Jacobs University Bremen

Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV)
www.clamv.jacobs-university.de

CLAMV Report 2002–2007

Compiled by the CLAMV Seminar and Editorial Committee

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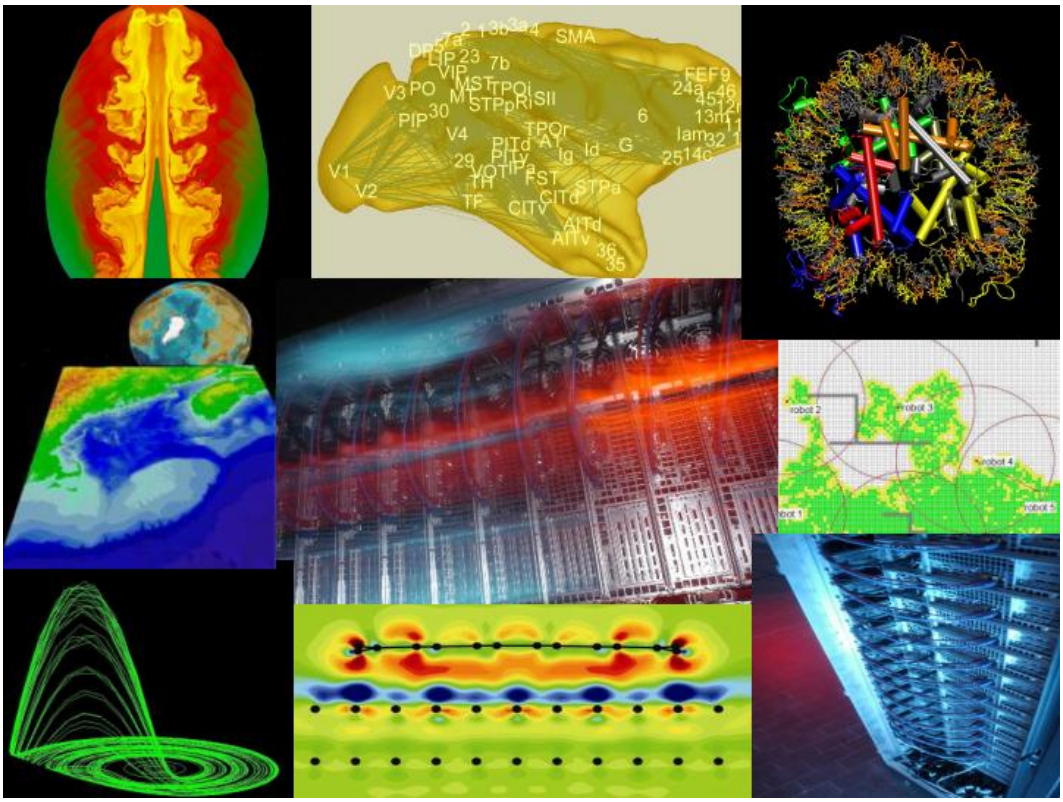

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1 Introduction

The *Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV)* is designed to be the umbrella and support initiative for all computationally oriented disciplines at Jacobs University Bremen. Since its foundation in April 2002, the laboratory has established itself within this university as a small but efficient institution to serve a large number of users in research and teaching. CLAMV users benefit from a shared infrastructure with workspaces for researchers and students as well as remote access to software, servers, and high-performance computing platforms. The laboratory is open to all scientists and students on campus. We support a broad spectrum of activities ranging from large-scale simulations on parallel computing platforms to undergraduate programming courses. A large selection of scientific computing software is available to the community through the CLAMV file and license server.

This report visits the various areas where CLAMV has been active over the first five years of its existence. A short history of events, the current state of services that we offer to the community, and a brief description of our future plans are given in section 2. As apparent from its name, CLAMV is designed to support computational research in the three methodological areas analysis, modeling, and visualization. These are illustrated by means of selected scientific projects in section 3. The bulk of research projects are described in four thematically organized sections 4–7 showing the diversity of subject areas that are served by CLAMV. Our involvement in teaching is summarized in section 8. Technical and organizational details are given in the appendix.

2 CLAMV Components and Services

Contributed by Achim Gelessus

2.1 The First Five Years of CLAMV

CLAMV started in summer 2002 with the installation of a 40-node dual-processor Linux cluster (100 MBit interconnect). The same year in fall the startup of the CLAMV Teaching Lab followed. 4 class rooms in building Research I were equipped with a total of 30 identical Linux computers. User and home account management was configured on a central server (SUN v880 server). In summer 2003 the local cluster performance was significantly enhanced by the installation of a 16-node GigaBit cluster for the computational chemistry group and a 16-node Myrinet cluster for the computational biology group. Both clusters were extended with additional local storage and computing nodes in summer 2004. For the increasing number of students in electrical engineering and computer science the Undergraduate Teaching Lab (CS-Lecture Hall) in building Research I was opened in January 2004. From the beginning the Undergraduate Teaching Lab was integrated into the CLAMV user administration; hardware and software for the lecture hall have been maintained by the IRC since then. For the then newly founded group for computational geoscience the GIS-Lab in Research III was taken into service between summer 2004 and summer 2005. At about the same time it became clear that the CLAMV Teaching Lab rooms in Research I were needed as offices for new students and faculty. Therefore the CLAMV Teaching Lab moved to newly renovated rooms in the Westhall basement during the summer break 2005. With the installation of a 24-processor shared memory server (SGI Altix) the situation for high performance computing users was significantly improved. In order to train users in programming skills a workshop for parallel programming in MPI and OpenMP was organized for August 2005. A second workshop with the same topic took place in January 2007. In February 2007 the computer hardware in the CLAMV Teaching Lab was replaced by new machines. For the newly founded groups in computational system biology and physics a fourth cluster with 40 nodes and combined GigaBit / Infiniband interconnect is currently installed. The scope of the software which is maintained by CLAMV has been growing steadily over the years and covers all computationally oriented disciplines at Jacobs University.

In summer 2002 a full time position was assigned to CLAMV for system administration. Later that position was upgraded to a system manager. The system manager has been supported by two student assistants for the last years. In September 2006 the GIS-Lab got a half time position for a system administrator.

2.2 Current Status of CLAMV Components and Services

The number of CLAMV users has been growing steadily for the last 5 years. In April 2007 there are about 750 users in total from faculty, staff and students who use CLAMV facilities. Most users (about 600 in April 2007) have a CLAMV account which

enables them to get access to the Linux based resources. There is another group of users (about 150 in April 2007) who benefit from the services for Windows and MAC OS software without actually having a CLAMV account.

CLAMV is open for all schools and center at Jacobs University. Not surprisingly the majority of users and requests come from the School of Engineering and Science. Table A.7 in the appendix lists all faculty members who have used CLAMV between 2002 and 2007.

The CLAMV components and services are subdivided into six groups according to their field of application. The six groups are:

Teaching,

Software,

High Performance Computing (HPC),

Storage,

WWW-Presentations,

Research Group Support.

The facilities for teaching and software are also called basic components. Basic components are actually commonly used for teaching and research. Many requests from faculty can be served with the basic components (s. table A.7). High Performance Computing, storage, WWW presentations and research group support are called advanced components. Advanced services are mainly or in some cases even exclusively used for research.

A schematic representation of the CLAMV components is given in Fig. 1.

Teaching

The CLAMV Teaching Lab is located in the Westhall basement. There are four class rooms with a total of 48 computer (Dell Optiplex, Dual Core Processor). The rooms are of different size; in three rooms (21,9,6 computer) the operating system SuSE Linux is installed. In the fourth room the operating system Windows XP is used. Direct access to the Teaching Lab rooms is possible for registered courses only. Remote access via the computer network to hardware and software resources is permanently possible. There is also a Linux terminal server for users who use the CLAMV resources only occassionally (lab rotation students, guests, ICTS members, . . .).

The user accounts are located on a central file server system. The file server system is a complete redundant configuration of two identical servers with direct optical interconnect for instantaneous data replication. Mutual monitoring of the services ensure high availability of the file server system.

The undergraduate lecture hall in building Research I is maintained by the IRC and the CLAMV. The user administration has been incorporated into the CLAMV user administration for providing an identical user environment (user login, home account)

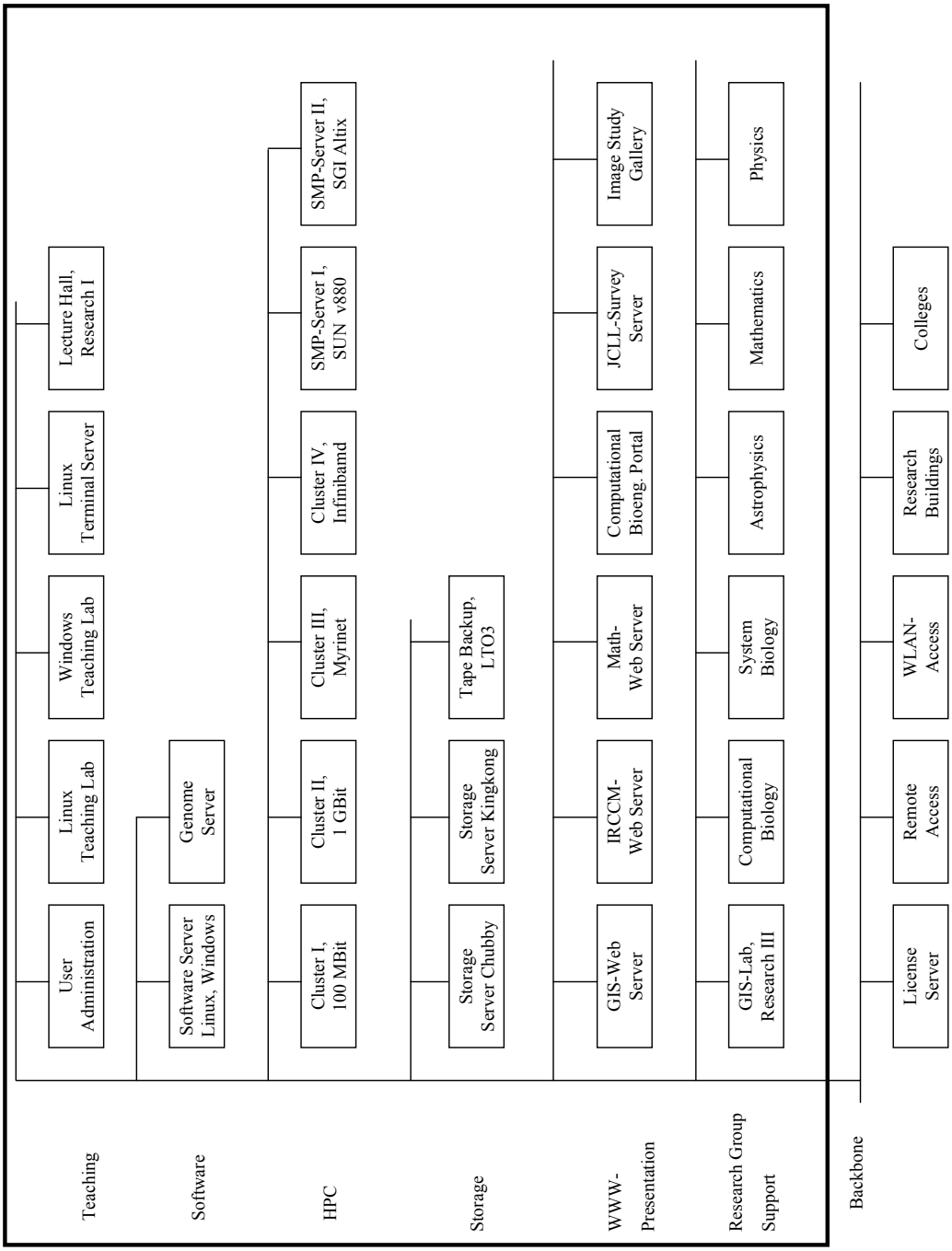

Figure 1: Overview of CLAMV services.

Figure 2: The largest computer lecture room of the CLAMV Teaching Lab in the basement of West Hall.

on the CLAMV teaching lab and the undergraduate lecture hall computers. The hardware maintenance of the undergraduate lecture hall is done by the IRC.

More details about the CLAMV Teaching Lab and how to access the resources can be found in the CLAMV Primer CLAMV primer (Achim Gelessus)[1] .

Software

CLAMV provides the community of Jacobs University with software which is essential for the daily work in a scientific environment. The focus of the software installation is on the Linux operating system but other operating systems like SUN Solaris, Microsoft Windows and MAC OS are also partially supported. Scientific computing and visualization software on CLAMV computer include commercial packages like Eagle, Gaussian, IDL, IVS Fledermaus, Maple, Mathematica, Matlab, PetroMod, Portland Compiler and Tecplot and a large number of free software packages. Commercial software packages are licensed as floating licenses where ever possible. CLAMV runs a software download page and also a software share where frequently requested Windows software can be found.

[1] http://www.clamv.jacobs-university.de/CLAMV/Publications/CLAMV-Primer.pdf

Figure 3: CLAMV Linux Clusters.

High Performance Computing (HPC)

For high performance computing (parallel computing) there are four Linux cluster with distributed memory and two shared memory server on campus. The clusters differ significantly with respect to their interconnect for data exchange; 100 MBit, 1 GBit, Myrinet and Infiniband are in use. For message passing in parallel jobs the Message Passing Interface (MPI) is used; on the shared memory server OpenMP is also available. The oldest cluster (Cluster I) and the SUN v880 shared memory server have been in permanent operation for nearly five years and are expected to be taken out of service in the near future.

Additional computing resources can be requested at the national computing centers. Currently two groups of Jacobs University use additional computing resources at national computing centers. Jacobs University cooperates closely with the Alfred Wegener Institute, Bremerhaven and University Bremen in the field of high performance computing. The Bremer Competence Center for High Performance Computing (BremHLR) is the platform where the three institutions coordinate and discuss their activities in HPC.

Storage

CLAMV has two servers which are used exclusively for data storage. Many simulation and data analysis projects require storage capacities which usually exceed locally available disk space. The storage server are connected to the high performance computing platforms to allow easy transfer of produced data. Access to the storage server is limited and granted only for dedicated projects.

WWW-Presentations

There have been several requests to CLAMV to run web services which have a scientific background. In many cases the web application includes server side actions like access to data bases or CGI triggered calculations. In order to limit the deployment of hardware the virtualization method Xen is applied. Xen allows the simultaneous operation of several servers on one hardware platform. For load sharing and to ensure availability of the web services also during hardware failures two Xen installations on identical hardware platforms are used. The following incomplete table shows which web presentations are running on CLAMV platforms:

GIS Web Server[2]

IRCCM Web Server[3]

Math Web Server[4]

Computational Bioengineering Portal[5]

JCLL Survey Server[6]

Image Study Gallery

Research Group Support

Several research groups at Jacobs University with UNIX/Linux desktop computers have requested for a tighter integration of their local systems into the CLAMV configuration. This has already been realized for the computational biology group, and partially for members of the system biology, geoastro and mathematics groups. Integration into the CLAMV configuration has been done by different methods (common user administration, thin client) and also for different systems (32Bit and 64Bit desktop computers).

The GIS lab (Geographic Information System) in building Research III consists of several computers with advanced visualization hardware (dual-head graphics adapters) and software for geoscience and statistical analysis. The GIS lab is intended to be used for geoscience projects, scientific visualization and large scale data analysis.

[2] http://gis-web.jacobs-university.de
[3] http://www.irccm.org
[4] http://www.math.jacobs-university.de
[5] http://map.jacobs-university.de
[6] http://survey.jacobs-university.de

Figure 4: Geochemical Modelling course in the GIS lab, November 2005.

2.3 The Next Five Years

It is expected that services for scientific computing will continue to be an important pillar for teaching and research at Jacobs University. The strategic concept consisting of the six areas discussed above is probably a robust basis for scientific computing services for the next years. In order to be reliable and attractive for potential users regular updates and replacements for hardware are needed. The maximum life time for hardware should be not more than five years. Quantitative changes of the available resources are likely for high performance computing and storage capacities. The number of research projects which are based partially or even completely on computer simulations is expected to grow. Many requests for resources in high performance computing can probably be answered by using standard cluster installations. Depending on the type of application more sophisticated hardware like shared memory architectures or vector machines might be necessary.

Currently a further development and growing of the offered services in scientific computing is limited by the number of personnel. More trained personnel is essential if new services are to be integrated to CLAMV or if existing servces are to be enhanced quantitatively. Examples of additional services which could be provided by CLAMV and which would be of great value for the whole community at Jacobs University are grid computing, cooperation with industrial partners and teaching activities in scientific programming.

3 CLAMV Research: Analysis, Modeling, and Visualization

Computationally oriented research at Jacobs University Bremen offers many facets and spans a variety of disciplines across the Schools and the Jacobs Center. Despite the diversity in themes and subjects, there is a lot of common methodological ground, and here CLAMV offers a platform to combine efforts and to join forces. As reflected already in its name, the three research pillars that CLAMV is designed to support and develop are *analysis, modeling, and visualization*.

This section is supposed to illustrate the three methodological areas by selected research projects. As explained in subsection 3.1, *analysis* and representation of modern scientific data often involve efficient management of large data sets of different formats and diverse nature. In subsection 3.2 a number of *modeling* projects in statistical physics are described. The art of scientific *visualization* is introduced in subsection 3.3.

3.1 Analysis and Management of Geoscientific Data using GIS

Contributed by Vikram Unnithan and Angela Schäfer

Over the past few years CLAMV has provided invaluable support to our Geoscience research, accommodated various project requests, supported and sustained the development of the GIS lab. The research group focuses on: (a) Understanding and modelling fluid flow processes on continental margins, (b) seismic interpretation and petroleum system's modelling of continental margins offshore Norway and Ireland and (c) geoinformatics, GIS and scientific visualisation. Of particular interest is the development of GIS methodologies, conceptual frameworks and techniques (MarineXML, SensorML) to capture, manage and analyse large volumes of real-time geodata. The main task of the GIS lab, with the help of CLAMV, is to facilitate and support these research activities.

Data Analysis, GIS and Visualisation Laboratory

In 2004, computer hardware and software was acquired within the framework of CLAMV and IRCCM. It included a number of high-end visualisation pc's equipped with dual monitors. These computers along with the dual-processor visualization server SISCOE formed the basis for the CLAMV–StatOil–IRCCM GIS and visualisation lab. The lab is physically located in R3, room 96. Funding for the above mentioned hardware (except SISCOE) was provided by IRCCM. Software support and maintenance is jointly provided by CLAMV and IRC. The computers in this lab are linked to the CLAMV infrastructure and make use of the Linux clusters, file and license servers. In addition, industry-standard software such as ArcGIS and Open Source GIS tools installed on the CLAMV teaching computers provide access to a wide range of tools to analyse data gathered by IRCCM and HERMES partners from continental margin sites such as the Norwegian Margin, North Sea and Irish Continental Margin.

In terms of software, over 1 million euro (commercial value) of software is installed in the GIS Lab. The main GIS software includes 25 classroom licenses of ArcGIS, ArcIMS and ArcSDE. The classroom licenses are maintained by the central license server of CLAMV. This provides not only an efficient license management infrastructure but also a service to all within IUB. Open source GRASS provides additional GIS resources on the teaching lab pc's.

Seismic interpretation, visualisation and modelling is facilitated by open source opendTect, gDb, SeismicUnix, Kingdom Suite (SMT) and Charisma. IUB has been granted a special university license worth 500.000 euro for Charisma. The software was installed in February 2005. IUB and IRCCM only pay for third party software used by this package. Charisma is an industry standard seismic interpretation and exploration tool used by most hydrocarbon exploration companies. Hydrocarbon System Modelling software PetroMod has also been donated to IUB and IRCCM. A new free license for 2005 was provided to IUB for academic use. This software is used for modelling oil and gas accumulations and migration through time.

2006 was another busy year for the GISLab in terms of establishing web and database servers, teaching and hosting web based services for several scientific research projects. The donation of a few old CLAMV teaching lab machines has substancially increased the capacity of the GIS lab. A new staff member – Florian Neu joined the team. He will work as the IT administrator for the GIS lab but will also support the CLAMV and Oceanlab with technical support.

The following is a brief description of the assessts of the GIS lab:

DESKTOP GEOGRAPHIC INFORMATION SYSTEM. On all three Win2000 computer the full range of ESRI Desktop GIS has been upgraded to the latest Version 9.1 with full access to the concurrent license versions of ArcInfo (2x), ArcView (2x), ArcEditor (2x), ArcInfo/Workstation (2x) and additional extensions of Network Analyst, 3D Analyst, Survey Analyst, ArcScan, Spatial Analyst, Geostatistical Analyst, Publisher and Maplex. As mentioned above, 25 classroom licenses of the ArcGIS can be accessed campus wide via the Sun license server.

GIS-DATABASE SERVER. A database server based on ESRI Spatial Database Engine and MS SQL Server has been installed in the GIS lab. This database can be accessed campus wide by desktop GIS applications.

WEB BASED GIS. Two linux based web servers are installed with ArcIMS 9.1 Internet Map Server, and Tomcat which provide a variety of interactive web mapping services for IUB projects (HERMES, IRCCM, guided research projects). One of these linux servers functions as a fall-back backup server. These map services provide live maps with a geodatabase (SDE/MS SQL Server) in the background. These online maps can be interactively queried and linked with existing web map services of other providers. Since 2004 IUB is an active University member of Open Geospatial Consortium (OGC).

VISUALISATION AND MODELLING SOFTWARE. Geoscientific modelling techniques are facilitated by PetroMod, Geochemical Workbench, SPSS and ArcGIS. The GISLab has three Fledermaus licenses for 3D visualisation, surface modelling and data integra-

tion. In addition a Geowall system has been installed and is currently being tested. A GeoWall provides an effective tool for passive 3D stereoscopic visualisation.

Selected Current Projects and Geo-Data Management

IRCCM information services are now in a position to maintain central program-wide web-based portals to facilitate exchange, delivery and monitoring of progress of stakeholders. An ArcIMS – Internet Map Server has been established in 2005 at IUB with IRC and CLAMV help. In order to facilitate these maps SDE-database has been expanded by labour-intensive data integration within student GIS projects supervised in the GISLab. Three main geodatabases implementing raster and vector data have been established in order to yield essential spatial data for ongoing research projects like HERMES and IRCCM and for overall geoscientific research and student projects at IUB: One database for worldwide and local bathymetry data in different resolutions and two database for geo/bio scientific data for the Black Sea and the northern European margin.

New projects have been established between the GISLab, the Computer Science department of IUB (Prof. Baumann) and the Alfred Wegener Institute in Bremerhaven (Prof. Thiede, Prof. Schlüter and M. Klages) in terms of web based raster data base integration and GIS, and sharing of general data integration for common EU-projects and the IRCCM. Students for internships and training have been exchanged between both institutes and departments.

Cooperation with the University of Tromsoe (Prof. Mienert) and Geosciences Department at University Bremen (Prof. Bohrmann and Prof. Wefer) have been established in terms of a forthcoming web based GIS and common data management within shared targets sites and projects.

Seabed observatories that provide online, real-time access to instruments generate a large volume of data. The implementation of a comprehensive and integrated data management strategy based on MarineXML (eXtended Markup Language) was started in 2005. As part of student projects in 2006, real-time data from CTD and methane sensors will be wrapped in a MarineXML metadata header complying with international ISO standards. This data package can be sent via the internet to users for direct analysis and to World Data Centres such as Pangaea for long-term storage in relational databases.

A close relationship between the GISLab and the World Data Center MARE (Dr. M. Diepenbroek, MARUM at University Bremen and Dr. H. Grobe, AWI) has been broadened within the project HERMES and in terms of combined proposal writing. Coupling WebGIS and the long-time data archive PANGAEA via automatically generated URL-addresses and linked web feature services is currently being implemented.

Within HERMES and the IRCCM two regional web based GIS for the Black Sea and the Norwegian margin are now established in the GISLab. Published and already available data and meta data are integrated and visualized as base information for data overlay, data query and data mapping in the target areas. These GIS databases will

help ongoing research activities within HERMES contributing to both an interactive web based working and education platform for public outreach.

GRANTS

HERMES (Black Sea and Norwegian Margin, regional GIS co-ordinators and involved in education and outreach)

IRCCM and Statoil (Grant 2006-2009)

Statoil Biomonitoring Project (Grant 2006-2009)

AWARDS, PRICES

Free software licenses and support have been awarded to IUB after negotiations with Geophysics and GIS software companies. The commercial value of these licenses is in the order of over 1.5 million euro which include our seismic interpretation licenses of Geoframe and Kingdom Suite. This is a great asset and will be used both for research and teaching purposes.

FUTURE RESEARCH PROJECTS

Some of the project planned for 2007 include:

- web based integration of raster data base techniques to GIS web map services,
- development of marine xml-standards for consistent on-line/real-time data transfer between seabed observatories,
- platform and web based GIS/database,
- establishing GIS and visualisation techniques for professional educational modules at Jacobs University Bremen,
- environmental monitoring of sediment and water in the Lesum.

GROUP MEMBERS: Yangze Fu (PhD Student), Jakob Hauschildt (PhD student), Angelica Garcia (Phd student), Anke Lederer (Diploma student), Florian Neu (IT technician).

3.2 Modelling of Complex Systems — Statistical Physics of Complex Networks

Contributed by Hildegard Meyer-Ortmanns

Nowadays a prototype of complex systems runs under the name of complex networks. Complex networks cover a broad range of different systems, ranging from genetic, metabolic, proteomic or neural networks in biology, via power grids, oscillators or (more abstract) spins in physics, to the world wide web and social systems of whole populations. In spite of this variety of systems there are common aspects, similarities

in their organizational structure, going along with similar topologies of the network graphs, consisting of nodes and edges, and similar dynamical processes on top of these graphs. It is physics, in particular statistical physics and the physics of nonlinear dynamical systems, that provides the theoretical background for appropriate modelling as well as a number of numerical and analytical tools for treating these systems. For example, spreading processes on these networks like virus spreading on the web or in human populations are described by percolation theory. Cooperation phenomena like the synchronization of oscillator ensembles can be controlled as a function of the coupling strength and the coupling connections between the oscillators, as well as the external input. The physical theory of phase transitions explains so-called tipping phenomena, or more generally, threshold phenomena, for which (not only the quantitative but also) the qualitative behavior of phases below and above the threshold is quite different.

In this context we focussed our research during the last three years on a number of projects dealing with dynamical processes on networks. They are described in the following sections.

Fractal structures on scale-free networks

Scale-free topologies are found over a wide variety of natural and artificial data sets, ranging from genetic networks to the internet (on the scale of routers). On the other hand, also fractal structures are ubiquitously found in nature. For some time, both characteristics, that is a scale-free degree distribution and self-similar features as in fractals, appeared as incompatible. As it turned out, with an appropriate way of calculating the fractal dimension, these concepts are compatible. In our contribution [3] we studied a further feature that seems to go along with scale-free and self-similar network structures. These networks seem to be disassortative, in addition. This notion comes from social science, here it refers to the degrees of network nodes, i.e. the number of edges emerging from nodes. In networks which are disassortative with respect to their degree, hubs are most likely not connected to hubs, it is rather unlikely that nodes with similar degrees are directly connected with each other. It remains a challenge to understand the disassortative, scale-free, and self-similar features in terms of biological mechanisms that are responsible for these interesting combinations.

Synchronization on Networks [P-SN]

We considered two prototypes of oscillators: Kuramoto oscillators as a prototype for limit-cycle behavior, and Rössler oscillators as a prototype for chaotic behavior.

KURAMOTO OSCILLATORS. Kuramoto oscillators are individually described just by a phase variable. In [4,5] we studied systems, either equipped with one pacemaker or homogeneous systems with a linear gradient on their natural frequencies, out of which the one with the largest frequency became the pacemaker in a dynamical way. The pacemaker entrained the other oscillators and locked up their frequencies with the result that clusters of various size were formed out of synchronized oscillators. To

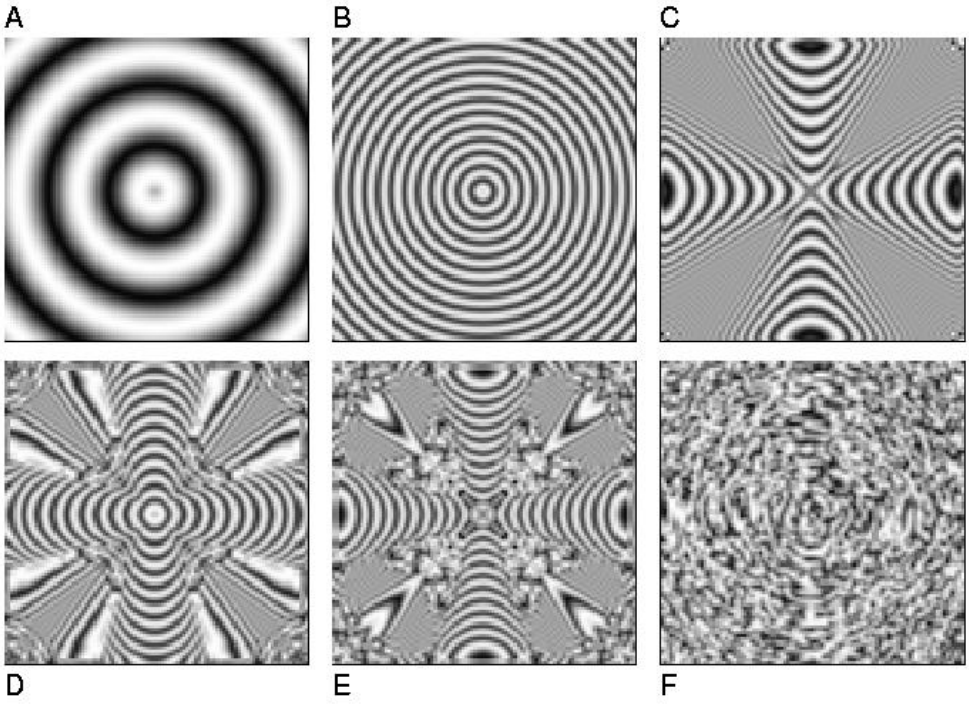

Figure 5: Stationary patterns in the phases of oscillators that are posed on a square lattice. The various snapshots correspond to different degrees of partial synchronization. [H. Meyer-Ortmanns]

mention a few of our results: For a system with one pacemaker we have shown that the mere closure of an open chain to a ring induced synchronization over a whole range of parameters for which no synchronization was possible for the open chain. This observation clearly demonstrated a case in which the network topology has an important impact on the dynamical behavior. Furthermore we have determined how the possibility of synchronization of an ensemble of oscillators depends on the so-called depth of the network, that is the average distance of oscillators from the pacemaker. This way it becomes possible to predict how many pacemakers are needed to entrain a given ensemble and where to optimally place them into the system. An example for stationary patterns in the phases of oscillators that are posed on a square lattice is shown in Figure 5.

RÖSSLER OSCILLATORS. Rössler oscillators can show chaotic behavior already on the individual level, and when interacting, may or may not show common chaotic behavior, that is, they may synchronize. We have shown [6] that synchronization on scale-free topologies (which are frequently realized on natural data sets) is facilitated by the number of loops, which simultaneously provide shortcuts in the system.

Evolutionary algorithms

THE APPROACH OF SOCIAL BALANCE [P-ASB]. The approach of social balance is a reinterpretation of an evolutionary algorithm applied to spin systems, in which the spins are assigned to the edges of the network. The spins can take values of $+1$ or -1, interpreted as relations between friends or enemies, respectively, assigned to the nodes. One of the stable states is the so-called paradise, in which all the individuals are mutually friends. The question of interest is as to whether a set of local dynamical rules can drive the system to reach paradise within a finite time, increasing logarithmically or power-like (but not exponentially) with the system size. The answer depends on a certain parameter p. As a function of this parameter the system undergoes a phase transition in the time it takes to reach the paradise, roughly speaking never or ever.

THE RELATION TO SATISFIABILITY PROBLEMS IN COMPUTER SCIENCE. Interestingly, we were able to map the approach to social balance to certain satisfiability problems of computer science, the so-called XOR-SAT problems. The problem there is to assign Boolean variables to the nodes of a network in a way that a given set of logical constraints between the variables is satisfied. In principle, such an assignment is always possible in XOR-SAT problems, but the challenge here is whether this solution can be found by a local stochastic algorithm in a finite time. Again, the answer depends on a certain parameter p of the algorithm and on the degree of dilution of the formerly used all-to-all topology, as we have shown in [7]. There are certain threshold values in the degree of dilution and the parameter p, which separate phase of qualitatively different behavior.

NEW UNIVERSALITY CLASS FOR A PERCOLATION PROCESS [P-NUC]. The network topology in the approach of social balance and in the context of satisfiability problems was either all-to-all or diluted random networks, respectively. Instead, in [8] we studied the same spin dynamics on a regular triangular topology. Here the algorithm drives the system always into an absorbing state, but there is a difference in the time it takes the system to reach the absorbing state, depending on the choice of the parameter p. In the vicinity of the critical threshold in p we determined the critical exponents that further characterize the singular behavior at the threshold (of the second-order phase transition) and found exponents that characterize a new universality class: it is neither that of directed percolation nor of parity conservation. Statistical physicists like to group dynamical behavior into universality classes. Models differing in their microscopic details but sharing the critical exponents, i.e. the singular behavior in a second-order phase transition, belong to the same universality class.

Algorithms with synchronous versus asynchronous updating rules

As suggested by the name, in synchronous updating rules all individual units are updated in the same time step, while a typical case of asynchronous updating is provided by the Metropolis algorithm, at which at each elementary time step just one unit, randomly chosen out of all units, is updated according to a certain prescription. In the context of Boolean network dynamics it was a topical discussion how the number of attractors (stable configurations to which the system converges) depends on

the size of the system and on the updating rules. Depending on the updating mode, the number of attractors may increase algebraically or exponentially with the system size. Motivated by this discussion, we started a systematic study of the dependence of the updating rules by interpolating between synchronous and asynchronous updating [9]. For simplicity we chose a chain of interacting Ising spins. Already in this very simple system we found a transition between absorbing and active steady states, depending on the degree of synchrony in the updating. Moreover we were able to identify the universality class of this transition as that of parity conservation. These results shed some light on the interpretation of stationary states as being representative for a certain dynamics. In general, it is the dynamics together with the order of updating events that lead to certain stationary states.

Former research: Phase separation in heavy-ion collisions

During the first two years (2002-2003) we used CLAMV-facilities for projects of our former field of research, that was phase structures in particle physics. We studied numerically the phase conversion in effective spin models for quantum chromodynamics [1,2]. The challenge there is to predict signatures for the phase conversion in heavy-ion collisions even if the conversion proceeds without true thermodynamic singularities at the transition point. There is some chance to see effects due to a fast cooling process after the collision if the cooling proceeds out-of-equilibrium. In heavy-ion collisions heavy ions are smashed against each other at relativistic energies. Such experiments are performed at the European Center for Nuclear Research (CERN) in Geneva, or in Brookhaven (U.S.A.), for example. For very short instants of time (of the order of $10^{-23}s$) exotic states of matter are created, made up of our basic truly elementary constituents, quarks and gluons, but deliberated during the smash due to the very high energy densities of the order of hundreds of MeV (corresponding to temperatures of the order of $10^{12}K$). Usually the quarks and gluons are confined into mesons and baryons. Otherwise these exotic states were realized only once in the very early evolution of our universe.

Further former projects which made use of CLAMV facilities are listed via the publications [10,11,12,13].

Future projects

As an extension of oscillatory dynamics considered in [P-SN] we will study excitable media on various distinguished network topologies. Excitable media are supposed to model, for example, neural systems. In excitable media stable states can get ”excited” if they are perturbed strongly enough. In such a case they make a long turn through phase space, fire, and finally return to their stable state. Here we will extensively use the facilities of CLAMV since apart from some aspects which can be treated analytically, many questions will be studied by extensive numerical simulations.

Computational Aspects

As typical examples we summarize the computational aspects of the projects [P-ASB], [P-NUC], and [P-SN] mentioned above. For the work reported in [P-ASB] we numerically studied networks of small size in the case of fully connected networks, since it was sufficient for testing the validity of our mean-field predictions. For diluted networks we performed several simulations in order to analyze whether the same transitions as in the case of k-XOR-SAT problems can be also found in the approach to social balance. The maximal size of the network was 10^3, the numerical results were averaged over 10^3 simulations. The maximal value of the typical CPU-time of a single simulation increases exponentially with the network size. So in our simulations, the maximal CPU-time was about 10 minutes. For the work reported in [P-NUC] the CPU-time was needed for a finite-size scaling analysis in order to numerically determine the critical threshold and the critical exponents of the percolation transition on two-dimensional triangular and square lattices. Here we extensively used the CLAMV-cluster resources. We analyzed lattices of maximal size of 256^2 nodes; for each choice of the parameters of our model we performed a number of realizations up to 10^4. The CPU-time of each simulation was very sensitive to the choice of the parameters of the simulations and the size of the lattice: the time needed for reaching a frozen configuration varied from a logarithmic dependence on the linear size of the lattice, away from the critical point, to a power-law dependence on the linear size at the critical point. The maximal CPU-time for a single simulation was about three minutes, for the maximal lattice size at the critical point, altogether it was of the order of days. Finally, the finite-size scaling analysis, reported in [P-SN] and required for the determination of the critical point and the critical exponents, needed a CPU-time of the order of minutes for a single simulation at the maximal lattice size of 10^4 and at the critical point, at which the time to reach the frozen configuration increases algebraically with the system size. Away from the critical point the time increases only logarithmically with the system size. Altogether we made about 10^3 simulations per specific choice of the parameters, summing up to a CPU-time of the order of days.

Technical Details

Again we choose as typical examples the projects [P-ASB], [P-NUC], and [P-SN] describe above and summarize the technical details in the following. We used the Intel C/C++ compiler as well as GNU-C compiler to generate the executable files from our source codes. The largest size of the systems that we analyzed was 256^2 [8], so the maximal memory used was $530MB$.

RESEARCH TEAM: Hildegard Meyer-Ortmanns (Professor), Xiang Li (Humboldt Fellow), Filippo Radicchi (PhD student), Daniele Vilone (Postdoctoral fellow).

GRANTS FOR POSITIONS WHICH MADE USE OF CLAMV

PhD-position, DFG-Grant ME 1332/10-2

Fellowship, Humboldt-Stiftung IV-CHN/1116658 STP

Two DAAD-grants (Germany-Korea): a) *Physics of Surface Growth*, b) *Neural Networks*

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3.3 Scientific Visualization

Contributed by Lars Linsen

Visualization is an inherently interdisciplinary field with application in many different areas. Scientific visualization deals with the visualization of data with spatial interpretation such as computer-generated data from numerical simulations (physics, chemistry) or measured data using scanning or sensoring techniques (medicine, life sciences, geosciences). Our efforts are to generate visualization methods that can handle large data sets efficiently, filter distinct features automatically or interactively, and display the relevant information in a comprehensive and intuitive fashion. The research focuses on segmentation and isosurface extraction, multi-variate data visualization, flow and tensor field visualization, and user interaction. In order to deal with large data sets in real time or even at interactive rates, the developed visualization methods need to be coupled with hierarchical data management techniques and should exploit parallelism. Parallelized visualization algorithms map directly to the CLAMV cluster or shared-memory machine hardware. Adaptively operating hierarchical methods support the computational load balance of the computational nodes.

The overarching goal of the visualization efforts at CLAMV is to incorporate data visualization into the computational loop of computationally intense applications. Data should be visualized, as soon as it is generated by the application, e. g. after every n iterations of a simulation. Doing so, the visualization output can be used to intervene and steer the simulations at any time. In the following, we describe visualization and data management methods we developed that can be used in this context. They address the visualization of (time-varying) volumetric scalar and vector fields defined over regular and irregular grids or even as scattered data.

Direct Isosurface Extraction from Scattered Volume Data

Isosurface extraction is a standard visualization method for scalar volume data and has been subject to research for decades. Nevertheless, no isosurface extraction method exists that directly extracts surfaces from scattered volume data without prior 3D mesh generation or reconstruction over a structured grid. We developed a method to extract surfaces from dense scattered data sets with many points, as they occur in particle simulations. To reduce the amount of pre-computations, we have developed a method based on spatial domain partitioning using a kd-tree and an indexing scheme for efficient neighbor search. Our approach consists of a geometry extraction and a rendering step. The geometry extraction step computes points on the isosurface by linearly interpolating between neighboring pairs of samples. The neighbor information is retrieved by partitioning the 3D domain into cells using a kd-tree. The cells are merely described by their index and bitwise index operations allow for a fast determination of potential neighbors. The output of the geometry step is a point cloud representation of the isosurface. The final rendering step uses point-based rendering techniques to visualize the point cloud. Our direct isosurface extraction algorithm for scattered volume data produces results of quality close to the results from standard isosurface extraction algorithms for gridded volume data (like marching cubes). In

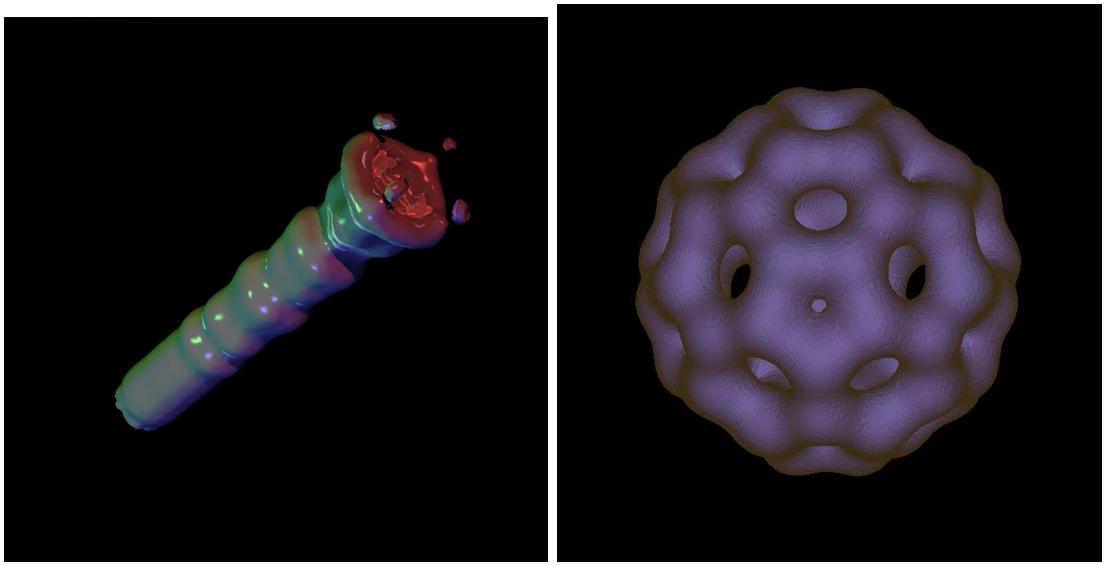

Figure 6: Left: Point-based ray tracing of isosurface directly extracted from scattered volume data. The scattered data set is a uniform random sampling of simulation data of fuel injection into a combustion chamber. Right: Exact dual isosurfacing using ray intersection applied to simulation of electron density inside a C-60 Buckminsterfullerene. [L. Linsen]

comparison to 3D mesh generation algorithms (like Delaunay tetrahedrization), our algorithm is about one order of magnitude faster for the examples used. [3,11]

Using Ray Intersection for Dual Isosurfacing

Isosurface extraction using dual contouring approaches have been developed to generate a surface that is dual in terms of the underlying extraction procedure used when compared to the standard Marching Cubes (MC) method. These approaches address some shortcomings of the MC methods including feature-detection within a cell and better triangles. One approach for preserving sharp features within a cell is to determine isosurface points inside each cell by minimizing a quadric error functions. However, this category of methods is constrained in certain respects such as finding just one isosurface point per cell or requiring Hermite data to calculate an isosurface. We have developed a simple method based on the MC method and the ray intersection technique to compute isosurface points in the cell interior. One of the advantages of our method is that it does not require Hermite data, i. e. the discrete scalar values at vertices suffice. We compute ray intersections to determine isosurface points in the interior of each cell, and then perform a complete analysis of all possible configurations to generate a look-up table for all configurations. Since complex features (e. g. tunnels) tend to be undersampled with dual points sufficient to represent sharp features and disjoint surfaces within the cell, we use the look-up table to optimize the ray intersection method to obtain minimum number of points necessarily sufficient for defining topologically correct isosurfaces in all possible configurations. Isosurface

points are connected using a simple strategy. Our approach operates locally on the cells of the grid, which allows for a parallel implementation. [12]

A Framework for Real-time Volume Visualization of Streaming Scattered Data

Scattered data reconstruction algorithms are often computationally expensive and difficult to implement. In order to visualize streaming scattered data, efficient approaches to scattered data reconstruction are required. We have developed a general framework for scattered data interpolation operating on discrete domains. The key idea for speeding up the reconstruction over an underlying grid is a re-factorization of the algorithm. The re-factorized version is designed such that it easily maps to graphics hardware architectures exploiting their performance and parallelism. Moreover, it naturally extends to applications for streaming data. As a proof of concept, we have implemented inverse-distance-weighted interpolation, natural neighbor interpolation, and radial Hermite interpolation using our general framework. In particular, the natural neighbor interpolation gained a major speed-up when exploiting geometrical properties of Sibson's interpolant, which reduces the d-dimensional interpolation problem to rendering d-dimensional spheres of known radii and blending them. We have applied the framework to two kinds of streaming data: progressive scattered data and real-time sensor data with moving sensors delivering asynchronous measurements. To account for the scattered spatial and temporal distribution of streaming sensor data, we use a four-dimensional extension of our framework, which elegantly handles representation of time-varying data and leads to reconstructions that are smooth in both space and time. [8,9]

Structure-accentuating Dense Flow Visualization

Vector field visualization approaches can broadly be categorized into approaches that directly visualize local or integrated flow and approaches that analyze the topological structure and visualize extracted features. Our goal was to come up with a method that falls into the first category, yet reveals structural information. We have developed a dense flow visualization method that shows the overall flow behavior while accentuating structural information without performing a topological analysis, which can be computationally rather expensive. Our method is based on a geometry-based flow integration step and a texture-based visual exploration step. The flow integration step generates a density field, which is written into a texture. The density field is generated by tracing particles under the influence of the underlying vector field. When using a quasi-random seeding strategy for initialization, the resulting density is high in attracting regions and low in repelling regions. Density is measured by the number of particles per region accumulated over time. We generate one density field using forward and one using backward propagation. The density fields are explored using texture-based rendering techniques. We generate the two output images separately and blend the results, which allows us to distinguish between inflow and outflow regions. We obtained dense flow visualizations that display the overall flow

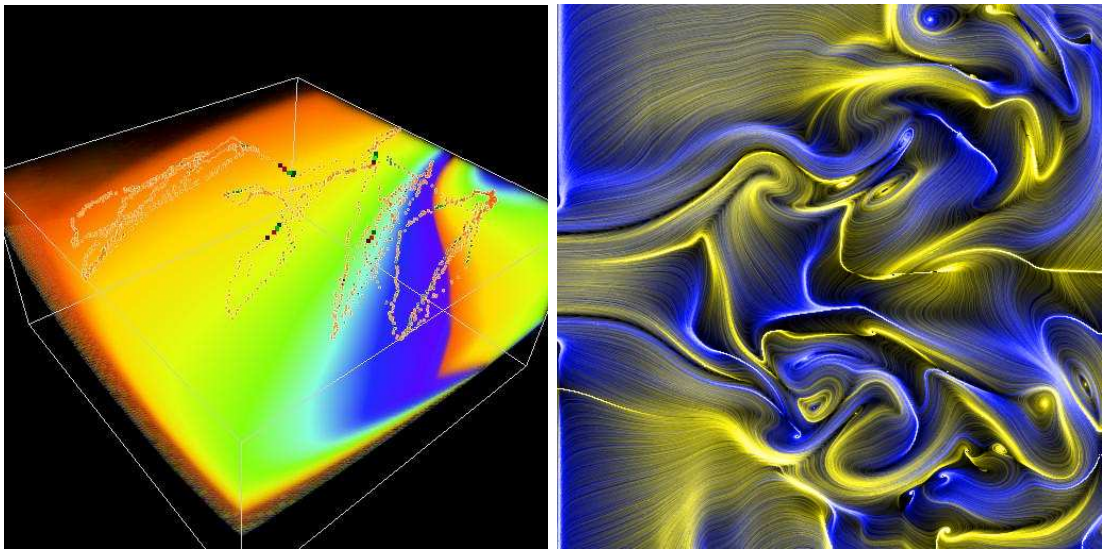

Figure 7: Left: Visualization of streaming temperature data in Monterey Bay scattered over time and space. A direct volume rendering of a three-dimensional time-orthogonal hyperplane after reconstruction over a $128 \times 128 \times 64 \times 1800$ grid (using natural neighbor interpolation) is shown. Right: Structure-accentuating dense flow visualization applied to 2D simulation of a swirling jet. [L. Linsen]

behavior, emphasize critical and separating regions, and indicate flow direction in the neighborhood of these regions. [6,7,10]

Wavelet-based Multiresolution with $\sqrt[n]{2}$ Subdivision

Multiresolution methods are a common technique used for dealing with large-scale data and representing it at multiple levels of detail. We have developed a multiresolution hierarchy construction based on $\sqrt[n]{2}$ subdivision, which has all the advantages of a regular data organization scheme while reducing the drawback of coarse granularity. The $\sqrt[n]{2}$-subdivision scheme only doubles the number of vertices in each subdivision step regardless of dimension n. We have constructed 2D, 3D, and 4D hierarchies representing surfaces, volume data, and time-varying volume data, respectively. The 4D approach supports spatial and temporal scalability. For high-quality data approximation on each level of detail, we use downsampling filters based on n-variate B-spline wavelets. We present a B-spline wavelet lifting scheme for $\sqrt[n]{2}$-subdivision steps to obtain small or narrow filters. Narrow filters support adaptive refinement, out-of-core data exploration techniques, and parallel implementations. [1,2,5,4]

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4 Life Sciences, Chemistry, and Biophysics

Computational Chemistry and Physics are established and rapidly growing disciplines at the interface of Computer Science and Physical and Chemical Sciences. Progress in computational power but also the development of new computational methods and algorithms in recent years allows for the analysis and modeling of structures and processes at high spatial and time resolution including. In the Life Sciences technological progress in many experimental areas has led to an enormous increase of data on biological sequences and biological structures. It is widely recognized that the development of computational methods of data analysis and modeling is a key technology to extract meaningful biological and medical relevant information out of the wealth of already available biological data. The challenge is taken by Computational Life Sciences, an emerging new scientific discipline, at the interface between Computer Science and Biology/Biochemistry. This extremely rapidly developing discipline has a growing influence on basically all aspects of the Life Sciences.

The Computational Laboratory for Analysis, Modeling and Visualization (CLAMV) has been of central importance for the development and application of computational methods in the Life Sciences, Chemistry and Biophysics at IUB. The applications use basically all computational resources of the CLAMV ranging form single workstations, clusters of workstations (teaching laboratory) and Linux-Cluster computers. A large area of interest is the understanding of the structure and dynamics of biomolecules at an atomic level of detail employing computational docking, molecular dynamics and quantum simulation methods. Especially applications in the area of quantum chemistry, quantum dynamics and molecular dynamics require powerful cluster computers available within the CLAMV. The cluster computers have, for example, been used for large-scale molecular dynamics simulation of ions moving through membrane channels or to study the folding kinetics of peptides and the influence of organic solvent on protein molecules. Other applications involve modeling and docking of proteins or the quantum mechanical study of organic molecules. The simulation studies have been performed in collaboration with experimental groups and have helped to better understand and interpret experimental results. One of the largest molecular dynamics simulations performed world-wide so far, a simulation of a complete nucleosome particle (the packing unit of eukaryotic DNA) including surrounding water molecules and ions, has been performed in part also on CLAMV cluster computers. In addition to computational studies at atomic resolution, the CLAMV resources are also used extensively to analyze and model cellular systems such as image analysis of enzyme distributions in cells or pattern formation in cellular systems. The availability of increasingly powerful computers and new computational methods within CLAMV will further broaden and expand the rapid growth of computational modeling and simulation in the area of the Life Sciences, Chemistry and Biophysics at IUB.

4.1 Imaging of Protease Functions

Contributed by Klaudia Brix

This project aims to elucidate the regulation of protease transport pathways in epithelial cells. In particular, we are interested in the localization, trafficking and functional role of cysteine cathepsins in epithelial cells of the thyroid gland to clarify the contribution of proteolysis to this organ's function. The main task of the thyroid gland is the production of thyroid hormones which are essential for growth, brain development, regulation of metabolic processes and thermoregulation. Disorders of the thyroid are frequently observed. Hypothyroidism and goiter may arise as a result of iodine deficiency, in severe cases of low-iodine diets the phenotype of cretinism still occurs. However, hyperthyroidism and thyroid cancers are similarly frequent and are accompanied by thyroid dysfunctions. Therefore, the understanding of the cellular and molecular mechanisms leading to maintenance of thyroid function is not only important for basic sciences but also contributes to the field of molecular medicine.

The central hypothesis of our project is that protein degrading enzymes must meet with their substrate at specific cellular and tissue locations and at distinct times to allow physiologically meaningful proteolysis to occur. Previously, we observed that cleavage of the thyroid prohormone for liberation of thyroid hormones is mediated by cysteine cathepsins which act on their substrate thyroglobulin in a highly regulated and consecutive fashion. Proteolysis of thyroglobulin starts extracellularly, i.e. within the thyroid follicle lumen, and it is enabled by the TSH-regulated secretion of cysteine cathepsins at the apical plasma membrane of thyroid epithelial cells.

The research group's work had shown that cysteine cathepsins B, K, and L are mainly responsible for thyroglobulin degradation and that their action is essential to maintain thyroid function. It was, however, not clear how the proteases would actually enter their shipping containers which transport them within thyroid epithelial cells and to the apical cell surface for subsequent secretion into the extracellular space. To answer this question, we have chosen an experimental approach, which combines biochemistry and molecular biology with cell biology. By including cathepsin-deficient animal models and tissue samples, we extend our work to a systemic context.

Cysteine cathepsins belong to the group of lysosomal enzymes. Their targeting to the compartments of the endocytic pathway is classically attributed to signals within the N-terminally located propeptide sequences and to the mannose-6-phosphate (M6P) receptor-mediated sorting pathway. However, previous work had shown that M6P-dependent trafficking cannot account for protein sorting in thyroid epithelial cells, because this signal is not recognized in this cell type. Therefore, we asked, whether intrinsic signals of proteases – other than mannose-6-phosphate – can direct the transport pathways of lysosomal cysteine cathepsins in thyroid epithelial cells.

For the trafficking studies, vectors encoding for green fluorescent protein (GFP)-tagged cathepsin B were constructed. One such vector was built with cathepsin B-coding cDNA isolated from a rat thyroid epithelial cell line, which was further modified by site-directed mutagenesis within its active site. The use of these vectors allowed us to distinguish between trafficking of the normal wild type versus the active-site-mutated

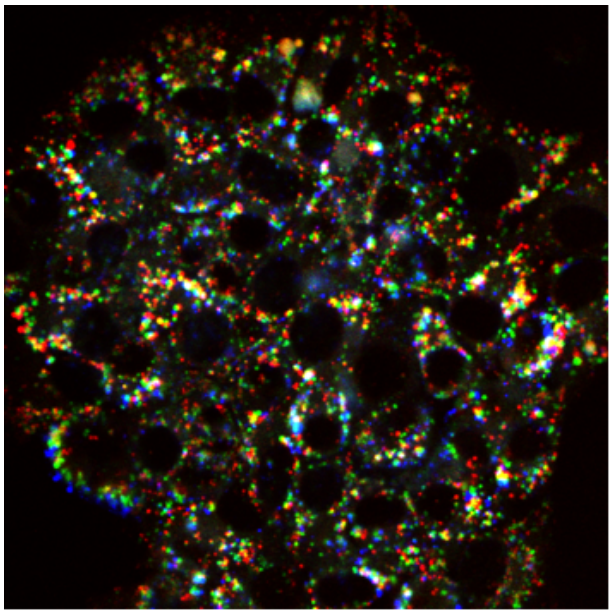

Figure 8: Cysteine protease cocktail of rat thyrocytes (FRTL-5 cells) visualized with the activity based probe GB111. Overlay represents localization of the proteases at three different time points of a 10-min live-cell imaging series in which color-coding depicts vesicle positions at 1 min (blue), 5 min (green) and 10 min (red). [K. Brix]

and proteolytically inactive cathepsin B in thyroid epithelial cell lines. Expression studies, fluorescence microscopy and immunolabeling of the compartments that were reached by the GFP-tagged proteins demonstrated that both cathepsin B-variants reached the same compartments, i.e. endosomes and lysosomes. Hence, both variants of the proteases were fully transport-competent.

Our observations on trafficking of GFP-tagged lysosomal proteases suggest that the primary sequence of properly folded proteases is sufficient to target the proteins into endocytic compartments. In addition, the results suggested that cellular transport decisions are most probably taken by the cells themselves rather than by the transported proteases, i.e. the cargo. The signals that determine destination of transport vesicles remain, however, elusive. Therefore, we continued in asking the question as to whether transport vesicles as well as endocytic organelles are loaded with an arbitrary mixture of proteases or if there might be selectivity in loading of proteases into cellular vesicles. This was hypothesized from the general concept that specific proteases are needed at distinct locations and in a timely fashion for proper processing of the substrate.

Using specifically designed activity based probes applied to living cells, their set of cysteine proteases was fluorescently tagged and could be visualized in terms of spatio-temporal localization. We observed that active cysteine cathepsins were contained within vesicles that did not contain GFP-tagged cathepsins and vice versa. This was true for wild type cathepsin B and for its active site mutant. These results suggested that active and inactive proteases followed the same routes in thyroid epithelial cells.

At present, we perform in vivo-analyses to directly visualize protease transport in living cells. In combination with the activity based probes, these experiments will enable us to visualize protease functions on the spot. Our hypothesis is that thyroid epithelial cells have the means to deliver distinct cocktails of proteolytic enzymes at the needed locations of thyroid follicles.

GROUP MEMBERS: Heiko Büth, Stefanie Dannenmann, Anna Dunkhorst, Sasa Jenko-Kokalj, Silvia Jordans, Meike Klepsch, Malgorzata Kubica, Kristina Mayer, Dr. Ulf Meyer-Grahle, Hong Qu, Maren Rehders, Lakshmi Settu, Ruxandra Sirbulescu, Brit Wolters.

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GRANTS

DFG Br 1308/6-1, 6-2 (in cooperation with FOR 367).

DFG Br 1308/7-1, 7-2, 7-3 (in cooperation with KFO 115).

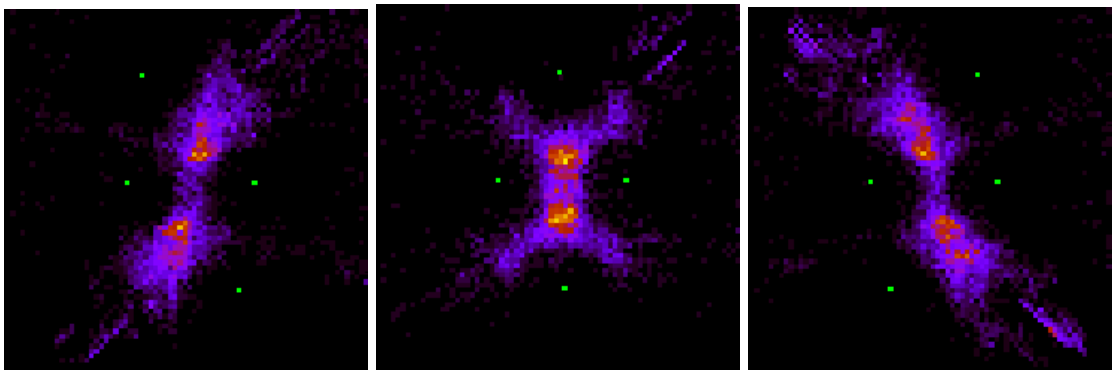

Figure 9: These pictures show the probability distribution of finding a spiral at any given spatial position, depending on three different choices of pacemaker locations (green dots), that are used to initiate the signaling process. The pacemakers are a very simple example of binary differences in cell properties. [M.-T. Huett and D. Geberth]

4.2 Influence of Biological Variability on Pattern Formation in *Dictyostelium Discoideum*

Contributed by Marc-Thorsten Hütt and Daniel Geberth

Research of the Computational Systems Biology group focuses on three key topics: biological networks, genome evolution and pattern formation. In the past year, we have mainly employed the CLAMV infrastructure for the computationally demanding simulation of self-organizing systems exhibiting pattern formation. Pattern formation is a ubiquitous phenomenon in nature. The movement of swarms of fishes and birds for example is based on the local knowledge of individual animals. In spite of the essentially local decision process, however, global patterns arise. The main focus was simulation of a system modeling the signaling behavior of the slime mold *Dictyostelium discoideum* (*Dd*), which widely serves as a model organism for pattern formation on a cellular level. *Dd* 'starts' its life cycle as a colony of single-cell amoebae, feeding on local food resources. Once these are used up, a signaling process is started that causes the amoebae to aggregate, forming a multicellular slug organism that has the capability to move over comparatively large distances. The different stages are accompanied by different types of patterns: spiral waves during cell-cell signaling and, later, aggregation streams. In our research we are concerned with the signaling and aggregation stages of Dd's life cycle, trying to uncover the rules behind the formation of *specific* structures from biological variability, a process which is not well understood yet.

We are interested in the dependence of the resulting spiral patterns on the purely geometric aspects of distributions of cell-cell differences. So far, we were able to show that some of the information stored in the cell property pattern is in fact conserved through the process of self organization, acting as a higher level of control of the spiral pattern, which is primarily influenced by specific firing patterns on the single run level, an example is shown in Figure 9. The main tool we employed to this end was the phase singularity recognition algorithm originally developed in the context of

atrial fibrillation, combined with filtering methods.

The results we found would not have been possible to obtain via lab experiments, because of the high stringency requirements imposed on the initial conditions necessary for detecting the influence of cell properties on phase singularity statistics. We hope, however, to be able to make experimental verification possible at a later stage. Here we aim at using simulations as a guiding scheme to understand, how a measured pattern of cell-cell differences may help predict the precise layout of spatiotemporal structures in *Dd* self-organization.

For 2007 we can see that the projects from the biological networks and genome evolution contexts will also enter a phase, where high computational power is an important ingredient for progress, and will thus use the CLAMV resources more extensively.

GROUP MEMBERS: Manuel Dehnert (Postdoc), Daniel Geberth (PhD Student), Carsten Marr (PhD Student), Mark Müller-Linow (PhD Student), Heike Hameister (Graduate Student), Niko Sonnenschein (Graduate Student).

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M. Dehnert, W.E. Helm, and M.-Th. Hütt (2006), *Informational structure of two closely related eukaryotic genomes*, Phys. Rev. E, 74:021913.

A.M. Freund, M.-Th. Hütt, and M. Vec (2006), *Selbstorganisation. Ein Denksystem für Natur und Gesellschaft*, Böhlau-Verlag.

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4.3 Phylogenetic Analyses and Protein Modelling

Contributed by Albert Jeltsch and T. Jurkowski

CLAMV computers have been used primarily for: generating multiple sequence alignment, protein structure prediction and phylogenetic analyses as well as for bioinformatics software development. We have prepared a phylogenetic tree of DNA-(cytosine-C5)-methyltransferases comprising several bacterial enzymes, representatives of plant and fungi DNA methyltransferases and examples of Dnmt1, Dnmt2 and Dnmt3 enzymes using the programs. The multiple sequence alignment was created in t-coffee and pcma programs and corrected manually. Phylogenetic trees were constructed

Figure 10: Phylogenetic analyses and protein modelling. [A. Jeltsch and T. Jurkowski]

using Phylip, Mega, PHYML, TreePuzzle, PROML. The multiple sequence alignment underlying the tree was well defined and most branch points in the tree were highly significant as deduced from bootstrap analyses. The tree is roughly separated into four branches, the Dnmt2 branch, the Dnmt3 branch, one branch of prokaryotic DNA methyltransferases (including M.HhaI and M.SssI) and one branch containing several prokaryotic DNA methyltransferases and the Dnmt1 related enzymes. It demonstrates that the closest homologs of Dnmt1 are prokaryotic DNA-(cytosine-C5)-methyltransfeases like M.HaeIII, and M.HgiDI, the plant Met1 enzymes and the Ascobulus immersus Masc1 enzyme. These results shed new light on the evolution of DNA methyltransferases. Currently we plan to correlate them to experimental findings.

In the future, the multiple sequence alignments and phylogenetic studies will be extended in cooperation with Prof. Glöcker to study the distribution of DNA methyltransferases in marine bacteria.

Protein structure prediction was performed through the Genesilico Meta Server

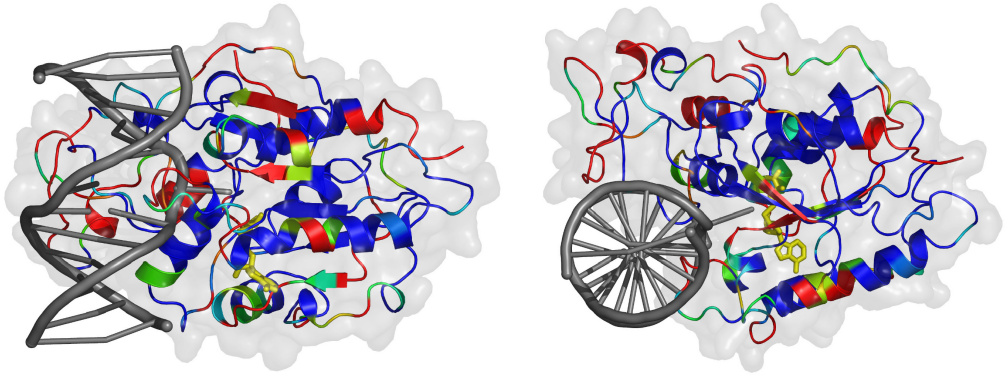

Figure 11: Phylogenetic analyses and protein modelling. Figure taken from Gowher et al. (2006). [A. Jeltsch and T. Jurkowski]

(http://www.genesilico.pl/meta) gateway using various publicly available services for fold-recognition like 3DPSSM, GenTHREADER, SPARKS and secondary structure prediction including PSIPRED, Jnet, and SAM-T02. The fold-recognition alignments reported by those methods were compared, evaluated and ranked by Pcons2 and Pcons5 servers. The best scoring alignments with different template structures reported by both Pcons servers were used as starting points for modeling of the tertiary structure of CD-Dnmt3a. Although the crystal structure of M.HhaI was reported as the best template for homology modeling all the other structures of m^5C methyltransferases (DNMT2 and M.HaeIII) reported by the servers were also used for model building.

In the absence of an experimentally determined 3D-structure of a protein, homology modeling can provide a basis for the interpretation of experimental data. We have modeled the tertiary structure of the catalytic domain of Dnmt3a using the "Frankenstein's monster" approach which combines various aspects of traditional homology modeling and fold-recognition protein structure prediction (Gowher et al., 2006). Crystal structures of all the DNA-(cytosine C5)-MTases reported by the threading servers (M.HhaI 6MHT, M.HaeIII 1DCT and Dnmt2 1G55) contributed (to different extent) to the creation of the final model. In our structural model, CD-Dnmt3a, like all DNA-(cytosine C5)-MTases, is composed of two domains. The large domain comprises conserved motifs I-VIII and X and contains the cofactor-binding and active sites. Due to the high level of sequence similarity between Dnmt3a and other MTases, a reliable model was obtained for this part of the molecule. This is indicated by the observation that all the contacts between the enzyme and the coenzyme, as well as the position of the catalytic residues are maintained as observed in the structural template. The small domain of Dnmt3a is formed by the TRD and motif IX. In the region of the variable domain (amino acid residues 218 - 298) the modeling is not very reliable due to the lack of appropriate template structures and very low sequence similarity. Although special care was taken to align the structurally conserved parts within the TRD (like the TL motif), the loops making the actual contacts to the DNA could not be reliably modeled due to restrictions of the method itself.

Homology modeling was performed according to the "Frankenstein's monster" ap-

proach, comprising cycles of model building by MODELLER and SWISS-MODEL and evaluation of the models by VERIFY3D (with 3 amino acids window) via the COLORADO3D server. The alignment in the low scoring regions (Verify3D score below 0.2) was realigned and next iteration of the model building was performed. At one time only one region in the alignment was shifted to avoid the interference of effects from different parts. The consensus model was created by combining the best scoring fragments (according to Verify3D score) from the initial models. Steric clashes in this hybrid model were relieved during rounds of energy minimization in GROMOS96 force field performed *in vacuo* as implemented in DeepView 3.7 http://www.expasy.org/spdbv/. During the optimization process the enzyme, the DNA and the AdoHcy molecule were allowed to move.

RELATED PUBLICATION

Gowher, H., Loutchanwoot, P., Vorobjeva, O., Handa, V., Jurkowska, R.Z., Jurkowski, T.P., and Jeltsch, A. (2006), *Mutational analysis of the catalytic domain of the murine Dnmt3a DNA-(cytosine C5)-methyltransferase*, J. Mol. Biol. 357, 928-41.

4.4 Computational Physics and Biophysics Group

Contributed by Ulrich Kleinekathöfer

Quantum dynamics in nanosystems

The research projects performed using CLAMV resources are within the area of chemical and biological physics, both on a classical as well as quantum mechanical level. Some of the projects concerned method development and applications for molecular quantum dynamics. For the calculation of nonlinear spectra of small molecules such as the iodine molecule in gas phase wave packet calculations are being performed to reproduce and interpret spectra obtained in the group of Prof. Materny. When including the rotation dynamics the calculations become CPU intensive. For dynamics within a liquid environment, dissipation effects have to be added to the quantum dynamics which is accomplished by the coupling to a thermal bath. The emerging density matrix formalism then allows for a simulation of electron and excitation transfer processes for example in DNA. Similar techniques can be used to derive quantum master equations for the transfer of electrons trough molecular wires. The developed formalism allows to treat the laser-matter interaction accurately. Scenarios are being developed in which ultrafast laser pulses control the current through the molecular wire. Since the involved basis set increases exponentially with the number of sites in the tight-binding model and since not only the system density matrices but also auxiliary density matrices have to be computed and stored, the problem quickly gets memory and CPU consuming.

Method development in this direction is already going on in our group for several years and we will certainly continue this work while using the computational resources of CLAMV.

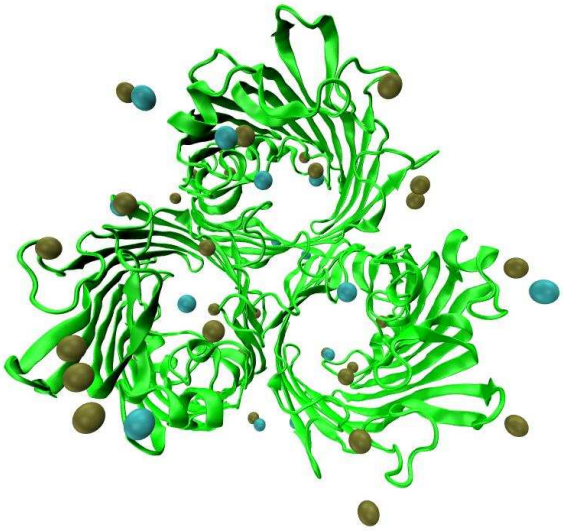

Figure 12: Ions moving through the OmpF protein consisting of three pores. [U. Kleinekathöfer]

Molecular dynamics simulations for biosystems

The research of our computational physics group in the direction of biological systems is twofold: large scale classical molecular dynamics simulations on one hand and quantum dynamical calculations for electron and excitation transfer processes on the other. Both types of projects can be very computational costly. The ion and antibiotics transport through the outer membrane protein F (OmpF) and the large domain motion within the molecular motor ATPase are, so far, simulated using purely classical molecular dynamics simulations. For these simulations we use the parallel code NAMD2 from the group of Prof. K. Schulten in Illinois. This code is latency tolerant and therefore does not require a very fast network, i.e. Gigabit Ethernet works well. Usually production jobs run on 20-30 CPU cores for several days. Quantum dynamical studies are used to investigate e.g. electron transfer within DNA. Combinations of classical and quantum mechanical methods are used to study the light-harvesting in purple bacteria. To perform an atomic level description of the light-harvesting process classical molecular simulations are complemented with quantum chemistry calculations and quantum modeling. For these quantum modeling we needed to do Monte Carlo disorder sampling. Using our own MPI code these jobs run on several tens of CPU cores in parallel making a good statistics possible.

Especially the large-scale molecular dynamics simulations will be extended in the coming years. Since each job easily uses more than 20 CPU cores for several days while no fast network is required, we will heavily depend on the Linux clusters of CLAMV.

GRANTS

Individual DFG grant on light-harvesting complexes, KL 1299/3-1

Project within DFG priority program SPP 1243 *Quantum transport at the molecular scale*, KL 1299/4-1

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M. Schröder, U. Kleinekathöfer and M. Schreiber (2006), *Calculation of absorption spectra for light-harvesting systems using non-Markovian approaches as well as modified Redfield theory*, J. Chem. Phys. 124, 084903.

S. Welack, U. Kleinekathöfer and M. Schreiber (2006), *Laser-driven molecular wires studied by a non-Markovian density matrix approach*, J. Lumin. 119 & 120, 91.

U. Kleinekathöfer, G.-Q. Li and M. Schreiber (2006), *Density matrix theory for reductive electron transfer in DNA*, J. Lumin. 119 & 120, 462.

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4.5 Geometrical Orientation of Adsobed Chiral Ligands on Nanoparticle Surfaces

Contributed by Ryan Richards

In the last decade, the synthesis of chiral pharmaceutical drugs has steadily increased and now represents one-third of all drug sales worldwide. Furthermore, it is estimated that 80% of all drug candidates presently being developed are chiral. This increased demand for enantiopure pharmaceutical drugs has elevated chiral alcohol synthesis into a high technology growth area by industry over the last 15 years. An excellent example of this is the class of drugs described as ACE inhibitors, of which there are no less than twelve, and include billion-dollar drug Lisinopril. The key step in the synthesis of these pharmaceutical drugs, many natural products, and some agrochemicals is the generation of a chiral alcohol. Less structurally complex chiral alcohols are frequently used as chiral ligands and chiral auxiliaries. Importantly, chiral alcohols are also used to synthesize the corresponding chiral amines because of significant methodology gaps in the field of chiral amine synthesis.

Amongst the various routes for obtaining enantiomerically pure products (chiral chromatography, classical resolution, etc.) use of enantioselective catalysts is not only promising, but is presently predominantly used in the pharmaceutical industry because a small amount of chiral catalyst can potentially generate a large amount of enantiomerically pure product in a cost effective manner.

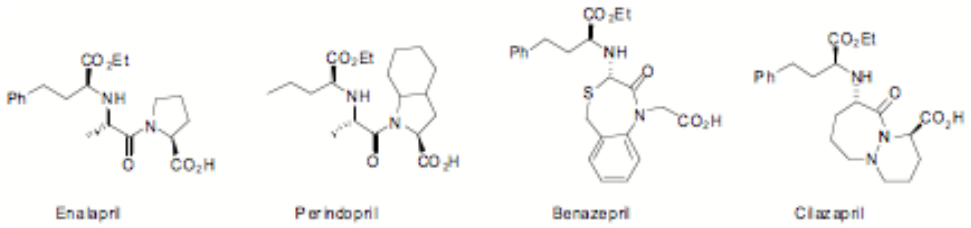

Figure 13: Examples of Ace Inhibitor Drugs Synthesized from Chiral α-Hydroxyesters. [R. Richards]

Although great advances have been made in the areas of biochemical and homogeneous enantioselective catalysis, heterogeneous systems offer the advantages of: low cost compared to homogeneous catalysts, ease of handling, simple removal, regeneration, and in many chiral modified surface instances simple reuse without loss of catalytic activity or enantioselectivity. Therefore, the study of heterogeneous catalytic systems provides a platform attractive to both academic and industrial applications.

Chiral ligand modification of transition metal surfaces represents one of the most promising approaches to heterogeneous enantioselective catalysis. Parallel independent studies have shown that the geometrical orientation of the chiral ligand is crucial to the catalytic activity and the induced enantioselectivity of the reaction. The Richards' group has developed a novel analytical method to study the geometrical orientation of various chiral ligands on Pt, Pd and Fe surfaces by combining nanoscale analytical techniques with computational modelling.

Several chiral ligand systems including cinchonidine, quiphos, diop, diphos, etc. have already been studied on Pt, Pd and Fe bulk and nanoparticle surfaces. We have successfully demonstrated that by using a combination analysis of DRIFTS (Diffuse Reflectance Infra-red Fourier Transform Spectroscopy) and geometrical optimization using Gaussian to obtain the vibrational frequencies of a molecule, we could determine its geometrical orientation of the ligand on a metal (and nanoparticle) surface.

With the data obtained from geometrical optimization and vibrational frequency calculations using Density Functional Theory (done on CLAMV, IUB), we could assign vibrational peaks of the free ligand molecule corresponding to its dipole moment. This data on the free molecule is further compared with data obtained via DRIFTS, which gives us the vibrational frequencies of the molecule on a metal surface. With the help of the metal-adsorption rule, which states that vibrations corresponding to the dipole moment of the ligand, which are perpendicular to the metal surface are enhanced upon adsorption of the ligand on the surface, we can thus determine the geometrical orientation of the ligand on the metal surface.

Thus far, we have successfully established the orientation of numerous ligands on both bulk and nanoscale surfaces. For example, our studies proved that in cinchonidine modified Pt nanoclusters, cinchonidine was found in both the 'flat' (Fig. 13) and two 'tilted' adsorption modes, the so called "α-H abstracted" and "N-lone pair bonded" (Fig. 14, since both tilted mode are similar, only last is shown). Furthermore, simul-

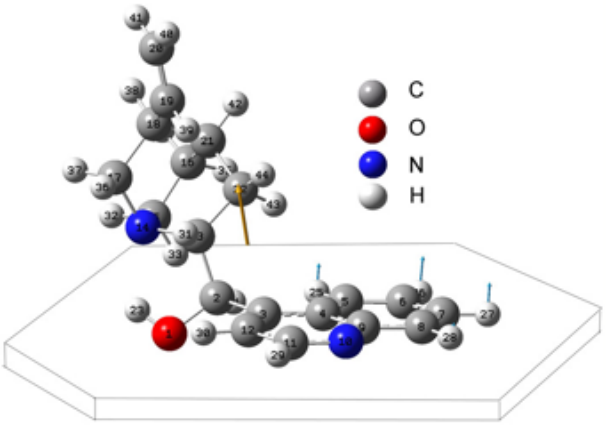

Figure 14: Flat adsorbed cinchonidine demonstrates vibration mode at 768 cm-1 with dipole moment (big arrow) orientated mostly perpendicularly to the metal surface. The most intensive displacement of atoms is shown by small arrows. [R. Richards]

taneous studies on catalytic activity have shown that the "flat" adsorption mode is more favorable for inducing enantioselectivity in the reaction products. These results are also in good agreement with similar research done by other independent research groups. However, we believe that the advantage we have over other analytical methods is that our method is efficient in terms of both cost and simplicity. In addition, our method allows us to work with 'real' catalytic conditions and thus our efforts have yielded several important molecular level insights that have directed us to prepare catalyst systems with numerous advantages over current technologies.

In the future, we plan to continue the use of this easy and yet accurate analytical method to determine the geometrical orientation of new organic modifiers on metal surfaces. Presently, we are pursuing a project in collaboration with the Nugent group. The Nugent group specializes in the synthesis of chiral amines, which we plan to use in the synthesis of novel man-made chiral ligands and utilize them as heterogeneous catalysts on metal supports in hydrogenation reactions. We plan to use the same analytical technique as described above to determine the geometrical orientation of the ligands on the metal surface. Moreover, since we would be dealing with completely new ligands, this technique not only helps to analyze the data from the ligand we synthesize, but also helps us in the planning of the synthesis of new ligands. From the results obtained thus, we can therefore not only same time in the laboratory, but also produce more efficient and effective results.

We would like to thank International University Bremen and EU-COST D24 for providing CLAMV computation hours, for facility and financial support.

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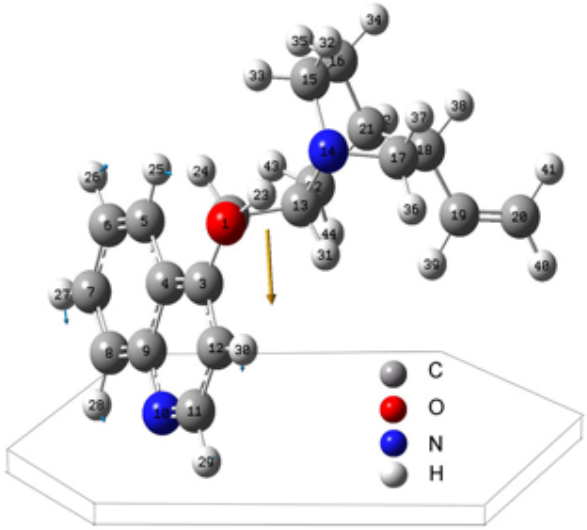

Figure 15: Tilted adsorbed cinchonidine demonstrates vibration mode at 1514 cm-1 with dipole moment (big arrow) orientated mostly perpendicularly to the metal surface. The most intensive displacement of atoms is shown by small arrows. [R. Richards]

DOI:10.1039/B615470K.

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Alexander Kraynov, Andreas Suchopar, Lawrence D'Souza and Ryan Richards (2006), *Determination of Geometric Orientation of Adsorbed Cinchonidine on Pt and Fe and Quiphos on Pt Nanoclusters via DRIFTS*, Physical Chemistry Chemical Physics, 8, 1321 - 1328.

Pending Grant Proposals

DFG, Co-applicants Thomas Nugent and Ryan Richards, *Design of New Chiral Heterogeneous Nanoscale Pt and Pd Catalysts for Asymmetric Hydrogenation of Ketoesters under low Hydrogen Pressure*, submitted August 2006.

Future Grant Proposals

VW Stiftung, *Innovative Methods for the Preparation of Functional Surfaces*, International Application planned with co-applicants, Vasile Parvulescu (University

Bucharest), Thomas Buergi (University Neuchatel), Jean Pierre Genet (University Paris), pre-proposal to be submitted February 2007.

EU 7th Framework STREP, Application planned with co-applicants, Vasile Parvulescu (University Bucharest), Thomas Buergi (University Neuchatel), Jean Pierre Genet (University Paris), Avelino Corma (Valencia). To be submitted 2007.

4.6 Computational Chemistry and Bioengineering

Contributed by Danilo Roccatano

The research interest of my group focusses mainly on theoretical investigation of structural and physico-chemical properties of molecular systems, in particular those of biological and nano-technological relevance. Our research involves the use of parallel computer facilities in CLAMV. A short description to various research highlights in my group is given below:

Study of non-aqueous solvents and their effects on molecular systems

Chemical environment (pH, salts, and co-solvents) plays a fundamental role in the stabilization of secondary structure-forming peptides and proteins in solution. The presence of organic co-solvents in aqueous solution can either enhance the structural stability or induce denaturation/conformational changes. As such, atomic level investigations of protein solvation can provide useful insights of the protein folding mechanism, aggregation, fibril formation etc. Among the co-solvents, alcohols (in particular fluorinated ones) are most commonly used as stabilizing or denaturing agents. Roccatano et al. have proposed new models of 1,1,1- trifluorethanol (TFE) [1] and 1,1,1,6,6,6-hexafluoropropan-2-ol (HFIP) [2] for MD simulations. These models have successfully reproduced the experimentally observed increase of stability for different secondary structure-forming peptides in TFE and HFIP/water mixtures [2,3,4,5].

Another interesting aspect of this research concerns the theoretical study of P450 BM-3 monooxygenase to understand and improve its catalytic activity in presence of organic co-solvents. This work is performed in collaboration with Prof. U. Schwaneberg and Dr. T. S. Wong. To date, the outcomes of this collaboration amount to four manuscripts, [5,6,7,8]. Among them, two were featured as cover page articles in scientific journals (see Figure 16). The most astonishing finding is the prediction, using Molecular Dynamics (MD) simulations, of the possible mechanism by which DMSO inactivates the enzymatic activity of P450 BM-3 [6]. MD simulations of P450 BM-3 with a few DMSO molecules present in the active site indicate the tendency of DMSO molecules to replace the water coordinating the heme iron. A subsequent determination of the crystal structure of P450 BM-3 heme domain in presence of DMSO (performed in collaboration with Prof. Wilmanns' group at EMBL Hamburg) has confirmed this theoretical hypothesis. A DMSO molecule was found to coordinate the heme iron, thus resulting in activity loss in presence of high DMSO concentration [8].

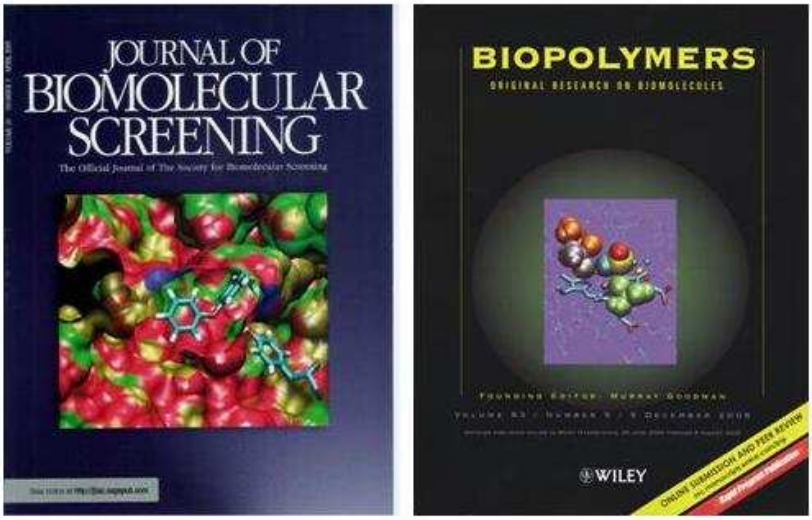

Figure 16: Cover pages of two P450 BM-3 publications. On the left: the cover picture shows the interaction of 3-phenoxytoluene with Tyr51 in the substrate binding pocket of P450 BM-3. On the right: a snapshot from the MD simulation of P450 BM-3 heme domain in DMSO/water mixture. The picture shows a DMSO molecule approaching the heme iron by displacing the iron-coordinating water molecule. [D. Roccatano]

The future endeavours are directed to studying the effects of other solvents (in particular ionic liquids) and conducting polymers on P450 BM-3 and its mutants.

Study of structural and dynamical properties of peptides in solution by comparing MD simulations to experimental FRET and time-resolved spectroscopic data.

The long-term goal of this project is providing an atomic model to interpret experimental data. These information offer the opportunity to analyze model of protein folding based on direct experimental observations. In retrospect, this approach provides the possibility of optimizing current force fields based on the experimentally obtained kinetic data using simple model systems.

We are carrying out these studies in collaboration with Prof. W. M. Nau, Dr. H. Sahoo and Prof. M. Zacharias. As an example, we are investigating the kinetic behavior of peptides with tryptophan as quencher and an amine derivative of 2,3-diazabicyclo[2,2,2]oct-2-ene (DBO) linked to the end of aspartate as fluorophore. This fluorophore has an unusually long singlet exited state lifetime in aqueous solution and high solubility in water. Thus, the tryptophan/DBO forms a unique probe/quencher pair characterized by a contact quenching mechanism which differentiates it from conventional fluorescence resonance energy transfer (FRET) donor/acceptor pairs. This offers the possibility to compare directly the time-resolved kinetic data with the indirect kinetic information extracted from steady-state fluo-

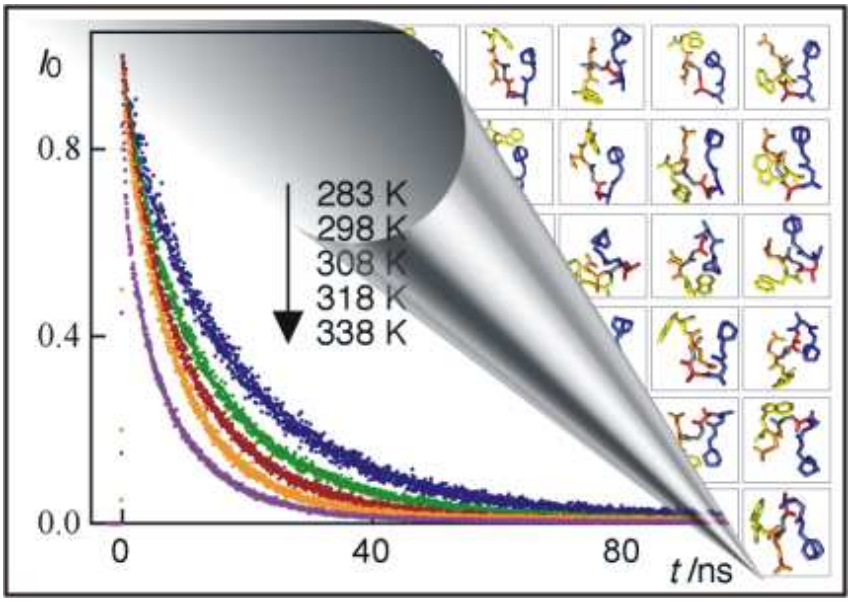

Figure 17: Experimental time-resolved kinetic data for the looping rate of the the Dbo-AlaGlyGlnTrp-NH_2 peptide. On the right site, representative structures of the peptide at different temperatures are reported. [D. Roccatano]

rescence intensity measurements. The collaboration resulted in three joint publications [9,10,11]. We have combined spectroscopic data and long time scale molecular dynamics simulations (> 100 ns) of peptides of different length and compositions. The end-to-end equilibrium distances obtained from MD simulations using GROMOS96 force field for different peptide lengths [10] are in good agreement with the FRET data. Furthermore, the comparison between experimentally obtained kinetic data from time-resolved spectroscopy and MD simulations have also shown a good agreement in term of temperature dependant rate constants [11] (see Figure 17). ¿From computational point of view, the encouraging results provide a benchmark for qualitative analysis of atomistic force field over long time scale simulations in flexible peptides [11].

Along the same research line, other works in the pipeline include studying flexible glycine/serine rich peptides and rigid polyproline peptides to analyze end-to-end distance and the looping kinetic (manuscript in preparations).

Computational Bioengineering Portal

In collaboration with Prof. U. Schwaneberg and Dr. T. S. Wong, we are actively involved in developing computational tools to support and improve mutagenesis experiments. Some of these tools are already available in the Computational Bioengineering Portal at Jacobs University Bremen (map.jacobs-university.de, see Figure 18). The portal is meant to provide different computational services to support protein engineering research. In particular, MAP (Mutagenesis Assistant Program) [12,13] (running since

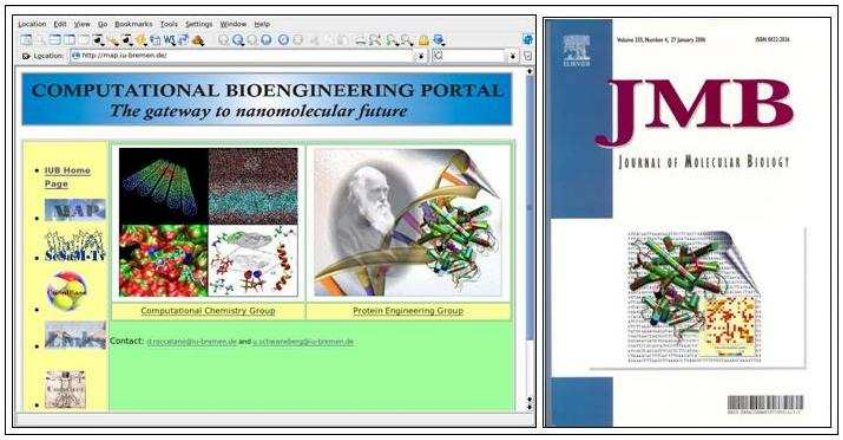

Figure 18: On the left: Computational Bioengineering Portal at Jacobs University Bremen (map.jacobs-university.de). On the right: cover page the JMB issue where the paper on the MAP program was published. [D. Roccatano]

the beginning of 2006) is a statistical tool that allows us to develop promising directed evolution strategies by comparing random mutagenesis methods. It provides, upon input of a DNA sequence, amino acid substitution patterns of 19 random mutagenesis methods. We have used this tool to explore the genetic code organization as well as the consequence of mutational bias [14,15].

The future prospect is to include two additional programs (SeSaMe-Tv and ExPoSeS) in the portal that extend and complement the information provided by the original MAP program.

Interfacial interaction of biomembranes and proteins with polymeric materials

These studies aim at investigating hybrid material at atomic and coarse-grained level for biomedical and biotechnological applications [16]. In collaboration with Dr. G. Milano (Univ. of Salerno), we are studying the interfacial interaction of biological membranes and proteins with polymeric materials. Synthetic polymers are extensively used to create new hybrid material that implement the possibility to tune physicochemical properties of the polymer with the biological function of the biomolecule. Their inert nature makes it possible to use these functionalized materials for medical applications, for instance drug delivery and gene therapy. The capability of tri-block polymers to encapsulate drugs, deliver, and release in the target tissue of the human body stimulates further demands of detailed investigations to understand the mechanism by which these processes occur. Recently, we have published a computational study of the interaction of a new model of polyethylenoxide (PEO) [17] with a DMPC membrane. In this report, we have analysed the barrier for the polymer penetration inside the bilayer using Steered Molecular Dynamics simulations (see Figure 19). The simulations have shown the presence of a barrier for PEO penetration in the hydrophobic core of the biological membrane in consistence with experimental

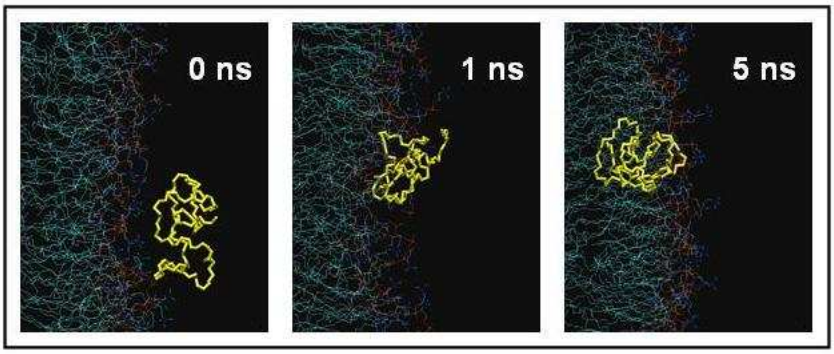

Figure 19: Sequence of snapshots from the SMD simulation showing the polymer penetration in the DMPC membrane. [D. Roccatano]

evidences. This new PEO model (and soon a new model for polypropilenoxide, PPO) will be used to model coarse-grained tri-block polymers (PEO-PPO-PEO) micelle in contact with biological membrane models.

Teaching Activity

The CLAMV teaching laboratories are constantly used for my courses on Computational Chemistry and Biochemistry and Advanced Computational Methods for Nanomolecular Science. Students in these courses are introduced to the use of Unix OS, computational chemistry programs (e.g. Gaussian03, gromacs) and molecular graphics tools (e.g. molden, VMD, rasmol) in their tutorial sessions and/or course projects.

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4.7 Structure-Function Relationship of Membrane Channels

Contributed by Mathias Winterhalter

The outer cell wall of Escherichia coli contains a number of channel forming proteins called porins. Such channels allow e.g. bacteria to harvest nutrients. Our main research focus is on the characterisation of transport across such membrane channels. For this our method of choice is to reconstitute membrane channels into planar lipid bilayers and characterise them by time resolved ion current. For example, previously we have been able to follow the translocation of single sugar molecules through Maltoporin. Maltose molecules diffusing into the channel will create typical fluctuations in ion conductance. An analysis of this “noise in the ion current” allows conclusions on the mode of translocation and the underlying molecular interaction. For example, we quantified the highly selective and efficient transport for maltose harvesting from the outside to the inside. How sophisticated nature had designed this uptake pathway is seen in the asymmetry of the transport: its four times faster than in the opposite direction.

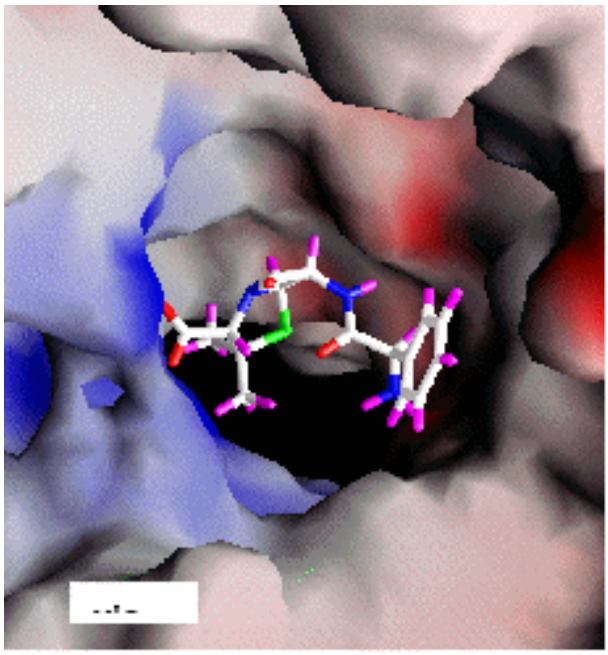

Figure 20: Molecular modelling of an antibiotic molecule (Ampicillin) in an OmpF channel. [M. Winterhalter]

A related question is to understand the pathway of antibiotics. For example OmpF, is a general diffusion porin allowing smaller molecule to permeate and is known to facilitate the translocation of antibiotics like Ampicillin. In collaboration with Dr. S.M. Bezrukov (NIH, Bethesda) we characterised the transport of a series of penicilins. Measureing the ion current fluctuation in presence of different concentrations of penicilins revealed a clear correlation between permeation and biological activity. The data serves as an input for the group of M. Cecarelli (University of Sardenia, Cagliari) to perform one of the most powerful nonequilibrium molecular dynamic simulations to elucidate the effect of molecular interaction during transport.

The use of CLAMV-resources will support us to perform simplified modelling at IUB. For the interpretation of the experimental results graphic programs allow to visualise the structure of the channels and facilitates the data interpretation.

GROUP MEMBERS: Dr. Karin Tuerk, Dr. L. Damian, Dr. K. Gelin, Dr. Y. Ramaye, M. Lindemann, J. Gomes, T. Mach

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Sukhorukov (coordinator, MPI Potsdam), A. L. Rogach (LMU Munich) and W. J. Parak (LMU Munich)

Powerzyme (Princeton): *Biofuel cell.*

Eureka 3271 *Nano to Bio* (PI L. Levy, Nanobiotix, Paris; J.F. Hochepied, Ecole des Mines, Paris).

PhD fellowship from the Ministere dEducation and support through 2 national programs on Nanoscience and on Proteomique for the group of Mathias Winterhalter at the Institut Pharmacologie et Biologie Structurale (UMR 5089, CNRS) Toulouse.

4.8 Biomolecular Simulation and Molecular Docking

Contributed by Martin Zacharias

The research areas of the Computational Biology Group at Jacobs University Bremen are the study of biomolecular structure formation and association using computer simulation approaches. We are especially interested in the role of conformational flexibility during molecular association. As the major computational tool we employ the molecular dynamics simulation method to investigate the structure and dynamics of proteins and nucleic acids at atomic resolution. We also develop new docking approaches to predict putative binding sites for ligands and inhibitors on the surface of biological target molecules. The prediction of putative ligand binding geometries and binding sites on a biomolecule is of great importance for the design of new drugs that can bind and interfere with the function of biomolecules. Focus of another research area is to improve comparative protein structure modeling. Improving the accuracy of structural modeling of proteins is also of central importance to use such structural models for drug design. In close collaboration with experimental groups the computational approaches are applied to several biologically important biomolecules.

During 2006 we used extensively the CLAMV Linux Clusters as well as the teaching lab computer resources. New methodological developments included improvements in our protein-protein docking software ATTRACT [1] and applications to several interesting docking applications [2-4] as well as the development of a new advanced sampling method [5]. In the area of free energy simulations structural transitions between substates of an RNA bulge motif have been characterized [6, see Figure N] and simulations of DNA minor groove opening [7] DNA twisting [8] and RNA kink-turn opening [9,10]. Simulations on the CLAMV resources were performed to understand the kinetics of peptide folding in close collaboration with the experimental group of Prof. Nau [11,12]. Ongoing collaborative projects with experimental groups involve the study of the effect of organic co-solvents on protein dynamics [13,14; together with Prof. Schwaneberg] and the dynamics of MHC class I molecules [15]. The CLAMV cluster computers were also used in part to simulate and analyse the dynamics of complete nucleosome core particles at atomic resolution and under realistic conditions with surrounding ions and solvent molecules [16]. The simulations were performed for more than 20 ns and are among the largest atomistic simulations so far performed

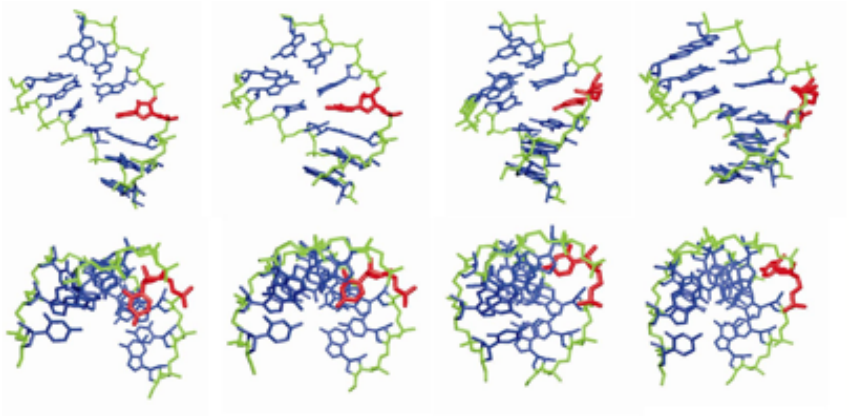

Figure 21: Looping out of an extra un-matched base (in red) in RNA during molecular dynamics free energy simulations [6]. The different phases of the looping out process are illustrated as four snapshots. The view is into the RNA major groove in the top panels and for the same snapshots along the helical axis in the lower panels. Nucleic acid backbone structure is shown in green and the base pairs in blue. [M. Zacharias]

on a complex biomolecular system. The simulation allowed us to characterize the nucleosome fine structure, dynamics and solvent motion at unprecedented spatial and time resolution.

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5 Geosciences and Astrophysics

Research in Geosciences and Astrophysics, or GeoAstro for short, focuses on the observation, evaluation and the physical modeling of natural phenomena on Earth and in the Universe. The different GeoAstro branches share many methodological similarities and the unique combination of expertise gathered within the GeoAstro group allows to address questions that require a holistic view of the physical world. Many of the research activities within GeoAstro are heavily computer-based and profit from the hardware and services provided by CLAMV. Scientific projects that rely on efficient management, analysis, and visualization of large and complex data sets in the geosciences are described earlier in this report (see the contribution by Vikram Unnithan and Angela Schäfer in subsection 3.1). In this section we present a series of research projects in computational modeling of astrophysical continua on a variety of spatial scales.

Until a few decades ago, *theoretical problems of space and astrophysics* were solved using analytical techniques. However, the complexity of most astrophysical phenomena has the consequence that accessible analytical techniques are more and more relegated to limiting – and often unrealistic – cases. In a realistic description of cosmic phenomena, one faces highly non-linear couplings between different kinds of interactions, including gravitational, electromagnetic, radiative, and gas dynamical processes. Assumptions in simplifying symmetries or equilibrium/stationary states are rarely justified. Consequently, computer simulations have become an indispensable tool to provide the theoretical framework within which the superb data, which are delivered by modern observational facilities on the ground and in space, can be interpreted and fully exploited. Numerical modeling holds the promise to dominate the theoretical methodology in space-/astrophysics well into the 21st century and beyond.

Our ability to model complex phenomena is on the one hand determined by our creativity to find suitable physical approximations and on the design of numerical techniques that are able to treat today's multi-physics and multi-scale challenges. On the other hand, this type of research heavily relies on the latest high-performance computer architecture and on our ability to make efficient use of it.

The *common theme in space-astro research* is the modeling of continua. These continua come in many different forms ranging from neutral, ideal gases over dilute, collisionless space plasmas to highly degenerate matter at supra-nuclear densities in neutron stars. On top, further physical effects such as magnetic fields, chemical or nuclear reactions and the cooling via either neutrino or photon radiation are often key ingredients of realistic models. Consequently, there is no such thing as "the method" but instead a large variety of different methods exists, each one with its specific strengths and shortcomings. It is part of the research to wisely choose the best computational approach for the question of interest.

Most fields of astrophysics, such as solar physics, star formation, stellar collisions and explosions and cosmology have benefited greatly from *hydrodynamical simulations* over recent years. There are two main approaches to the numerical solution of

the equations of hydrodynamics that are commonly used in astrophysics: grid-based ("Eulerian") and particle-based ("Lagrangian") methods (in astrophysics a very popular method is the so-called Smoothed Particle Hydrodynamics method, SPH). In the first approach the equations are discretized on a computational mesh and flows between grid-cells are calculated. The latter method avoids the notion of a mesh and instead moves discretized portions of the flow ("particles"). Both methods have different strengths and weaknesses, the "right choice of method" usually depends very much on the problem to be solved. Generally, sharp continuities are easier to resolve with a grid-based method while the particle methods have advantages in numerically conserving quantities that are physically conserved (such as energy or angular momentum). In the space- and astrophysics at Jacobs University Bremen we employ both types of methodologies. In recent times *magnetic fields* have become key ingredients in several of the simulations performed by members of the space-astrophysics group.

Codes that are regularly used are the adaptive mesh-refinement code FLASH (from the Center for Astrophysical Thermonuclear Flashes at Chicago), the grid-based MHD-codes PENCIL (Brandenburg and Dobler) and BATS-R-US (developed at the University of Michigan), the smoothed particle hydrodynamics code GADGET (Springel) and the smoothed particle magnetohydrodynamics code MAGMA developed for compact objects (Rosswog and Price).

5.1 The Large-Scale Structure of the Universe

Contributed by Marcus Brüggen and Elke Rödiger

Recent observations show a multitude of physical effects that occur when powerful jets launched by supermassive black holes interact with the surrounding medium. While these effects are widely believed to be crucial for the formation of structure in the universe, they are still poorly understood. Clusters of galaxies are excellent laboratories for studying the interaction between active galactic nuclei (AGN) and diffuse gas. Recent observational evidence demonstrates that the lives of AGN and their environment are closely intertwined. This complex pattern of processes has been simulated with unprecedented realism by our group at the Jacobs University Bremen using CLAMV resources, in particular the MASTER cluster and the KINGKONG system for the data analysis.

Interactions of AGN jets with dynamic cluster atmospheres

We performed our simulations in three dimensions in Cartesian geometry using the adaptive mesh refinement code FLASH (version 2.4). The FLASH code was developed by the Department of Energy-supported ASCI/Alliance Center for Astrophysical Thermonuclear Flashes at the University of Chicago. FLASH is a modular block-structured AMR code, parallelised using the Message Passing Interface (MPI) library. It solves the Riemann problem on a Cartesian grid using the Piecewise-Parabolic Method (PPM).

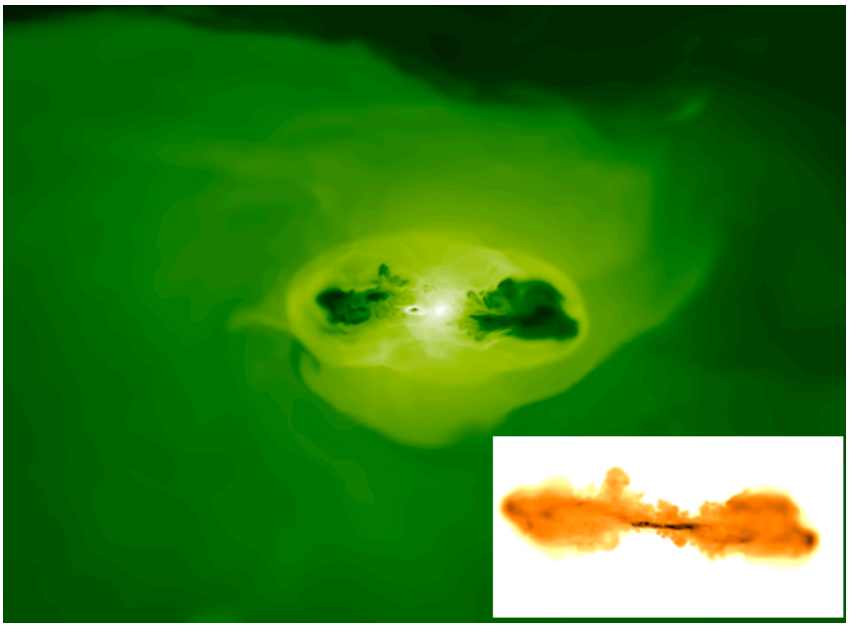

Figure 22: Snapshot of the gas density in a simulation of a jet in a cluster of galaxies. One can see how the jet drives shocks into the intracluster medium. The inset shows the simulated radio emission from this jet. [M. Brüggen]

It uses a criterion based on the dimensionless second derivative of a fluid variable to refine or derefine the grid. Collsisionless matter, i.e. stars and dark matter, were represented by particles that interact gravitationally with each other and the gas. Our initial models were extracted from cosmological SPH simulations and typically included around 700,000 dark matter and star particles. We modified the FLASH code to follow the central black hole and modelled the jet as inflow boundary conditions that lie within the computational domain. Moreover, we developed a fast multigrid gravity solver in order to be able to simulate the galaxy cluster for more than 300 Million years.

This code allowed us to study the interaction of the jet with its environment, for the first time taking into account the dynamic nature of the cluster gas. The simulations successfully reproduce the observed morphologies of radio sources in clusters (Fig. 22). We find that cluster inhomogeneities and large-scale flows have significant impact on the morphology of the radio source.

PUBLICATIONS

Heinz, S.; Brüggen, M.; Young, A.; Levesque, E., The answer is blowing in the wind: simulating the interaction of jets with dynamic cluster atmospheres. MNRAS, 373L, 65

Influence of AGN-blown cavities on metal abundance profiles in clusters

The hot, diffuse gas that permeates clusters of galaxies, the intra-cluster medium (ICM), has a metallicity of about 1/3 of the solar value. Meanwhile, the total amount of iron in the ICM is huge: it is larger than the total iron mass in all cluster galaxies. Galaxy clusters can be grouped into two categories depending on their X-ray surface brightness profiles: (i) clusters with a central peak in the X-ray surface brightness, i.e. clusters with a cool core and (ii) clusters without a cool core. Interestingly, these two groups show a different spatial distribution of metals. The clusters without cool cores have a nearly uniform spatial distribution of metals, while clusters with cool cores have a strongly peaked abundance profile.

Stellar mass loss from the central cluster galaxy through supernovae and stellar winds appears to be the prime source for the metals observed in the inner parts of galaxy clusters. However, the observed metallicity profiles are much broader than the stellar light profiles of the central galaxy. Hence, the differences in the light and metal distributions are interpreted as the result of transport processes that have mixed the metals into the ICM. While it appears to be established that the metals produced by the central galaxy are dispersed into the ICM to form the broad abundance peaks, it remains unclear what the mechanism is via which the metals are transported.

As one likely mechanism of metal transport, we have studied the effect of bubble-induced motions on metallicity profiles. The central galaxies of cooling core clusters host active galactic nuclei (AGN). Connected with the dynamics of AGN are relativistic jets. When these jets interact with the intracluster medium, they blow up bubbles. These bubbles are filled with a hot, underdense gas and thus rise buoyantly through the ICM, transporting gas outwards in their wakes.

We have simulated this process with the hydrodynamical adaptive mesh refinement code FLASH (version 2.5). We start the simulations with a hydrostatic ICM, using a "tracer" fluid to follow the evolution of the metal distribution. This tracer fluid records the injection of metal-rich gas from a central galaxy as well as the evolution due to motions in the ICM. In each simulation, we generate a series of bubbles. While the bubbles rise through the cluster atmosphere, they drag metal-rich gas from the inner regions outwards, thus broadening the metallicity profiles. Moreover, the resulting metal distribution becomes very elongated along the direction of the bubbles, as is shown in Fig. 23.

The simulations for this project are mainly run on the Linux Cluster MASTER. A typical simulation took about 800CPUh, we ran 12 simulations with different parameters. Each simulation produces 5-6GB of data. The data analysis and visualisation is done with the software IDL, which is also provided by CLAMV. Moreover, we use the CLAMV storage service for our data.

The next step in this project is to combine the two models described above, i.e. to study the evolution of the metal distribution in clusters where AGN-jets interact with a dynamic cluster atmosphere. The rich structure of ambient motions may help to isotropise the resulting metal distribution. This work is already in progress.

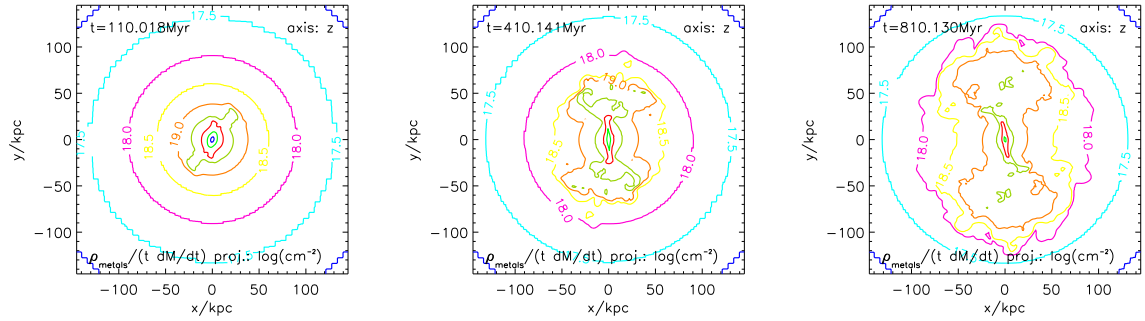

Figure 23: Projected metal density in the galaxy cluster for different timesteps. The metal density is normalised to elapsed time and total injection rate for easier comparison between single timesteps. The rising bubbles produce an elongated metal distribution and reduce the central metal density. [E. Rödiger]

PUBLICATIONS

E. Roediger, M. Brüggen, P. Rebusco, H. Böhringer and E. Churazov, Metal mixing by buoyant bubbles in galaxy clusters. MNRAS, 2007,375,15

5.2 The Radio Universe

Contributed by Matthias Hoeft

Most of the Universe is filled by very tenuous plasma, i.e. ionized gas with a background or self-generated magnetic field. Sudden energy releases can initiate magnetic or hydrodynamic waves in the plasma, which may steepen into collisionless shocks. They are capable to accelerate some particles to very high energies, e.g., by an electric field inherent to the front or by reflecting a particle to and fro across the front. The resulting supra-thermal electrons and ions may interact with the plasma and excite plasma radiation or simply loose their energy by gyro-synchrotron radiation. These radiation can be detected with ground or space telescopes observing in the radio band, i.e. form ~ 1 MHz to ~ 10 GHz.

Radio observation are a powerful diagnostic tool for a multitude of space and astrophysical processes. We focus here on two topics: First, rather close events, namely solar coronal mass ejections (CME) and, secondly, the physics of shock fronts in the plasma of galaxy clusters. In linear size the latter are as different from our solar system as the Earth from a grain of sand. However, the plasma conditions at the shock front are rather similar. Therefore, studying the physics of the interplanetary space will help a great deal to understand the physics of the intra-cluster medium. More precisely, space crafts have shown already the complexity of collisonless shocks for both the magnetopause around the Earth and for CME related interplanetary shocks. Those studies allow us to set up a model for the electron and proton acceleration at a shock front, a process which cannot be emulated on Earth.

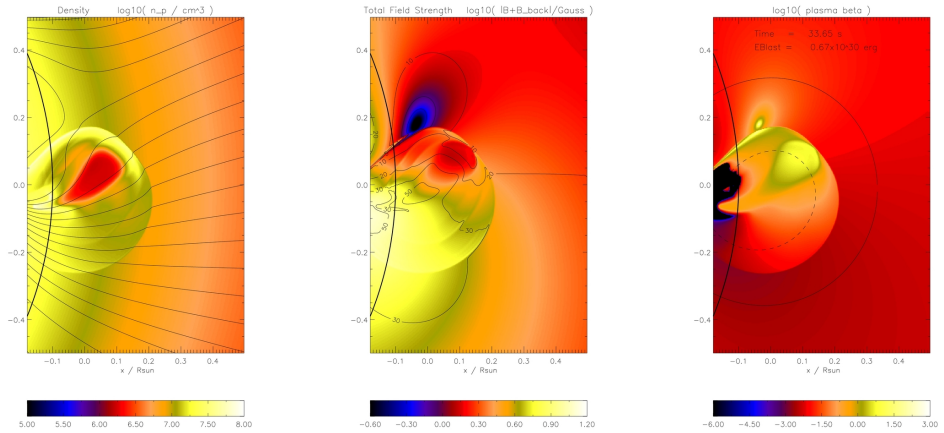

Figure 24: A blast wave in the solar corona. Magnetic reconnection may release large amounts of thermal energy which causes a blast wave. The resulting shock front may generate supra-thermal electrons which excite plasma radiation seen in dynamical radio spectra. [M. Hoeft]

Our aim is to simulate the formation of shock fronts in both the solar corona and in the intra-cluster medium. The former are related to CMEs, see Fig. 24, and the signature of the shock fronts can be seen in dynamic radio spectra which show how the CMEs propagate into the interplanetary space. Moreover, radio imaging telescopes, as the Nancay Radio telescope, provide images at several fixed frequencies above 160 MHz. In near future the situation will dramatically improve with the upcoming radio telescope LOFAR. Its capability to observe down to 30 MHz will allow to follow the evolution of the shock fronts to much larger distance from the Sun. Moreover, since the telescope is 'shaped' digitally, imaging can take place with a much smaller distance in frequency space. Hence, for the first time the propagation of the radio emission can be followed, this may shed new light on origin of the still enigmatic substructure in radio spectra and how CMEs are launched.

We combine the research on the radio signature of shocks in the solar corona with study of the formation of galaxy clusters. We have shown that diffuse radio objects, found in the periphery of clusters, see Fig. 25, can be consistently explained by particle acceleration at strong shock fronts. By the help of large simulations of the structure formation in the Universe we have shown that shock fronts in galaxy clusters are generally arranged in a 'onion' structure. The fronts trace the growth history of the clusters, i. e. when a cluster has merged with another one. At the moment only the most luminous emission at shock fronts has been observed. The upcoming radio telescopes as LOFAR and SKA will beyond doubt detect a large number of new radio objects. With the detection of those objects we will observe directly how the intra-cluster medium gets to its high temperature. Moreover, the origin of the magnetic field in the intra-cluster medium is still enigmatic. A very likely source are also the strong shocks surrounding clusters of galaxies. The abundance, the spectrum, and the polarization of the resulting radio emission in comparisons to its properties expected from simulations may allow us to conclude for the magnetic field generated at

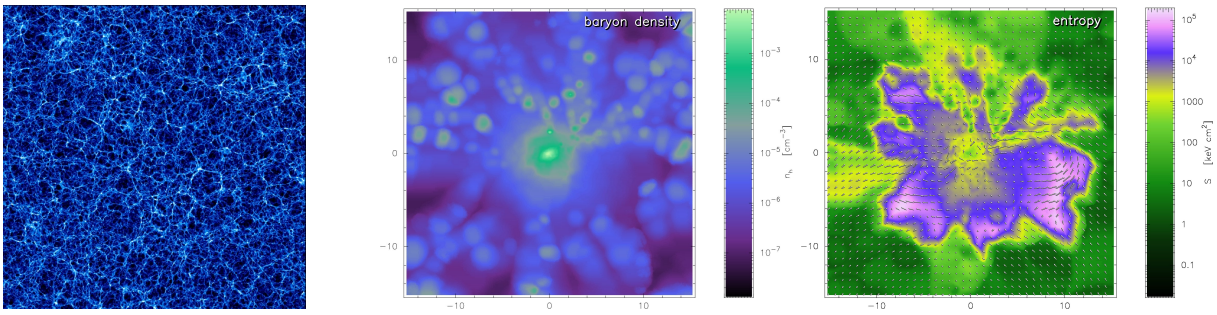

Figure 25: We study the formation of cosmological structures by the help of very large simulations. The left panel shows the matter distribution in cube of more than a billion light years. The right panels show the density and entropy distributions in small sub-regions. The edge length of these amounts to 1/20 of the large box. High entropy is generated by structure formation shocks which will be observable with next generation radio telescopes. [M. Hoeft]

those shocks.

To carry out the necessary simulation powerful computing resources are needed. For instance, to model the shock propagation in the solar corona a magnetohydrodynamic simulations with adaptive mesh-refined are required. A comparison with observed dynamic radio spectra is only useful if a three dimensional simulation has been carried out. Depending on the resolution, the code, the setup of the problem, and the communication speed between the processors in the computer cluster up to several hundred processors have to be used in parallel to simulate the necessary physical time span. For those very large simulations we use computing time at the national or international computing centers, e. g. the John von Neumann-Institut for Computing, Jülich, Germany or the Barcelona Supercomputing Center, Spain. However, those large simulations need an intense preparation for which the resources of CLAMV are indispensable.

5.3 Galaxy Evolution in Different Environments

Contributed by Elke Rödiger

Galaxies populate different environments in the universe, ranging from isolated field regions to dense galaxy clusters. Depending on environment, the properties of galaxies change: In denser regions the galaxies tend to contain less neutral gas, show a weaker star formation activity and redder colours than galaxies in sparse regions. Several processes have been proposed to explain these features. One idea are gravitational interactions among the cluster galaxies. But besides galaxies, clusters also contain a large amount of dilute gas - the intra-cluster medium (ICM). The presence of the ICM leads to ram pressure stripping, another process that can affect cluster galaxies. As galaxies move through a cluster, they also move through the ICM. The ram pressure they experience hereby can push out (parts of) their gas disks.

We simulated this process with the hydrodynamical adaptive mesh refinement code

FLASH (version 2.5). Its modularity makes is suitable for a large variety of problems. We modified the FLASH code in order to simulate the evolution of the gas disk of a galaxy moving through a cluster. For this purpose we need to include the gravitational potential of the galaxy. If the galaxy's gravity is strong enough, it can prevent the gas disk from being stripped.

Previous work – investigation of some aspects with a simplified model

In a first step, we have simulated the interaction between the gas disk and the ICM using a constant galaxy velocity and ICM density. We focussed on the question how the stripping effect depends on the inclination angle between the galaxy's rotation axis and the ICM wind direction. We found that the inclination angle does not play a major role for the amount of gas loss from the galaxy as long as it is not moving close to edge-on. However, with increasing inclination angle, the stripping proceeds more and more asymmetrical.

Inspired by the observation of a ~ 100 kpc long tail of neutral gas behind the spiral galaxy NGC 4388 in the Virgo cluster, we ran a few simulations in a large simulation box to follow the evolution of the galaxy's wake. The tail of NGC 4388 shows an S-shape and a flaring width. In our simulations, we could reproduce S-shaped tails, but the simulated tails are wider than the observed case.

Current work – Galaxies orbiting in clusters

Currently, we are running ram pressure stripping simulations of a galaxy orbiting in a cluster, i.e. now the galaxy is exposed to changing ICM conditions (ICM density and galaxy velocity). Moreover, the galaxy is affected by the gravitational potential of the galaxy cluster. Our simulations with constant ICM conditions have shown that ram pressure stripping cannot unbind the galaxy's gas from the galaxy's gravitational potential instantaneously, but this process takes a few 100 million years. This implies that in order to remove that gas from the galaxy, the ram pressure does not only need to be strong enough, but also the time intervall of strong ram pressure must be long enough. Now, in our improved simulations, we will be able to investigate these relations in detail. A different aspect deals with the impact on the ICM. The galactic gas is enriched with heavier elements ("metals"), and as this gas is lost from the galaxy, it enriches the ICM with metals. Our simulations will show where the galaxy leaves which amount of enriched gas. A very first result is shown in Fig. 26: The density of galactic (i.e. enriched) gas at the end of the simulation is shown in a slice through the cluster. The black line marks the orbit of the galaxy. It is remarkable that the galaxy has spread its gas all along the orbit. The "tail" is densest close to the galaxy cluster (at coordinates $(0, 0, 0)$), i.e. where the ram pressure was strongest, but the galaxy has lost gas on its way into the cluster as well as on its way out.

The simulations for this project are mainly run on the Linux Cluster MASTER. E.g. the simulation described in Fig. 1 took approx. 3000CPUh, i.e. it ran for five days on 24 processors. It produced 22 GB of data (in compressed format). We will need at

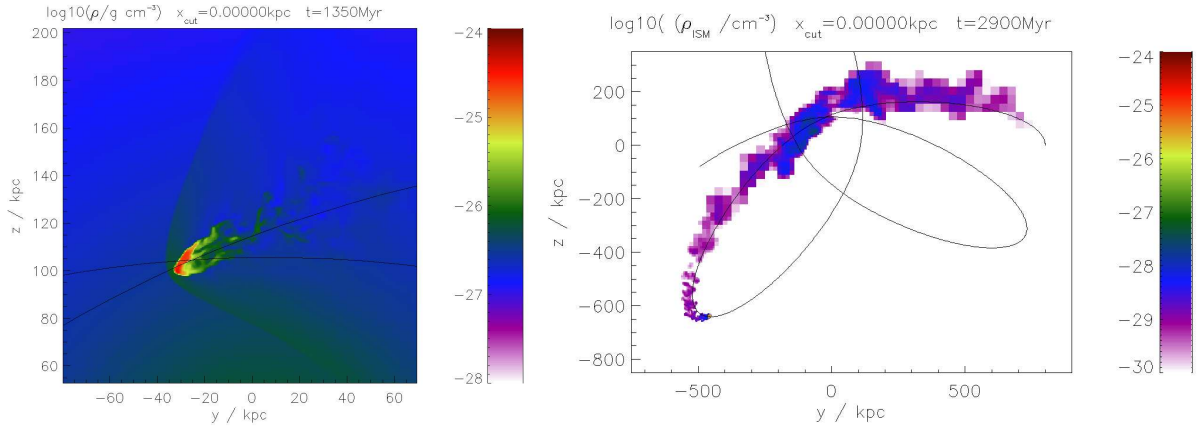

Figure 26: Cuts through the simulation box. The left panel shows the galaxy in the stage of strongest stripping, i.e. when the galaxy passes near the cluster centre. The galaxy is moving supersonically, as indicated by the bow shock. The colors code the gas density. The right panel shows the distribution of gas originating in the galaxy after the galaxy has gone through the cluster once. The black line marks the orbit of the galaxy. The galaxy has been heaviliy stripped, and, remarkably, it lost gas not only in the vicinity of the cluster centre, but all along its orbit. [E. Rödiger]

least 10 simulations to probe the parameter space sparsely, plus some simulations with higher resolution. The data analysis and visualisation is done with the software IDL, which is also provided by CLAMV. Moreover, we use the CLAMV storage service for our data.

PUBLICATIONS

E. Roediger and M. Brüggen, Ram pressure stripping of disc galaxies. The role of the inclination angle, MNRAS, 2006, 369,567

E. Roediger, M. Brüggen and M. Hoeft, Wakes of ram pressure stripped disc galaxies. MNRAS, 2006, 371,609

5.4 Collisions Between Compact Stellar Objects

Contributed by Stephan Rosswog

Coalescence of neutron stars with black holes

Binary systems consisting of two compact objects, either two neutron stars or a neutron star and a stellar-mass black hole, are among the most promising sources for gravitational waves that could be detected in the near future by ground-based detector facilities. The gravitational waves carry away energy and angular momentum

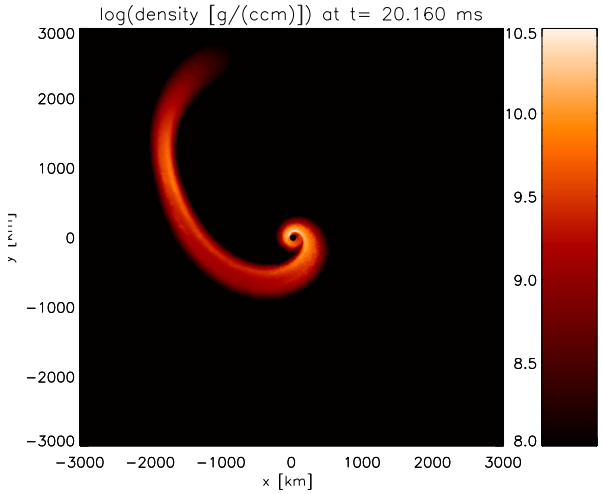

Figure 27: Snapshot of the tidal disruption process of a 1.4 solar mass neutron star by a black hole of 14 solar masses. Color-coded is the column density through the neutron star debris. [S. Rosswog]

from the binary system, therefore the two components of the system will slowly drift towards coalescence.

This final coalescence releases a tremendous amount of energy: more than 10^{53} ergs, more than the energy our Sun could emit during the whole age of the Universe, are released in fractions of a second. Such coalescences seem to be responsible [1,3,4,6,11,13,15] for a good fraction of the most violent explosions in the Universe since the Big Bang: gamma-ray bursts, tremendously violent explosions that emit copious amounts of gamma-rays.

We have simulated the last milliseconds in the life of a neutron star black hole binary system. For technical reasons we have started this investigation focusing on the high-mass end of the expected black hole mass distribution, i.e. we focused on Black Holes with masses larger than 14 $\mathrm{M}_\odot$. Black holes possess a so-called *innermost stable circular orbit* at a radius R_{ISCO}, inside of which no particle can revolve around the hole in a stable, circular fashion. Our recent simulations [14] show that the neutron star, once it has come close enough to the black hole, transfers a large portion of its mass directly into the hole. Only after that stage an accretion disk can form. However, none of our investigated cases formed the hot (several 10^{10} Kelvin) and massive ($\approx 0.1\ \mathrm{M}_\odot$) accretion disk that is needed to launch a gamma-ray burst. Instead, the disk that finally forms has only a relatively small mass. Most of it resides inside the innermost stable circular orbit and is therefore falling rapidly towards the hole without having enough time to heat up. A small amount of the initial neutron star mass takes up a lot of the orbital angular momentum and transports it outward in rapidly expanding tidal tail. A snapshot of such a disruption process is displayed in Fig. 27, movies can

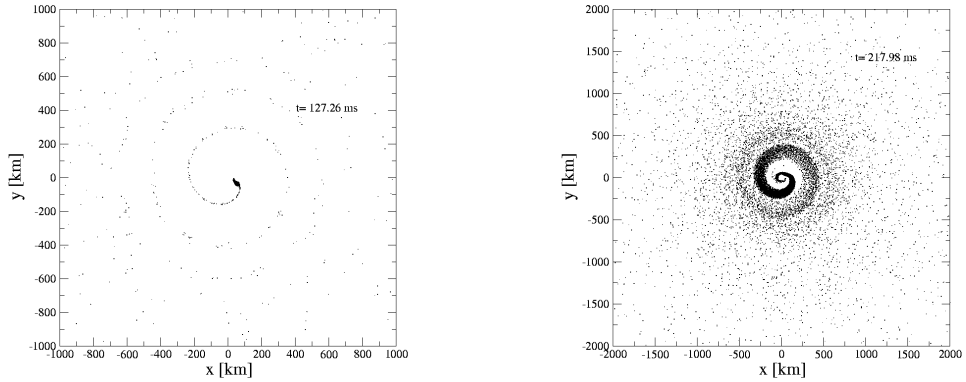

Figure 28: Dynamical evolution of a neutron star black hole system that undergoes episodic mass transfer. [S. Rosswog]

be found at http://www.faculty.jacobs-university.de/srosswog/movies.html. We have also explored the lower black hole mass range [16] in which case we found long-lived, episodic mass transfer occuring for dozens of orbital periods, see Fig. 28.

The high mass end of the distribution that we began our study with does not seem to be promising for the central engine of gamma-ray bursts, but the low mass end of the black hole mass distribution could produce bursts of moderate strength. So if many of these systems do not produce a gamma-ray burst how else would they make themselves known? They will definitely be a strong source of gravitational waves. The tidal tails also hold some promise for observation. Depending (quite sensitively) on the mass of the black hole, up to 0.2 $\mathrm{M}_\odot$ of the neutron star get thrown out into space with velocities of about half the speed of light. This material initially has very high densities where nature favors very large nuclei containing hundreds of neutrons and protons. As this material expands very rapidly, the physical conditions and therefore the preferred nuclei change continuously. This leads to a constant transmutation/decay of the present nuclei and goes along with constant electromagnetic emission. This could (like a type Ia Supernova) lead to an electromagnetic emission that is powered by radioactive decays. It will produce a flash with a maximum intensity in the optical/near infrared band [14].

Moreover it could be shown that, contrary to the common prejudice, long-lived accretion processes continuing for hours are a natural consequence of compact binary mergers [17].

Collisions of magnetised objects: the MAGMA code

Most stars possess magnetic fields and these can be extremely large compared with the Earth's magnetic field ($\sim$ 0.5 G): new-born neutron stars have field strengths of $\sim 10^{12}$ G, a particular breed of neutron stars, so-called magnetars, even have field strengths of $\sim 10^{15}$ G. Motivated by this fact and the desire to understand the physics

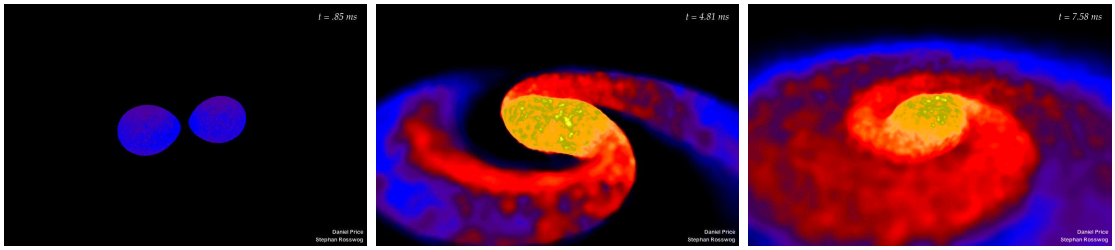

Figure 29: Computer simulation of the last stages of a double neutron star coalescence: short after contact the stars shed mass into spiral arms that subsequently form a hot torus. The central object will probably at some stage collapse to a black hole. Figure from Price, D. & Rosswog, S. (2006), Science 312, 5774. [S. Rosswog]

behind gamma-ray burst explosions, I have started with Daniel Price from Exeter, UK to write a completely Lagrangian, particle-based magnetohydrodynamics (MHD) code called MAGMA. The particular difficulty in this approach is to find a particle representation that enforces the $\nabla \cdot \vec{B} = 0$ ("no magnetic monopoles") constraint. This was done using so-called Euler-potentials, α and β, via

$$\vec{B} = \nabla\alpha \times \nabla\beta. \tag{1}$$

This formulation is equivalent to a vector potential approach and therefore fulfils the $\nabla \cdot \vec{B} = 0$ constraint by construction. The code MAGMA further benefits from a slew of recent numerical improvements in comparison with other smoothed particle hydrodynamics implementations. It incorporates an artificial viscosity oriented at Riemann solvers, see [5], with time dependent parameters [7,12] consistent accounting of the effects of the so-called "grad-h"-terms [8] and a consistent implementation of adaptive gravitational softening lengths [10]. This code will become the main workhorse of future (magneto-)hydrodynamic investigations.

The first application was the collision of magnetised neutron stars, see Fig. 29 [9], which allowed to investigate the evolution and amplification of the magnetic field during the coalescence.

White dwarf explosions triggered by tidal compression

As most stars in the Universe have masses comparable to that of our Sun, the most common remains after a stellar lifetime are white dwarfs. In a Globular cluster about 10 % of the disrupted stars are white dwarfs [2]. A star passing a black hole will be disrupted if the tidal forces overwhelm the self-gravity of the star. As we want to know whether a white dwarf can be compressed enough to trigger a thermonuclear explosion, we are interested in the strongest possible encounters with the distance of closest approach being much smaller than the tidal radius where the star becomes disrupted. Such requirements cannot be met by all types of black holes as for the most massive ones, such as the one in the center of our Galaxy, the white dwarf would be swallowed by the black hole before it can be disrupted. Therefore for this study only black holes with masses smaller than 10^4 $M_\odot$ are interesting.

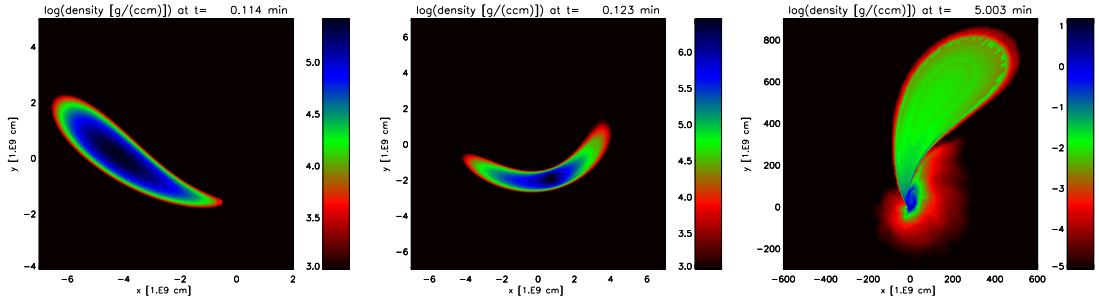

Figure 30: Tidal ignition and detonation of a white dwarf as it passes an intermediate mass black hole (located at the origin). As the Helium white dwarf passes the point of maximum compression (panel 2) it heats up to about $5 \cdot 10^9$ K and ignites its nuclear fuel. During the passage more than its entire gravitational binding energy is released via nuclear burning processes, therefore the white dwarf blows up in a violent explosion. The parts that have passed closest to the hole are captured and form via an angular momentum redistribution shock an accretion disk around the hole. [S. Rosswog]

In a good fraction of the investigated cases the white dwarfs become strongly enough compressed so that the temperatures rise beyond 10^9 K. At the end of their normal stellar lifetimes white dwarfs had stopped nuclear burning as there was no means to reach high enough temperatures to ignite the ashes form previous burning stages (mostly Helium, Carbon or Oxygen). In such a fly by, however, a white dwarf can reach much higher temperatures than ever before in its life. They are large enough to ignite the ashes the white dwarf is made of and the nuclear reactions that now set in can become extremely fast: more than 10^{51} ergs, more than the energy our Sun would radiate in a billion years, will be released within fractions of a second. A white dwarf cannot react on this short time scale by expanding and thus slowing down the nuclear reactions, it has to take up all this thermonuclear energy and then blow up in a violent detonation.

An example of a thermonuclear explosion induced by tidal compression is shown in Fig. 30. A 0.2 $M_\odot$ white dwarf composed of pure Helium passes close to a 1000 solar mass black hole. At the point of maximum compression more than $5 \cdot 10^9$ K are reached which explosively ignites the white dwarf. The deposition of more than 10^{51} ergs results in a violent thermonuclear explosion.

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5.5 Space Plasma Physics

Contributed by Joachim Vogt

Being a magnetized obstacle in the supermagnetosonic solar wind plasma, the Earth carves out of the interplanetary medium a cavity known as the magnetosphere. Threaded by magnetic field lines of terrestrial origin, the magnetosphere acts as a shield against high-energetic particles of cosmic and solar origin. Spacecraft observations in combination with ground-based measurements established the controlling influence of solar wind fluctuations on short-term magnetospheric dynamics and space weather. On geological time scales, variations of the internal geomagnetic field can affect the Earth's magnetosphere even stronger and contribute to what may be called space climate.

Paleomagnetospheric processes

The DFG funded project *Studies of paleomagnetospheric processes* dealt with the magnetosphere during geomagnetic polarity transition periods. In the context of the DFG Priority Programme SPP 1097 *Geomagnetic Variations*, paleomagnetospheric processes were investigated by project groups first at the TU Braunschweig, and later also at the International University Bremen. Over the past six years, we have studied

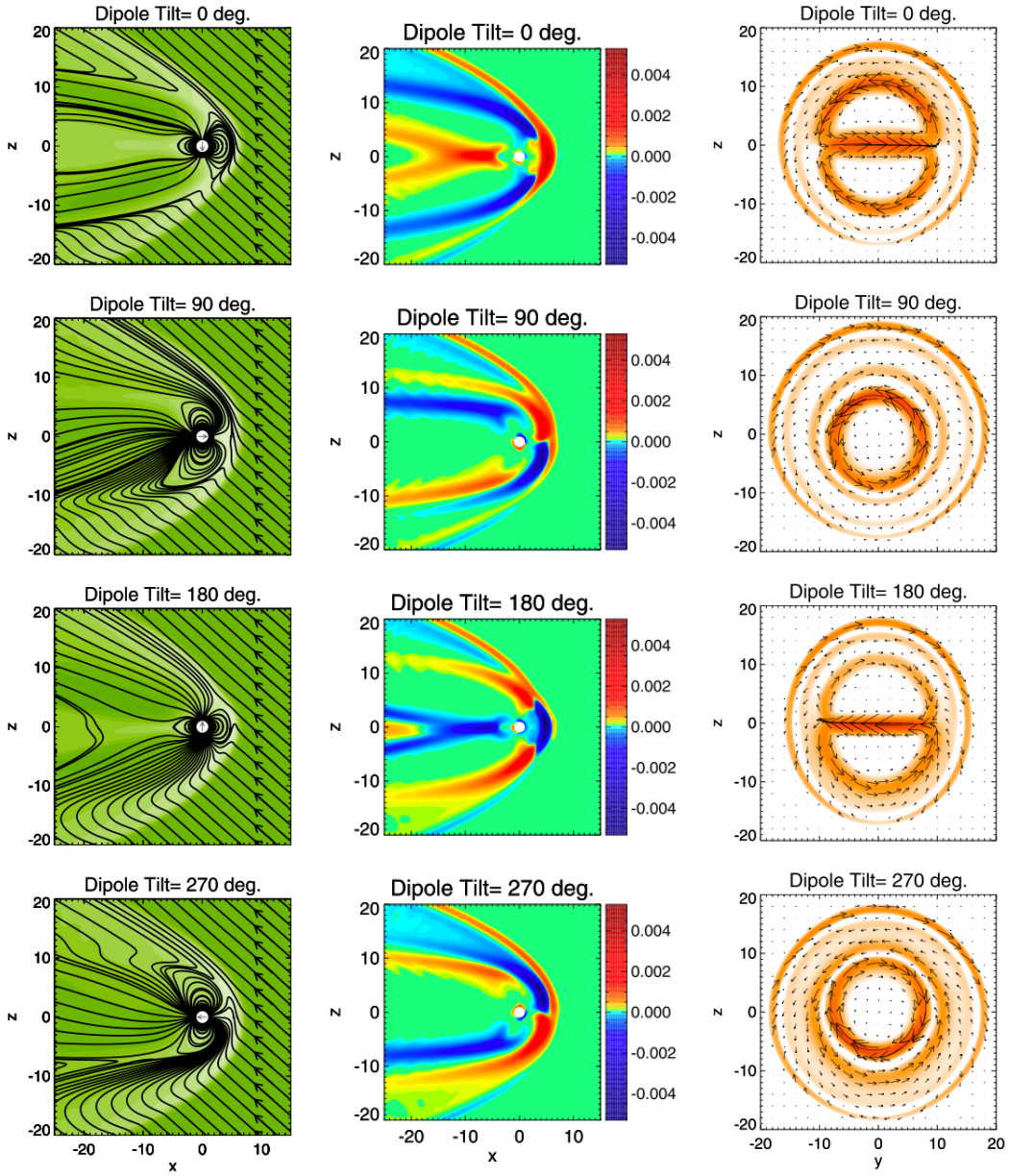

Figure 31: Diurnal variations in an equatorial dipolar paleomagnetosphere. Figures taken from Zieger et al. (2004). Left: Magnetic field lines and pressure distribution. Center: Currents flowing across the equatorial plane. Right: Tail current systems. [J. Vogt and B. Zieger]

structural aspects of paleomagnetospheres using theoretical concepts of magnetosphere formation, a potential field approach to model magnetopause shielding, and magnetohydrodynamic simulations. High-energetic particle fluxes into the Earth's upper atmosphere were obtained through the integration of large numbers of charged particles in the model paleomagnetospheres. The types of geomagnetic variations considered here include changes of the dipole moment magnitude and excursions of the dipole axis. Quadrupolar paleomagnetospheres were studied to assess the rich variety of non-dipolar configurations.

During an excursion event, the angle between the dipole axis and the Earth's rotation axis is large. The orientation of the dipole axis with respect to the solar wind flow direction changes significantly during one day, leading to global reconfigurations on time scales of several hours. We briefly refer to such a configuration as an equatorial dipolar magnetosphere. Magnetohydrodynamic (MHD) simulations of such a configuration were carried out by Zieger et al. (2004). The interplanetary magnetic field was assumed to follow a Parker spiral in the away sector which is one of the two most probable IMF directions of the solar wind. Figure 31 displays how the magnetic field line topology and large-scale magnetospheric current systems change as the dipole axis rotates in the course of one day. The dipole tilt is the angle between the dipole axis and the z-axis in the geocentric solar-magnetospheric coordinate system (GSM), where the x-axis points towards the Sun and the dipole axis is in the plane defined by the x and z axes. Thus in an equatorial dipolar magnetosphere the z (GSM) axis points from dawn to dusk. If the dipole tilt angle is 0 degrees (first row in figure 31), there is no reconnection at the dayside magnetopause but only in the cusp regions, and the overall configuration is essentially a closed-type magnetosphere. The tail current configuration is Θ-shaped with the tail magnetopause currents closing through the neutral sheet current. After six hours the dipole axis points towards the Sun (90 degrees dipole tilt, second row in figure 31), and the field line topology has changed completely. The magnetosphere opens up in response to reconnection at the nose of the magnetopause, and open field lines are convected towards the tail at the dawn side of the magnetosphere. The tail magnetopause current is detached from the neutral sheet current. Both current systems close on themselves and flow on cylindrical surfaces in opposite directions. After another six hours, the dipole tilt is 180 degrees (third row in figure 31), the perpendicular component of the IMF is antiparallel to the geomagnetic field at the dayside magnetopause, thus yielding an open-type magnetosphere with magnetic flux transport over both poles and reconnection in the tail. The tail current system is again Θ-shaped. A dipole tilt of 270 degrees (fourth row of figure 31) gives again rise to cylindrical tail current systems and marks the transition to the closed-type field line configuration at the beginning of the daily cycle.

Higher-order multipoles are likely to come into play during geomagnetic polarity reversals. Numerical geodynamo simulations can be used to obtain a representative set of geomagnetic coefficients to study the formation of a reversal magnetosphere and the impact of energetic particles into the Earth's upper atmosphere. Fig. 32 shows the the regions on the globe which become accessible to 256 MeV protons before and during the transition.

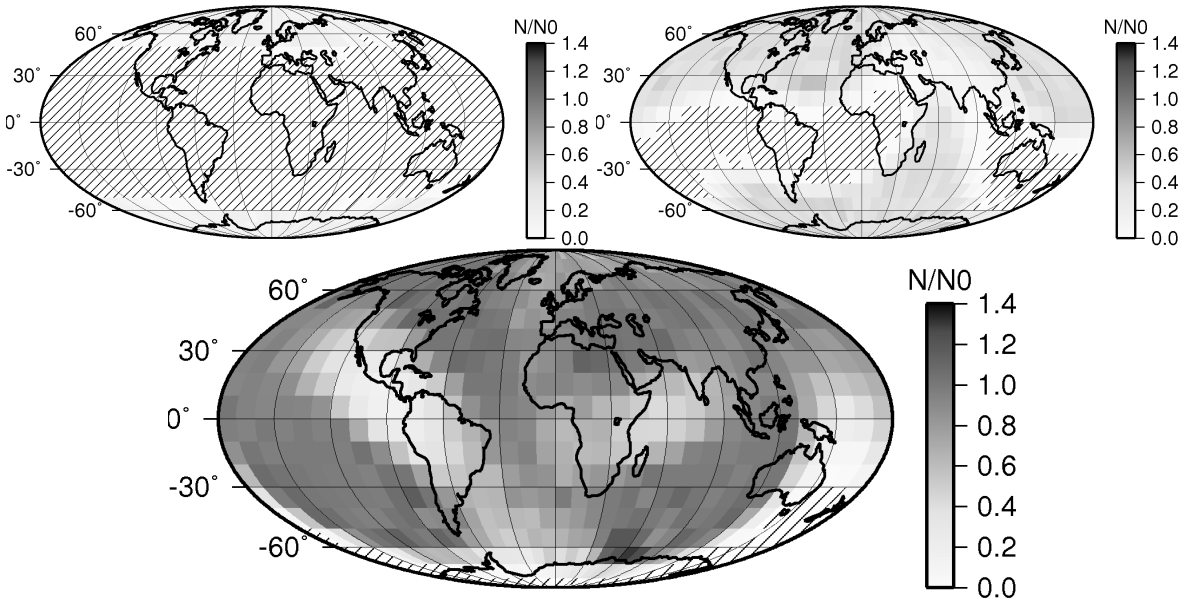

Figure 32: Regions on the globe that become accessible to 256 MeV protons before and during the simulated polarity reversal (see text). Figures taken from Vogt et al. (2007). Top left: 15 000 years before the reversal. Top right: 1 000 years before the reversal. Bottom: At the time of the reversal. [J. Vogt and A. Stadelmann]

Solar radio emissions

In a second DFG funded space plasma project (jointly with Marcus Brüggen and Matthias Hoeft), we are planning to model radio emissions of coronal mass ejections which happen on time scales like hours or days, and lead to space weather phenomena like geomagnetic storms and substorms. The project started in August 2006.

GROUP MEMBERS: Anja Stadelmann (PhD student at TU Braunschweig, graduation in November 2004), Bertalan Zieger (PostDoc, from October 2002 until January 2007), Joachim Schmidt (PostDoc, from January 2004 until January 2006), Matthias Hoeft (PostDoc, since August 2006).

GRANTS

DFG VO 855/1 (2000–2006, J. Vogt and K.-H. Glassmeier): *Studies of paleomagnetospheric processes*.

DFG VO 855/2 (2006–2007), J. Vogt and M. Brüggen: *The CME source region in LOFAR related simulations*.

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6 Mathematical and Computer Sciences

To solve scientific problems with the aid of computers, both efficient algorithms and hardware are required. Hence scientific computation has roots in mathematics and in computer science. In this section selected research projects from those areas are presented. Two further projects that contribute to those subject areas are presented in an earlier section of this report, see subsections 3.2 and 3.3.

6.1 GALEON and Other Data Services

Contributed by Peter Baumann

GALEON (Geo-interface to Atmosphere, Land, Earth, Ocean netCDF)

The Open GeoSpatial Consortium (OGC)[7] is the main standardization body worldwide for interoperable geo services. OGC has published a series of standards for diverse data structures and application fields, such as the widely used WMS (Web Map Service) and, more recently, the WCS (Web Coverage Service) which allows to request and subset n-D raster data "cubes".

Interoperability Experiments (IEs) are an OGC mechanism to validate specifications by means of demonstrating, in a collaborative effort of several independent partners, communication between different implementors' clients and servers. The GALEON IE undertakes to test the WCS 1.0.0 specification on a particular data, namely 4-D/5-D climate model data hitherto stored in the NetCDF data format. As such, GALEON addresses several innovative aspects in addition to evaluating the WCS standard:

- use of data structures beyond the 2-D maps currently receiving main attention in the geographic domain of OGC,
- particularly high-volume data (a single ECHAM T42 climate simulation, which is relatively low-resolution, occupies several Terabytes),
- serving of such data not in files (as all other servers currently do), but in a standard, open-source database (PostgreSQL); this is IUB's particular contribution.

Under the leadership of Unidata/UCAR a large number of participants contribute to GALEON, among them NASA, CadCorp, Jet Propulsion Laboratory, University of Florence, and IUB.

More information about GALEON can be found at http://my.unidata.ucar.edu/content/projects/THREDDS/OGC/[8].

[7] http://www.opengis.org
[8] http://my.unidata.ucar.edu/content/projects/THREDDS/OGC/

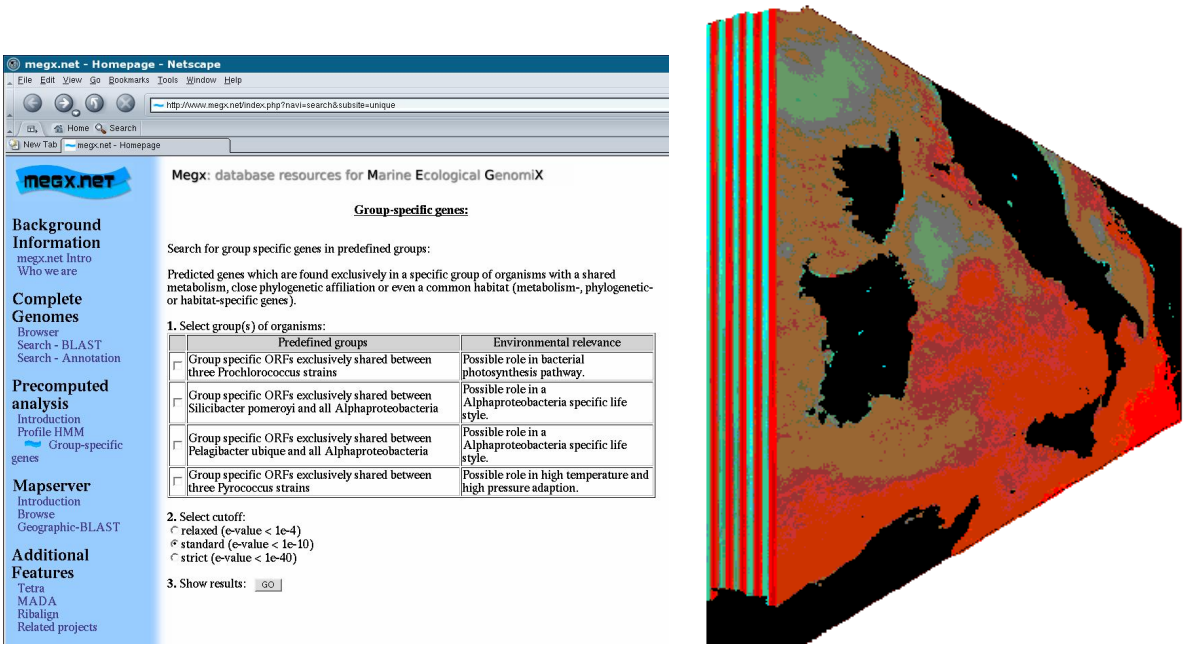

Figure 33: Scientific data services. [P. Baumann]

Scientific Data Services for IRCCM

In the course of the joint IRCCM activities, an OGC Web Map Service (WMS) has been set up which allows browser-based navigation on images of the mid-Atlantic ridge taken by an underwater robot in more than 1,000m depth. The area is geophysically interesting due to its mud volcanos. This service is the first one of a series for different data, which will be included as they become available via IRCCM; the main issue to solve concerns intellectual property rights.

6.2 Multi-Robot Exploration under Constraints of Wireless Networking

Contributed by Andreas Birk and Martijn N. Rooker

Exploration is a core issue for many robotics applications. Obviously, the usage of multi-robot systems is a very interesting option for exploration as it can lead to a significant speed-up and increased robustness. A popular basis for multi-robot exploration is the Frontier-Based Exploration algorithm introduced by Yamauchi in 1997, which was extended by himself in 1998 as well as later by Burgard et.al.in 2000 to deal with multiple robots. These extensions suffer the drawback that perfect communication between the robots is assumed. When it comes to real multi-robot systems, communication is based on wireless networks with a limited range posing a severe limit on the usefulness of the aforementioned algorithms. In this article we present a new exploration strategy that takes the range limits into account and that is therefore more suited for real application scenarios.

In the Frontier-Based Exploration algorithm, a frontier is defined as regions on the boundary between open space and unexplored space. A robot moves to the nearest frontier, which is the nearest unknown area. By moving to the frontier, the robot explores new parts of the environment. This new explored region is added to the map that is created during the exploration. In the multi-robot approach different robots are moving stochastically over to the frontier, respectively in a coordinate manner such that multiple robots will not move to the same position. When we assume a realistic communication model for a multi-robot system, there is a limit to the communication range of each robot. This is not taken into account in previous approaches where nothing prevents the robots from moving further and further away from each other.

We extend the Frontier-Based exploration such that exploration takes place while the robots maintain a distributed network structure which keeps them in contact with each other through ad-hoc networking. This *communicative exploration* algorithm is based on a utility function which weights the benefits of exploring unknown territory versus the goal of keeping communication intact. In our experiments that are partially done on CLAMV, we show that this algorithm yields results that are very close to the theoretical upper bound of coverage while constantly maintaining communication between the robots.

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6.3 Cellular & Wireless Communications (CWC)

Contributed by Harald Haas and the CWC group

Research within the Cellular and Wireless Communications (CWC) Group at Jacobs University Bremen is centred around the development of technologies, algorithms and protocols for existing and new emerging wireless systems such as WiMAX, the European IST WINNER 4G (fourth generation) system concepts, etc.. The core of the CWC group comprises of nine PhD students and four research staff all of whom primarily work on externally funded research projects. In addition and attached to the CWC group, every year on average five semester research projects within the graduate program *Communications, Systems, and Electronics (CSE)* and five guided research

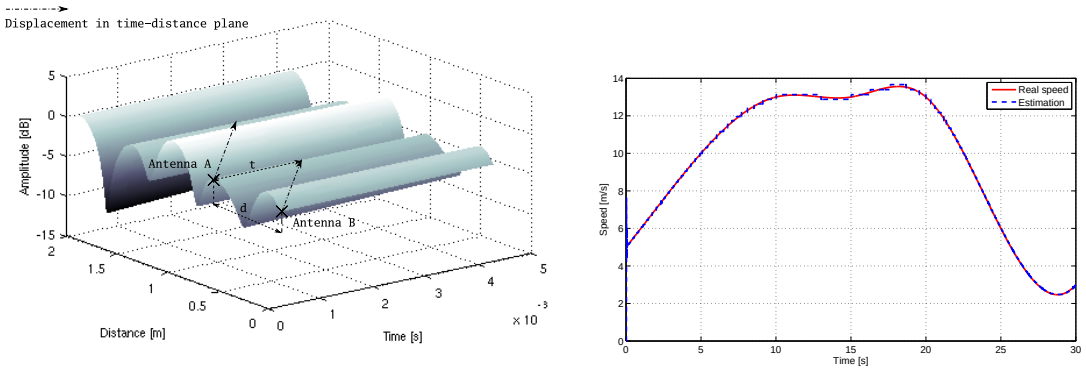

Figure 34: MPOS project within the CWC group. Left: Multipath channel in time and space simulated for a carrier frequency of 474MHz (DVB-T) and a speed of $1.5\mathrm{ms}^{-1}$. After t seconds, *antenna B* is where *antenna A* was and experiences the same channel response that *antenna A* experienced t seconds ago. As the distance, d, between the antennae is known, the speed is easily estimated as $v = d/t$. Right: Simulation of the speed estimation algorithm for an inter-antenna distance of $15\mathrm{cm}$. Results indicate that the scheme is highly accurate and effective. [H. Haas]

projects (BSc thesis) in the Electrical Engineering & Computer Science (EECS) major are conducted. The main CLAMV resource required for all these projects is MATLAB. In the following a few projects are listed.

LIST OF CONTRIBUTORS: Mostafa Afgani, Zubin Bharucha, Ellina Foutekova, Birendra Ghimire, Denis Kolyuzhnov, Raed Mesleh, Hrishikesh Venkataraman.

Indoor Mobile Positioning (MPOS)

GPS (Global Positioning System) is great for the outdoors but what about indoors? Due to the lack of a direct line of sight to GPS satellites from sheltered locations, it is impossible to obtain reliable location information using conventional GPS end-user equipment. Solutions utilising existing cellular infrastructure are able to provide approximate location fixes but the accuracy is hardly satisfactory. The goal of the MPOS project is to develop a working PDR (Pedestrian Dead Reckoning) hardware solution that will fill this gap.

PDR requires estimates of the user's speed and direction. During the first phase of the project, a speed estimation algorithm utilising RF (Radio Frequency) signature matching will be developed. The speed can be easily estimated from a knowledge of the fixed distance between two antennae and the time it takes for the trailing antenna to experience the same channel conditions (RF signature) as the leading antenna (see Fig. 34). Then, during the second and final phase, sensor fusion techniques will be applied to combine the device with an existing solution utilising inertial sensors for step length estimation – resulting in a product that is able to provide reliable and accurate location information.

Pathloss Distribution in a Circle

The general aim is to assist in the derivation of pathloss distribution in a circular scenario. Until now, pathloss computation involved uniformly distributing nodes and then running loops to calculate the distance and therefore pathlosses between them. An analytical approach to the problem eliminates the need for the additional computation. Furthermore, the effects of different parameters on the distribution of pathloss can be studied easily.

The derivation of the pdf of pathloss distribution is taken one step further by analytically deriving the probability of finding at least on star-node from a uniformly distributed group of nodes in a circular scenario. A star-node is defined as that node which is connected to n or more other nodes with pathlosses below a certain predefined threshold.

Pathloss is generally represented as some power of distance (γ) plus a random variation about this power law due to shadowing. Beyond some close-in distance d_0, the pathloss (in dB) can be written as

$$L = a + 10\gamma \log_{10}(d/d_0) + \xi;\ d \geq d_0, \tag{2}$$

where a is an intercept which is given by the free-space pathloss formula and is the decibel pathloss at distance d_0. ξ is the shadow fading variation about the linear relationship and is a zero-mean, normally distributed random variable with standard deviation σ, i.e., $\mathcal{N}\left(0, \sigma^2\right)$. For the sake of convenience, in (2), we make the substitutions $b = 10\gamma$ and $X = d/d_0$. Thus the pathloss between two points separated by Xd_0 meters is written as

$$L = a + b \log_{10}(X) + \xi. \tag{3}$$

The pdf (probability density function) of pathloss distribution in a circle of radius R is analytically found to be

$$f_L(l) \ = \ \frac{(\ln 10)}{bR^2} \exp\{C\} \times \{1 - \operatorname{erf}\{D\}\};\ \forall l, \tag{4}$$

where

$$\begin{aligned} C &= \frac{2(\ln 10)(l-a)}{b} + \frac{2\sigma^2(\ln 10)^2}{b^2} \qquad \text{and} \\ D &= \frac{l\ b - a\ b - b^2 \log_{10} R + 2\sigma^2(\ln 10)}{\sqrt{2}b\sigma}. \end{aligned}$$

This is verified through Monte Carlo simulations as shown in the left panel of Fig. 35.

UL/DL Load Balancing for OFDM Cellular Systems using Inter Cell Relaying

Among the most significant problems of time division duplex (TDD) systems is the base station (BS)-to-BS interference due to the high probability of line of sight (LOS).

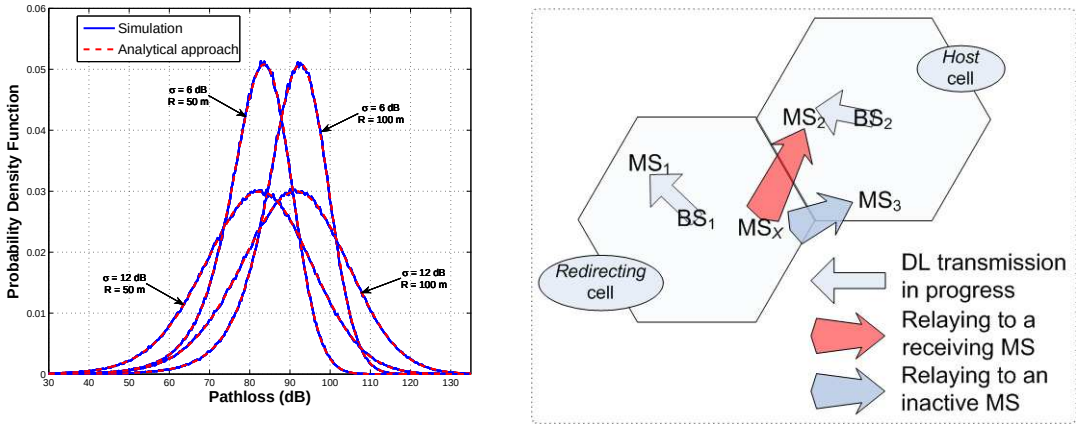

Figure 35: Projects of the CWC group. Left: Pathloss distribution in a circle. Pdfs of pathloss distribution in a circle for different values of log-normal shadowing standard deviation and varying radii. Right: UL/DL Load Balancing for OFDM Cellular Systems using Inter Cell Relaying. During a DL time slot a MS in the redirecting cell has UL traffic to transmit and is not receiving. The UL traffic can be accommodated by transmitting to a MS from a neighbouring cell (host cell). The SP:s of the cells are synchronised, thus both cells are in DL. The MS from the host cells could be either receiving or idle. [H. Haas]

The most straightforward way to resolve this problem is to synchronise the switching points (SP) of the individual cells, such that they are in uplink (UL)/downlink (DL) at the same time, thus no BS-to-BS interference occurs. This solution, however, handicaps the TDD system: its main advantage, namely to dynamically adapt to the UL/DL traffic demands of individual cells, is not utilised.

Here an idea is proposed (in the context of orthogonal frequency division multiple access (OFDM-FDMA)-TDD) to retain the properties of TDD and attend to the traffic needs of the individual cells, while avoiding BS-to-BS interference. The key feature is that free DL resources of a certain cell with high UL load (which cannot be supported by the allocated resources) are used to redirect UL traffic, and thus increase the UL capacity of the cell. In other words, during a DL time slot, a mobile station (MS), which has UL traffic to transmit and is not being served in DL can redirect the UL traffic to a near-by MS (to act as a relay station) from a neighbouring cell. The idea is illustrated in the right panel of Fig. 35. Ultimately the load in the system is balanced among the cells, which leads to more efficient bandwidth utilisation and increase in capacity.

Power Control and Link Scheduling

Investigation of the joint optimisation between power control and link scheduling for CDMA and OFDMA uplink system is the field of active research. Good link scheduling scheme should provide elimination of the interference and hence minimise transmit power. In order to find optimum solution between power control and link scheduling

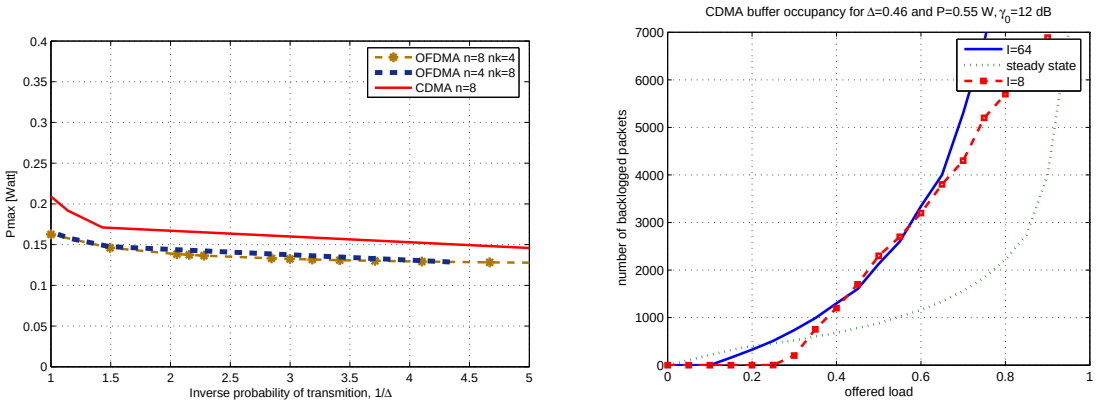

Figure 36: Power control and link scheduling project of the CWC group. Left: Pareto optimal curves for CDMA and OFDMA, obtained for the same N_c number of subcarrier per system. Right: Mean buffer occupancy for CDMA uplink. [H. Haas]

Pareto optimal curves were obtained. This is huge optimisation problem with a lot of variables. Therefore, CLAMV was used to run a number of simulations for optimisation problem simultaneously (CVX for Matlab, Figure 36).

In order to provide investigation of delay analysis for CDMA and OFDMA uplink, Markov chains simulations were carried out by the means of CLAMV (MATLAB). The states in the Markov chain describe the number of back-logged packets. The number of back-logged packets can increase, decrease and stay the same. After construction of the transaction matrix, the steady state probability vector is obtained and used for further delay analysis.

Interference Avoidance using the Busy Tone Concept

The typical data rates expected from third generation (3G) cellular networks was 144 kbps in vehicular, 384 kbps in outdoor-to-indoor and 2 Mbps in indoor and picocell environment. In fourth generation (4G) systems, typical data rates envisioned are 100Mbps for mobile and 1 Gbps for fixed wireless links. For increasing the data rates for 4G systems, the bandwidth of almost an order of magnitude larger than that of 3G system is allocated, such high data rates can be achieved only by reusing the spectrum as much as possible.

Reusing the spectrum leads to interference among the users and therefore degrades the system performance. Interference awareness is the key to ensure that such collisions are minimised. To achieve this, the channel reciprocity in time division duplex (TDD) systems is exploited to signal to the potential interferer the amount of interference it would cause to the system if it were to transmit. The medium access control (MAC) frame is divided into timeslots. For signalling back the interference, the timeslots are further divided into data mini-slot and busy tone mini slot. If the ongoing transmission in the data mini-slot meets the SINR requirements, a busy tone

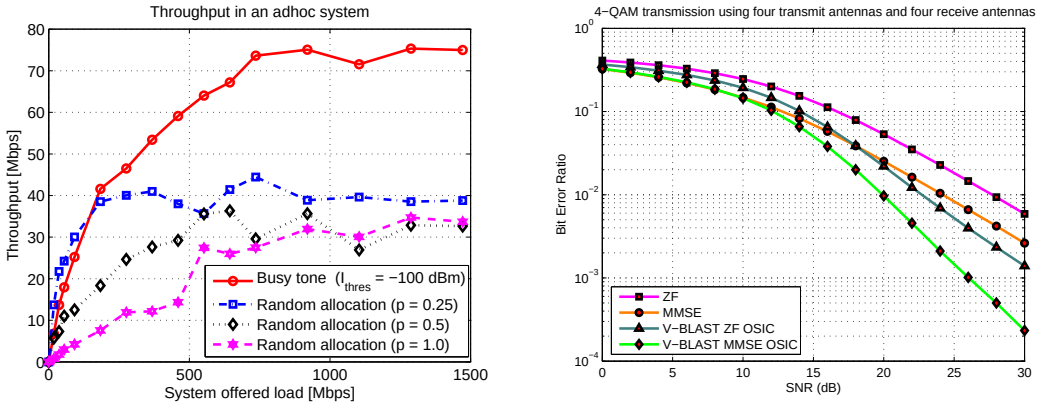

Figure 37: Projects of the CWC group. Left: Interference avoidance using the busy tone concept. Comparison of throughput in different channel allocation scheme. Right: MIMO systems. BER vs. SNR for 4-QAM spatial multiplexing transmission using four transmit and receive antennas. [H. Haas]

is transmitted by the unit receiving data in the busy tone mini-slot. This signals the transmitter (of data) that the transmission was successful. If any other unit wants to commence transmission, it must listen to the busy tone. If the signal received during the busy tone mini-slot is lower than a certain threshold, it will be allowed to proceed. Otherwise, it must refrain from transmitting as it would cause too much interference to ongoing transmissions.

A typical result from simulation of busy tone signalling mechanism for interference avoidance and channel allocation is shown in the left panel of Fig. 37. The results obtained show that busy tone signalling mechanism performs better than a p-persistent random allocation scheme taken as a benchmark system.

MIMO Systems

One of the projects CLAMV is used for is to run V-BLAST algorithm simulations with several configurations, i.e. several number of transmit and receive antennas. V-BLAST is a spatial multiplexing technique in MIMO systems. The detection of V-BLAST is considered to be highly computational due to matrix inversions in iterative ways. In the right panel of Fig. 37 a bit error ratio (BER) plot of V-BLAST algorithm is shown.

A system simulation with four transmit and four receive antennas is shown. The simulation is carried out over flat Rayleigh fading channels. At the receiver, zero forcing (ZF) and minimum mean square algorithms are implemented to detect the symbols. V-BLAST uses iterative detection based on the post SNR information of the received symbols and therefor perform better.

Performance analysis of multihop hybrid *ad hoc* cellular networks

The CLAMV machines have been used from August 2005 to January 2007 for this thesis research project. There were 2 major simulation stages for this project for which the CLAMV was used extensively.

CALCULATIONS FOR MULTIHOP AD HOC NETWORK. This part of the project considered a multihop wireless network with no central base station. A TDMA system was considered in the system design. An interference avoidance Protocol Model was considered and the multihop system was designed such that the available resources could be spatially reused. The cumulative distribution function (CDF) of the number of simultaneous communication pairs, the increase in mean and variance of the packet throughput with an increase in the number of time slots in the time frame and the average system throughput were computed through computer simulations. The multihop system were shown to provide a much higher system throughput as compared to a single-hop network.

MULTIHOP HYBRID CELLULAR NETWORKS. A multihop design is considered in a cellular network where a base station is located at the centre of every cell. The number of hops between the mobile station and the base station is varied from 2 hops to as high as 5 hops and the system performance is evaluated. A novel cluster based model for a multihop cellular network is also simulated and its performance is evaluated against other state-of-the-art methods.

6.4 Computational Fluid Dynamics in Marine Environments

Contributed by Arzhang Khalili

Over the past decade research in the fields of computational fluid dynamics connected with the field of porous medium has advanced the understanding of natural systems, namely, the marine and aquatic environment. In marine systems, there is a variety of situations where this approach has been used.

The CLAMV computing facilities have served us to account for mathematical simulation of these complex phenomena, from which two examples are shown below.

Marine aggregates and their nutrient exchange with ambient fluid

Marine aggregates (coagulated organic material from dead or decomposed plants and animals) which sink continuously from water surface of oceans and seas to the seabed, are known as a source for the vertical energy transfer in seas and oceans. The existing model in the literature [Kiørboe et al. (2001), *Mar. Ecol. Prog. Ser. 211*, 1-13] departs from a solid aggregate. However, transmission electron microscopy images have shown that marine aggregates have porous structure. Hence, modeling the flow percolating through porous aggregates plays an important role in understanding the nutrient distribution in aquatic systems.

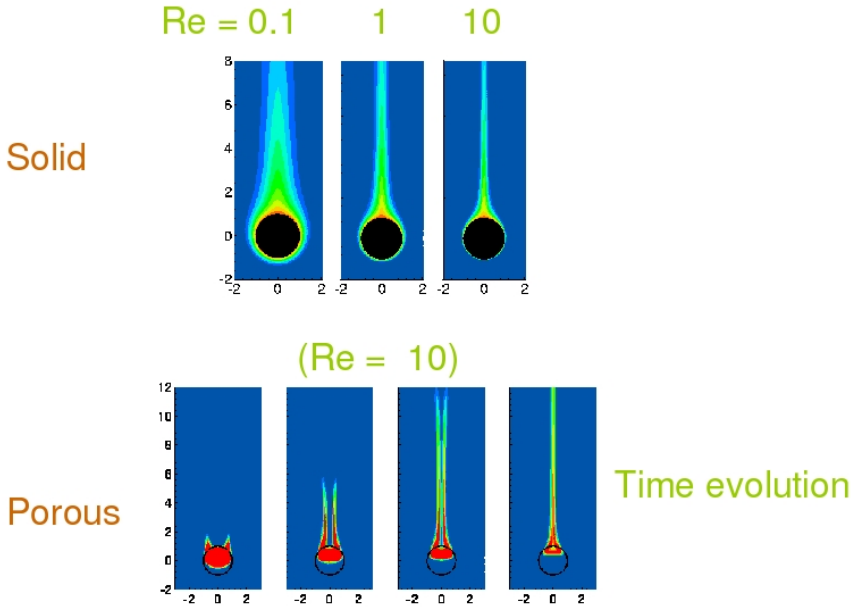

Figure 38: Comparison of fluid flow around a solid aggregate vs the same through and around a porous one. [A. Khalili]

As the comparison shows, the difference between the existing model of Kiørboe et al. (2001) and our porous model is drastic [1].

Flow instabilities in hydrothermal vent systems

A specific problem of our interest is flow instability in hydrothermal vents that are openings in the sea floor through which super"=heated water and other materials are rapidly discharged into the surrounding seawater. Submarine hydrothermal vents occur in both deep and shallow waters. In hot vents, complex hydrodynamical, chemical and sedimentological processes occur simultaneously. Through the interaction of these processes, high temperature discharges of different chemical compositions are produced in the form of plumes. Worldwide, great efforts are made to highlight important processes involved. The biogeochemistry of hydrothermal vents depends very much on the advective and convective flows as well as the interaction between porewater and seawater. In this connection, flow instabilities due to salinity and temperature disturbances play an important role in transfer of heat, mass and chemical species. Using rigorous numerical simulations, we found out mechanisms leading to buoyancy-opposed mixed convection in a sediment layer exposed to a vertical temperature as well as solute gradients, given in hydrothermal vent systems [2].

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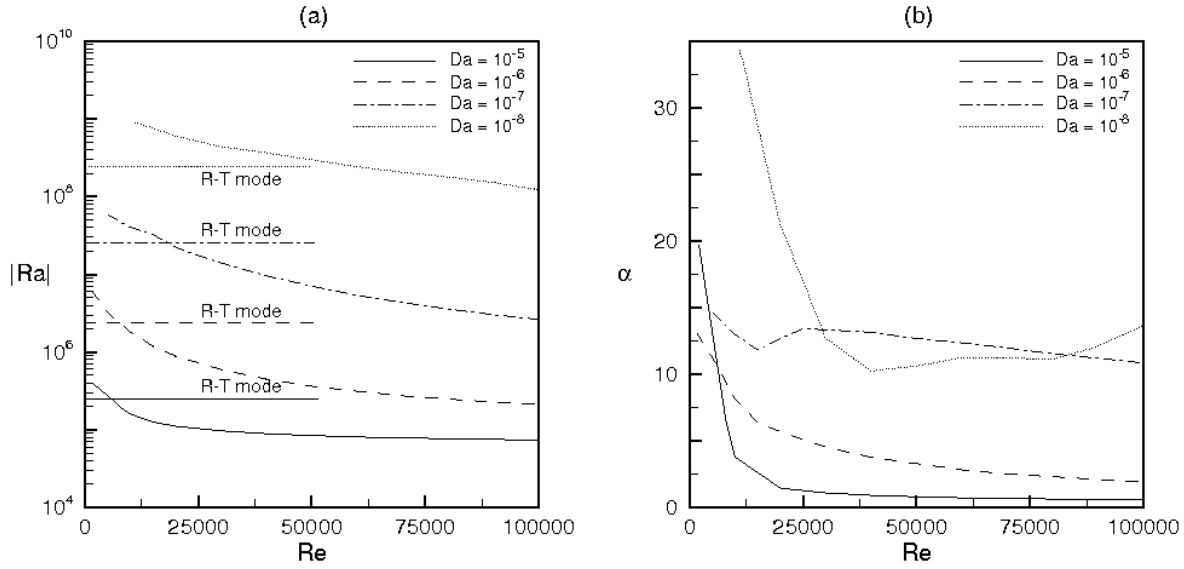

Figure 39: Dependence of the critical Rayleigh number (a) and wave number (b) on Re for different Darcy numbers at Pr = 7. [A. Khalili]

through a porous cylinder, *Chem. Eng. Sci. 61*, 4451-4461.

[2] Bera, P., and A. Khalili (2006), Influence of Prandtl number on the stability of mixed convective flow in a vertical channel filled with a porous medium, *Physics of Fluids 18*, 124103-1–124103-10.

6.5 ODE/PDE Numerics (Fluid Dynamics)

Contributed by Marcel Oliver

The project concern numerical benchmarking of a family of conservative asymptotic models for shallow water flow in the limit of fast rotation. Recent theoretical work has shown that there is a distinct member of this family for which the vorticity-streamfunction inversion is an elliptic operator of order four (where order two is typical in two-dimensional hydrodynamics). The project aims at numerically testing the conjecture that fourth order inversion leads to improved stability, both in the sense of numerical time-stepping and in the context of quantifying modeling errors for well-prepared initial data.

PUBLICATIONS

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6.6 Uncertainty Principles on Finite Abelian Groups

Contributed by Götz Pfander

Heisenberg's uncertainty principle implies that functions defined on the real line cannot be arbitrarily well localized in time and frequency simultaneously. In the case of functions defined on finite abelian groups, the uncertainty principle states that the product of the number of nonzero entries in a vector and the number of nonzero entries in its Fourier transform is not smaller than the order of the group. This result can be improved for cyclic groups of prime order: the sum of nonzero entries in a vector and the number of nonzero entries in its Fourier transform exceeds the order of the group. In a recent project we considered uncertainty principles for time-frequency representations of functions defined on finite abelian groups. Within this project, we examined all finite abelian groups of order less than or equal to 16 and determined all possible pairs composed of the number of nonzero entries in a vector and the number of nonzero entries in its Fourier transform. That is, for groups of order up to 16, we answered the following Question: For a given finite Abelian group G and integers $1 \leq m, n \leq |G|$, does there exists a vector f with m nonzero entries and whose Fourier transform $\hat{f}$ has nonzero entries.

The numerical computations are very involved and they were performed over a span of a few weeks, using multiple CLAMV CPUs. For example, the computations showing that there is no function (vector) on $\mathbb{Z}^2 \times \mathbb{Z}^2 \times \mathbb{Z}^2 \times \mathbb{Z}^2$ with six nonzero entries and whose Fourier transform has nine nonzero entries includes the calculation of the singular values of $\begin{pmatrix} 16 \\ 9 \end{pmatrix} \begin{pmatrix} 16 \\ 5 \end{pmatrix} = 49969920$ nine by nine matrices.

PUBLICATIONS

F. Krahmer, G.E. Pfander, and P. Rashkov (2007). *Uncertainty principles for timefrequency representations on finite abelian groups.* In preparation.

J. Lawrence, G.E. Pfander, and D. Walnut (2005). *Linear independence of gabor systems in finite dimensional vector spaces.* J. Fourier Anal. Appl., 11(6):715726.

6.7 Rational Points on Curves

Contributed by Michael Stoll

In 2006, I have used several thousand hours of CPU time on the CLAMV Teaching Lab machines in order to do computations in Arithmetic Geometry. The software used was MAGMA (developed by a group at the University of Sydney), on a personal licence.

The computations were done in continuation of a project undertaken in collaboration with Nils Bruin (Simon Fraser University, Vancouver); see last year's report for a description. The recent computations were done in order to obtain some statistical data on genus 2 curves of the form

$$y^2 = f_6x^6 + f_5x^5 + f_4x^4 + f_3x^3 + f_2x^2 + f_1x + f_0$$

with integral coefficients f_j, in relation to $N = \max\{[f_j|\}$. For the computations, we considered N up to 50.

The curves fall into four categories:

1. Curves with a rational point (this means that f_6 is a square — this corresponds to a rational point "at infinity" — or there are rational numbers x and y satisfying the equation);
2. Curves that fail to have a real point (solution in real numbers) or a p-adic point for some prime p (solution mod p^n for n sufficiently large);
3. Curves not in the first two sets that can be proved not to possess rational points by a so-called "2-descent";
4. The rest.

One point of interest is the proportion of curves that fall into the second set; here we found quite good agreement already for small N with the predicted value of ca. $15\,\%$. However, our main interest lies in the proportion of curves that fall into the fourth set, since these are the curves for which we need to employ more sophisticated and computationally involved methods in order to decide whether they have rational points or not. (See the paper [1] or last year's report for a description.) Our results seem to indicate that this proportion stabilizes for $N \geq 20$ at a value between 7 and $8\,\%$. This would imply that only a fairly small part of all genus 2 curves needs these more sophisticated methods. The results will be included in the paper [2] and are mentioned in [1].

[1] N. Bruin and M. Stoll, *Deciding existence of rational points on curves: an experiment*, accepted (modulo minor revisions) by Experimental Mathematics.

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7 Computing Projects in the SHSS and the JCLL

CLAMV is open to all academic units at Jacobs University Bremen. Several projects in psychology and social sciences require access to software which is provided by CLAMV. Other projects need access to large storage capacities which can be provided through the storage servers. The video studies from the JCLL are examples for projects producing large data volumes. CLAMV runs also a web server for public surveys for the JCLL. Originally the server was used for a survey about the birdflu disease. For the EU-funded workshop Mathematical and Computational Models of Attention, Decision and Action an integrated environment of mathematical and statistical software was needed which could be easily offered with the CLAMV Teaching Lab. An increasing number of requests by SHSS and JCLL for access to the Teaching Lab is expected for the future because the newly opened Windows Teaching Lab makes it possible to fulfill requirements from Windows trained users.

7.1 Modeling Projects in Psychology

Contributed by Adele Diederich

Stochastic models to account for phenomenon in human behavior: Modeling the effects of payoff on response bias in a perceptual discrimination task

Sequential sampling models seek to account for both response time and accuracy data. They assume that the stimuli (or choice alternatives) can be mapped onto a hypothetical numerical dimension representing the instantaneous level of activation, evidence, or preference. Further, they assume some random fluctuation of this value over time in the course of information accumulation. Therefore, sequential sampling can be described as a stochastic process. In particular, diffusion processes (e.g., Wiener process, Ornstein–Uhlenbeck process) with two absorbing boundaries are powerful approaches to model human information processes in a variety of psychological tasks. Two quantities are of foremost interest: (1) the probability that the process eventually reaches one or the other boundary for the first time (the criterion to initiate a response), the *first passage probability*; (2) the time it takes for the process to reach one of the boundaries for the first time, the *first passage time*. The former quantity is related to the observed relative frequencies, the latter usually to the observed mean choice response times.

Three hypotheses, hereafter labeled *bound–change hypothesis*, *drift-rate-change hypothesis* and *two-stage-processing hypothesis* are proposed to account for data from a perceptual discrimination task in which three different response deadlines were involved and three different payoffs were presented prior to each individual trial. The research shows how the three different hypotheses incorporate response biases into a sequential sampling decision process; how payoffs and deadlines affect choice probabilities; and the hypotheses' predictions of choice times and choice probabilities. The

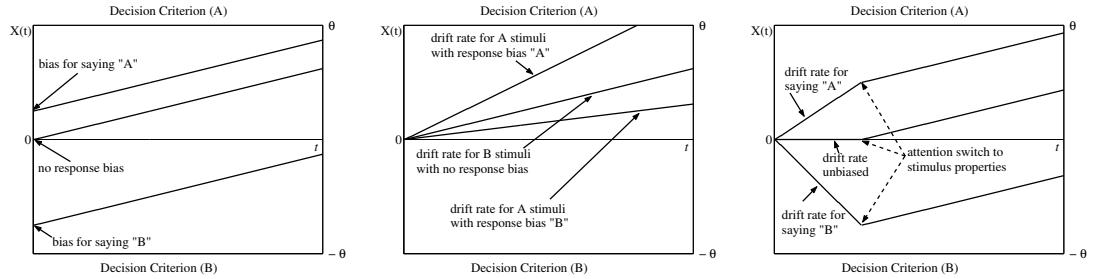

Figure 40: Left: *Bound–change hypothesis*. The payoff matrix induces an a priori bias. The slope of the mean drift rate is the same regardless of the payoffs. Center: *Drift–rate–change hypothesis*. The response bias is mapped onto the mean drift rate. The slope indicates the respect bias. Right: *Two–stage–processing hypothesis*. The entire process consists of two subprocesses, the first one processing the payoffs, the second the stimulus properties. The process is non–time–homogeneous. [A. Diederich]

basic process is a Wiener process with two absorbing boundaries; the specific hypotheses are demonstrates in Figure 40. The boundaries refer to choice criteria for alternatives A and B, respectively.

The quantitative predictions of the diffusion processes are calculated using Markov chain approximation (utilizing the sparse matrix function of MATLAB). Models are fitted to data by using optimisation procedures such as the OPTMUM toolbox of MATLAB.

Results. The two–stage–processing hypothesis gave the best account, especially for the choice probabilities whereas the drift–rate–change hypothesis had problems predicting choice probabilities as a function of deadlines.

Modeling spatial effects in visual-tactile saccadic reaction time

Saccadic reaction time (SRT) to visual targets tends to be faster when non-visual stimuli are presented in close temporal or spatial proximity even when subjects are instructed to ignore the accessory input. The present study investigated visual-tactile interaction effects on SRT using a focused attention paradigm. Saccadic responses to bimodal stimuli were reduced by up to 30 ms compared to responses to unimodal visual targets. In contrast to previous findings with visual-auditory stimulation, the amount of multisensory facilitation was not decreasing with the physical distance between target and non-target but depended on (i) whether both stimuli were presented ipsi- or contralateral, (ii) the eccentricity of the stimuli, and (iii) the frequency of the vibrotactile non-target. A recent time-window-of-integration (TWIN) model (Colonius & Diederich, 2004) allowing to separate effects of peripheral processing differences from multisensory interaction effects is presented and tested on the data.

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bias in a perceptual discrimination task: Threshold-bound, drift-rate-change, or two-stage-processing hypothesis, Perception & Psychophysics.

Akerfelt, A. Colonius, H. & Diederich, A. (2005). *Visual-tactile saccadic inhibition*, Experimental Brain Research.

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Colonius, H., Diederich, A., (2004), *The time-window-of-integration model: Visual-tactile interaction in saccade generation*, Journal of Cognitive Neuroscience.

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DFG, DI 506/8-1 (from July 2005), *Experimentelle und theoretische Untersuchung räumlicher und zeitlicher Regeln der multisensorischen Integration*.

DFG, DI 506/8-1 (until June 2005), *Experimentelle und theoretische Untersuchung räumlicher und zeitlicher Regeln der multisensorischen Integration*.

DFG, International Graduate School for Neurosensory Science and Systems.[9].

7.2 Models of Human Performance

Contributed by Ben Godde and Claudia Voelcker-Rehage

Our research at the Jacobs Center for Lifelong Learning focus on identifying mechanisms underlying cortical plasticity and the structure-function relationships between cognitive, sensory, and motor performance and learning. The human brain remains plastic even at high age. However, plastic capacity declines with age. In this context the ability to facilitate plasticity is of high significance for the elder learner. We have developed three complimentary, yet distinct, lines of research:

First, within the sensory domain we are interested in the plastic-adaptive competencies related to tactile processing of younger and older adults. Using functional MRI we investigated the cortical topography of tactile perception [1]. In another study we could show how tactile perceptual learning can be facilitated or rather gated by transcranial magnetic stimulation revealing new insights into the cortical mechanisms of perceptual learning [2].

Second, physical fitness is assumed to not only preserve cognitive functioning but also learning abilities in the elderly. Following an interdisciplinary view on human performance that compromises motor, neurophysiological, and psychological expertise and methods, during the last year we have designed a longitudinal study to investigate the influence of aerobic and acrobatic exercise on cognitive performance and

[9] http://www.physik.uni-oldenburg.de/Docs/medi/projects/eurogk/index.html

well-being across the lifespan. In pilot experiments we began to develop a training program and to collect cross-sectional data regarding the influence of physical activity in older adults (65 years and older) on well-being and cognition. We also investigated the correlation between motor and cognitive performance in kindergarten children [3].

In a third line of research we examined age-related differences in force control, practice effect on force modulation [4], and age-related differences in dual-task performance [5]. Force control of the upper extremities is an elementary component of movement production of many daily activities and its assessment provides insight into movement control and coordination. Further, using electroencephalography, we investigated which cortical networks are involved in performing learned motor tasks and how motor abilities learned with one hand can be transferred to the opposite hand [6]. In a recent study we now test the sensory-motor coupling and determine if tactile stimulation/practice influences fine motor performance.

For data analysis and the generation and control of experimental stimuli we use the software packages Matlab and IDL as provided by CLAMV. Moreover, for our research the computing facilities of CLAMV are of particular importance for computation with large data sets as obtained during brain imaging.

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[6] Lange R.K., Braun C., Godde B. (2006), *EEG-correlates of intermanual transfer from the nondominant left towards the right Hand*, Exp Brain Res, 168(4): 547-556.

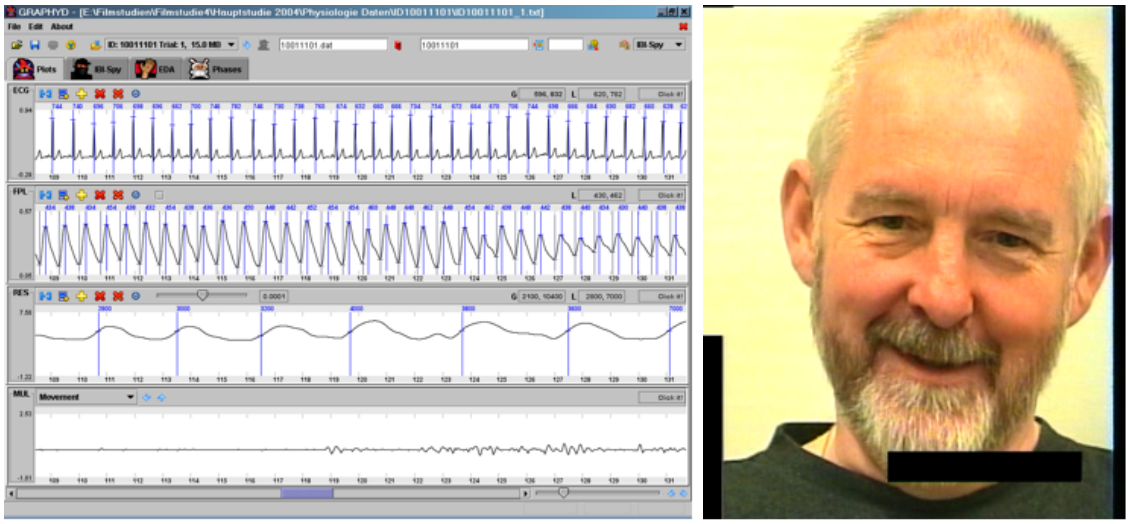

Figure 41: Adult development of socioemotional competencies. Left: Example of one step in the processing of the autonomous activity data conducted in our experiments. Right: The storage capacities of CLAMV enable us to conduct video recordings of facial expressions in very good quality. [U. Kunzmann]

7.3 Adult Development of Socioemotional Competencies

Contributed by Ute Kunzmann

Our research group is interested in adult development and aging. Our research approach is characterized by an emphasis on individual and contextual variations in developmental processes and outcomes. Our projects examine four realms of psychological functioning: emotional competence (emotional reactivity, regulation, and understanding), knowledge about the meaning and conduct of life (wisdom-related knowledge), social behavior (empathic concern and accuracy), and subjective well-being (the frequent experience of positive affect and the absence of negative affect over time). The purpose of our research is to describe and understand age-related gains and losses in each of these four realms of functioning. We are also interested in the ways in which cognitive, emotional, and social competencies interact and together facilitate or hinder personal growth and happiness. Our present experimental work is focused on age differences in emotional reactivity, regulation, and understanding. We study these facets of emotional competence by examining emotional reactions activated by video based stimulus material on three different levels: self-reported subjective feelings, observed facial expressions, and autonomous activity.

The storage facilities of CLAMV are of major importance for dealing with the huge amounts of data generated through the recording of the autonomous activity of the participants. An example of one step in the processing of the autonomous activity data is shown in the left panel of Fig. 41. Big storage capacities are also needed for the recording of facial expressions shown by the participants during our experiments. The right panel of Fig. 41 shows the very good quality of the video recordings of the

facial expressions enabled through the storage capacities of CLAMV.

7.4 The Interaction of Reflexive and Volitional Attention

Contributed by Bettina Olk

Attention research distinguishes between reflexive and volitional orienting. Orienting towards sources of information is a key prerequisite for an efficient interaction with our stimulus-rich environment. The function of reflexive orienting is to guide attention quickly to areas of interest as they might constitute sources of reward or threat. Importantly, however, the allocation of attention is not only subject to reflexes. Top-down factors and purposeful processing require the inhibition of reflexes and directing of attention to a stimulus in a volitional fashion.

A current project investigates the interaction between reflexive and volitional attention by systematically varying the degree to which each type of processing is required for a given task. We are using MATLAB for the presentation of the displays and for data recording. Young and elderly healthy persons as well as persons who have suffered a stroke are taking part in the study. The studies allow us to characterize the normal integration between attentional processes as well as the impact of brain injuries.

SELECTED RELEVANT PUBLICATIONS

Olk, B. and Harvey, M. (2006), *Characterizing exploration behavior in spatial neglect: Omissions and repetitive search*, Brain Research, 1118, 106-115.

Shimozaki, S. S., Kingstone, A., Olk, B., Stowe, R., & Eckstein, M. P. (2006), *Classification images of two right hemisphere patients: A window into the attentional mechanisms of spatial neglect*, Brain Research, special issue on Attention and Awareness, guest editor, Barry Giesbrecht, 1080, 26-52.

Olk, B., Chang, E., Kingstone, A. and Ro, T. (2006), *Modulation of Antisaccades by Transcranial Magnetic Stimulation of the Human Frontal Eye Field*, Cerebral Cortex, 16, 76-82.

Olk B. and Kingstone A. (2005), *Ausprägung und zeitlicher Verlauf des "disengage deficits" bei Patienten mit rechtshemisphärischen Läsionen*, Zeitschrift für Neuropsychologie 16 (Suppl.), 20-21.

Olk B., Wee J., and Kingstone A. (2004), *The effect of hemispatial neglect on the perception of centre*, Brain and Cognition,55, 365-367.

Hunt A., Olk B., von Mühlenen A., and Kingstone A. (2004), *Integration of competing saccade programs*, Cognitive Brain Research, 19, 206-208.

Olk B. and Kingstone A. (2003), *Why are antisaccades slower than prosaccades? A novel finding using a new paradigm*, NeuroReport, 14, 151-155.

Olk B., Cameron B. and Kingstone A.F. (2003), *Measuring components of volitional and reflexive spatial attention*, Abstracts of the Psychonomic Society, 8, 1073.

Olk B. and Harvey M. (2002), *Effects of visible and invisible cueing on line*, 282-290.

GRANTS

Integration of reflexive and volitional orienting: Comparing visual attention and eye movement control. Funded by the German Academic Exchange Service (DAAD), 2006-2007.

Integration of reflexive and volitional orienting: Comparing motor systems. Funded by The Royal Society, 2006-2008.

7.5 Risk Perception, Bird Flu, and Social Curiosity

Contributed by Britta Renner

Unrealistic Risk Perceptions

The goal of our ongoing experimental research program on risk perception is to develop more effective risk communication which allows recipients to make informed decisions. For optimizing health promotion efforts, it is especially important to understand how individuals construe the risk of a certain health threat. Usually, health campaigns for risk reductions only list risk factors impersonally, or show high-risk persons. Our research group examines from a social psychological perspective how risk stereotypes influence risk perceptions, in particular unrealistic optimistic risk perceptions for the self. Previous studies have focused on downward comparison, involving the image of a "high risk stereotype" as comparison target that permits the person to feel better about his or her risk (Weinstein, 2003).

Extending previous research, our research examines not only what people consider as risky (high risk stereotype) but also what they consider as safe (low risk stereotype). This approach allows testing the hypothesis that it is the ratio of the low risk stereotype, the self, and the high risk stereotype which determines risk perception (Renner & Schwarzer, 2003; Renner & Schupp, 2005). In experimental studies participants' behavioral profile and stereotypical beliefs are assessed and used as basis for online feedback as well as for the generation of adaptive risk behavioral profiles in the context of HIV. This has been realized through a web-based adaptive assessment tool box based on a SQL-database located at the CLAMV.

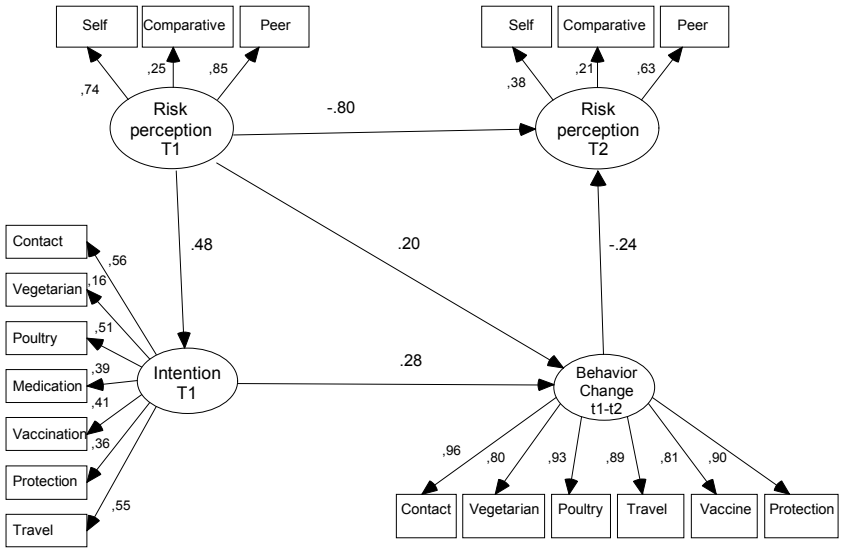

Figure 42: Risk perception and behaviour change in the context of H5N1. [B. Renner]

Do you CARE about the bird flu? An online survey on risk perception of avian influenza in Germany

In spring 2006, the first cases of avian influenza occurred in Germany. The CARE study examined the relation between preventive behavior change and accuracy of risk perceptions related to the H5N1 avian influenza. Participants in a longitudinal web-based survey were asked to report in their behavioral responses and their perceived risk for contacting H5N1 and other related diseases. Cross-sectional analyses at both measurement points showed that participants who demonstrated a low level of preventive behavior felt more at risk than those reporting comparably higher levels of preventive behaviour, indicating relative accuracy. These results suggest that people realize when their behaviour is risky. More importantly, risk estimates also showed adaptive accuracy from a change perspective. In particular, an increase in preventive behavior from T1 to T2 was significantly associated with a decrease in perceived risk between T1 and T2. See figure 42.

The use of CLAMV resources allows us to start new waves of data collection within a short period of time, and to reach many participants quickly and efficiently.

Social Curiosity and Interpersonal Perception

Curiosity has been conceptualized as a desire for new information and knowledge. Given the importance of curiosity for learning and development, personality theorists developed various measures to assess individual differences in curiosity. Most current measures for trait curiosity explore the desire to gain knowledge or sensory experience. However, to function efficiently in a changing and complex social environment humans require information about those around them. Social curiosity has been de-

fined as the interest in the thinking, feelings and actions of other people (Renner, 2006). We developed and tested a measure for assessing interindividual differences in social curiosity. Through the facilities of CLAMV we were able to conduct online-surveys with high geographical coverage and over 400 participants.

In a second line of research we are interested in the behavioral impact of social curiosity. In particular, we are interested in how social curiosity influences the process and the accuracy of personality judgements and social interactions. We will apply different methods for assessing the accuracy of personality judgements (self-other-agreement, other-other-agreement and behavioral observations). Of particular crucial importance for this study are social interactions between two unacquainted persons which are videotaped. These videotaped interactions will be presented to independent judges who will evaluate the target personality and behavior during the interaction. For this research the facilities of CLAMV are indispensable for storing and editing this large video data set.

PUBLICATIONS

Renner, B. & Hartung, F.-M. (2007). *Soziale Neugier und Gossip: Zusammenhänge und Funktionen [Social curiosity and gossip: Correlations and functions.].* Paper to be presented at 9th Conference of the German Personality Psychology and Psychological Assessment Chapter in the DGPs, Vienna, Austria.

Hartung, F.-M. & Renner, B. (2007). *Neugierig oder nicht? Selbst- und Fremdeinschätzung von Neugier [Curious or not? Self- and other-ratings of curiosity.].* Paper to be presented at 9th Conference of the German Personality Psychology and Psychological Assessment Chapter in the DGPs, Vienna, Austria.

Oeberst, A. & Renner, B. (in press). *Stereotypes as warrants of apprehension in HIV-risk perception?* Psychology & Health Supplement.

Renner, B., Panzer, M., Oeberst, A. & Hartung, F.-M. (in press). *Risk Perceptions and Behaviour Change related to H5N1 Avian Influenza.* Psychology & Health Supplement.

Renner, B. (2006). *Curiosity about people: The development of a social curiosity measure in adults.* Journal of Personality Assessment, 87, 305316.

Oeberst, A. & Renner, B. (2006). *Die Alltags-Arithmetik des Risikos: Wie Stereotype die Risikowahrnehmung beeinflussen [Everyday-arithmetics of risk: How stereotypes influence risk perception.].* Poster presented at the 45th conference of the DGPs, Nrnberg, Germany, Sept. 17th to 21st.

8 Teaching

The CLAMV is primarily designed as a computational laboratory for graduate and faculty research but its resources are also used for undergraduate teaching and research. Course work and student projects take place in the CLAMV Computer Teaching Lab (CTL) in basement in West Hall, and in the GIS Lab in Research III.

The CLAMV CTL hosts graduate as well as advanced undergraduate courses to provide hands-on instruction on how to use a broad spectrum of computational tools. Furthermore, the computers are heavily used for computing jobs during times when there is no teaching, e.g., for guided research projects, and also student projects at the graduate and PhD level. The computer workplaces of the CLAMV CTL were initially located in four separate rooms in the building Research I. In August 2005, the CLAMV CTL moved to the basement of West Hall. In February 2007, after more than four years of intensive use, the computers were replaced by a total number of 50 new dual-processors machines. Courses that made use of the CLAMV CTL are listed in tables 1 (spring semester) and 2 (fall semester).

The GIS Lab in the building Research III became fully operational in 2005. The set-up is described in section 2. Mainly financed through contributions from industry, the GIS Lab serves as an example for how CLAMV can help to integrate third-party funded facilities into the IUB infrastructure. The use of the GIS Lab for teaching and student projects is explained below in section 8.3.

8.1 Undergraduate Programs

The CLAMV CTL facility (i.e., the teaching lab Linux PCs as well as the network and file server for license management and file storage) served computational courses and natural science lab units in Mathematics, Computational Science, Computer Science, Electrical Engineering, Computational Physics, Bioinformatics and Computational Biology, Computational Chemistry and Biochemistry, and Geosciences and Astrophysics. Examples of special uses of the CLAMV as a teaching facility are given below.

Furthermore, a number of undergraduate guided research projects relied on CLAMV resources, including access to multiple machines for extended compute jobs, software, and terminal access in the teaching lab. These projects addressed scientific problems of rather different nature, e.g., image interpretation and feature extraction, time series analysis, and numerical modeling.

Database and Web Applications

Contributed by Peter Baumann

In this course 3rd-year undergraduate students are introduced to database and Web/Internet technology. In the integrated project work students have to implement

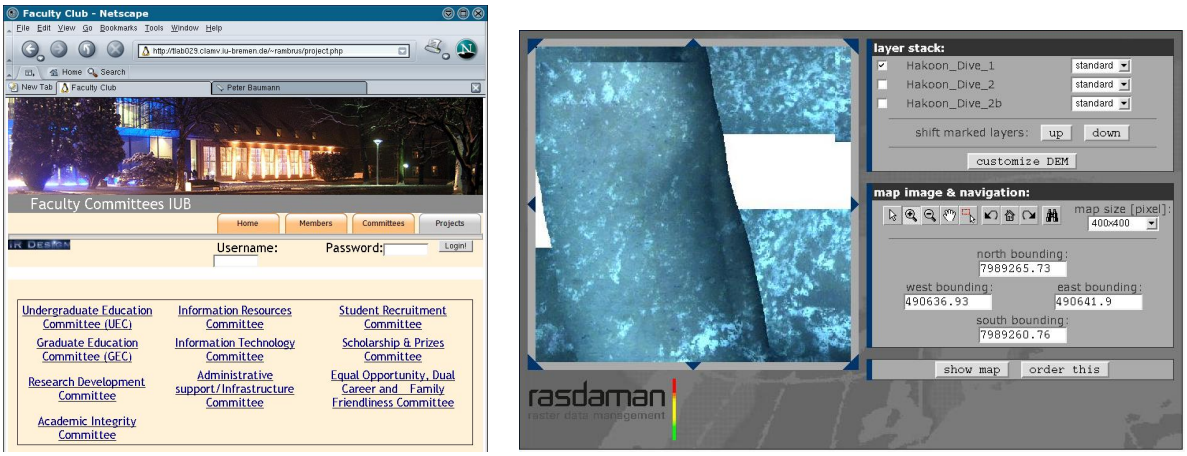

Figure 43: Screenshots obtained in the courses on *Database and Web Applications* and *Semantic Web Engineering*. [P. Baumann]

the core part of a Web service based on LAMP (Linux, Apache, MySQL, PHP). Implementation is done on CLAMV machines to ensure a well-working, homogeneous environment. Students can choose their individual topic and form teams to specify and implement the service. Among the services implemented in Fall 2005 were Web presences of CODATA Germany, the IUB Faculty Committee, and IUB Student Government. As can be seen – and students actually are encouraged to do so – topics are drawn from practical needs, and several services go into operational use after the semester has ended.

International Collegiate Programming Contest (ICPC)

Contributed by Stefano Carpin

Since 1977, the Association for Computer Machinery (ACM), the world's first educational and scientific computing society, organizes the annual International Collegiate Programming Contest (ICPC) to foster the creativity and the capabilities of young students to develop challenging software under pressure. The competition is limited to undergraduate students or graduate students with no more than one year of graduate studies. Participants are allowed to form groups of up to three persons. Thanks to the commitment of IBM, which got involved in 1997, the competition became very popular. In 2003, about 23000 students from 1329 universities from 68 countries participated to the different stages. One of the reasons of the fast growth is that students can participate to the qualification stage from everywhere, provided an Internet connection and a workstation are available.

The contest is structured as follows. The organizers post a set of problems on a web site and an evaluation server is started. Participants have to solve problems and submit the source code to the evaluation server, which will compile and run the program over a set of undisclosed test cases. Only when the program correctly answers all the

Figure 44: CLAMV on the move: The IUB team on the way to the International Collegiate Programming Contest in Lund, Sweden. [Stefano Carpin]

test cases the problem is considered solved and the team is given credit. Typically, a contest runs for 5 hours in which 8 problems have to be solved.

On September 27, 2003, the local IUB contest was held in the CLAMV teaching lab, in order to select the best two teams for the regional competition. Although the competition took place on a Saturday evening starting at 19.00, about 20 students participated. The contest was won by Mathias Goerner, Michael Thon, and Andreas Pfeil. As the second place resulted in a draw, CLAMV hosted a second local contest the following Saturday. This second contest was won by the students Vlad Vicol, Dan Popovici and Ioan Sucan. The two winning teams, together with their coach, Dr. Stefano Carpin, went to the Northern Europe regional competition, which took place at the Lund Institute of Technology, Sweden, on November 23, 2003. The IUB teams ranked on positions 16 and 26 out of more than 50 teams.

The BICB experience

Contributed by Frank-Oliver Glöckner

In the emerging field of Bioinformatics and Computational Biology (BICB) lab courses in CLAMV are essential for practical ”hands on” education of the students. In each semester the students assemble in the CLAMV lab two times a week to get basic skills in programming, molecule modelling and sequence analysis. The BICB lab courses are taught by Martin Zacharias and Frank Oliver Glckner, Professors for Computational Biology and Bioinformatics, respectively. In 2004 a genome server has been integrated in the CLAMV system to support enhanced sequence- and genome analysis and phylogenetic reconstructions. The new server is equipped with two Xeon 2.8 GHz

processors and 4 GB of main memory and is running with SuSE-Linux Professional as operating system. Specific command line software tools like BLAST, signal peptide, transmembrane helices and transfer RNA prediction are installed for batch processing of DNA and protein sequences. Furthermore the two software suites GenDB and ARB are available. GenDB[10] is an open source software system for genome annotation developed by the University Bielefeld. It is able to run all kinds of similarity and pattern based tools for assigning potential functions to predicted genes. All data are stored in the relational database system MySQL for data mining and graphical visualisation. Search and retrieval of specific data can be done via an API (applications programmer interface). For the students CLAMV is a perfect environment to get the principles to process large amounts of sequence data as well as to store and retrieve them.

The second software suite now available is ARB. ARB[11] (latin: arbor, tree) is a comprehensive software package for phylogeny which had primarily been developed for ribosomal RNA (rRNA) data, but can be used for any kind of sequence data. The rational behind the program design was to arrange a database of sequences and any other additional information according to the phylogenetic relationships of the corresponding organisms. This phylogenetic tree can be visualized on the screen and be used for walking through the database by mouse click. ARB integrates all kinds of distance matrix, parsimony and maximum likelihood based phylogenetic reconstruction programs under a common graphical user interface (GUI). Access to the data via a database management system as well as an enhanced sequence editor and probe design functions are also implemented. The students are able to import their own sequences, align them and reconstruct phylogenetic trees with different methods. ARB is a good model to illustrate students how large software systems are created, maintained and improved by the scientific community over years.

Semi-Automatic Picture Retrieval

Contributed by Peter Ludes

In the spring semester 2004 Prof. Peter Ludes (IUB/SHSS) and Prof. Otthein Herzog (Universitt Bremen/Technologiezentrum Informatik TZI) gave a USC *Olympic Key Visuals and Semi-automatic Picture Retrieval*. Methods from Mass Media Communication were combined with the latest technological development in semi-automatic image retrieval such as the Video Content Manger VCM or the PictureFinder, both developed at the TZI. To give the students the opportunity to work with those tools a server version of the VCM was installed within the CLAMV surrounding. The VCM required an installation of MySQL-Server 4, Java J2SDK 1.4, Apache Jakarta Tomcat 4/5, Apache Webserver with PHP-support, Postnuke Phoenix 0.726 which is provided by the CLAMV. This environment enabled the students to upload any mpg1 video to the server, where it was automatically analyzed for shot boundaries. The extracted Key Frames allowed new methods of comparison.

This server has also been used by members of our research project on key visuals,

[10] www.cebitec.uni-bielefeld.de/groups/brf/software/
[11] www.arb-home.de

which cooperates with universities in Brazil, China, Germany and the USA and was honored by the Ernst A.C. Lange prize for innovative cooperation between universities in Bremen. The upcoming detailed analysis of annual TV reviews from four countries needs a reliable server environment, provided by the CLAMV.

Psychology Lab Course II

Contributed by Bettina Olk

Lab course II is taught each fall as part of the psychology program. The course is also open to students pursuing other majors than psychology. In this course students design, carry out and analyze psychology experiments in small groups. In fall 2004 the carried out experiments dealt with a range of different topics and for each study MATLAB was used to present the stimuli and record the responses of the participants.

Computational Partial Differential Equations

Contributed by Peter Oswald

The lecture “Computational Partial Differential Equations”, taught by Prof. P. Oswald (AWI) in spring 2005, was attended by 12 undergraduate and graduate students from various majors (Computational Science, Mathematics, Physics). The course covered finite difference and finite element methods for partial differential equations, with emphasis on stationary linear elliptic problems in the larger part of the semester. The lectures offered a mix of theoretical (construction principles, solvability, stability and error estimates) and practical information (matrix assembly, quadrature rules, matrix structure, linear solvers) on these numerical schemes.

Besides homework and standard programming assignments, the course also required project work in groups of 2-3 students towards the end of the semester (weeks 8-13). The topic ”Adaptive multiscale finite element solution of elliptic boundary value problems” extended the material covered in the lectures. The students were challenged to study some (mostly publicly available) software packages and research codes, and apply them to model linear and semi-linear elliptic problems, including the Poisson-Boltzmann equation, with solution singularities. Supported by A. Gelessus, currently available versions of PLTMG (R. Bank, UCSD), MClite (M. Holst, Caltech/UCSD), ALBERT (A. Schmidt et al., Uni Bremen), as well as trial versions of DiffPack resp. FemLab were installed on the CLAMV server, and made accessible to the student groups. Due to time constraints, the actual use was restricted to PLTMG and MClite for which tutorial sessions in the CLAMV Teaching Lab were offered, programming interface, I/O formats, coarse mesh generation, and scope of the packages were explained. The students experimented with various parameters influencing grid refinement and solution quality, and presented their findings in a Lab session complemented by a written report.

Figure 45: USC Mathematics and Democracy on May 25, 2003: Members of the coverage group studying the latest projection of the Bremen state elections in the CLAMV teaching lab. [D. Schleicher]

USC Mathematics & Democracy

Contributed by Dierk Schleicher and Johannes Rückert

University Studies Courses (USCs) are jointly taught by at least two professors from different fields with the aim of demonstrating how methods from the one field can be used to solve problems in the other. Student involvement in these IUB-typical courses is usually very high.

The USC *Mathematics & Democracy* was taught in Spring 2003 by Max Kaase, Professor of Political Science and Dean of the School of Humanities and Social Sciences, and Dierk Schleicher, Professor of Mathematics. The course consisted of two parts. In the first, theoretical part, students analyzed different election models from sociological and mathematical points of view, and examined their influence on the power structures of political entities.

The second, practical part, was centered around the election to the Bremen state parliament on May 25, 2003. Before the election, students conducted a professional telephone poll of the voters' intentions. On election day, students went out to observe the polling process and gathered data to predict the outcome. For some students from countries with emerging or non-existent democracies this was a unique and defining experience.

About 50 IUB students were active that Sunday. When the ballot boxes closed at 18:00 hours, 40 students—augmented by volunteers from faculty and staff—were present at 66 voting precincts, statistically selected from a total of about 500. Election staff had been informed about their visitors in cooperation with the *Statistisches Landesamt*

Courses	**Year(s)**	**Instructors**
Advanced Bioinformatics	2004–2007	M. Zacharias, F.O. Glöckner
Graphics and Visualization	2004–2007	H. Kenn, L. Linsen
NatSciLab Computer Science	2003	S. Carpin
NatSciLab GeoAstro	2003	M. Brüggen, J. Vogt
NatSciLab Symbolic Software	2003–2007	P. Bangert, M. Comerford, G. Pfander
Numerical Methods II	2005–2006	P. Oswald
Computational PDE	2005–2006	P. Oswald
Computational Neuroscience	2005–2007	C. Hilgetag
Computational Fluid Dynamics	2004–2007	A. Khalili
Database and Web Applications	2005–2007	P. Baumann
Experimental and Theoretical Physics B II	2007	U. Kleinekathöfer
Open lab sessions	2003–2006	CLAMV personnel

Table 1: Spring semester courses that made use of the CLAMV CTL facility.

Bremen. Here the students had the opportunity to watch volunteers count the ballots.

Back at IUB, the coverage group was holed up in the CLAMV teaching lab. The IRC had installed several telephones for receiving incoming poll data, which was immediately entered into the browser-based election software. Every two minutes, the software collected newly arrived data over the CLAMV network and recalculated the predicted seat allocation. The results were automatically displayed as pie-charts on the site `www.wahl.iu-bremen.de` All programs, including two mathematical prediction models, were developed by students of the USC under the supervision of Dierk Schleicher and Johannes Rückert.

The project was a tremendous success: in contrast to the official projections of the major German television stations ARD and ZDF, the IUB project used data from only half as many precincts (66 compared to 150) and was conducted entirely by students with no previous experience in election projection. Still, the IUB projection was accurate within a variation of just one seat compared to the official end result. The web site received about 800 hits on election night alone and several newspaper articles have appeared covering the project.

The project would not have been possible without access to the CLAMV: A networked set of workstations and a web server was essential for the simultaneous entering and processing of the incoming data. While this project was certainly unusual for the CLAMV, it added to the diverse and transdisciplinary education at IUB, and was a defining experience for many students.

Courses	Year(s)	Instructors
Computational Logic Lab	2004	M. Kohlhase
Database and Web Applications II	2005, 2006	P. Baumann
GeoAstro Lab, Field and Data Analysis Project II	2002–2006	J. Vogt, S. Rosswog
NatSciLab GeoAstro	2003–2006	M. Brüggen
Advanced Bioinformatics I	2004–2006	M. Zacharias
Computational Chemistry and Biochemistry	2004–2006	D. Roccatano, F. Müller-Plathe
Computational Physics	2004–2006	M. Rohlfing
Numerical Methods I	2004–2006	M. Oliver, P. Oswald
General Mathematics and Computational Science I	2004–2006	M. Oliver
NatSciLab Numerical Software	2003–2006	P. Oswald, P. Bangert
Scientific Computing	2004	W. Hiller
Time series analysis	2004	J. Freund
Principles of Modeling Dynamics in Biology	2006	M.-T. Hütt
Open lab sessions	2002–2006	CLAMV personnel

Table 2: Fall semester courses that made use of the CLAMV CTL facility.

8.2 Graduate Programs

A growing number of graduate students at IUB take advantage of the hardware and software environment provided by the CLAMV. Many of the student research projects are implicitly covered in the contributions to sections 4, 5, 6, and 7. The following example shows how the CLAMV CTL can be used for graduate courses.

Semantic Web Engineering

Contributed by Peter Baumann

Goal of this graduate course is to make students familiar with the state of the art in Web-enabled information systems, with particular emphasis on database technology, so that they will be successful database/Internet professionals in IT industry or, alternatively, have a sound knowledge base to specialize towards a scientific career in the field.

The project work in the year 2005 focused on implementing a Web Coverage Service (WCS) according to the published standard of the Open GeoSpatial Consortium (OGC)[12] as part of the GALEON project (cf. section 6.1). By the end of the semester the students had set up Web-based navigation on 4-D climate simulation data.

[12] http://www.opengis.org

Courses	Instructors
Lab Data Management, GIS & Visualization (211461)	V. Unnithan, A. Schäfer
Advanced Geographic Information Systems (211441)	A. Schäfer, V. Unnithan
Guided research projects (210351/2, 210371/2)	V. Unnithan, A. Schäfer
Introduction to GIS (Intersession 2006)	A. Schäfer, V. Unnithan
Geochemical Modelling (211432)	A. Koschinsky

Table 3: Spring and fall semester 2005 and 2006. Courses using GIS Lab facilities and instructors.

8.3 Teaching and Instruction in the GIS Lab

Contributed by Vikram Unnithan and Angela Schäfer

The computers at the GIS-Lab provide access to undergraduate, graduate and PhD students to all software within the CLAMV. Instruction and classes are provided in this lab. This lab is used intensively for GIS training on ArcGIS products, Geochemical Modelling, and Petroleum Basin Modelling. A basic overview of teaching and instruction is provided below.

1. GIS (Guided research projects, MSc thesis work, visualisation, webservices for Hermes and IRCCM projects)
2. Petroleum Basin Modelling (Guided research project, PhD thesis work)
3. Geochemical Modelling software training (Undergraduate, MSc and non-IUB staff)

Students and researchers of Jacobs University as well as cooperative researchers from other institutes have been trained in the GIS Lab at various levels in GIS techniques and geodata management during classes, workshops, intersession and internships. The use in the years 2005 and 2006 is summarized in Table 3. A variety of courses in applied GIS, modelling and visualisation techniques for IUB students and researcher are planned for the future. The GIS Lab has become an integral part of geoscience education at Jacobs University. It provides training and skills that are currently in high demand and that employers consider to be valuable assets while hiring personnel.

8.4 Workshops

The CLAMV hosted a number of workshops over the years 2002-2007.

Parallel computing workshops

Two workshops entitled *Parallel Programming in MPI and OpenMP* were hosted by CLAMV, one in August 2005 (four days) and the second one in January 2007 (five

days). Organized through the Bremer Competence Center for High Performance Computing (BremHLR), the workshop took place in the CS lecture hall in Research I. Workshop instructors were W. Baumann and H. Stüben from the Konrad-Zuse-Zentrum für Informationstechnik in Berlin. A total number of more than 60 participants from the Alfred-Wegener-Institut, Universität Bremen and Jacobs University attended the two workshops.

When the new shared memory machine SGI Altix arrived on campus in Spring 2005, a small workshop was offered to introduce the local user community to the new compute server.

Geoscience workshops

The CLAMV helped organize and host several workshops in the geosciences.

1. GIS Workshop (January 2005) for "Advanced GIS, Map ServerTechniques and GeoData Management" hosted jointly at AWI and IUB. Instructors: Dr. A Schäfer, Prof. V. Unnithan, and Prof. M. Schlüter.
2. Petroleum Basin Modelling (PetroMod) Workshop (2004) held by instructors from the company IES.
3. Advanced Petroleum Systems Modelling Workshop (May 2005), instructor: Prof. Vikram Unnithan.
4. Hermes GIS workshop (October 2005).
5. Introduction to Geographic Information Systems, Intersession Course January 2007.

For further information see http://www.irccm.de/[13].

Erasmus IP Seminar

In January 2007 a 12 days EU-supported Erasmus program with the title Mathematical and Computational Models of Attention, Decision and Action took place on campus. More than 30 students from 9 European countries were trained in up-to-date application of mathematical and computational models in cognitive psychology. Courses took place in lab3 and in the CLAMV Teaching Lab. The program was organized by Prof. Adele Diederich.

Introduction to IDL

In December 2004 the CLAMV organized a technical workshop for the software IDL. Participants got an overview about the features of IDL and had the chance to discuss user specific topics with trained personnel from the German IDL distributor Creaso GmbH.

[13] http://www.irccm.de/

International Collegiate Programming Contest

In 2003 and 2004, the training for the International Collegiate Programming Contest (ICPC) was held in the CLAMV CTL. See section 8.1 for a description of this activity.

8.5 CLAMV Seminar

The CLAMV seminar is the research seminar of the CLAMV, primarily serving the community of IUB computational scientists and researchers from adjacent disciplines. The general goals are:

- providing a forum where faculty and researchers can introduce themselves, present their results, discuss ideas, and initiate collaborations particularly across disciplines,
- introducing a certain number of external speakers to an interdisciplinary audience, with approximately one distinguished guest per year,
- informing IUB users on practical issues such as availability and access to computer resources, or the use of important software packages, and
- inviting computational researchers from industry both to present their work, but also to inform faculty and students about career options outside of academia.

A detailed seminar schedule can be found in Appendix A.4.

A Appendix

A.1 Organisation

Steering and Policy Committee (SPC)

The role of CLAMV within IUB and how the laboratory should interact with other university bodies is defined and controlled by the Steering and Policy Committee (SPC). Meetings of the SPC are called and chaired by the CLAMV Director. The SPC consists of all members of the CLAMV Operations Team, the chairpersons of the CLAMV committees, the Deans of the two Schools and the Jacobs Center, the IRC Chief Technology Officer, and a representative of Business and Administration.

CLAMV Management (Operations Team)

DIRECTOR: Joachim Vogt (until June 2005: Ronny Wells).

The CLAMV Director is responsible for the representation of the CLAMV to the Academic Council and within IUB in general.

EXECUTIVE DIRECTOR: Martin Zacharias (until June 2005: Joachim Vogt).

The CLAMV Executive Director is responsible for the management of daily operations and the coordination of CLAMV committee work.

SYSTEMS MANAGER: Achim Gelessus (Chair).

The CLAMV Systems Manager is responsible for the administration and support of all CLAMV hardware facilities and software repositories. He furthermore serves as an interface between IUB and scientific computing groups at partner institutions.

Two more persons have standing invitations to all meetings of the CLAMV Operations Team: (1) Heinrich Stamerjohanns (Head of CS Lab), and (2) Torge Schmidt (IRC Chief Technology Officer).

CLAMV committees

The following committees are supposed to collect input from the CLAMV Community in dedicated areas.

SCIENTIFIC COMPUTING COMMITTEE (SCC): Stephan Rosswog (Chair), Marcus Brüggen, Adele Diederich, Achim Gelessus, Hildegard Meyer-Ortmanns, Götz Pfander, Joachim Vogt, Martin Zacharias.

Responsibilities include the definition, allocation, and coordination of hardware and software resources for scientific computing.

COMPUTER EDUCATION COMMITTEE (CEC): Adalbert Wilhelm (Chair), Andreas Birk, Claus Hilgetag, Marcel Oliver.

Responsibilities include the definition of hardware and software resources for graduate and advanced undergraduate teaching.

SEMINAR AND EDITORIAL COMMITTEE (SEC): Joachim Vogt (Chair), Achim Gelessus, Lars Linsen, Peter Oswald (until September 2005: Marcel Oliver), Stephan Rosswog (until September 2005: Michael Rohlfing), Martin Zacharias.

The SEC is responsible for the organisation of the CLAMV Seminar and coordinates the editorial process of the CLAMV Annual Report.

A.2 Hardware

CLAMV Computer Teaching Labs

48 DELL OPTIPLEX GX620; TLAB036 - TLAB082, TLABTERM

- Intel Pentium D processor (3.00 GHz, 800 MHz FSB, 2 x 2 MB Cache)
- 2048 MByte RAM
- 80 GByte SATA harddisk
- 10/100/1000 MBit Ethernet
- Onboard Intel Media Accelerator 950 graphic adapter
- OpenSuSE Linux 10.2 Operating System (tlab036 - tlab071, tlabterm)
- Windows XP Professional SP2 (tlab072 - tlab082)

2 IBM INTELLI STATION, TLAB034 - TLAB035

- 2 Intel Pentium Xeon processor 2.80 GHz
- 1024 MByte RAM
- 36 GByte, 72 GByte harddisk
- 100 MBit Ethernet
- Matrox G450 graphic adapter
- SuSE Linux 9.3 Operating System

UNDERGRADUATE TEACHING LAB, RES. I

- 2 SUN Server v440
- 16 GByte RAM per server
- 45 SUN ThinClients
- SUN Solaris 10 Operating System

The Undergraduate Teaching Lab in Research I is completely integrated into the CLAMV configuration. Administration of the Undergraduate Teaching Lab is done by the IT-Support.

CLAMV Fileserver for data and software

2 DELL PE2900 SERVER

- 1 Intel Xeon 5150 processor (2.66 GHz, 1333 MHz FSB, 4 MB Cache)
- 4096 MByte RAM
- PERC5i SAS RAID Controller, 8 x 300 GByte SAS Disks (RAID5)
- PERC5i SAS RAID Controller, 2 x 300 GByte SAS Disks (RAID1)
- 1 GBit Ethernet
- Direct optical 1 GBit Ethernet interconnect
- SLES 10 Operating System
- Steeleye LifeKeeper Software (6.1) incl. data replication

CLAMV High Performance Computing equipment

CLAMV LINUX CLUSTER I

- 40 computer nodes
- 2 Intel Pentium Xeon 2.20 GHz processors per node
- 1.0 GByte RAM per node
- 100 MBit Ethernet interconnect
- RedHat Linux Operating System
- OpenPBS Queuing System

CLAMV LINUX CLUSTER II

- 32 computer nodes
- 16 nodes with 2 Intel Pentium Xeon 2.80 GHz processors
- 16 nodes with 2 Intel Pentium Xeon 3.20 GHz processors (2 MByte Cache)
- 30 nodes with 1 GByte RAM
- 2 nodes with 4 GByte RAM
- 1000 MBit Ethernet interconnect
- RAID system, 8 x 160 Gbyte
- RedHat Linux Operating System
- OpenPBS Queuing System

CLAMV LINUX CLUSTER III

- 24 compute nodes
- 2 Intel Pentium Xeon 2.80 GHz processors per node
- 1.0 GByte RAM per node
- Myrinet2000 interconnect

- RAID system, 8 x 160 Gbyte
- RedHat Linux Operating System
- OpenPBS Queuing System

CLAMV LINUX CLUSTER IV

- 40 compute nodes
- 2 Intel Quad-Core Xeon E5345 (2.33 GHz, 1333 MHz FSB, 2 x 4 MB Cache) processors per node
- 8.0 GByte RAM per node
- GigaBit and Infiniband interconnect
- RAID system, 15 x 500 Gbyte (2 x RAID5)
- SuSE Linux 10 Operating System
- Torque Queuing System
- ParaStation Software

CLAMV SMP-SERVER I, SGI ALTIX

- SGI Altix 3700Bx2 Server
- 24 Itanium2 processors (Madison9M) 1.6 GHz / 6 MByte Cache
- 96 GByte shared memory
- RAID system TP900, 4 x 146 GByte
- RAID system TP9300, 14 x 400 GByte
- SLES 9 / ProPack Operating System
- PBSPro Queuing System

CLAMV SMP-SERVER II, SUN FIRE V880

- 8 SUN Sparc-3 processors 900 MHz
- 16 GByte RAM, shared memory
- 2 * 80 GByte harddisk
- SUN Solaris 8 Operating System

CLAMV Data Storage

CLAMV STORAGE SERVER I

- 2 AMD Opteron 265 Dual Core-CPUs, 1.8 GHz / 2 MByte Cache
- 16 GByte memory
- RAID system: SATA2, Areca-Controller, 24 x 500 GByte
- 1 GBit Ethernet
- SuSE Linux 10.0 Operating System

CLAMV STORAGE SERVER II

- 2 AMD Athlon MP2400+ processors
- 1.0 GByte memory
- RAID system: 8 x 250 GByte
- 1 GBit Ethernet
- SuSE Linux 10.0 Operating System

CLAMV BACKUP SERVER

- Dell Precision 490 Server
- Intel Xeon 5110 (1.66 GHz, 1066 MHz FSB, 4 MB Cache) processor
- 2048 GByte memory
- 2 x 750 GByte SATA2 harddisks
- 1 GBit Ethernet
- LTO3 400/800 GByte SCSI tape drive
- SuSE Linux 10.2 Operating System

CLAMV WWW Presentations

2 DELL PE1950 SERVER FOR VIRTUALIZATION WITH XEN

- Intel Xeon 5130 (2.0 GHz, 1333 MHz FSB, 4 MB Cache) processor
- 4096 GByte memory
- 146 GByte SAS harddisk
- 1 GBit Ethernet
- Direct 1 GBit Ethernet interconnect
- SuSE Linux 10.2 Operating System / Xen3

GIS-WEB SERVER

- 2 Intel Pentium IV 3.00 GHz processors
- 1024 GByte memory
- 146 GByte harddisk
- SLES 9 Operating System

Research Group equipment

CLAMV GIS LAB
The CLAMV GIS Lab is located in Research III and consists of four PC with the following specifications.

- Intel Xeon processor 3.2 GHz

- 2.0 GByte memory
- 80 GByte harddisk
- Matrox Parhelia-512 / nVidia Quadro4 980 graphic adapter
- Windows 2000 Operating System

A.3 Software

Software on the central server (Linux)

GENERAL SOFTWARE PACKAGES FOR MATHEMATICS AND ANALYSIS: IDL, Maple, Mathematica, MatLab incl. 22 Toolboxes, Tecplot

SOFTWARE PACKAGES FOR MOLECULAR VISUALIZATION: gOpenMol, Molden, Molekel, Molmol, RasMol, Swiss PDB Viewer, VMD

COMPUTATIONAL CHEMISTRY MODULE: Gaussian03, Ghemical, Gromacs, Jmol, YASP.

COMPUTATIONAL BIOLOGY AND NEUROSCIENCE MODULE: Arb, ClustalX, Emboss, Genesis, Modeller, Neuron, Statistical Parametric Mapping (SPM5, MatLab), ViennaRNA.

ELECTRICAL ENGINEERING AND COMPUTER SCIENCE MODULE: CVX (Matlab), Eagle, ns-2 Simulator.

GEOASTRO MODULE: GDI, GMT, iGMT, MB-System, OpendTect, PetroMod, Seismic UNIX

Software locally installed on the CLAMV TeachingLab computers (Linux)

COMPILER, LANGUAGES: C (GNU, Intel, Portland), C++ (GNU, Intel, Portland), Fortran (GNU, Intel, Portland), Java, Mono, Perl, Prolog, Python, Ruby, Smalltalk, Tcl/tk.

PARALLEL COMPUTING: Local Area Multicomputer (LAM), Message Passing Interface (MPICH), Parallel Virtual Machine (PVM).

TOOLS: Concurrent Version System (CVS), Front end for the GNU profiler (kprof), GNU debugger (gdb), Intel debugger (idb), Graphical interface to gdb (kdbg), Revision Control System (RCS), Subversion System.

DATABASES: MySQL.

EDITORS: Ed, Emacs, Gvim, Jedit, Joe, Nano, Pico, Texmacs, Vim, Xemacs, Yzis.

GRAPHICS: Blender, Chemtool, Gimp, Gnuplot, Opendx, Povray, Q-CAD, Xfig, Xmgrace, Xv, Yafray.

OFFICE: OpenOffice.

PUBLISHING: Acroread, Bibview, Gv, Lyx, Tetex (Latex), Xpdf.

SCIENTIFIC SOFTWARE: Basic Linear Algebra Subprograms (BLAS), BioPerl, Fastest Fourier Transformation in the World (FFTW), GNU Scientific Library (GSL),

Grass GIS, Linear Algebra Package (Lapack), Octave, R-Statistics, Scientific Calculator.

WWW: Lynx, Konquerer, MozillaFirefox.

Software locally installed on the CLAMV TeachingLab computers (Windows XP)

AUXILLARY PROGRAMS: FileZilla, Putty, TightVNC, WinSCP

OFFICE: Acrobat, GhostView, MS Office, MikTex, WinEdt

SCIENTIFIC SOFTWARE: ArcView, Grass GIS, IDL, Maple, Mathemaica, Matlab, SPSS, Tecplot

A.4 CLAMV Seminar Schedules

CLAMV Seminar 2002

08/10/2002 Patrick Bangert, *Magnetic Field Topology in the Solar Corona: Computational Challenges*

15/10/2002 Michael Schreiber, *Numerical Investigations of the Metal-Insulator Transition in Disordered Materials*

22/10/2002 Adalbert Wilhelm, *Visual Exploration of Large Data Sets*

29/10/2002 Götz Pfander, *The crest factor of trigonometric polynomials: Computation, analysis, modeling, and visualisation*

05/11/2002 Tijana Janjic, *Error due to unresolved scales in atmospheric data assimilation*

12/11/2002 Andreas Birk, *On the origins of cooperation*

19/11/2002 Thanos Antoulas, *POD and model reduction*

26/11/2002 Klaudia Brix, *Imaging of cells*

05/12/2002 Xinyuan Wu (Nanjing University), *Extended Runge–Kutta formulae*

10/12/2002 Ahmed Hujeirat (MPI for Astronomy, Heidelberg), *A robust self-adaptive solver for modelling radiative MHD flows*

CLAMV Seminar 2003

07/02/2003 Georg Gottwald (University of Sydney), *A new test for chaos*

11/02/2003 Adele Diederich, *Decision making under Conflict: Decision Time as a Measure of Conflict Strength*

18/02/2003 Stefano Carpin, *Advanced Techniques for Randomized Robot Motion Planning*

25/02/2003 Herbert Jaeger, *Blackbox modeling of dynamical systems*

04/03/2003 Ken Kennedy (Rice University), *High Performance Computing without a Degree in Computer Science*

11/03/2003 Florian Müller-Plathe, *Computational Polymer Science: What we do and how we do it*

01/04/2003 Michael Köhne, *CLAMV: a moving target*

08/04/2003 Marcus Brüggen, *Looking into the sun*

22/04/2003 Claus Hilgetag, *Analyses of brain connectivity*

29/04/2003 Alfred Schmidt (Uni Bremen), *Adaptive finite element methods for phase transition computations*

06/05/2003 Bertalan Zieger, *Large-Scale MHD Simulation of the Earth's Magnetosphere*

13/05/2003 Special Event: Computational Science at IUB. *Presentation of the undergraduate major in Computational Science to students and faculty*

20/05/2003 Rein van der Hout (Leiden University), *Nematic liquid crystals and harmonic maps*

18/09/2003 Melvin Leok (Caltech), *Generalized Galerkin variational integrators for multiple scales*

23/09/2003 Martin Zacharias, *Computer simulation of biomolecular structures and complexes*

30/09/2003 Marcel Oliver, *Introduction to variational and quasi-variational integrators*

07/10/2003 Götz Pfander, *The crest factor of trigonometric polynomials*

14/10/2003 Ulrich Kleinekathöfer, *Quantum and classical molecular dynamics calculations on clusters*

28/10/2003 Matthias Hoeft, *Radio relics in clusters of galaxies*

04/11/2003 Jun Tian, *Reversible Information Hiding and Its Application to Scalable Content Access Control*

11/11/2003 Rein van der Hout (Leiden University), *Liesegang bands: a model involving a Stefan problem*

18/11/2003 Wolfgang Hiller (AWI Bremerhaven), *FoSSi: The Family of Simplified Solver Interfaces – a framework for fast parallel solution of large linear systems*

25/11/2003 Holger Kenn, *Ad-hoc networks for control*

CLAMV Seminar 2004

17/02/2004 Antje Boetius, *Coordinated Growth of Microbial Consortia: Microbiology needs Mathematics*

02/03/2004 Michael Kohlhase, *European Connexions: Content Markup Techniques for E-Learning*

09/03/2004 Joachim Schmidt, *Interactions of Coronal Mass Ejections with the radial interplanetary magnetic field or with themselves*

16/03/2004 Matthias Görner, *Introduction to Blender and POV-Ray or: How I annimated Escher's Relativity*

30/03/2004 Oliver Junge (Paderborn), *Dynamical system methods in space mission design*

13/04/2004 Arzhang Khalili, *On Brinkman Boundary Layer in Permeable Sediments*

20/04/2004 Matthias Bode, *Pattern Formation in Reaction-Diffusion Systems*

27/04/2004 Jerry Marsden (Caltech), *From Poincare to the EPDiff Equations*

04/05/2004 Stephan Rosswog, *Collisions of Compact Stars*

11/05/2004 Michael Beck (Bayer CropScience), *Support of agro-chemical research by first-principle quantum chemical calculations*

21/09/2004 Neville de Mestre (Bond University), *Mathematical modeling in sport*

28/09/2004 Michael Rohlfing, *Electrons, holes, and their dynamics: Ab-initio electronic-structure theory for excited states*

05/10/2004 Herbert Jaeger, *Honing raw power: Learning to train observable operator models efficiently*

12/10/2004 Mathias Lindemann (Uni Bremen and IUB), *Besov spaces and wavelet expansions with general dilation matrices*

19/10/2004 Max Wardetzky (Konrad-Zuse-Zentrum Berlin and Mental Images), *Topics in applied geometry - surface optimization and mesh compression*

26/10/2004 Niklas Grip, *Wavelets: an application-oriented introduction with some new results on wavelet prefiltering*

02/11/2004 Danilo Roccatano, *Understanding the mechanisms of large scale protein motion using molecular dynamics*

09/11/2004 Peter Oswald, *Polarization control: Mathematical model and computational challenges*

16/11/2004 Joachim Vogt, *Analysis methods for multi-spacecraft data*

23/11/2004 Peter Deuflhard (Konrad-Zuse-Zentrum and Freie Universität, Berlin), *From molecular dynamics to conformation dynamics in drug design*

30/11/2004 Michael Stöhr (MPI for Marine Microbiology, Bremen), *Laboratory studies on solute transport in marine sediments induced by rising gas bubbles*

07/12/2004 Onno Bokhove (Twente University) *A (dis)continuous finite element model for generalized 2D vorticity dynamics*

CLAMV Seminar 2005

01/03/2005 Hanno Teeling (MPI for Marine Microbiology, Bremen), *How genome linguistic approaches can be used to tackle the fragment identification problem in metagenomics*

15/03/2005 Charles Doering (University of Michigan and IUB), *Birth, death, epidemics & extinction: modeling and analysis of some basic processes in population dynamics and epidemiology*

05/04/2005 Jörg Schumacher (Marburg University), *Polymer stretching in turbulent flow*

12/04/2005 Don H. Johnson (Rice University and IUB), *Information Theory and Neural Coding in the Auditory System*

19/04/2005 Werner Kozek (Siemens AG), *Nonexistence of Nash equilibria in practical network management*

26/04/2005 Nicolas Neuß (IWR Heidelberg), *Numerical methods for multiscale problems*

03/05/2005 Meheboob Alam (JNCASR Bangalore and MPI for Marine Microbiology, Bremen), *Instability-induced ordering and universal unfolding of pitchfork bifurcations in granular Couette flow*

17/05/2005 Ulrike Wacker (AWI Bremerhaven), *Simulation of mixed phase clouds with a numerical weather prediction model*

20/09/2005 Jörn Sesterhenn (TU Munich), *Interaction Of turbulence With weak oblique shock waves*

11/10/2005 Xiang Li (Shanghai Jiao Tong University and IUB), *Complex Networks: Models, Synchronization, and Control*

13/10/2005 Jörn Behrens (TU Munich), *Adaptive atmospheric modeling: basic principles and algorithmic realizations*

25/10/2005 Dan Price (University of Exeter), *Simulating astrophysical magnetic fields with particle methods*

29/11/2005 CLAMV Keynote Speaker: Michael Griebel (Bonn University), *A parallel level-set approach for two-phase flow*

06/12/2005 Jason Frank (CWI Amsterdam), *Symplectic discretization of atmospheric flows*

CLAMV Seminar 2006

04/04/2006 Tim Kröger (CeVis, Uni Bremen), *Numerical Simulation of Radio Frequency Ablation for Hepatic Tumors: Difficulties and Current Workarounds*

09/05/2006 Margarita Petkova, *Visualization of scientific data with tecplot*

31/10/2006 CLAMV Keynote Speaker: Zavisa Janjic (NOAA/National Weather Service), *Numerical Tools in Climate and Weather Studies and Forecasting*

23/11/2006 Tobias Preusser (CeVis, Uni Bremen), *Joint image denoising and optical flow extraction*

30/11/2006 Julian Illies , *Cluster analysis for large data sets*

A.5 Charter of the CLAMV

This document defines the objectives and the organisational structure of the Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV) at International University Bremen (IUB).

Objectives

The *Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV)* is an umbrella and a support initiative for all computationally oriented disciplines at IUB. CLAMV's mission is to create a community of users that cooperate in technical and scientific aspects of computing, to provide a shared infrastructure with workspaces for researchers and students, and to constitute a virtual laboratory for remote access to software, servers, and high performance platforms.

CLAMV Community

The CLAMV is open to all IUB scientists and students who are interested in computationally oriented research. Support is provided for a broad spectrum of activities with a focus on scientific computing and graduate teaching as well as advanced undergraduate teaching. New IUB faculty members, researchers, and students can join the CLAMV Community quickly and unbureaucratically at any time.

Once a year CLAMV associated faculty and staff are expected to provide a short description of their CLAMV related activities that will be included in the CLAMV Annual Report.

CLAMV associated faculty meets twice per year to discuss and decide on formal issues. Topics to be addressed at the CLAMV Spring Assembly are: report of the CLAMV Operations Team, presentation and approval of the CLAMV Activity Report, initiation of the budget definition process, and the choice of representatives. Topics to be addressed at the CLAMV Fall Assembly are: report of the CLAMV Operations Team, presentation of the submitted budget, and initiation of the CLAMV Activity Report editorial process.

Steering and Policy Committee (SPC)

The role of CLAMV within IUB and how the laboratory should interact with other university bodies is defined and controlled by the Steering and Policy Committee (SPC). Meetings of the SPC are called and chaired by the CLAMV Director. The SPC consists of all members of the CLAMV Operations Team, the chairpersons of the CLAMV committees, the Deans of the two Schools and the Jacobs Center, the IRC Chief Technology Officer, and a representative of Business and Administration.

CLAMV Operations

The CLAMV Operations Team is organized as follows.

Director: Responsible for the representation of CLAMV to the Academic Council and within IUB in general. Appointed by the Academic Council after consultation of CLAMV Community representatives and supported by a dedicated assistant.

Executive Director: Responsible for the management of daily operations and the coordination of CLAMV committee work. Interface between the CLAMV Community and the CLAMV Operations Team. Chosen by CLAMV associated faculty for a period of one year, re-nominations are possible.

Systems Manager: Responsible for the administration and support of all CLAMV hardware facilities and software repositories. Interface between IUB and scientific computing groups at partner institutions. Employed by IUB through the IRC, and assigned to CLAMV.

The CLAMV Operations Team may invite individual CLAMV members to participate in team meetings on a permanent or temporary basis.

The IRC Chief Technology Officer has a standing invitation to all CLAMV Operations Team meetings to ensure coordinated actions between the IRC and the CLAMV.

CLAMV Committees

The following committees are supposed to collect input from the CLAMV Community in dedicated areas. Committee members are chosen by CLAMV associated faculty for a period of one year, re-nominations are possible. The members of a committee appoint a chairperson who acts as the interface to the CLAMV Operations Team.

Scientific Computing Committee (SCC): Responsibilities include the definition, allocation, and coordination of hardware and software resources for scientific computing.

Computer Education Committee (CEC): Responsibilities include the definition of hardware and software resources for graduate and advanced undergraduate teaching.

Seminar and Editorial Committee (SEC): The SEC is responsible for the organisation of the CLAMV Seminar and coordinates the editorial process of the CLAMV Annual Report.

The members of the CLAMV Operations Team have standing invitations to the meetings of the CLAMV committees.

Approval of and changes to the CLAMV Charter

Changes to the CLAMV Charter require the approval of the CLAMV Community and the Academic Council.

The CLAMV Charter was approved at the CLAMV Spring Assembly on March 23, 2004, and by the Academic Council on April 21, 2004.

A.6 Abbreviations

AWI Alfred-Wegener Institut, Bremerhaven[14]
GIS Geographic Information System
ICBM Institut fuer Chemie und Biologie des Meeres, Universitaet Oldenburg[15]
IRCCM International Research Consortium on Continental Margins[16]
JCLL Jacobs Center for Lifelong Learning[17]
NIC John von Neumann - Institute for Computing at Forschungszentrum Juelich[18]
SES School of Engineering and Science[19]
SHSS School of Humanities and Social Sciences[20]

A.7 CLAMV People

Table 4 lists the faculty members who have been using CLAMV resources in the years 2002-2007.

The people mentioned in this report are listed in the index.

[14] http://www.awi-bremerhaven.de
[15] http://www.icbm.de
[16] http://www.irccm.de
[17] http://www.jacobs-university.de/schools/jacobs
[18] http://www.fz-juelich.de/nic/index-e.html
[19] http://www.jacobs-university.de/schools/ses
[20] http://www.jacobs-university.de/schools/shss

Name	School, Center	Teaching Lab	Software	HPC	Storage	WWW	Research Group
Athanasios C. Antoulas	SES		x				
Patrick Bangert	SES	x	x		x		
Peter Baumann	SES	x	x		x		x
Andreas Birk	SES	x	x				x
Mathias Bode	SES		x				x
Klaudia Brix	SES				x		x
Marcus Brüggen	SES	x	x	x	x		
Stefano Carpin	SES	x	x				
Mark Comerford	SES	x	x				
Adele Diederich	SHSS	x	x				
Marcelo Fernandez-Lahore	SES		x				
Frank Oliver Glöckner	SES	x	x				
Benjamin Godde	JCLL		x				
Harald Haas	SES	x	x				
Werner Henkel	SES	x	x				
Claus Hilgetag	SES	x	x				
Marc-Thorsten Hütt	SES	x	x	x	x		x
Herbert Jaeger	SES	x	x		x		
Albert Jeltsch	SES	x	x				
Vadim Kaimanovich	SES				x		
Holger Kenn	SES	x	x				
Arzhang Khalili	SES	x	x				
Ulrich Kleinekathöfer	SES	x	x	x	x		x
Dietmar Knipp	SES		x				
Michael Kohlhase	SES	x	x				
Ute Kunzmann	JCLL				x		
Lars Linsen	SES	x	x	x			
Peter Ludes	SHSS	x					
Bendick Mahleko	SES		x				
Keivan Mallahi-Karai	SES		x				
Arnulf Materny	SES		x				
Hildegard Meyer-Ortmanns	SES	x	x	x			
Florian Müller-Plathe	SES	x	x	x			
Marcel Oliver	SES	x	x			x	x
Bettina Olk	SHSS		x				
Peter Oswald	SES	x	x				
Götz Pfander	SES	x	x		x		
Britta Renner	JCLL				x	x	
Ryan Richards	SES	x	x				
Danilo Roccatano	SES	x	x	x	x	x	x
Michael Rohlfing	SES	x	x	x			
Stephan Rosswog	SES	x	x	x	x		x
Dierk Schleicher	SES	x					
Klaus Schömann	JCLL		x				
Jürgen Schönwälder	SES	x	x				
Heinrich Stamerjohanns	SES	x	x				
Michael Stoll	SES	x	x				x
Konstantin Styrkas	SES	x					
Stefan Tautz	SES	x	x				
Laurenz Thomsen	SES		x			x	
Vikram Unnithan	SES	x	x		x	x	x
Joachim Vogt	SES	x	x	x			x
Veit Wagner	SES	x	x				
Jon Wallace	SES		x				
Matthias Winterhalter	SES		x				
Isabel Wünsche	SHSS					x	
Martin Zacharias	SES	x	x	x	x		x

Table 4: CLAMV usage in the years 2002–2007.

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