] Shaw-Reid, C.A.; Munshi, V., Graham, P., Wolfe, A., Witmer, m.; Danzeisen, R., Olsen, D.B.; Carroll, S.S.; Embrey, M.; Wai, J.S.; Miller, M.D.; Cole, J.L. and Hazuda, D.J.: Journal of Biological Chemistry 2003, 278, 2777-2780.
[181] Steitz, T. A. and Steitz, J. A. Proceedings of the National Academy of Sciences of the United States of America 1993, 90, 6498-6502.
[182] Steitz, T. A. and Steitz, J. A.: Proceedings of the National Academy of Sciences of the United States of America 1993, 90, 6498-6502.
[183] Shi, J. and Tomasi, C.: Good features to track, in Proceedings of Computer Vision and Pattern Recognition, IEEE, 1994
[184] Shin M. and Arnon D.I.: (1965) J. Biol. Chem. 240: 1405-1411.
[185] Simon, J.: PC² Benchmarking Center, http://wwwcs.uni-paderborn.de/pc2/about-us/staff/jens-simons-pages/benchmarkingcenter.html
[186] Smiatek, J.; Allen, M.P. and Schmid, F.: Europ. Phys. J. E 26, 115 (2008)
[187] Smiatek, J.; Sega, M.; Schiller, U.D., Holm, C. and Schmid, F.: J. Chem. Phys. 130, 44702 (2009)
[188] Steinbuch Centre for Computing. Karlsruher Institute of Technology. About High Performance Computing as a Service. [Online]. Available: http://www.scc.kit.edu/forschung/4942.php
[189] Steenken, D.: Multiobjective Optimization and Sensitivity Evaluation of IC Standard Cells Using Set-oriented Numerical Methods, Diploma thesis, University of Paderborn, 2009
[190] Sulpizi M.; Raugei S.; VandeVondele J.; Carloni P. and Sprik M.: (2007) J. Phys. Chem. B 111: 3969-3976.
[191] Tamm, M.; Petrovic, D.; Randoll, S.; Beer, S., Bannenberg, T.; Jones, P.G. and Grunenberg, J.: Org. Biomol. Chem. 2007, 5, 523; b) Petrovic, D.; Hill, L.M.R.; Jones, P.G.; Tolman, W.B. and Tamm, M.: Dalton Trans. 2008, 887; c) Panda, T. K.; Hrib, C.G.; Jones, P.G.; Jenter, J.; Roesky, P.W. and Tamm, M.: Eur. J. Inorg. 2008, 4270.
[192] Tanese, N. and Goff, S. P.: Proceedings of the National Academy of Sciences of the United States of America 1988, 85, 1777-1781.
[193] The ARMINIUS Cluster at PC²: http://pc2.uni-paderborn.de/hpc-systems-services/available-systems/arminius-cluster/
[194] The International Go Federation) http://www.intergofed.org/
[195] The MathWorks – MEX-files Guide, Website http://www.mathworks.com/support/tech-notes/1600/1605.html?BB=1
[196] The SMP Server at PC²: http://pc2.uni-paderborn.de/hpc-systems-services/available-systems/smp-server/
[197] Thielemans, K.: et. al., STIR: Software for Tomographic Image Reconstruction Release 2 Proc. IEEE Medical Imaging Conference 2006, San Diego, CA.
[198] Tomasi, C. and Kanade, T.: Detection and Tracking of Point Features, in CMU Techreport, 1991
[199] Uchiyama, Y.; Miura, Y.; Inoue, H.; Ohtsuka, E.; Ueno, Y.; Ikehara, M. and Iwai, S.: Journal of Molecular Biology 1994, 243, 782-791.

[200] Uhlherr, A.; Leak, S.J.; Adam, N.E.; Nyberg, P.E.; Doxastakis, M.; Mavrantzas, V.G. and Theodorou, D.N.: Large scale atomistic polymer simulations using Monte Carlo methods for parallel vector processors, Computer Physics Communications 144(1), 1, 2002
[201] Vanderbilt, D.: Phys. Rev. B (Rapid Communications), 1990, 41, 7892
[202] Valiev, M.; Garrett, B. C.; Tsai, M. K.; Kowalski, K.; Kathmann, S. M.; Schenter, G. K. and Dupuis, M.: Journal of Chemical Physics 2007, 127, -.
[203] Valiev, M.; Kawai, R.; Adams, J. A. and Weare, J. H.: Journal of the American Chemical Society 2003, 125, 9926-9927.
[204] Vomweg, T.W., Mayer, D.; Maciak, A.; Rösler, T. and Mattiuzzi, M.: CADMRM A full automatic Breast Cancer Diagnosis Tool in CE MRM and Image Processing, Framework for Construction of CAD System, in ECR, 2008
[205] Walther, D.; Kuzmin, P. and Donath, E.: Brownian dynamics simulation of the lateral distribution of charged membrane components, Eur. Biophys. J. 24, 125, 1996
[206] Web-page PG VSC:
[207] Weiser, S.; Meier, T.; Möbius, J.; Euteneuer, A.; Mayer, E.J., Stolz, W.; Hofmann, M.; Rühle, W.W.; Thomas, P. and Koch, S.W.: Phys. Rev. B 61, 13088 (2000).
[208] West, B.; Brown, F.L.H. and Schmid, F.: Membrane-Protein Interactions in a Generic Coarse-Grained Model for Lipid Bilayers, Biophysical Journal 96, 101, 2009
[209] West, B. and Schmid, F.: Properties of Lipid Membranes in the Fluid and the Gel State: A Coarse-Grained Monte-Carlo Study, Soft Matter, submitted
[210] Wittmann, H.; Schorm, A., Sundermeyer, J.: Z. Anorg. Allg. Chem. 2000, 626, 1583; b) Oakley, S. H.; Soria, D. B.; Coles, M. P. and Hitchcock, P. B.: Polyhedron 2006, 25, 1247; c) Wittmann, H.; Raab, V., Schorm, A.; Plackmeyer, J. and Sundermeyer, J.: Eur. J. Inorg. Chem. 2001, 1937; d) Aoki, S., Iwaida, K.; Hanamoto, N.; Shiro, M. and Kimura, E.: J. Am. Chem. Soc. 2002, 124, 5256; e) Ishikawa, T. and Kawahata, M.: EP 1752451A1, 2007.
[211] Wörl, S.; Hellwinkel, D., Pritzkow, H.; Hofmann, M. and Krämer, R.: Dalton Trans., 2004, 2750.
[212] Wortmann, R.; Herres-Pawlis, S., Flörke, U. and Henkel, G.: Manuscript in preparation.
[213] WS-Agreement specification: http://www.ogf.org/documents/GFD.107.pdf
[214] www.quantum-espresso.org
[215] Wu, J.; Yu, T.-L.; Chen, C.-T. and Lin, C.-C.:Coord. Chem. Rev. 2006, 250, 602
[216] Wu, H. J.; Lima, W. F. and Crooke, S. T.: Journal of Biological Chemistry 2001, 276, 23547-23553.
[217] Xu, W.; Dong, M.; Gersen, H.; Rauls, E.; Vazquez-Campos, S.; Crego-Calama, M.; Reinhoudth, D.N., Stensgaard, I.; Laegsgaard, E.; Linderoth, T.R. and Besenbacher, F.: ”Influence of Alkyl Side Chains on Hydrogen-Bonded Molecular Surface Nanostructures”, Small 4, 1620 (2008)
[218] Yalagandula, P.; Sharma, P.; Banerjee, S.; Basu, S. and Lee, S.J.: S3: A scalable Sensing Service for Monitoring Large Networked Systems, INM '06: Proceedings of the 2006 SIGCOMM workshop on Internet network management, 2006
[219] Yang, W.; Lee, J. Y. and Nowotny, M.: Molecular Cell 2006, 22, 5-13.

[220] Yu, M.; Yi, Y.; Rexford, J. and Chiang, M.: Rethinking Virtual Network Embedding: Substrate Support for Path Splitting and Migration, SIGCOMM Comput. Commun. Rev., 2008
[221] Zentrales Innovationsprogramm Mittelstand, Website: http://www.zim-bmwi.de
[222] Zhu, Z. and Ammar, M.: Overlay network assignment in PlanetLab with NetFinder, Technical Report GT-CSS-06-11, 2006