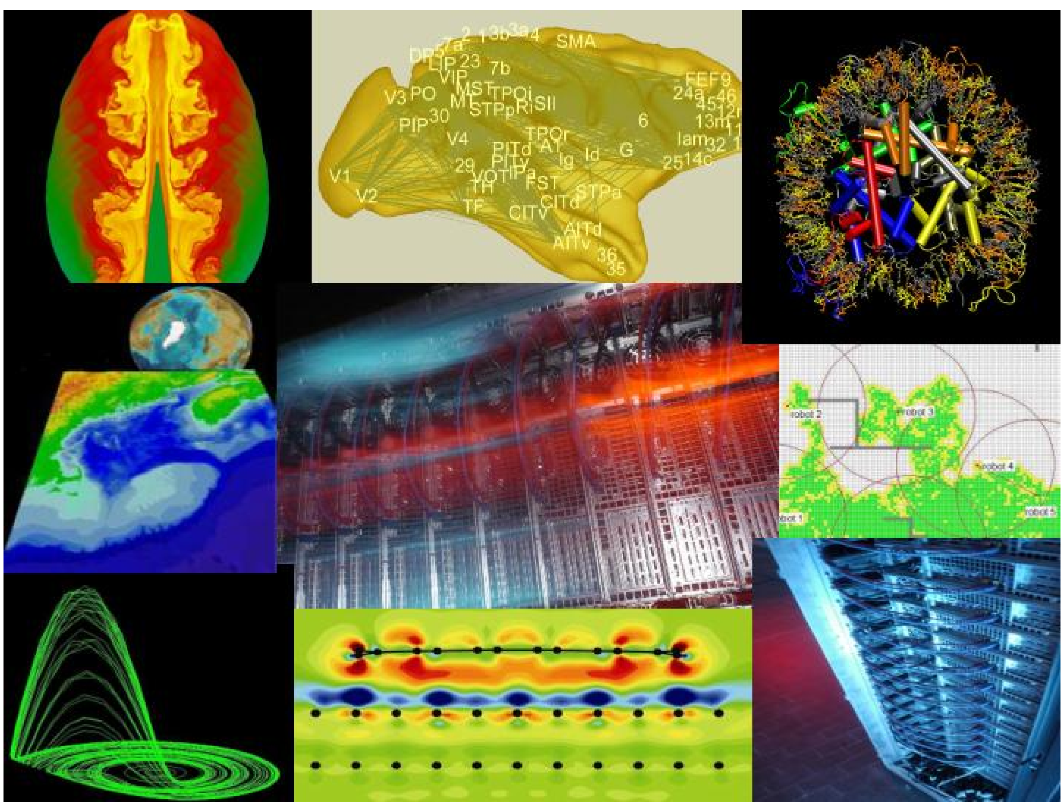
International University Bremen (IUB)

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

CLAMV Activity Report 2005

Compiled by the CLAMV Seminar and Editorial Committee

A. Gelessus, P. Oswald, S. Rosswog, J. Vogt, M. Zacharias



Contents

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 International University Bremen (IUB). Its hardware and software infrastructure serves large parts of the IUB community. CLAMV users cooperate in technical and scientific aspects of computing. They benefit from a shared infrastructure with workspaces for researchers and students as well as remote access to software, servers, and high performance computing platforms. Since its foundation in April 2002, the laboratory has established itself within IUB as a small but efficient institution to serve and maintain a large number of users in the areas of computationally oriented research and teaching.

The remainder of this section will introduce the CLAMV community, available resources, and CLAMV's interaction with other university bodies and institutions outside IUB. The following sections discuss the CLAMV activities in the year 2005, with particular emphasis on research projects in scientific computing (section 2) and the involvement in teaching (section 3). Service, consulting, and new facilities are addressed in section 4). Technical and organizational details are given in the appendix (section A).

The CLAMV Activity Report 2005 was compiled by the CLAMV Seminar and Editorial Committee.

1.1 CLAMV Community

CLAMV is open to all IUB scientists and students who are interested in computationally oriented research. We support a broad spectrum of activities ranging from large-scale simulations on parallel computing platforms to undergraduate programming courses. Approximately 400 students and more than 100 scientists in about 35 research groups have been served in the year 2005.

CLAMV is designed to include new IUB faculty members and researchers in a fast and unbureaucratic way. A large selection of scientific computing software is immediately available to new members of the IUB community through the CLAMV file and license server. The performance of different kinds of computer architectures (shared memory, Linux clusters, visualization workstations) can be explored. If the available facilities should not be sufficient for the purposes of a new faculty member, qualified CLAMV personnel help obtaining offers from different vendors, testing new hardware, applying for third-party funding, and cooperating with IUB partner institutions in and around Bremen.

It is easy to become part of the CLAMV community: One should make use of CLAMV facilities and services. In return, we expect a short report of activities associated with CLAMV of the kind listed in section 2.

1.2 Available Resources

CLAMV hardware resources for scientific computing include three Linux clusters and two parallel compute servers of shared memory architecture which are also partially used for file service and user administration. A computer teaching lab for advanced undergraduate and graduate teaching consisting of 35 visualization workstations is located in the basement of West Hall. A small GIS Lab in Research III is also supported by CLAMV personnel.

Scientific computing and visualization software on CLAMV computers include commercial packages like Matlab, Mathematica, Maple, IDL, LEDA, GAUSSIAN, NAG libraries, SUN HPC libraries, the SUN EduSoft package, PetroMod, TecPlot, and a large number of free software packages.

The CLAMV Systems Manager Achim Gelessus gives support and provides service to the IUB community in many different ways: administration and maintenance of the CLAMV facilities, account and software management for computer lab courses, integration of various parallel computing platforms, planning of new computer infrastructure, consulting of new faculty members in the process of defining and purchasing scientific computing equipment, and coordination of activities with scientific computing departments at IUB partner institutions such as AWI Bremerhaven and Universität Bremen. The CLAMV Systems Manager is supported by currently two student assistants.

1.3 Cooperation

The primary university body that CLAMV interacts with is the *Information Resource Center (IRC)*. CLAMV complements the general information services provided by the IRC in well-defined and specific areas, namely, graduate teaching and computationally oriented research. The CLAMV Systems Manager has his office in the IRC which guarantees optimum interaction. The IRC Chief Technology Officer has standing invitations to all CLAMV Ops Team Meetings where daily CLAMV issues are discussed. The IRC is represented in the CLAMV Steering and Policy Committee which is responsible for the mid- and long-term strategic planning and for the optimum embedding of CLAMV in the university.

The CLAMV is IUB's interface to scientific computing departments at partner institutions like the Alfred-Wegener-Institut in Bremerhaven and Universität Bremen. This close cooperation is formalized in the *BremHLR*. The BremHLR coordinates scientific computing activities in the Bremen area, helps to make efficient use of available resources at different institutions, and organizes the access to the high-perfomance computing facilities in Hannover and Berlin.

IUB and a number of partner institutions from academia and industry are organized in the *International Research Consortium on Continental Margins (IRCCM)*. Here IUB aims at a leading role in the fields of data management and modeling. CLAMV provides hardware and software for IRCCM related project work.

1.4 Organisational and Technical Changes in the Year 2005

In 2005 the founding father of the CLAMV, Ronny Wells, stepped down not only from his position as Vice-President of IUB but also as the first CLAMV Director. His vision and his engagement brought this laboratory into existence, and his continuous support was essential during the built-up phase. The CLAMV Community thanked Ronny for his work at the Fall Assembly in September 2005. We would like to take this opportunity to express again our appreciation for his initiative, and our hopes that he will stay in touch with CLAMV.

At the same assembly Martin Zacharias was nominated the new CLAMV Executive Director, after Joachim Vogt had been appointed the new CLAMV Director.

The year 2005 also saw a few technical changes. To make additional office space for an increasing number of graduate students available in the building Research I, the CLAMV Teaching Lab was relocated to the basement of West Hall. A new shared memory computer of type SGI Altix with 24 processors became operational on campus in Spring. The Linux Cluster of the former computational chemistry group was fully integrated into CLAMV in Fall.

1.5 Outlook

CLAMV will enter its fifth year of existence after April 2006. Parts of the initial hardware have already started to become less reliable and will require increasing attention from CLAMV personnel. To maintain the high quality of the computational infrastructure provided by CLAMV, and to keep system administration at a reasonable level, it will be necessary to renew parts of the initial hardware configuration in the near future. CLAMV representatives are currently working on a proposal to get third-party funding for the renewal of the teaching lab facility through the CIP program.

The resources and services offered to students and researchers on campus through CLAMV have considerably increased over the years, and the community is still growing. The existing personnel (Systems Manager and student assistants) will have difficulties to meet the growing demand, and further professional support will be needed. We strongly suggest to establish the position of an additional *CLAMV Systems Administrator*.

2 Scientific Projects

The hardware infrastructure and the software environment provided by the CLAMV enter a large number of scientific projects carried out at IUB. We support activities in areas such as numerical modeling, the analysis of observational data, and the visualization of simulation results. Numerical modeling and simulation projects are the most challenging ones in terms of hardware resources and very often call for parallel computing platforms. Data analysis and visualization projects require a broad spectrum of software products and often also personal consulting and maintenance by the CLAMV personnel.

Selected projects that were using CLAMV resources in 2005 or are currently planning to do so are listed in the following table.

Project scientist(s)	**Field**	**Page**
P. Baumann	Computer Science	10
A. Birk, M. Rooker	EECS	10
K. Brix et al.	BCCB	11
M. Brüggen	Astrophysics	12
A. Diederich	Psychology	14
B. Godde, C. Voelcker-Rehage	Human Performance	17
H. Haas et al.	Electrical Engineering	18
M. Hoeft	Astrophysics	21
H. Meyer-Ortmanns et al.	Physics	23
B. Olk	Psychology	22
R. Richards, A. Kraynov	Chemistry	26
E. Rödiger	Astrophysics	27
M. Rohlfing	Physics	30
S. Rosswog	Astrophysics	35
M. Stoll	Mathematics	39
V. Unnithan, A. Schäfer	Geoscience	40
J. Vogt et al.	Space Physics	44
M. Winterhalter et al.	Biophysics	46
M. Zacharias et al.	Computational Biology	49

The technical specifications of the hardware resources provided by the CLAMV can be found in the appendix (cf. Sec. A.2). Three Linux-operated PC clusters with a total number of almost 200 processors are administered by the CLAMV, and also two shared memory computers (8 nodes and 24 nodes). The visualization PC's of the CLAMV Teaching Lab can be accessed from remote and are used also off-hours for smaller computing jobs that do no require a parallel architecture.

The software environment provided by CLAMV (cf. Sec A.3) is used in many different contexts which include advanced undergraduate or graduate teaching, student projects, the work of individual scientists or research groups, and scientific collaborations with partner institutions. Standard tools like compilers and debuggers as well as numerical or technical libraries are managed and maintained. Of particular importance are scientific software packages like Matlab, IDL, Mathematica, Maple, VMD, and Gaussian.

The hardware and software infrastructure is maintained by the CLAMV Systems Manager Dr. Achim Gelessus and currently two student assistants.

2.1 GALEON and Other Scientific Data Services

Prof. Dr. Peter Baumann (Computer Science)

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

The Open GeoSpatial Consortium (OGC)[1] 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.

GALEON will deliver its results to OGC beginning 2006. As a preliminary outcome, a substantial list of change requests to the WCS specification have been collected

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

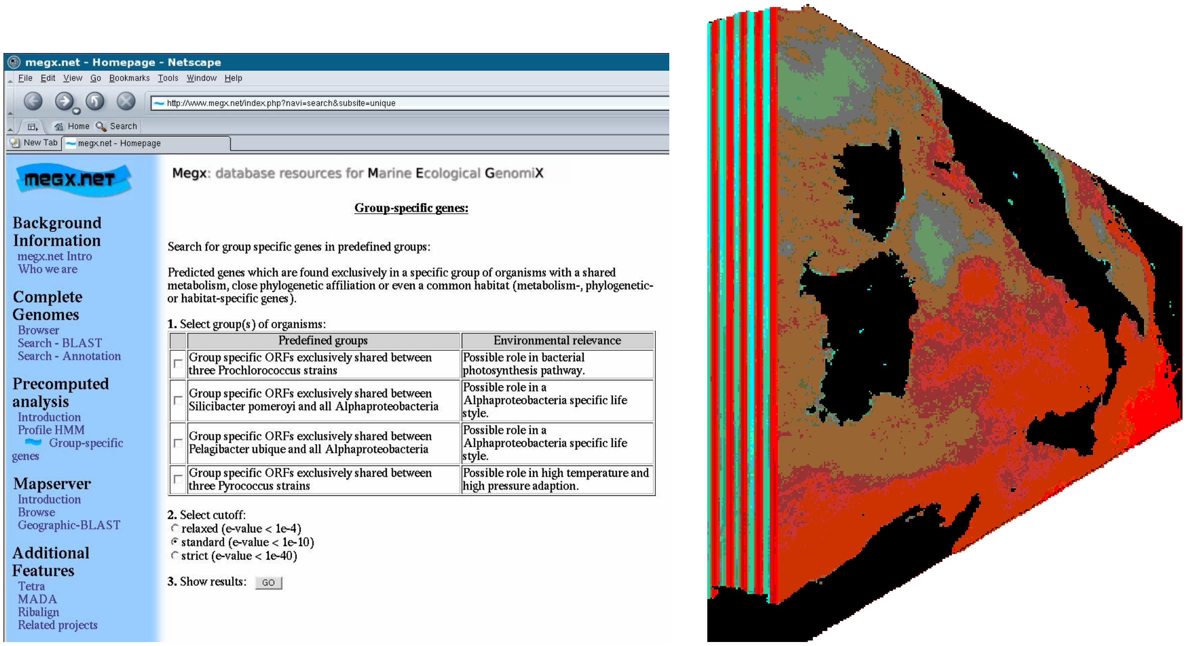


Figure 1: Scientific data services. [P. Baumann]

which will be considered by the WCS group for version 1.1 of the standard. IUB, being both actively engaged in the WCS group and GALEON, provides liaison between both, which has led to several improvements in the standard itself already.

More information about GALEON can be found at http://my.unidata.ucar.edu/content/projects/THREDDS/OGC/[2].

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.

[2] http://my.unidata.ucar.edu/content/projects/THREDDS/OGC/

2.2 Multi-Robot Exploration under the Constraints of Wireless Networking

Prof. Dr. Andreas Birk and Martijn N. Rooker (Electrical Engineering and Computer Science)

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.

PUBLICATIONS

Martijn Rooker and Andreas Birk (2006), *Communicative Exploration with Robot Packs*, RoboCup 2005: Robot Soccer World Cup IX, Springer, LNAI, Noda et al. (Eds.).

Martijn Rooker and Andreas Birk (2005), *Combining Exploration and Ad-Hoc Networking in RoboCup Rescue*, RoboCup 2004: Robot Soccer World Cup VIII, Springer, LNAI, Nardi et al. (Eds.), pp.236-246.

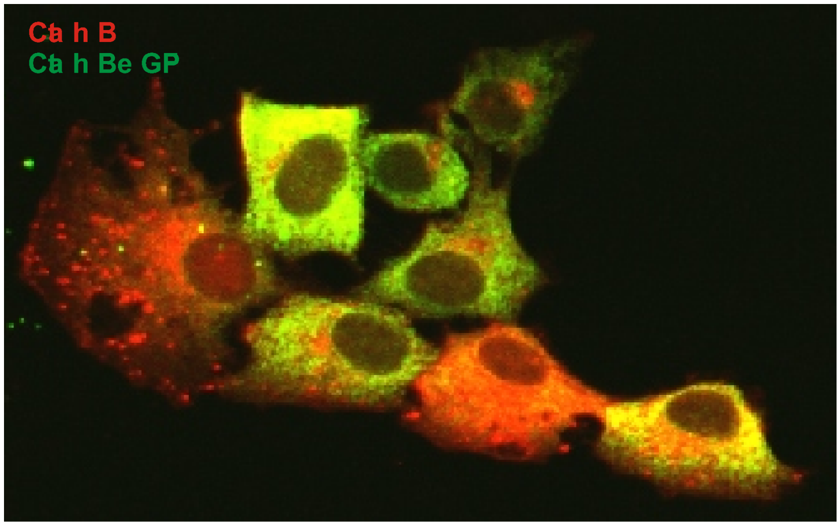


Figure 2: Thyroid epithelial cells expressing green fluorescent protein-tagged cathepsin B (green) that is in part co-localized (yellow) with the endogenous lysosomal cysteine protease (red). [K. Brix et al.]

Martijn Rooker and Andreas Birk (2004), *Communicative Exploration in Dangerous Environments*, Second International Workshop on Advances in Service Robotics.

2.3 Visualization of Protease Trafficking

Prof. Dr. Klaudia Brix, (Biochemistry and Cell Biology)

Our group is interested in the biological significance of cysteine protease-mediated proteolytic processes that enable migration of keratinocytes, maintain thyroid hormone homeostasis, and that contribute to the induction of local inflammatory events as a result of surgery. We concentrate on cysteine cathepsins, the major group of lysosomal enyzmes, which are secreted from epithelial cells under certain physiological and pathological conditions. To better understand their *in situ* importance, we analyze targeting, transport, and trafficking of the proteases by tagging with green fluorescent protein. In addition, we used activity based probes to visualize cysteine protease acitivities in living cells. Our results demonstrated that epithelial cells sort distinct proteases into particular transport containers that deliver the enzymes at specific locations in cells and tissues, where they can perform proteolytic tasks when needed [Brix and Jordans, 2005]. Our plans include the 4-dimensional visualization of protease trafficking and analysis of proteolytic activities *in vivo*, a project for which CLAMV resources will be helpful.

GROUP MEMBERS: Heiko Büth, Stefanie Dannenmann, Silvia Jordans, Malgorzata Kubica, Kristina Mayer, Dr. Ulf Meyer-Grahle, Hong Qu, Meike Klepsch, Brit Wolters.

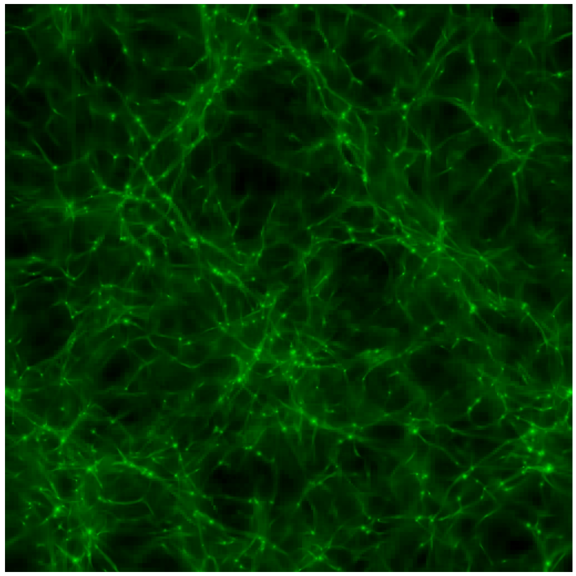


Figure 3: The projected gas density of the simulated part of the universe. The comoving box size is 128 Mpc h^{-1} which corresponds to ~580 million light years. The filamentary density structure is also called *cosmic web*. [M. Brüggen]

PUBLICATIONS

Brix, K. and S. Jordans (2005), *Watching proteases in action*, Nature Chem. Biol. 1, 186-187.

GRANTS

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

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

2.4 Simulations of Large-Scale Structures in the Cosmos

Prof. Dr. Marcus Brüggen (Astrophysics)

Galaxy clusters are the largest gravitationally bound objects in the cosmos and are useful in many ways to unravel the history of the Universe. For example, the statistics of X-ray clusters of galaxies can serve as an excellent probe of cosmology. By comparing observed cluster properties with the results of cosmological simulations of structure formation, one can try to determine the fundamental cosmological parameters that describe the evolution of the Universe. Examples of these parameters are Hubble's constant, that describes the expansion speed of the Universe, or the dark matter density. Most interestingly, galaxy clusters are thought to provide firm evidence for the existence of so-called dark energy.

Together with third-year student Margarita Petkova, who does her Guided Research Project on this topic, we critically examine this evidence for dark energy. The line of argument hinges on a number of assumptions that we will try to validate using massive computer simulations. To this end, we are studying the temperature, density, entropy and other profiles and scaling relations of simulated galaxy clusters and compare them to the analytical and empirical values. The latter have been obtained from measurements by x-ray satellite missions such as Chandra and XMM-Newton.

The computer simulations are based on a code that solves the equations of Eulerian hydrodynamics plus the interaction of dark matter on an adaptive mesh in an expanding space-time. An adaptive mesh means that the grid is automatically refined in regions of space where more resolution is needed, and de-refined in regions that are very smooth. Our simulations are run on 16-32 nodes of the GAMBO cluster managed by CLAMV. An example of the density distribution is shown in the figure 3.

A second project was concerned with the origin of large-scale magnetic fields in the cosmos. The origin of cosmic magnetic fields is still an enigma. There is ample evidence for magnetic fields that pervade the Universe on all scales, from stars to clusters of galaxies. Magnetic fields are germane to almost all branches of astrophysics, yet their provenance and physical effects remain largely unclear. Magnetic fields affect, both, radiation and gas processes. They are essential for synchrotron emission, they relax dilute media, such as the intergalactic medium, they suppress thermal conductivity and viscosity, they alter the paths of cosmic rays, and they may affect cosmic structure formation.

A great number of observations, based on starlight polarisation, Zeeman splitting, Faraday rotation and synchrotron emission confirm the presence of magnetic fields in our Galaxy as well as in other galaxies. The magnetic fields are typically toroidal, have coherence lengths of kiloparsecs and strengths of μG which makes the magnetic pressure comparable to the cosmic-ray pressure.

The intergalactic magnetic field within filaments should be less polluted by magnetised outflows from active galaxies than magnetic fields in clusters. Therefore, filaments may be a better laboratory to study magnetic field amplification by structure formation than galaxy clusters which typically host many more active galaxies. We have published highly resolved cosmological adaptive-mesh simulations of magnetic fields in the cosmos and made predictions about the evolution and structure of magnetic fields in filaments. Comparing our results to observational evidence for magnetic fields in filaments suggests that amplification of seed fields form the early Universe by gravitational collapse is not sufficient to produce IGM fields. We also discussed implications for cosmic ray transport.

GROUP MEMBERS: Dr. Matthias Hoeft, Dr. Elke Rödiger.

PUBLICATIONS

Roediger, E. and M. Brueggen (2005), *Ram pressure stripping of disc galaxies: The* *role of the inclination angle*, MNRAS accepted, ArXiv Astrophysics e-prints, astro-ph/0511401.

Iapichino, L., M. Brueggen, W. Hillebrandt, J. Niemeyer (2005), *The ignition of thermonuclear flames in Type Ia supernovae*, Astronomy & Astrophysics accepted, ArXiv Astrophysics e-prints, astro-ph/0512300.

Brüggen, M., M. Ruszkowski, A. Simionescu, M. Hoeft, and C. Dalla Vecchia (2005), *Simulations of Magnetic Fields in Filaments*, Astrophys. J. Lett., 631, L21-L24, doi 10.1086/497004.

Brüggen, M., M. Ruszkowski, and E. Hallman (2005), *Active Galactic Nuclei Heating and Dissipative Processes in Galaxy Clusters*, Astrophys. J., 630, 740-749, doi 10.1086/432112.

Roediger, E. and M. Brueggen (2005), *3D simulations of the ISM-ICM interaction of disk galaxies in cluster*, Astronomische Nachrichten, 326, 509.

Brueggen, M. and M. Hoeft (2005), *Simulations of magnetic fields in the cosmos*, Astronomische Nachrichten, 326, 610.

Hoeft, M., M. Bruggen, and G. Yepes (2005), *Radio relics in a cosmological cluster merger simulation*, Astronomische Nachrichten, 326, 613-614.

Brüggen, M., M. Hoeft, and M. Ruszkowski (2005), *X-Ray Line Tomography of AGN-induced Motion in Clusters of Galaxies*, Astrophys. J., 628, 153-159, doi 10.1086/430732.

Hoeft, M., and M. Brüggen, *Heating of the ICM Due Fossil Plasma*, in X-Ray and Radio Connections (eds. L.O. Sjouwerman and K.K Dyer), published electronically by NRAO[3].

2.5 Modeling Projects in Psychology

Prof. Dr. Adele Diederich (Psychology)

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

[3] http://www.aoc.nrao.edu/events/xraydio

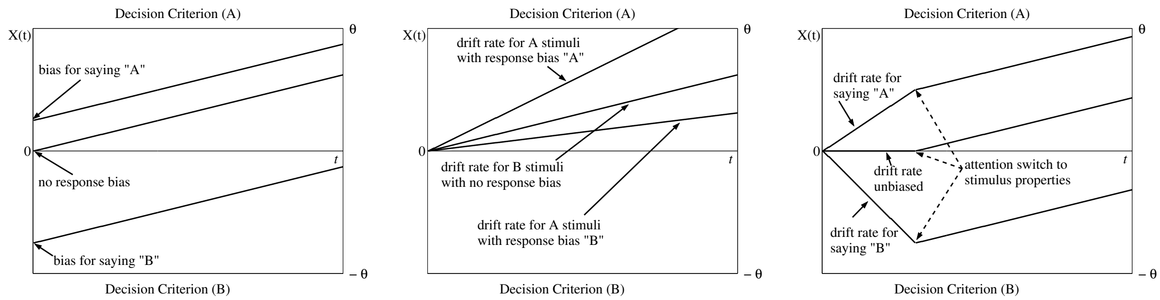


Figure 4: Left: *Bound–change hypothesis*. The payoff matrix induces an a priori bias. The slope of the mean drift rate is the same regardless of the payoffs. Center: *Drift–rate–change hypothesis*. The response bias is mapped onto the mean drift rate. The slope indicates the respect bias. Right: *Two–stage–processing 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]

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 hypothesis, 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 basic process is a Wiener process with two absorbing boundaries; the specific hypotheses are demonstrates in Figure 4. 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.

PUBLICATIONS

Diederich, A. & Busemeyer, J.R. (2005), *Modeling the effects of payoff on response 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.

Busemeyer, J.R., Townsend, J.T., Diederich, A., & Barkan, R. (2005), *Contrast effects of loss aversion?*, Comment on M.Usher and J.L.McClelland (2004), Psychological Review, 112, 1, 253–255.

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

GRANTS

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.[4].

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

2.6 Models of Human Performance

Prof. Dr. Ben Godde, Dr. Claudia Voelcker-Rehage (Neuroscience and Human Performance)

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 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.

PUBLICATIONS

[1] Godde B., Braun C., Wuehle A., Li Hegner Y., Diamond M.E. (2005), *The somatosen-*

sory cortical processing of regular and noisy vibrotactile stimuli as revealed by fMRI, Program No. 173.11, 2005 Abstract Viewer/Itinerary Planner, Washington, DC: Society for Neuroscience, 2005. Online.

[2] Karim A.A., Schueler A., Li Hegner Y., Friedel E., Godde B. (2006), *Facilitating effect of 15 Hz repetitive transcranial magnetic stimulation (rTMS) on tactile perceptual learning*, J Cogn Neuroscience, in press.

[3] Voelcker-Rehage, C. (2005), *The correlation between motor and cognitive development in early childhood*, Journal of Sport & Exercise Psychology, 27, 155.

[3] Voelcker-Rehage, C. (2005), *Der Zusammenhang zwischen motorischer und kognitiver Entwicklung im frühen Kindesalter - Ein Teilergebnis der MODALIS-Studie*, Deutsche Zeitschrift für Sportmedizin, 56, 358-363.

[4] Voelcker-Rehage, C. & Alberts, J. L. (2005), *Age-related changes in grasping force modulation*, Experimental Brain Research, 166, 61-70.

[5] Voelcker-Rehage, C., Stronge, A. J. & Alberts, J. L. (2006), *Age-related differences in working memory and force control under dual-task conditions*, Aging, Neuropsychology, and Cognition, in press.

[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.

2.7 Cellular and Wireless Communications (CWC)

Prof. Dr. Harald Haas (Electrical Engineering)

A new analytical framework has been developed for the analysis of intercellular timeslot allocation over TDMA (time division multiple access) based air-interfaces using TDD (time division duplexing). The analysis is used to evaluate the performance of an adaptive decentralized intercellular interference mitigation technique that exploits the inherent channel reciprocity of TDD. The main principle is that receivers upon successful transmission of a packet transmit a busy burst on a succeeding minislot. Potential transmitters in neighbouring cells sense the minislot prior to signal transmission. With this mechanism, intercellular interference to the existing link is avoided. The performance of this new and patented MAC (medium access control) protocol is compared against conventional timeslot allocation. The new MAC protocol is shown to facilitate network self-organization, offering superior delay, throughput and coverage compared to the state of the art, with a minimum overhead and complexity requirement.

The network model consists of a large service area, with a very "large" number of randomly positioned cells surrounding a central "tagged" cell as shown in Fig. 5. Therefore, cells are irregularly shaped but a maximum cell radius of R_{cell} is assumed.

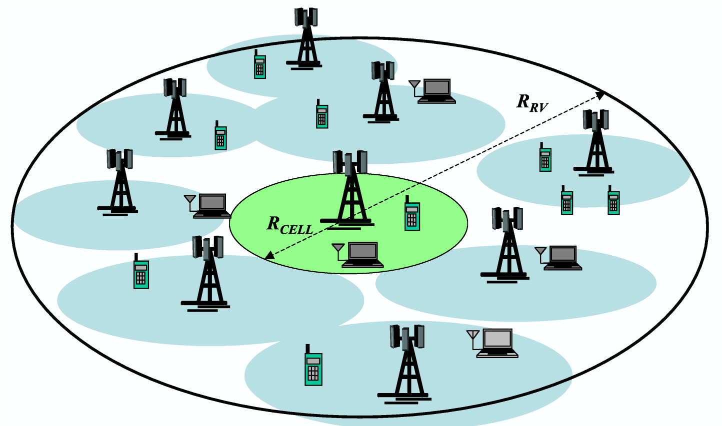


Figure 5: Network deployment [H. Haas et al.]

Furthermore, due to the propagation pathloss, a receiver experiences negligible interference from transmitters outside the "receiver vulnerability" radius R_{RV}, where, typically, $R_{RV} >> R_{\text{cell}}$. Universal frequency reuse is assumed. It is envisaged that this models a typical 4G (4th generation) network deployment scenario, lacking in any network planning, and presents fundamental challenges for intercellular interference mitigation.

The delay performance, when observing an arbitrary timeslot in the tagged cell, is that of a discrete time $M/G/1$ queue, where M indicate a Poisson arrival process, G indicates that service times have an arbitrary statistical distribution, and '1' indicates that it is a single server queue. The mean arrival rate into the slot is λ packet bursts per frame, where a frame consists of one or more timeslots. The mean delay of a packet burst in the $M/G/1$ queue, including the transmission time is given by the Pollaczek–Khinchin formula,

$$D_q = \mathrm{E}\left\{w_{\text{serv}}\right\} + \frac{\lambda \mathrm{E}\left\{w_{\text{serv}}^2\right\}}{2(1 - \lambda \mathrm{E}\left\{w_{\text{serv}}\right\})}. \quad (1)$$

The packet burst service time w_{serv} is modeled as the sum of two independent random variables, $w_{\text{serv}} = w_{\text{vac}} + w_{\text{tx}}$, namely the intercellular timeslot allocation delay (or server "vacation") time w_{vac} experienced by a packet burst at the head of the queue before transmission, and its uninterrupted transmission time w_{tx}. Based on these basic assumptions an analytical model is developed and the results are presented in Fig. 6.

Fig. 6 shows the throughput-delay plots of the new medium access technique compared to state-of-the-art solutions, FSA (fixed slot assignment), and RTSO (random time slot opposing) for R_{cell} equal to 1 km. First, analysis and simulation results match closely. Second, as a reference an idealized scenario, labeled "ideal" with zero intercellular timeslot allocation delay w_{vac} and zero packet loss from interference, is also included. It can be found that the performance of the new technique is very close to the optimum performance which is a significant result.

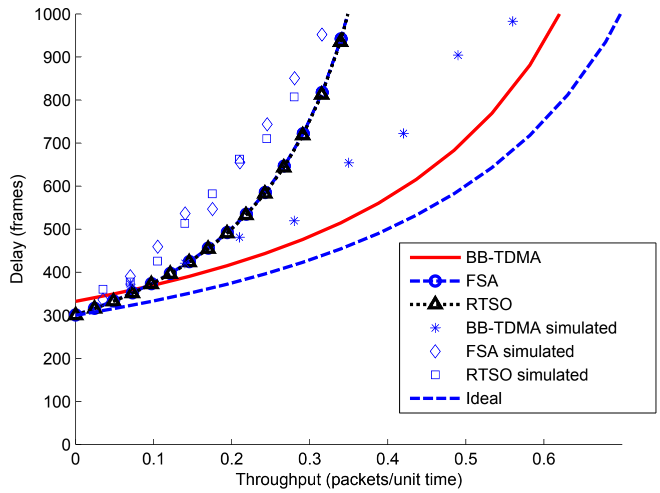


Figure 6: Throughput-delay results of new medium access control (MAC) protocol for hybrid cellular and *ad hoc* 4th generation wireless networks. [H. Haas et al.]

GROUP MEMBERS: Dr. Peter Omiyi, Dr.-Ing. Van Duc Nguyen, Dr. Nedko Nedev, Hrishikesh Venkataraman, Raed Mesleh, Shameem Chaudhury , Denis Kolyuzhnov , Atli Lemma Gebretsadik

PUBLICATIONS

K. Hassan and H. Haas (2005), *User Scheduling for Cellular Multi User Access OFDM System Using Opportunistic Beamforming*, Proceedings of the 10th International OFDM Workshop InOWo'05, Hamburg, German, August 31 – September 1 2005, pp. 26 – 30.

V. D. Nguyen, P. E. Omiyi, and H. Haas (2005), *Decentralised Dynamic Channel Assignment for Cellular OFDM/TDD Networks*, Proceedings of the 10th International OFDM Workshop (InOWo'05), Hamburg, German, August 31 – September 1 2005, pp. 255 – 259.

H. Haas (2005), *Air-interface Requirements of Mobile Data Services*, The Handbook of Information Security, H. Bidgoli (ed.), John Wiley & Sons, New York.

P. K. Jain and H. Haas (2005), *Analysis of User Distributions in CDMA Systems*, Proceedings of the 16th International Symposium on Personal, Indoor and Mobile Radio Communications (PIMRC 2005), Berlin, Germany: IEEE, September 11 – 14 2005, pp. 5 pages on CD–Rom.

P. Omiyi and H. Haas (2005), *Distributed Intercellular Interference Management in 4th Generation TDMA TDD Cellular Mobile Wireless Communications*, Proceedings of the

16th International Symposium on Personal, Indoor and Mobile Radio Communications (PIMRC 2005), Berlin, Germany: IEEE, September 11 – 14 2005, pp. 5 pages on CD–Rom.

H. Venkataraman, H. Haas, Y. Lee, S. Yun, and S. McLaughlin (2005), *Performance Analysis for Hybrid Wireless Networks*, Proceedings of the 16th International Symposium on Personal, Indoor and Mobile Radio Communications (PIMRC 2005), Berlin, Germany: IEEE, September 11 – 14 2005, pp. 5 pages on CD–Rom.

R. Mesleh, H. Haas, Y. Lee, and S. Yun (2005), *Interchannel Interference Avoidance in MIMO Transmission by Exploiting Spatial Information*, Proceedings of the 16th International Symposium on Personal, Indoor and Mobile Radio Communications (PIMRC 2005), Berlin, Germany: IEEE, September 11 – 14 2005, pp. 5 pages on CD–Rom.

C. Evers, R. Esmailzadeh, H. Haas, and M. Nakagawa (2005), *Performance of a hybrid TDD-CDMA system with random slot allocation (RSA) in comparison with an equivalent FDD-CDMA system*, Proceedings of the 14th IST Mobile & Wireless Communications Summit, Dresden, Germany, June 19–23 2005, pp. 5 pages on CD–Rom.

GRANTS

DFG Ha 3570/2-1 (H. Haas), *Dynamic Spectrum Sharing for Asymmetric Services in UMTS Using a Hybrid Ad-Hoc and Cellular Approach.*

DFG Ha 3570/1-1, (H. Haas), *DCA Algorithms and MAC Protocols for COFDM Based Cellular Ad-Hoc Systems Using Carrier Sensing Time Division Multiple Access.*

Bremen T.I.M.E. Grant (H. Haas), *Mobile Discovery System (MDS).*

2 Research Grants from industrial partners.

2.8 Galaxy formation

Dr. Matthias Hoeft and Prof. Dr. Marcus Brüggen (Astrophysics)

Galaxies came apparently into being. Relic microwave radiation shows unambiguously that the early Universe was –almost– homogeneous. The tiny fluctuations of the matter distribution can also be determined by the relic radiation. During the evolution of the Universe those fluctuations grow and collapse by gravitational attraction to galaxies or large assemblies of galaxies. From a numerical point of view we are in a favorable position: We know precisely the initial conditions and we know the governing physical processes. However, those simulations still fail to reproduce the richness of –in particular large– spiral galaxies in the Universe. Since the evolution beyond galactic scales is well under control in those simulations, neglected processes in the galaxies, as supernova feedback, seems to play a crucial role for galaxy formation.

We study the formation of individual galaxies in a cosmological environment using smoothed-particle-hydrodynamics simulation. The environment which provides the realistic tidal fields is represented by a coarsely resolved mass distribution. In contrast, the galaxies itself are resolved with hundred thousand or even up to one million particles (for both dark matter and gas). This allows us to study in very much detail how galactic progenitors are formed and how they merge to the final galaxy. The very high resolution allows us in particular to study processes in small sub-clumps which fall after deceleration by dynamical friction into the central host galaxy. It is believed that the existence of those substructures hampers significantly the formation of a disk. In simulations where those substructures are smeared out large disks can be formed easily. Our main goal is to study how supernova feedback may help to reduce the destructive effect of galactic substructures on the disk formation. It is observationally evident that supernova winds remove gas in particular from small galaxies. Metalicity in the inter-galactic medium is a clear attestor for expelling galactic material. However, even with the best resolved simulations those processes need to relay on sub-resolution models for star formation and stellar feedback. To model realistic galaxies in a cosmological environment a suitable sub-resolution model has to be found.

This project is done in cooperation with several other research groups in Potsdam (Germany), Madrid (Spain), and Paris (France). Large simulations are carried out at national supercomputing facilities, in particular at John von Neumann-Institute for Computing (Jülich, Germany) and at Mare Nostrum supercomputer (Barcelona, Spain). However, those large computations would not be possible without extensive model development and parameter studies which are done to a large extent at the CLAMV facilities.

2.9 The Interaction of Reflexive and Volitional Attention

Prof. Dr. 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 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.

2.10 Network Dynamics

Prof. Dr. Hildegard Meyer-Ortmanns (Physics)

1. Disassortativity in Self-similar Scale-free Networks

(Work in collaboration with S.-H.Yook and F. Radicchi (IUB))

Recently, applications of statistical physics to networks became quite topical. The networks range from genetic, proteomic, metabolic and neural systems to social systems as well as artificial ones like the worldwide web and the internet. Apart from static properties there are also dynamical processes in common to these networks like spreading or cooperation phenomena or self-organization of individual units. For example, spreading viruses may refer to diseases in social systems as well as to computer viruses spreading in the internet. An example for cooperation and self-organization is the formation of synchronized clusters in an ensemble of oscillators, similar to an ensemble of clocks.

In our group we are studying such dynamical processes on a variety of network topologies like regular, small-world or scale-free networks. Networks with so-called scale-free degree distributions are frequently found in natural data sets. In such networks the typical number of edges, which is assigned to nodes, can vary over a large range, so that it is not unlikely to find hubs as well as almost isolated nodes at the same time. On the other hand, self-similar features are well-known from fractals and critical phenomena and attract the attention of theoreticians to explain their origin. For a long time both properties, the scale-free topology and the self-similarity, seemed to be incompatible in networks. Only recently it was found that both features can be identified in natural data sets if an appropriate tiling procedure for calculating the fractal dimension is applied. We wanted to obtain a deeper understanding of the simultaneous occurrence of these features. In view of that we analyzed correlations between the number of ingoing and outgoing edges of certain subsets of nodes and tested on properties called the assortativity or disassortativity of the network. (In assortative networks it is, for example, likely that nodes with similar degrees are connected, while a connection with very different numbers is most likely in disassortative ones.) As result we found out that the exciting combination of scale-free and self-similar properties usually leads to disassortative behavior. It is still quite challenging to explore the corresponding features translated into biological terms, which may be a favor for interactions between complementary units rather than similar ones, as it is known to occur in the immune system, for example. The results were published in Phys.Rev.E under Rapid Communications in 2005.

COMPUTATIONAL ASPECTS: The datasets corresponding to the various networks have the size of several hundred MB, the largest one was 429 MB. These sets had to be analyzed via partitioning them according to certain rules and iterating this procedure a number of times. The number of nodes in the network was up to 400000 and the number of edges up to 3×10^7. For our analysis we had to measure several local quantities like the degree of the nodes before and after the tiling. The procedure was comparable to iterating the renormalization group in spin systems.

TECHNICAL DETAILS: We used Intel C/C++ compiler as well as GNU-C compiler to generate the serial codes. Each code required around 3 days of CPU time. For the relationship between the self-similarity and (dis)assortativity of complex networks we had to analyze real network datasets. The largest dataset was the actor network whose size is around 429 MB. The required CPU times for small datasets including biological interaction datasets were 2 or 3 days of CPU time, but, for example, the box counting in the actor network took around 11 days of CPU time. We used up to 15 processes at the same time.

2. Synchronization of Kuramoto Oscillators on Regular Network Topologies

(Work in collaboration with F. Radicchi (IUB))

Synchronization phenomena are ubiquitous in nature, ranging from applications in biological systems like genetic and metabolic networks, social systems, physical systems like ensembles of clocks, to unwanted synchronization between nerve and muscle cells in Parkinson's disease. One prototype model that exhibits global synchronization between limit cycle oscillators is the Kuramoto model. We generalized this model to include a continuously varying interaction range from next-neighbor short-range interactions to all-to-all interactions and studied the phase transition from a synchronized phase to a desynchronized phase for various network topologies, i.e. for rings, chains, square lattices and Cayley trees. As it turned out, torus and ring topologies facilitate synchronization in contrast to open chains or non-periodic boundary conditions in higher dimensional lattices.

These results could be derived analytically only in the limiting cases of next-neighbor and infinite-range coupling, for all other type of couplings they were obtained numerically by solving the differential equations with the fourth order Runge Kutta algorithm. We observed an interesting phenomenon, a so-called reentrance of the synchronization transition as a function of the interaction range. This means that there is an intermediate interaction range for which the global synchronization of the system becomes very difficult or impossible while for smaller or larger interaction range it is possible. Moreover it turned out that the distinguished oscillators, called pacemakers, which differ from the rest of the system by having a much larger eigenfrequency, act as topological defects in an otherwise homogeneous system. The limit behavior of the other oscillators is very sensitive to their spatial distance from the pacemakers. This work led to one paper that was just submitted for publication and a second one that is under progress.

Furthermore we changed the continuous type of interaction of Kuramoto oscillators to so-called pulse-coupled oscillators that provide a more realistic description of networks where the interaction is mediated via pulses as in neural networks. Here the synchronization pattern and the existence of a finite synchronization threshold depends sensitively on the normalization of the coupling parameter. Work in this direction is in progress.

COMPUTATIONAL ASPECTS: The work on Kuramoto oscillators for intermediate coupling range and on pulse coupled oscillators was purely numerical work. We considered ensembles of up to 100 Kyramoto oscillators and up to 1000 pulse-coupled oscillators. The typical transient time until the final stable state was reached increased exponentially with the system size for Kuramoto oscillators and linearly with the system size for pulse coupled oscillators. The variation of the parameter, tuning the interaction range, of the coupling strength and the system size and the measurements of different order parameters for indicating the state of synchronization were CPU-time consuming. For further details see the technical aspects below.

TECHNICAL DETAILS: We used the same CLAMV-facilities as under 1, the CPU-time for typical runs was about 10 hours.

3. Future Plans

Our main focus of future research will remain Statistical Physics of Networks with applications to systems of biology and information science. The dynamics of such systems is modeled via cellular automata or differential equations, which are integrated numerically. Also in 2006 my collaborators (one post-doc, one PhD-student, and one Humboldt fellow) will need the CLAMV-facilities. I expect some students for guided research, who are interested in simulating aspects of population dynamics. They will need CLAMV facilities for restricted periods of time (of the order of three months each). For a future project on the analysis of metabolic networks I have applied for a grant from the VW-foundation asking for support of one further post-doc position.

GRANTS

One PhD-student (F.Radicchi) is supported by a DFG (Deutsche Forschungsgemeinschaft)-grant since June 2004. Parts of his PhD-thesis are numerical simulations of dynamical processes on networks.

Since June 2005 we have a Humboldt-fellow (Dr.X.Li) from China (University of Shanghai), who graduated in Computer Science and joins our group for one year, working on networks. His contributions are almost exclusively numerical work. He will use the facilities of CLAMV in future projetcs.

PUBLICATIONS

B. Berg, H. Meyer-Ortmanns, and A. Velytsky (2005), *Model A dynamics and the deconfining transition*, Nucl.Phys.B (ProcSuppl.) 140 , 571-573.

S. H. Yook, F. Radicchi and H. Meyer-Ortmanns (2005), *Self-similar scale-free networks and disassortativity*, cond-mat/0507198, Phys.Rev.E 72, 045105, Rapid Communications.

X. Li, H. Meyer-Ortmanns and X. Wang (2005), *Chaotic and periodic spreading dynamics in discrete small-world networks*, IEEE Int. Symposium on Circuits and Systems (ISCAS 2005), May 23-26, 2005, Kobe, 280.

S. H. Yook and H. Meyer-Ortmanns (2006), *Synchronization of Rössler oscillators on scale-free topologies*, cond-mat/0507422, submitted for publication.

F. Radicchi and H. Meyer-Ortmanns (2006), *Kuramoto oscillators on chains, rings and Cayley trees*, cond-mat/0508611, submitted for publication.

2.11 Geometry of Adsorbed Chiral Ligands on Nanoscale Pt, Pd and Fe

Prof. Dr. Ryan Richards, Alexander Kraynov (Chemistry)

Chiral ligands modifying transition metal surfaces (primarily Pt and Pd) represent one approach towards asymmetric heterogeneous catalysis. Since it has been effectively demonstrated that the orientation of the modifier is critical to the induced enantioselectivity of the heterogeneous systems, we have decided to investigate the geometry of cinchonidine adsorbed on Pt and Fe nanoclusters and the manmade ligand quiphos on Pt. Here, we report a combined DRIFTS (Diffuse Reflectance Infra-red Fourier

Transform Spectroscopy)-geometry optimization modeling study that demonstrates the ability of these methods to determine the geometrical orientation of modifiers on nanocluster systems and thus insight into these complex catalytic systems. We have investigated the geometry of cinchonidine adsorbed on Pt and Fe nanoclusters and the manmade ligand quiphos on Pt (Fig. 7).

Hence, since the optimized geometry of cinchonidine molecule and vibration modes with corresponding dipole moments orientation were found from DFT calculations (which have been performed on the CLAMV of IUB), it is possible to establish the orientation of the cinchonidine molecule with respect to the metal surface. This has been done for every observed vibrational frequency.

From analysis of the DRIFT spectrum (Fig. 8) of cinchonidine modified Pt nanoclusters it was concluded that cinchonidine was found in both the 'flat' (Fig. 9) and two 'tilted' adsorption modes, the so called 'α-H abstracted' and 'N-lone pair bonded' (Fig. 9, since both tilted mode are similar, only last is shown). In the case of the IR spectrum of cinchonidine on Fe (Fig. 8) the two strong peaks at 763 cm-1 and 1105 cm-1 indicate the 'flat' adsorption mode, the medium peak at 1566 cm-1 indicates 'flat' and/or 'tilted' mode and a shoulder at 1585 cm-1 indicates the 'tilted' mode. From this data it is possible to conclude that cinchonidine on Fe nanoclusters was definitively found in the 'flat' adsorption mode for and possibly in the 'tilted' mode, since the shoulder does not seem conclusive. All observed peaks corresponding to IR vibrations of quiphos adsorbed on Pt (Fig. 8) demonstrate two orientations of the dipole moment: mostly perpendicular to the quinoline ring and mostly perpendicularly to the phenyl ring. This leads us to propose two orientations of adsorbed quiphos on Pt. In the first mode, quiphos is adsorbed on Pt via the quinoline anchor (Fig. 10), in the similar way as cinchonidine does, but, possibly more tilted; in the second mode – via the phenyl group (Fig. 10) and possibly via 3,4N and/or P atoms. Some degree of tilt is also possible in both cases. In contrast to the cinchonidine, quiphos can not be adsorbed in a tilted orientation mode, for example, through the nitrogen in quinoline part without significant changes in geometry.

Authors thank International University Bremen and EU-COST D24 for providing CLAMV computation hours, for facility and financial support; Prof. Gerard Buono and Dr. Didier Nuel of Université Aix-Marseille III, France for providing the quiphos ligand.

2.12 Ram pressure Stripping of Disk Galaxies

Dr. Elke Rödiger (Astrophysics)

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

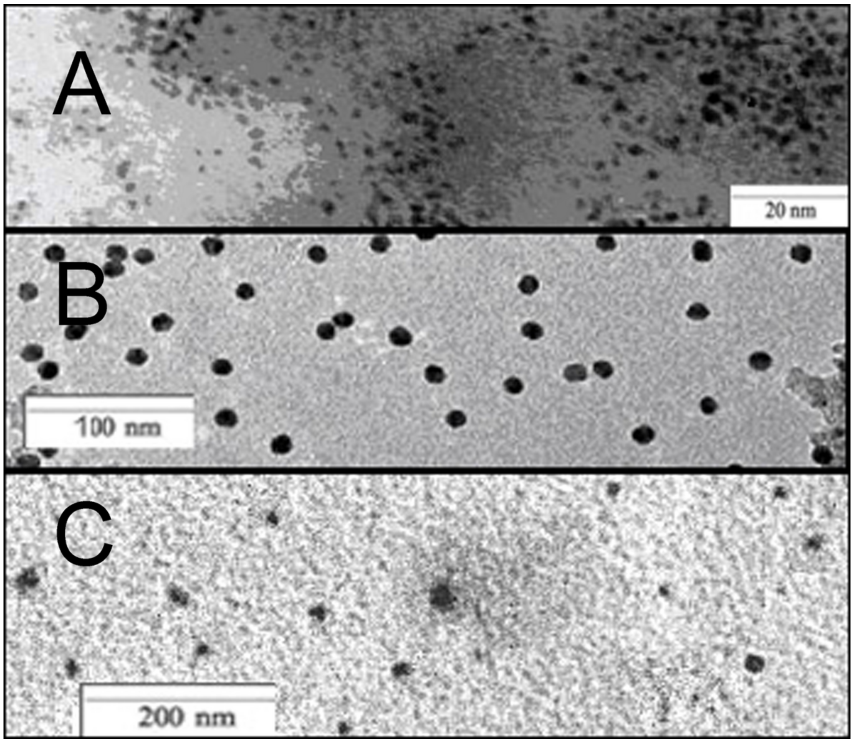


Figure 7: TEM image of Pt nanosized particles modified by cinchonidine (A), cinchonidine on Fe (B), quiphos on Pt (C). [R. Richards and A. Kraynov]

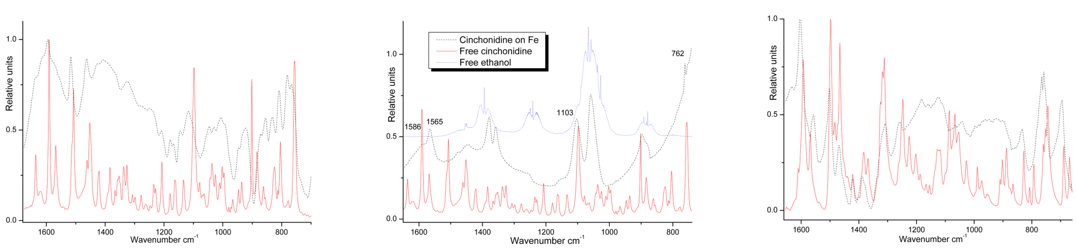


Figure 8: Left: IR spectrum of free and adsorbed on Pt cinchonidine. Solid line - free cinchonidine, dash - sample 1. Center: IR spectrum of ethanol, free and adsorbed on Fe cinchonidine. Solid line - free cinchonidine, dot - ethanol, - dash sample 2. Right: IR spectrum of free and adsorbed on Pt quiphos. Solid line - free quiphos, dash - sample 3. [R. Richards and A. Kraynov]

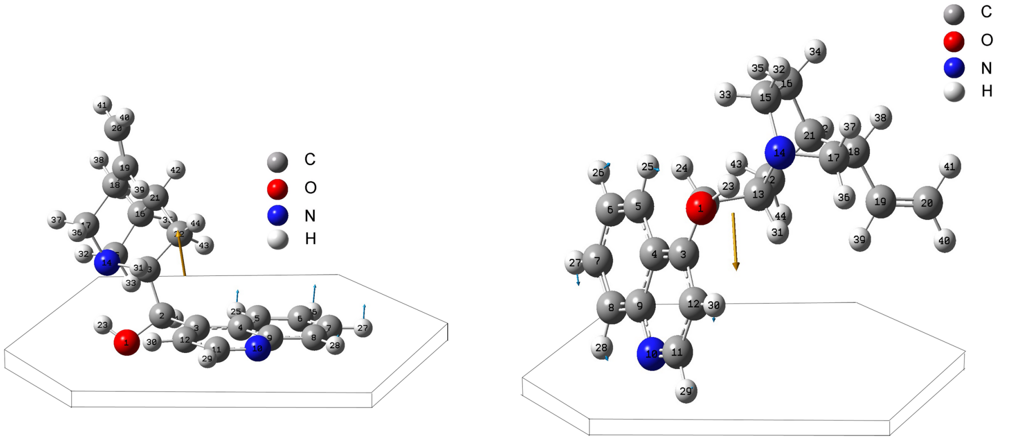


Figure 9: Left: Flat adsorbed cinchonidine demonstrates vibration mode at 768 cm-1 with dipole moment (big arrow) orientated mostly perpendicularly to the metal surface. Right: Tilted adsorbed cinchonidine demonstrates vibration mode at 1514 cm-1 with dipole moment (big arrow) orientated mostly perpendicularly to the metal surface. In each diagram, the most intensive displacement of atoms is shown by small arrows. [R. Richards and A. Kraynov]

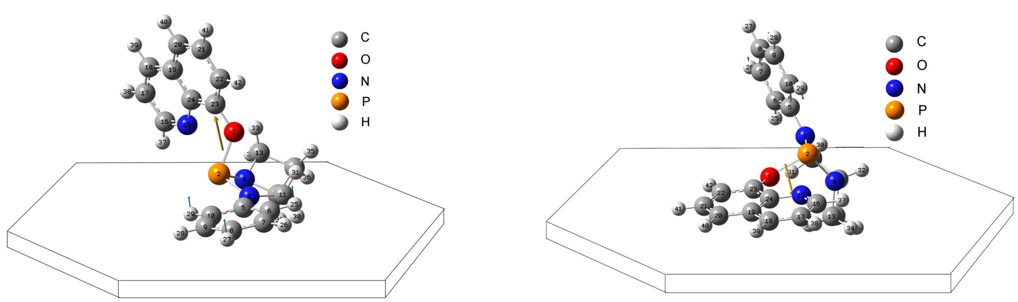


Figure 10: Right: Flat adsorbed quiphos demonstrates vibration mode at 1604 cm-1 with dipole moment (big arrow) orientated mostly perpendicularly to the metal surface. Right: Flat adsorbed quiphos via phenyl ring demonstrates vibration mode at 696 cm-1 with dipole moment (big arrow) orientated mostly perpendicularly to the metal surface. The most intensive displacement of atoms is shown by small arrows. [R. Richards and A. Kraynov]

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). This code was developed by the ASC/Alliances Center for Astrophysical Thermodynamical Flashes. Its modularity makes is suitable for a large variety of problems. We modified the FLASH code in order to simulate the evolution of a galactic gas disk in an ICM wind (i.e. we study ram pressure stripping in the rest frame of the galaxy). 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.

In our recent work, we have focused on the question how the stripping effect depends on the inclination angle between the galaxy's rotation axis and the ICM wind direction. We find 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 (inclination angle $i = 90°$). However, with increasing inclination angle, the stripping proceeds more and more asymmetrical. Figure 11 shows the gas density in slices through the simulation box for two different cases. In both cases, the ICM wind can strip the outer part of the galactic gas disk, but in the edge-on case the remaining gas disk is larger and more asymmetrical.

Interestingly, we find that in the initial stripping phase the tail of gas stripped from the galaxy does not necessarily point exactly in a direction opposite to the galaxy's direction of motion. Therefore, the observation of a galaxy's gas tail may be misleading about the galaxy's direction of motion.

PUBLICATIONS

E. Roediger and M. Brüggen, Ram pressure stripping of disc galaxies. The role of the inclination angle, submitted to MNRAS, 2005, astro-ph/0512365

2.13 Excited Electronic States

Prof. Dr. Michael Rohlfing (Physics)

The focus of our work is on excited electronic states in condensed matter. Such states and their spectra play a key role in understanding optical properties, in characterizing materials, for optoelectronic mechanisms, and more. Of particular interest are systems that are characterized by quantum-mechanical states on the length scale of the atomic bond. The properties of such nanostructured materials go far beyond those of the extended solid. They require a microscopic theory which takes the single

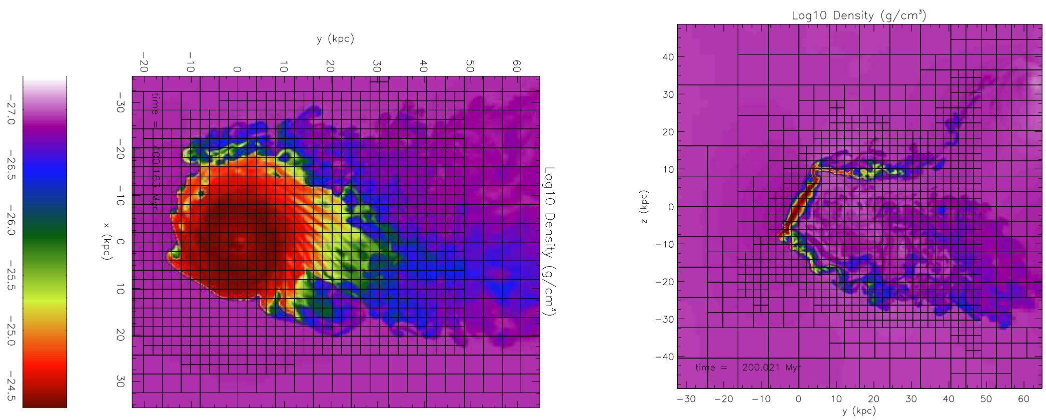


Figure 11: Cut through the simulation box, showing the colour-coded gas density in the x-z-plane. For two different inclinations of the galactic disk: $i = 90^\circ$ (left, the disk is seen face-on), $i = 30^\circ$ (right). The ICM wind is flowing along the y-axis (from left to right) in both cases. The outer parts of the gas disk are stripped by the ICM wind. In the 90° case, the stripping proceeds asymmetrical. The squares demonstrate the adaptive refinement of the resolution: One square corresponds to one block with 8^3 grid cells. [E. Rödiger]

atom and its orbitals as the smallest unit, and which is formulated as an ab-initio theory, without adjustable parameters. In addition, electronic states and their spectra are significantly affected by many-body effects (in particular, electronic correlation effects) whose careful treatment by many-body perturbation theory constitutes one of the main aspects of this field.

An important part of our work is given by the symbiosis between fundamental physical concepts and numerical methods, i.e. by the realization of many-body perturbation theory in efficient computer algorithms. Employing this software we investigate interesting topics of various material classes. The approach can thus be classified as belonging to the boundary between fundamental many-body physics, computational physics, and materials science.

Simulation of Scanning Tunneling Microscopy (STM) images

One current project of studying excited states is given by the simulation of scanning tunneling microscopy (STM) imaging. The tunneling process as such, in which electrons are removed from or added to a material by the STM tip, constitutes an excitation of the material's electronic structure: the number of electrons is changed by ± 1, and the associated energy and STM image correspond directly to the band-structure energy and quantum-mechanical wave function of the respective quasiparticle excitation. This poses a significant problem to simulation. On the one hand, the material's electronic structure must be treated as a true many-body problem, which can be achieved within many-body perturbation theory (MBPT) and the GW approximation for the electron self-energy operator. On the other hand, the numerical realization of such an MBPT approach for a tip-surface system is more difficult than for a bulk system. Most importantly, the exponential decay of the wave functions into space makes it difficult to evaluate them at the position of the STM tip, which can be as much as 10 Angstrom outside. At such distances, the relevant electronic wave functions can have decayed to only 10^{-5} of typical values inside a material, which is difficult to evaluate with the necessary precision. One main part of the project is thus devoted to the numerical evaluation of such spatial decay, which is achieved by decomposing the wave functions into two-dimensional Fourier components, extending those to the desired tip position, and reconstructing the entire wave function by Fourier summation.

STM simulation of the Si(111)-(2$\times$1) surface

Si(111)-(2$\times$1) constitutes an important semiconductor surface, which — even after 30 years — is still of high interest for fundamental research. In close cooperation with experimental colleagues from Göttingen (M. Wenderoth and R. Ulbrich) we are aiming at understanding important spectral features of the clean surface, as well as surface defects. For illustration, Fig. 12 shows STM data of the Si-atom Pandey chains that terminate the surface (running from left to right, as indicated in the panels on the right).

The most striking feature visible here is that at positive and negative tunneling voltage, completely different electronic states are probed. At positive voltage, addressing empty states above the fundamental band gap, the so-called D_{down} surface state is excited, which is given by orbitals at the low-lying (=down) atoms of the Pandey chain (indicated by the smaller circles in the figure). At negative voltage, on the other hand, the so-called D_{up} state (which has energies below the band gap and is occupied) is addressed, which is composed from orbitals at the high-lying (=up) atoms of the chain (protruding into the vacuum, indicated by the large circles in the figure).

Molecules on metals: PTCDA on Ag(111)

Adsorbate systems composed of organic molecules deposited on metal substrates constitute a fast-growing field of research. Potential applications include ballistically-controlled charge-transfer contacts and molecular electronics. Here we aim at a detailed undertanding of the structure and dynamics of such systems, of which STM is an invaluable part.

In the case of PTCDA on Ag(111), the calculation of STM images allows for a systematic comparison with experimental data gained in the group of S. Tautz (IUB). Such a

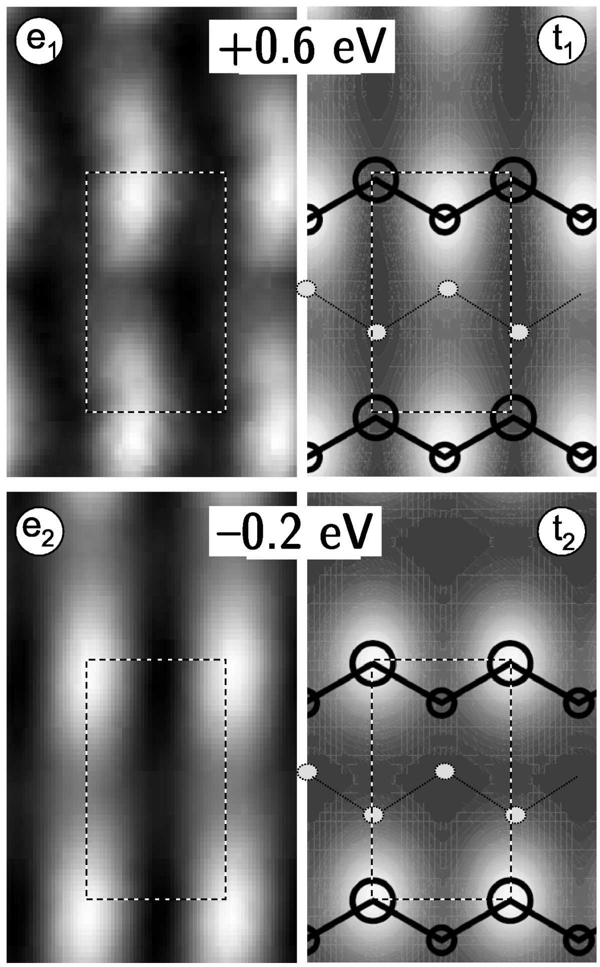


Figure 12: Measured (left) and simulated (right) STM images of the Si(111)-(2×1) surface. The images in the upper (lower) panels have been recorded for positive (negative) STM voltages, thus addressing the empty (occupied) electronic states.
[M. Rohlfing et al.]

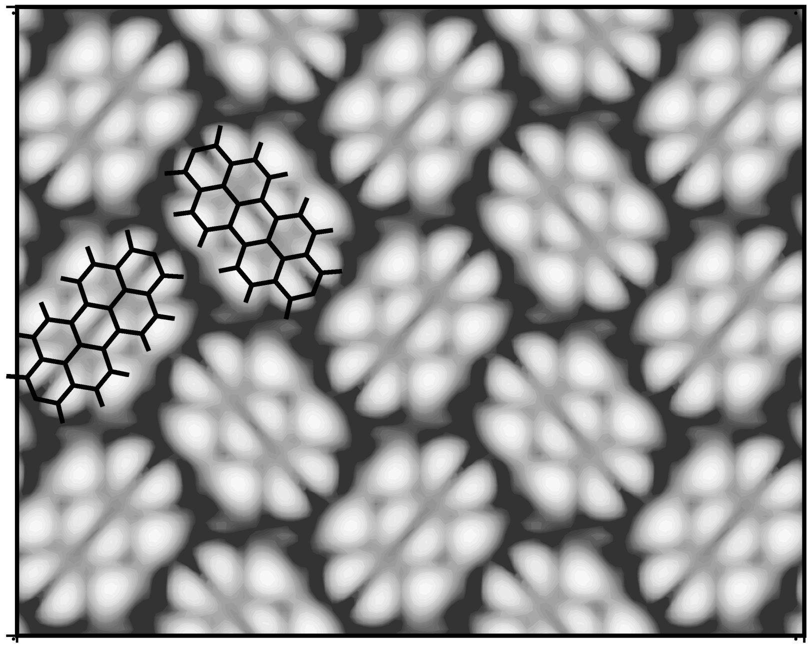


Figure 13: Calculated STM topographic image of a monolayer of PTCDA adsorbed on a silver (111) surface. The calculations are based on density-functional theory, combined with a specific wave-function expansion approach to the position of the STM tip. Tunneling voltage –1.0 eV, tip height 7.1 Å above Ag(111). [M. Rohlfing et al.]

comparison enabled us to identify the preferred adsorption site of PTCDA on Ag(111) (bridge position) with a lateral accuracy of only about 0.2 Å, which had not been possible before. In addition, the analysis of the voltage-, height-, and tip-dependence of the images yields deep insight into details of the electronic structure of this prototypical adsorbate system. Many aspects of the competition between adsorbate-substrate interaction and adsorbate-adsorbate interaction are still poorly understood, and our studies open a path to address such issues.

Fig. 13 shows some characteristic results of our simulation. In the current case, an ordered monolayer of PTCDA on Ag(111) is considered, leading to the well-known herring-bone structure (with two molecules per unit cell) clearly visible in the figure. More detailed inspection reveals that the intramolecular contrast is primarily given by the lowest unoccupied molecular orbital (=LUMO), which becomes partly populated upon adsorption and thus contributes to (and dominates) the STM image at moderately negative voltages.

Selected publications

R. Oszwadowski, M. Reichelt, T. Meier, S. W. Koch, and M.Rohlfing (2005), *Nonlinear optical response of the Si(111)-(21) surface exciton: Influence of biexciton many-body correlations*, Phys. Rev. B 71, 235324.

T. A. Niehaus, M. Rohlfing, F. Della Sala, A. Di Carlo, and Th. Frauenheim (2005), *Quasiparticle energies for large molecules: A tight-binding-based Green's-function approach*, Phys. Rev. A 71, 022508.

M. Weinelt, M. Kutschera, R. Schmidt, Ch. Orth, Th. Fauster, and M. Rohlfing (2005), *Electronic structure and electron dynamics at Si(100)*, Appl. Phys. A 80, 995.

A. Hauschild, K. Karki, B. C. C. Cowie, M. Rohlfing, F. S. Tautz, and M. Sokolowski (2005), *Molecular Distortions and Chemical Bonding of a Large pi-Conjugated Molecule on a Metal Surface*, Phys. Rev. Lett. 94, 036106.

N.-P. Wang, M. Rohlfing, P. Krüger, and J. Pollmann (2005), *Femtosecond dynamics of excited states of CO adsorbed on MgO(001)-(1x1)*, Phys. Rev. B 71, 045407.

J. K. Garleff, M. Wenderoth, K. Sauthoff, R. G. Ulbrich, and M. Rohlfing (2004), *2x1 reconstructed Si(111) surface: STM experiments versus ab initio calculations*, Phys. Rev. B 70, 245424.

GRANTS

DFG RO 1318/4-3, *Excited states of adsorbed molecules on semiconductor and insulator surfaces.*

2.14 Simulation Studies of Compact Stellar Objects

Prof. Dr. Stephan Rosswog (Astrophysics)

In spring 2005 a 24 processor SGI Altix shared memory computer has been installed on the IUB campus. It was funded to 50% by IUB and 50% by a HBFG-proposal submitted by myself.

My Smoothed Particle Hydrodynamics (SPH) code with various physics modules (Rosswog and Davies 2002, Rosswog and Liebendörfer 2003, Rosswog et al. 2003) that has been developed mainly to simulate compact stellar object encounters, has been ported and adapted to this new computer. The code scales very well: for SPH particle numbers in excess of a 10^6 particles the code speeds up nearly linearly up to the whole machine. Figure 14 shows a realistic scaling test (oscillations of an isolated neutron star modelled by 2 000 000 particles): on 24 processors a speedup of about 21 is reached. The projects described below have substantially profited from this in-house supercomputing facility.

My research is focussed on the physics and astrophysics of compact stellar objects like White Dwarfs, Neutron Stars and black holes. The involved questions range from the formation of elements in the cosmos over gravitational waves to stellar explosions such as Supernovae or Gamma-ray bursts.

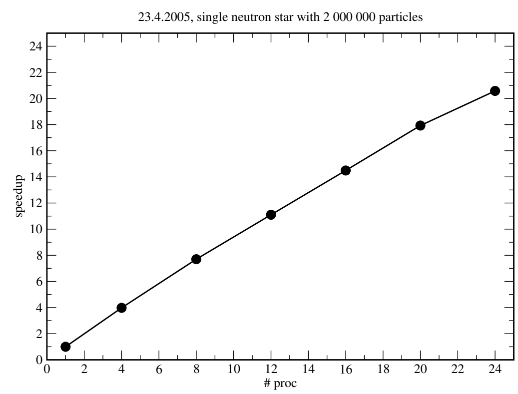


Figure 14: Speedup of the smoothed particle hydrodynamics code developed for neutron star collisions. [S. Rosswog]

Most of these processes are intrinsically three-dimensional, they involve the interplay of various physical processes (hydrodynamics, nuclear burning, neutrino emission/diffusion etc.) and they are highly time dependent (explosions!). It is close to impossible to find meaningful analytical treatments, therefore one has to resort to high-performance computations.

Tidal disruptions of neutron stars by stellar mass black holes

Neutron star black hole binary systems are thought to produce one of the most violent explosions in the Univesre since the big bang: (short) Gamma-ray bursts. Moreover, they are one of the strongest sources of gravitational waves and they are expected to be among the first events that will be detected by ground-based gravitational wave detectors such as LIGO or GEO600.

I have performed a large set of 3D-simulations of such encounters between a neutron star and a black hole. Most of these simulations made use of the JUMP supercomputer located at the Höchstleistungsrechenzentrum Jülich. CLAMV was used as a development platform and most of the data analysis and visualisation was done on the CLAMV facilities.

It could be shown that black holes with masses larger than about 14 $M_\odot$ will not be able to produce a gamma-ray burst (GRB), as the accretion disks that form for these cases (such as panel 3, Fig. 15) are deep inside the innermost stable circular orbit of the black hole. Therefore, very hot and dense disks that are required for large neutrino fluxes and the subsequent neutrino-antineutrino annihilation cannot be build up. An example of such an encounter is shown in Figure 15. If short GRBs really do come

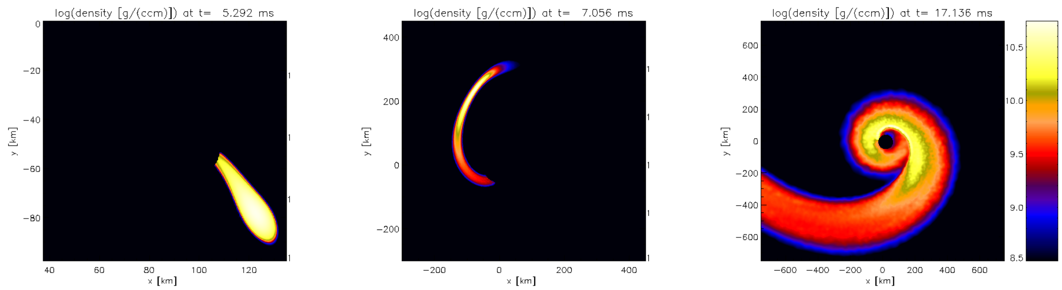


Figure 15: Tidal disruption of a neutron star with 1.4 $M_\odot$ by a 14 $M_\odot$ black hole ($M_\odot$= 1 solar mass). [S. Rosswog]

from neutron star black hole binaries, they have to be produced by lower mass black holes. Results from this study have been published in Rosswog 2005.

Mergers of magnetized neutron stars

Questions similar to those that are raised in the context of black hole neutron star systems also arise for coalescences of double neutron stars.

Neutron stars are highly magnetized objects: at birth a typical neutron star has a field strength of about 10^{12} Gauss. So far, however, it has not been possible to perform simulations of the collision of two *magnetized* neutron stars. In an effort together with Dr. Daniel Price, University of Exeter, UK, we have implemented magnetic fields into my Smoothed Particle Hydrodynamics code via so-called Euler-potentials:

$$\vec{B} = \nabla\alpha \times \nabla\beta. \tag{2}$$

The first calculations of magnetized neutron star mergers have been performed at the end of 2005 on the local SGI Altix supercomputer. The first results (Price and Rosswog 2006) are shown in Figure 16.

A new type of supernova explosion: Tidally induced detonations of White Dwarfs

In places with high stellar densities, such as the center of galaxies or in the core globular clusters, collisions/close encounters of stars/black holes occur quite frequently. We (S.R. and Dr. Enrico Ramirez-Ruiz, IAS, Princeton, USA) have focussed in

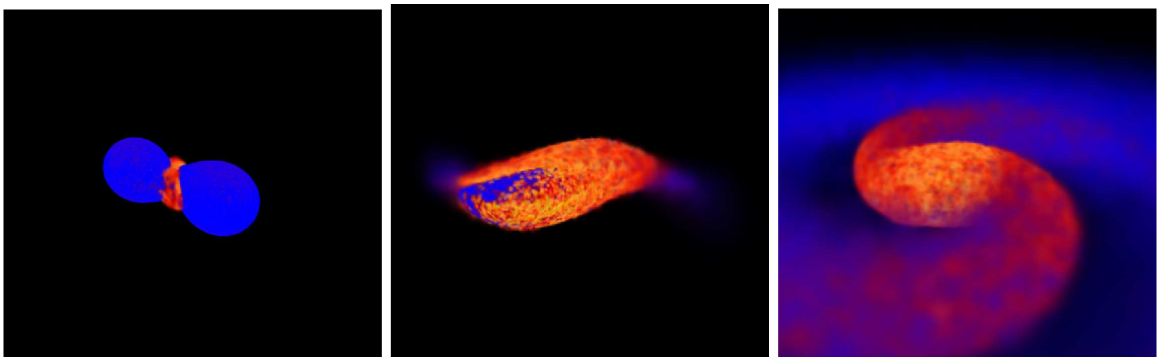


Figure 16: Shown are the milliseconds before and after the coalescence of two magnetized neutron stars. The stars have gradually moved towards each other and then merge in a "plunging phase" within about one orbital period (panel one and two). This object sheds mass into spiral arms that are subsequently wrapped around the central object to form a hot torus (panel three). Colour-coded is the strength of the magnetic field at the surface. The snapshots are taken at 1.85, 3.29 and 4.07 milliseconds after the simulation start. The velocity shear between the stars amplifies the magnetic field within one millisecond by orders of magnitude. [S. Rosswog]

this project on White Dwarf stars as they, being made of '"α-nuclei" such as Helium, Carbon or Oxygen, have the potential to release a lot of nuclear binding energy, provided that temperatures can be reached that are high enough to overcome the mutual Coulomb-repulsion between the nuclei.

To simulate such an ecounter I have taylored a minimal nuclear reaction network (based in the work of Hix et al. 1998) that is now coupled in an operator-splitting way to a Smoothed Particle Hydrodynamics code (a special version that includes the modules relevant for the physics of White Dwarfs). All the simulations have been performed on IUB's new SGI Altix shared memory supercomputer.

We found that in some cases a fly-by at a black hole can provide enough tidal compression, so that the White Dwarf can be thermonuclearly ignited and this results in a violent detonation in which about 10^{51} ergs of nuclear binding energy are released. Such a detonation would look like a peculiar type Ia supernova. An example of a tidal disruption is shown in Figure 17.

PUBLICATIONS

Hix et al., ApJ 503, 332 (1998)

D. Price and S. Rosswog, submitted (2005)

S. Rosswog, Astrophysical Journal, 634, 1202 (2005)

S. Rosswog, Il nuovo cimento C, 28, 607 (2005)

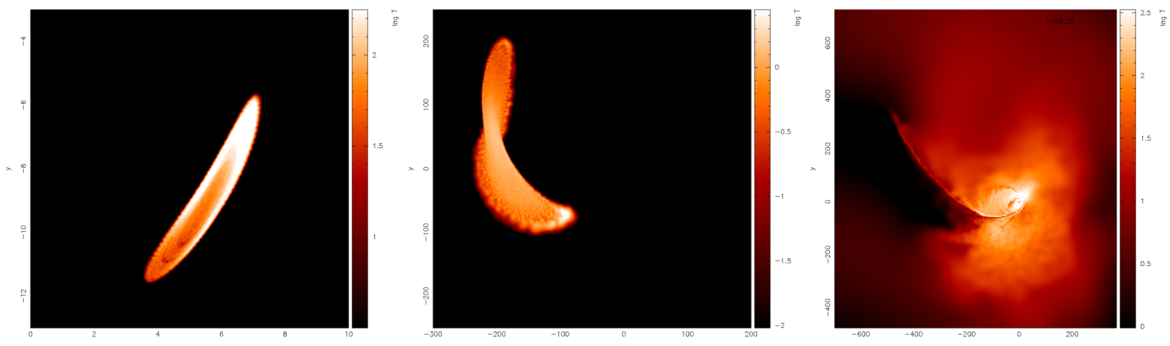


Figure 17: Tidal disruption of a 0.6 solar mass Carbon-Oxygen White Dwarf close to a black hole of 10000 solar masses. Colour-coded is T_6, the temperature in units of 10^6 K. [S. Rosswog]

S. Rosswog, M.B. Davies, MNRAS, 334, 481 (2002)

S. Rosswog, M. Liebendörfer, MNRAS, 342, 673 (2003)

S. Rosswog, E. Ramirez-Ruiz, M.B. Davies, MNRAS 345, 1077 (2003)

2.15 Rational Points on Curves

Prof. Dr. Michael Stoll (Mathematics)

In 2005, I have used some 2000 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 the context of a project undertaken in collaboration with Nils Bruin (Simon Fraser University, Vancouver). The goal of the project was to gather experimental evidence on the question to what extent it might be possible to decide if a given (smooth, projective) algebraic curve (defined over the rational numbers) possesses rational points. To this end, we looked at all curves of genus 2 that are given by an equation of the form

$$C : y^2 = f(x) = f_6x^6 + f_5x^5 + \ldots + f_1x + f_0$$

with f a squarefree polynomial of degree 6 with integral coefficients $f_0, \ldots, f_6$ of absolute value at most 3. On a representative of each of the about 230 000 isomorphism classes of curves thus obtained, we tried to either find a (small) rational point (i.e., a solution to the above equation in rational numbers; as a special case, C is considered to have rational points "at infinity" if f_6 is a square), or else to prove by various methods that they do not have a rational point. After checking "local solubility" (are there solutions in real numbers and solutions modulo n for every integer n?) and performing a so-called 2-descent on the remaining curves, roughly 1500 curves remained.

On these, we wanted to apply a third method, known as “Brauer-Manin obstruction” or “Mordell-Weil sieve”. The method used is based on a suitable embedding of the curve C into its Jacobian variety J (an abelian variety of dimension 2). In a first step, the group of rational points on J (the so-called Mordell-Weil group) had to be computed. Existing algorithms were extended to achieve this. Part of these computations involved the search for rational points on certain 2- and 3-dimensional varieties; some of these computations were done on the CLAMV machines.

The knowledge of the Mordell-Weil group can then be used to compute necessary conditions for rational points in J to be in the image of C. These conditions are obtained by comparing the image of the “mod-p” points on C with the image of the Mordell-Weil group in the “mod p” points of J, for many prime numbers p. In the end one hopes to obtain a contradiction, proving that C does not have rational points. These computations can be time- and space-consuming (there is a combinatorial explosion effect). Again, these computations were carried out in part on the CLAMV machines. In the end, we were able to deal with all the curves we were considering. This encouraging result lends convincing evidence to the conjecture that the existence of rational points on curves should be decidable.

Several papers reporting on the methods used and on the results of the experiment are in preparation.

2.16 Geoscience Modelling, GIS and Data Management

Prof. V. Unnithan, Dr. Angela Schäfer (Geoscience)

During 2005, CLAMV has provided invaluable support to IUB’s IRCCM modelling research, accommodated our HERMES contribution and supported the development of the GIS lab. The hardware and software setup of the GIS lab is explained in section 4. Related teaching activities and workshops are described in sections 3.3 and 3.4, respectively. In the following we summarize research projects in the areas of geoscience modelling and data management.

Geoscience modelling projects

The modelling efforts of the group in 2005 have focused on gas hydrate modelling with a particular emphasis on the theoretical and numerical aspects. Examples of the research conducted by Jakob Hauschildt and Feng Ding (PhD students) are detailed below.

PhD project of Jakob Hauschildt – current status

For the estimation of abundance and properties of worldwide gas hydrate occurrences analytical and numerical one-dimensional models have successfully been applied.

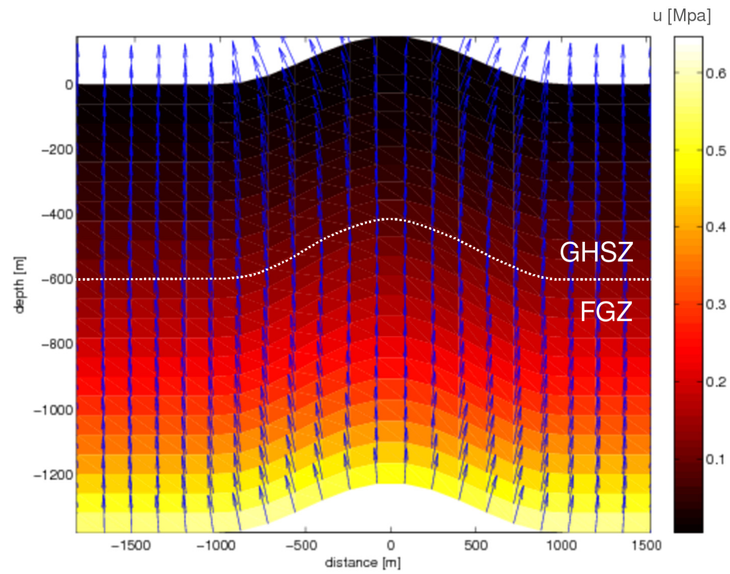


Figure 18: Overpressure and fluid flow induced in a ridge structure by continuous sedimentation. [J. Hauschildt]

These models are based on the assumption that the lateral fluid flow imposes no significant contribution to the transport of solutes and energy. The objective of this study is to substantiate this assumption and to quantify deviations in the resulting hydrate profile in areas with complex bathymetry, exemplified by a ridge structure.

In a sediment volume buried under constant sedimentation including organic matter, the pressure field resulting from compaction according to Athys Law is evaluated to provide the fluid flow driving the transport of dissolved methane, which is converted from the organic matter mediated by bacterial activity. In the gas hydrate stability zone (GHSZ) and the free gas zone (FGZ) methane in excess of its solubility in seawater undergoes a phase transition into the hydrate phase or vapour phase, respectively, and reduces the porosity and influences the hydraulic properties.

While the ridge geometry can significantly affect the flow field, especially if the vertical length scale is not small compared to the lateral extend, the additional deviation caused by reduced permeability due to dispersed hydrate formation is confirmed to be negligible for a hydrate fraction below 10%.

PhD project of Feng Ding – current status

The modelling of hydraulic overpressure was carried out using the commercial basin modelling software PetroMod (IES GmbH). The models are 2D and their geometries were obtained from a 2D multichannel seismic profile (10 km across, 1.5 km thick), shot across a pockmark in the vicinity of ODP site 889/890. Thermal and hydrological data from this ODP drill were used to calibrate the models. The modelling work assumes gas hydrate formation decreases permeability of the host sediments. This in turn can produce hydraulic overpressure inside or below the hydrate zone, and thus mechanically weaken the sediments by reducing their effective stress. Such process should be one of the candidate mechanisms for gas hydrate layer fraction and periodical gas discharge.

The results show that when sedimentation rate of 41.5 cm/kyr, sediment permeability of 0 log mD and gas hydrated sediment permeability of $-1 \log$ mD is assumed, the hydraulic overpressure in the sediment column is very small, far below the fracture threshold. A range of sedimentation rates, sediment permeability and hydrated sediment permeability values were used for model sensitivity testing. The results from these simulations show that even with rather rapid sedimentation rate (340 cm/kyr) the influence of hydraulic overpressure is still rather limited. On the other hand, significant overpressure occurs when the permeability of the hydrated sediment is lower than a fixed value ($-3.5 \log$ mD). Regardless of the sediment permeability (tested -2.5 to $1 \log$ mD), when the permeability of the hydrated sediment is set to be $-3.5 \log$ mD the hydraulic pressure reaches lithostatic (in spite of the fact that the hydrated sediment is fractured). If the hydrated sediment permeability is $-3 \log$ mD, hydraulic pressure is nearly hydrostatic. This result indicates that in this area, the hydration of sediment cannot reduce the sediment permeability over a fixed lower limit.

Further 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 GIS Lab. 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 GIS Lab, 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 Tromsø (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.

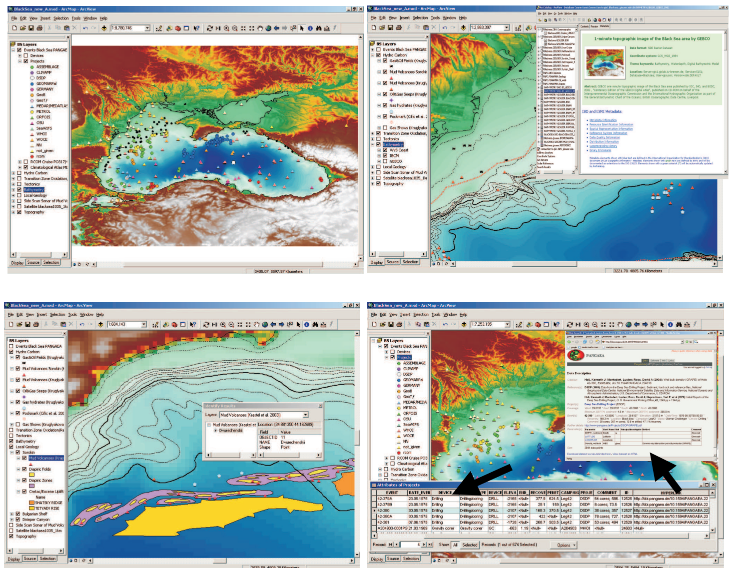


Figure 19: Examples of Black Sea GIS data management at IUB GIS-Lab: top) data visualisation, metadata query; bottom) online data retrieval from IUB's GIS to the World Data Center MARE via common Web browser techniques. [V. Unnithan, A. Schäfer]

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 stared 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 GIS Lab. 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.

Future research projects

Some of the project planned for 2006 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 IUB
- Environmental monitoring of sediment and water in the Lesum.

GRANTS

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

IRCCM and Statoil (Grant 2003-2005)

Projects submitted to ESA and BIA still under consideration i.e. Earthlook (with Peter Baumann), LEMP (Lesum Environmental Monitoring Project with Laurenz Thomsen & Peter Baumann)

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.

2.17 Computational Space Plasma Physics

Prof. Dr. Joachim Vogt (Space Physics)

The interaction of the geomagnetic field with the plasma of the solar wind leads to the formation of a magnetic cavity in near-Earth space that is commonly referred to as the Earth's magnetosphere. The highly variable solar wind causes magnetospheric dynamics on short timescales of hours to days which leads to space weather phenomena like geomagnetic storms, auroral emissions, failures of communication satellites, and electrical power disruptions on the ground. On geological timescales, variations of the geomagnetic core field are expected to have a strong effect on the magnetospheric structure and on the behavior of energetic particles in near-Earth space. At IUB, magnetosphere formation and other space plasma processes are studied using plasma theory, data from spacecraft, and large-scale magnetohydrodynamic (MHD) simulations.

The magnetosphere during geomagnetic polarity transition periods is investigated at IUB in detail in the context of a DFG-funded project entitled *Studies of paleomagnetospheric processes*. The MHD simulation code BATS-R-US was used to carry out a parametric study on the large-scale electrodynamic coupling of the magnetospheric boundary layer to the ionized part of the upper atmosphere (the ionosphere). We investigated the variation of the transpolar potential and the total field-aligned currents with changing geomagnetic dipole moment, ionospheric conductance, and the solar wind magnetic field. The main field-aligned current system is shown in Figure 20. We could reproduce the phenomenon of transpolar potential saturation observed from the ground and gave estimates of transpolar potentials and field-aligned currents for paleomagnetospheres with strongly decreased dipole moments. In general, a fairly good agreement was found between the MHD simulation results and the predictions of the analytical Hill model of transpolar potential saturation. Some corrections to the dipole scaling relations in the Hill model were suggested. This finding was investigated further in a second study (submitted to the Journal of Geophysical Research). We compared our MHD simulations with an empirical model for the size and the shape of the magnetospheric boundary layer (magnetopause) and found very good agreement within the validity range of this model. Outside this range our MHD simulations offer a more complete description of the magnetopause shape and size in terms of solar wind parameters and the geomagnetic dipole moment.

On much shorter timescales like hours or days, the magnetosphere responds to changes in solar wind parameters and yields space weather phenomena like geomagnetic storms and substorms. Most dramatic solar wind variations are induced by coronal mass ejections (CMEs) which are transient solar events that carry huge amounts of solar material (up to 10^{16} g) at large velocities (between 100 and 2000 km/s) from the solar corona into space. CME associated radio emissions are planned to be observed for space weather prediction studies by new generation radio facilities such as the Dutch LOFAR. A MHD simulation project to prepare LOFAR observations of CMEs was defined in collaboration with Marcus Brueggen, and a successful proposal was submitted to the DFG. The project will start in 2006. The parallel computing platforms of the CLAMV will be used to carry out the MHD simulations.

GROUP MEMBERS: Bertalan Zieger, Ph.D., Dr. Joachim Schmidt.

PUBLICATIONS

Zieger, B., J. Vogt, A. J. Ridley, and K.-H. Glassmeier (2005), *A parametric study of magnetosphere-ionosphere coupling in the paleomagnetosphere*, Adv. Space Res.

Zieger, B., J. Vogt, and K.-H. Glassmeier (2006), *Scaling relations in the paleomagne-*

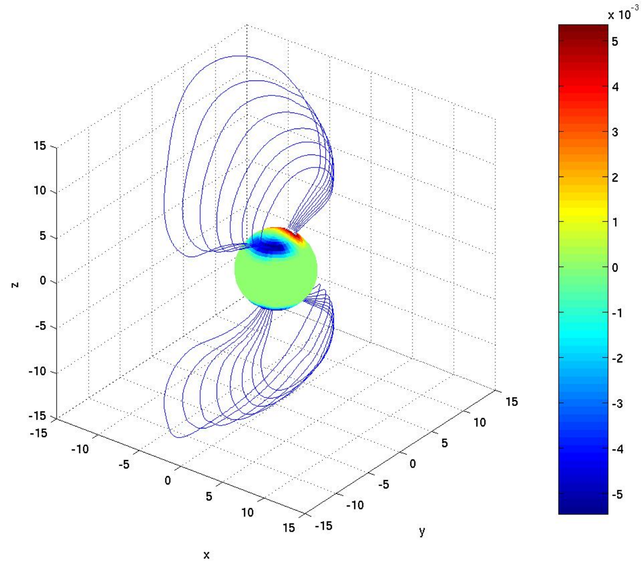


Figure 20: Field-aligned currents connecting the ionized upper atmosphere (ionosphere) with the magnetospheric boundary layer (magnetopause). [B. Zieger, J. Vogt]

tosphere derived from MHD simulations, J. Geophys. Res., submitted.

GRANTS

DFG VO 855/1-3 (2004–2006, 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.*

2.18 Structure-Function Relationship of Membrane Channels

Prof. Dr. Mathias Winterhalter (Biophysics)

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,

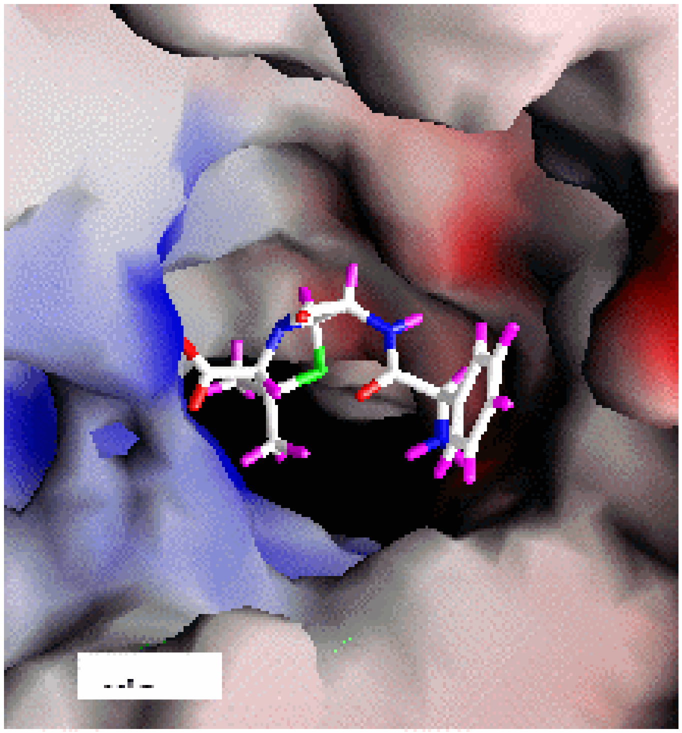


Figure 21: Molecular modelling of an antibiotic molecule (Ampicillin) in an OmpF channel. [M. Winterhalter]

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.

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

PUBLICATIONS

Neves P, Berkane B, Gameiro P, Winterhalter M, Castro B (2005), *Interaction between quinolones antibiotics and bacterial outer membrane porin OmpF*, Biophys. Chem. 113, 123.

Sukhorukov GB, Rogach AL, Zebli B, Liedl T, Skirtach AG, Köhler K, Antipov A, Gaponik N, Susha AS, Winterhalter M, Parak WJ (2005), *Nanoengineered polymer capsules. Tools for detection, controlled delivery and site specific manipulation*, Small 1, 194.

Berkane E, Orlik F, Charbit A, Danelon C, Fournier D, Benz R, Winterhalter M (2005), *Nanopores. Maltoporin channel as a sensor for maltodextrin and Lambda-Phage*, J. Nanobiotechnology 3, 3.

Damian L, Fournier D, Winterhalter M, Paquereau L (2005), *Determination of thermodynamic parameters of Xerocomus chrysenteron lectin interactions with N-acetylgalactosamine and Thomsen-Friedenreich antigen by isothermal titration calorimetry*, BMC Biochem. 6, 11.

Ruysschaert T, Marque A, Duteyrat JL, Lesieur S, Winterhalter M, Fournier D (2005), *Liposome retention in size exclusion chromatography*, BMC Biotechnol. 5, 11.

Ruysschaert T, Sonnen AF, Haefele T, Meier W, Winterhalter M, Fournier D (2005), *Hybrid nanocapsules. interactions of ABA block copolymers with liposomes.*, J Am Chem Soc. 127, 6242-7.

Germain, M, Balaguer, P, Nicolas, JC, Lopez F, Esteve JP, Suhorukov GB, Winterhalter M, Richard-Foy H, Fournier D (2005), *Mammalian cell encapsulation in a polyelectrolyte shell. Preserving cellular metabolism.*, Biosensors and Bioelectronics., in press.

Danelon C, Nestorovich EM, Winterhalter M, Ceccarelli M, Bezrukov SM (2005), *Interaction of Zwitterionic Penicillins with the OmpF Channel Facilitates their Translocation*, Biophys. J., in press.

Winterhalter, M, Sonnen A. (2006), *Stable bubbles*, Angewandte Chemie In. Ed., in press.

Kullman, L, Gurnev, P.A., Winterhalter, M, Bezrukov, S.M. (2006), *Functional Sub-Conformations in Protein Folding: Evidence from Single-Channel Experiments*, Phys. Rev. Lett., in press.

Chaize, B, Nguyen, M, Ruysschaert, T, Le Berre, V, Trevisiol, E, Caminade, AM, Majoral, JP, Pratviel, G, Meunier, B, Winterhalter, M, Fournier, D (2006), *Microstructured liposome array*, Bioconjungate Chem.

Berkane E, Orlik F, Stegmeier JF, Charbit A, Winterhalter M, Benz R (2006), *Interaction of bacteriophage lambda with its cell surface receptor: An in vitro study of binding of the viral tail protein gpJ to LamB (maltoporin)*, Biochemistry.

GRANTS

EU Training network *Molecular origin of antibiotic translocation*, PI M. Winterhalter. This project is performed in collaboration with N. Fertig (München), H. Vogel (Lausanne), J.M. Pages (Marseille), P. Gameiro (Porto), M. Page (Basel).

Volkswagen Foundation *Complex Materials: "Cooperative Projects of the Natural, Engineering, and Biosciences": Nanoengineered polymer capsules: Detection and manipulation for nanoreactors and controlled delivery.* (I/80 051) in collaboration with G. B. 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.

2.19 Computer Simulation of Biomolecules

Prof. Dr. Martin Zacharias (Computational Biology)

The research focus of the Computational Biology group is the study of biomolecular association and conformational flexibility using computer simulation approaches. The simulation studies are aimed to better understand structure formation of biomolecules and the mechanism of ligand-receptor 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 that allow 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.

We use extensively the CLAMV Linux Clusters as well as the teaching lab computer resources. During 2005 we have considerably improved our protein-protein docking software ATTRACT [1] to include now efficiently various levels of flexibility of the binding partners [2-5, see Fig. N]. Extensive simulations on the CLAMV resources of an important structural motif in RNA have been performed that included the calculation of free energy differences between conformational substates [6]. In collaboration with the group of U. Schwaneberg (Biochemical Engineering) and A. Gelessus a Web resource on the efficiency prediction of various mutagenesis methods has been started [7]. Together with the same group we studied the influence of organic cosolvents on the industrially important enzyme P450 BM-3 and on mellitin using molecular dynamics simulations [8,9]. Ongoing collaborative projects with experimental groups include modelling studies using CLAMV computers on protein-ligand interactions [10,11] and on RNA molecules [12,13].

PUBLICATIONS

[1] M. Zacharias (2005), *ATTRACT: Protein-Protein Docking in CAPRI Using a Reduced Protein Model*, Proteins 60, 252-256.

[2] K. Bastard, Prevost, C., and M. Zacharias (2006), *Accounting for loop flexibility during protein-protein docking*, Proteins, in press.

[3] A. May, and M. Zacharias (2005), *Accounting for global protein deformability during protein-protein and protein-ligand docking*, Biochem. Biophys. Acta, 1754, 225-231.

[4] N. Riemann and M. Zacharias (2005), *Refinement of protein cores and protein-peptide interfaces using a potential scaling approach*, Prot. Engineering 18, 465-476.

[5] M. Zacharias (2005), *Vorhersage von Protein-Protein Wechselwirkungen durch Docking-Simulationen*, Bioforum 2/2005, 38-39.

[6] A. Barthel, and M. Zacharias (2006), *Conformational Transitions in RNA Single Uridine and Adenosine Bulge Structures: A Molecular Dynamics Free Energy Simulation*, Study. Biophys. J. in press.

[7] S. Wong, D. Roccatano, M. Zacharias and U. Schwaneberg (2006), *A Statistical Analysis of Random Mutagenesis Methods Used for Directed Protein Evolution*, J. Mol. Biol. 355, 858-871.

[8] D. Roccatano, M. Fioroni, M. Zacharias, and G. Colombo (2005), *Effect of hexafluoroisopropanol alcohol on the structure of Melittin: a molecular dynamics simulation study*, Prot. Sci. 14, 2582-2589.

[9] D. Roccatano, T.S. Wong, U. Schwaneberg, and M. Zacharias (2005), *Structural and dynamic properties of cythocrome P450 BM3 in pure water and in DMSO/water mixture*, Biopolymers, 78, 259-267.

[10] D. Imhof, Wieligmann K, Hampel K, Nothmann D, Zoda MS, Schmidt-Arras D, Zacharias M, Bohmer FD, Reissmann S. (2005), *Design and biological evaluation of linear and cyclic phosphopeptide ligands of the N-terminal SH2 domain of protein tyrosine phosphatase SHP-1*, J. Med. Chem. 48, 1528-1539.

[11] A. Szymoszek, and M. Zacharias (2005), *Structure prediction of segments with low target-template similarity in comparative protein modelling using a reduced protein model*, IE J. of Mol. Design 4 (electronic Journal).

[12] Y. Ihle, O. Ohlenschlager, S. Hafner, E. Duchardt, M. Zacharias, S. Seitz, R. Zell, R. Ramachandran, and M. Gorlach (2005), *A novel cGUUAg tetraloop structure with a*

conserved yYNMGg-type backbone conformation from cloverleaf 1 of bovine enterovirus 1 RNA, Nucleic Acids Res. 33, 2003-2011.

[13] H. U. Göringer, M. Homann, M. Zacharias, A. Adler (2005), *RNA aptamers as potential pharmaceuticals against infections with African trypanosomes* H. of Experimental Pharmacology, 173, 375-393.

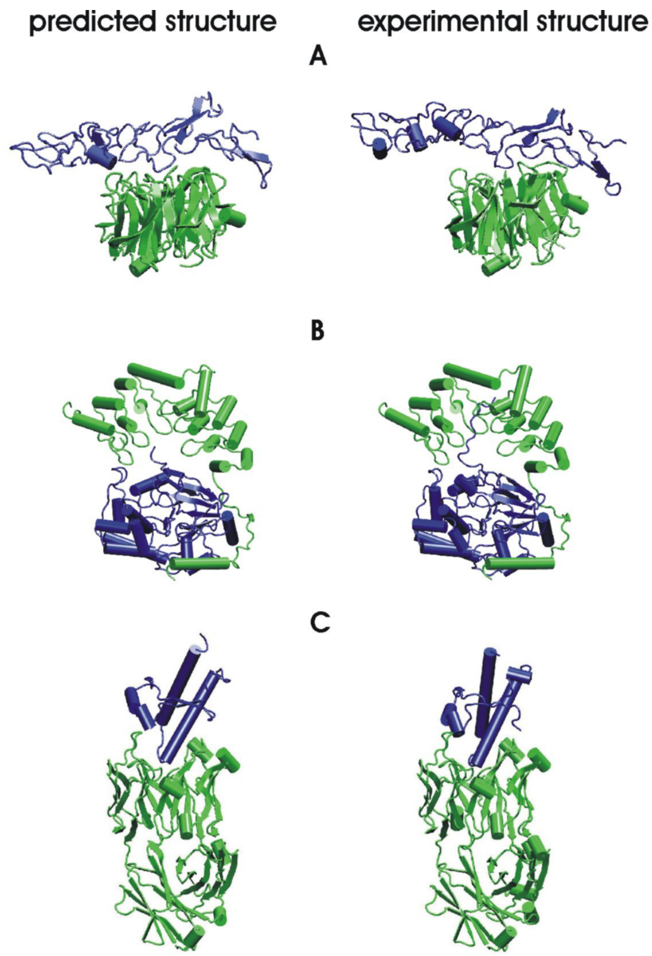


Figure 22: Protein-protein docking predictions of the Zacharias group at the CAPRI docking prediction challenge (http://capri.ebi.ac.uk/, see reference 1). Predictions were made before the experimental structures became available using our docking program ATTRACT [1]. Protein complexes are shown as a side-by-side comparison of predicted (left panels) and experimental (right panels) structures for three docking targets (cartoon representation). (A) Target 8: Laminin modules III3-5 (blue) in complex with nidogen (green). (B) Target 14: Protein phosphatase 1 (blue) in complex with myosin phosphatase targeting subunit (green). (C) Target 19: Ovine prion protein (blue) in complex with an antibody FAB fragment (green). For target 8 and 14 top ranking predictions and for target 19 the prediction with rank 9 is shown. [M. Zacharias]

3 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) and in the GIS Lab.

In August 2005 the CLAMV CTL was moved from the building Research I to the basement of West Hall, and enlarged to currently 35 single and dual processor Linux PC workplaces. This infrastructure improvement has led to more opportunities to provide hands-on instruction using computational tools throughout IUB for graduate and advanced undergraduate courses, guided research projects, and by research groups. Courses that made use of the CLAMV CTL are listed in tables 1 (spring 2005) and 2 (fall 2005).

In the relocated CLAMV CTL open sessions were offered on Wednesday afternoons. This new service received a very positive response from undergraduate students, and will be extended in 2006.

The GIS Lab in the building Research III became fully operational in 2005. The set-up is described in section 4. 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 3.3.

3.1 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. As an example, the guided research project of an undergraduate student in physics is described at the end of this section.

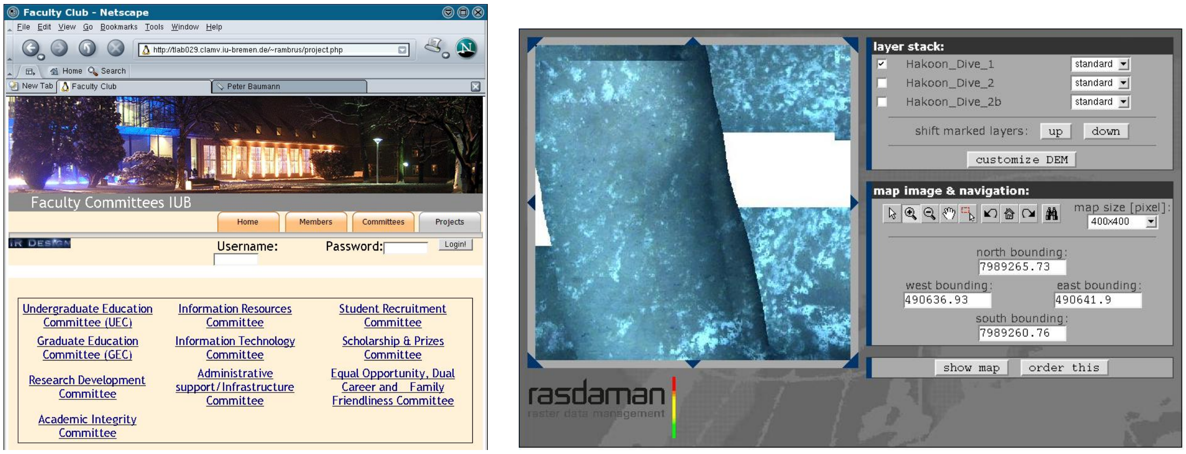


Figure 23: Screenshots obtained in the courses on *Database and Web Applications* and *Semantic Web Engineering*. [P. Baumann]

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 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.

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.

Language Development

Guided research project of T. Tesileanu; text contributed by Hildegard Meyer-Ortmanns (Physics).

The evolution of language has attracted the attention of linguists for many years, but more recently also neuro- and computer-scientists as well as physicists entered this field of research. It concerns basic questions as the origin of speech, the role of mimicry and movement, fine and rapid motor control, but also language development. Language development refers to the individual level during childhood and to the global level as language evolution of mankind. The evolution of a single language as a function of time may refer to a transformation of this language, say from ancient Latin to modern Italian. In the guided research project we focused on language evolution or language development, development in the sense of spreading, competition, extinction and dominance of languages as a function of mutation and adaptation rates that characterize the individual speakers. Similarly to the evolution of cultural traits for various cultural features to a homogeneous or multicultural polarized state, we studied how an initially multilingual population evolves: do the languages of individuals converge to a common “lingua franca” in the very end, or is a fragmentation into many coexisting language clusters the final state? In our model the individuals can change their mother tongue during their lifespan, pass on their language to their offspring and finally die. The languages are described by bitstrings, their mutual difference is expressed in terms of their Hamming distance. Language evolution is determined by mutation and adaptation rates. In particular we considered the case where the replacement of one language by another one is determined by their mutual Hamming distance. As a function of the mutation rate we found a sharp transition between a scenario with one dominant language and fragmentation into many language clusters. The transition was also reflected in the Hamming distance between the two languages

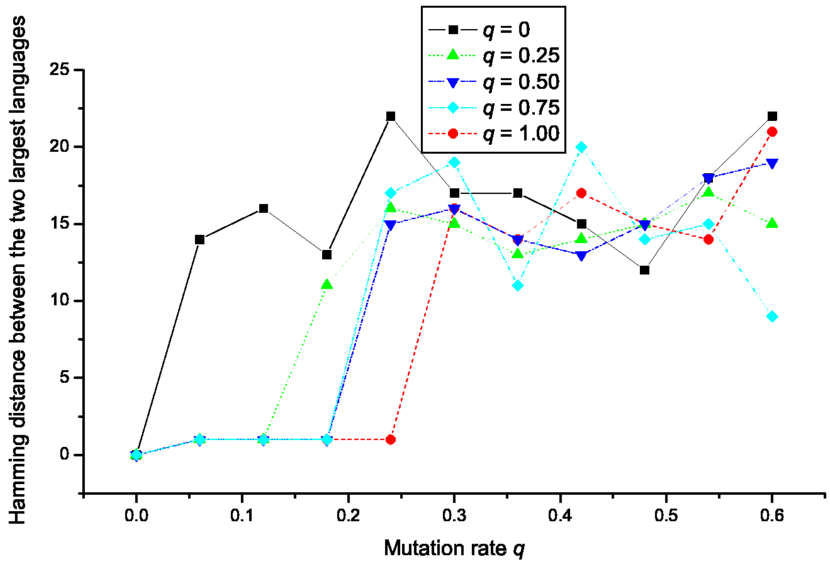


Figure 24: Hamming distance of the two largest languages versus the mutation rate. Guided research project of T. Tesilaneu, supervised by H. Meyer-Ortmanns.

with the largest and second to largest number of speakers. We also considered the case where the population is localized on a square lattice and the interaction of individuals restricted to a certain geometrical domain. Here it was again the Hamming distance that played an essential role in the final fate of a language of either surviving or being extinct.

COMPUTATIONAL ASPECTS: In our models the bitstrings had a typical length of 32 bits. The population size was varied between 1000 and 100000 individuals in steps of 10. Each simulation was run for 1000 time steps and various observables were measured every 10th step. The simulations had to be repeated for different initial conditions to test on the dependence on the initial language distribution. The complexity of these computations turned out to be linear in the populations size. A second part of the simulations made use of square lattices for localizing the individuals of the population. These two-dimensional lattices had a linear extension of up to 400 sites, and the language evolution was visualized to illustrate the appearance, change, size and extinction of language boundaries.

TECHNICAL DETAILS: We used GNU-C++ and Bash scripts to do batch runs of language simulations. The CPU time varied between several minutesand several hours per simulation.

PUBLICATION: T. Tesileanu and H. Meyer-Ortmanns (2006), *Competiton of languages and their Hamming distance*, physics/0508229, to be published in Int. J. Mod. Phys. C17, issue 3.

Courses	Instructors
Advanced Bioinformatics	M. Zacharias, F.O. Glöckner
NatSciLab Symbolic Software	P. Bangert
Numerical Methods II	P. Oswald
Computational PDE	P. Oswald
Computational Fluid Dynamics	A. Khalili
Database and Web Applications	P. Baumann
Open lab sessions	CLAMV personnel

Table 1: Spring semester 2005 courses that made use of the CLAMV CTL facility.

3.2 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 section 2. 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.

This year's project work focused on implementing a Web Coverage Service (WCS) according to the published standard of the Open GeoSpatial Consortium (OGC)[5] as part of the GALEON project (cf. section 2.1). By the end of the semester the students had set up Web-based navigation on 4-D climate simulation data.

3.3 Teaching and Instruction in the GIS Lab

Contributed by Vikram Unnithan and Angela Schäfer

The computers at the GIS-Lab provides access to GeoAstro 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 (Fig. 25) and Petroleum Basin Modelling. The lab is also

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

Courses	Instructors
Database and Web Applications II	P. Baumann
GeoAstro Lab, Field and Data Analysis Project II	J. Vogt, S. Rosswog
NatSciLab GeoAstro	M. Brüggen
Advanced Bioinformatics I	M. Zacharias
Computational Chemistry and Biochemistry	D. Roccatano
Computational Physics	M. Rohlfing
Numerical Methods I	M. Oliver
General Mathematics and Computational Science I	M. Oliver
NatSciLab Numerical Software	P. Oswald
Open lab sessions	CLAMV personnel

Table 2: Fall semester 2005 courses that made use of the CLAMV CTL facility.

Courses	Instructors
Lab Data Management, GIS & Visualization	V. Unnithan, A. Schäfer
Advanced Geographic Information Systems	A. Schäfer, V. Unnithan
Guided research projects	V. Unnithan, A. Schäfer
Introduction to GIS	A. Schäfer, V. Unnithan
Geochemical Modelling	A. Koschinsky

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

used for Astrophysics modelling and instruction is provided by Joachim Vogt. 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, November 2005)

IUB students and researchers 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 (Table 3). A variety of courses in applied GIS, modelling and visualisation techniques for IUB students and researcher are planned for 2006. The GIS Lab will become an integral part of geoscience education at IUB. It provides training and skills that are currently in high demand and that employers consider to be valuable assets while hiring personnel.

Figure 25: Geochemical Modelling course in the GIS lab, November 2005.

3.4 Workshops

In 2005 the CLAMV was again involved in the organisation of several workshops.

Parallel computing workshops

A 4-days workshop entitled *Parallel Programming in MPI and OpenMP* was hosted by CLAMV in August 2005. 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. More than 30 participants from the Alfred-Wegener-Institut, Universität Bremen and IUB attended the lectures.

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 organise and host a two-day workshop on “Advanced Petroleum Systems Modelling” in May 2005. This workshop provided scientists from various Northern German geoscience institutes hands-on experience with the Petroleum System’s Modeling Software – PetroMod. Other workshops include:

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 Workshop (May 2005) ”PetroMod Workshop - modelling hydrocarbon generation, migration and accumulation”. Instructor: Prof. Vikram Unnithan
3. Hermes GIS workshop (October 2005)

For further information see http://www.irccm.de/[6].

3.5 CLAMV Seminar

The CLAMV seminar was continued as the research seminar of the CLAMV, primarily serving the community of IUB computational scientists and researchers from adjacent disciplines. The general goals of

- 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

for the CLAMV seminar were followed also in 2005. Although the seminar always draws a diverse audience of faculty, post-doctoral researchers, graduate and increasingly undergraduate students, the overall number of seminars as well as attendance have been slightly lower than in previous years. This was partly triggered by the

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

consolidation of research groups on campus which run their own seminars, and the reduced number of newly hired faculty resulting in fewer talks by IUB research staff.

In 2005, one guest speaker from industry (Dr. Werner Kozek, Siemens AG) was invited, the keynote speaker was Prof. Michael Griebel, Institute for Scientific Computing, University Bonn. The proportion of technical talks and speakers from outside Bremen has further increased. A detailed seminar schedule can be found in Appendix A.4.

For the 2006 CLAMV seminar series, it is planned to put greater weight on the introduction and popularization of new software tools for visualization and scientific computing available through CLAMV (Tecplot, Povray, Portland Compiler, ...) to students and faculty. Some events will be used to more systematically support the interaction and synergies with local partners such as MeVis, AWI, Uni Bremen, etc.

4 Service, Consulting, and new CLAMV Facilities

In the year 2005 the CLAMV infrastructure was modified and enhanced in a number of aspects. The CLAMV Teaching Lab was moved to the basement of West Hall, a new shared memory computer arrived on campus, the GIS Lab in Research 3 became fully operational, and the Linux Cluster of the former computational chemistry group was fully integrated into CLAMV. These changes are explained in the following text.

4.1 Relocation of the CLAMV Computer Teaching Lab

Since the foundation of CLAMV in April 2002 the CLAMV Teaching Lab was located on the upper floor in Research I. In order to make additional office space available for the growing number of students and researchers in Mathematics and EECS, in August 2005 the CLAMV Teaching Lab was moved to the newly renovated rooms in the basement of West Hall. The new location offers more total floor space and can accommodate groups with up to 21 users in a single room. There are three teaching rooms of different sizes (6/8/21 users) and two project rooms for 4 users each. Computer equipment from the former computational chemistry group (F. Müller-Plathe) could be integrated into the CLAMV environment. Now 35 computer desktops can be offered for teaching purposes. Since there have been several requests by classes there are now regular open sessions on Wednesday afternoons (2 pm until 6 pm) which are supervised by a student assistant. In June 2005 the CLAMV office moved to its new location in the Campus Center (6-257).

4.2 New Servers for Shared Memory Parallel Computing and Storage

In April 2005 a shared-memory server (Silicon Graphics Altix3700Bx2) for high performance computing was installed in lab 1 (server room) on the IUB campus. The server is reserved for memory demanding jobs and parallel applications that can not be run on the Linux clusters. 50 % of the total performance is reserved for the group of S. Rosswog (astrophysics). The server was delivered and installed in April 2005. A 2-days user training accompanied the installation. The TP9300 RAID- system consisting of 14 harddisks (400 GByte / disk) was delivered and installed in June 2005.

For the analysis of large data sets (e.g. from computer simulations) the existing storage capacities at IUB were not sufficient. In November 2005 a new storage server with a RAID-array of 24 disks (500 GByte / disk) was taken into service. Research groups can get disk space assigned if necessary which also can be increased upon request.

4.3 New Software Tools

In 2005 several new software packages or upgrades of existing software packages were installed. The main intention was to offer a well maintained Linux environment for the CLAMV users. The very popular mathematics and visualization packages IDL, Maple, Mathematica and Matlab are now also available for 64Bit Linux system allowing the full exploitation of the hardware features of the above mentioned storage server. For Matlab additional toolboxes were purchased and for Maple the software maintenance service was reactivated. The very popular C and Fortran compilers for Linux from Portland Group Inc. were made accessible on a server license basis. For the analysis and visualization of fluid dynamics data the program tecplot including CFD-Analyzer is now available.

4.4 Further Services

Besides the regular work to maintain and improve the computer environment for its users, CLAMV personnel has participated in other computer infrastructure projects. There were several requests for support and consulting from the research groups. The majority of the requests is related to the UNIX/Linux operating system and how to integrate the local computer equipment into the CLAMV environment. In fall 2005 CLAMV initiated a workgroup together with IRC-IT in order to set up a general strategy for the configuration of UNIX/Linux-systems in the resarch groups. This process is still in progress. All technically possible solutions have to be monitored also from the additional workload they create and the available personnel.

4.5 The GIS Lab – a new Facility for Teaching and Research

Contributed by Vikram Unnithan and Angela Schäfer (Geoscience)

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 SISCOE (a visualisation server funded through a DFG project managed by J. Vogt) formed the basis for the CLAMV–StatOil–IRCCM GIS and visualisation lab. The lab is physically located in R3, room 156. 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 continetal 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.

2005 was a busy year for the GIS Lab in terms of establishing web and database servers, teaching and hosting web based services for several scientific research projects. The GIS Lab computers were provided a separate sub-net 'gislab' within the IUB network.

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-

Figure 26: Mr. Fleckenstein, CEO of Wintershall testing the GeoWall during a visit to IUB

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 (Fig. 26.

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 Brueggen, Adele Diederich, Achim Gelessus, Hildegard Meyer-Ortmanns, Goetz 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): Peter Oswald (until September 2005: Marcel Oliver – Chair), Achim Gelessus, Stephan Rosswog (until September 2005: Michael Rohlfing), Joachim Vogt, 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 Lab

30 COMPAQ EVO DESKTOP, TLAB001 - TLAB030

- Intel Pentium IV processor 2.26 GHz
- 512 MByte RAM
- 40 GByte Ultra ATA-100 harddisk
- 100 MBit Ethernet
- nVidia GeForce4 Ti 4200 graphic adapter
- SuSE Linux 9.3 Operating System

5 IBM INTELLI STATION, TLAB031 - TLAB035

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

CLAMV Linux Cluster

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

	Number of nodes	Number of processors	Theoretical performance (GFlops/s)
Cluster I	40	80	352
Cluster II	32	64	382
Cluster III	24	48	268
Sum			1004.8

Table 4: Comparison of the three CLAMV Linux Clusters

- Operating System RedHat Linux
- Queuing System PBS

Cluster I is not dedicated to a specific research group.

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
- Operating System RedHat Linux
- Queuing System PBS

Cluster II is not dedicated to a specific research group.

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
- Operating System RedHat Linux
- Queuing System PBS

Cluster III is dedicated 66.6% to the computational biology group.

CLAMV Servers

CLAMV SHARED MEMORY COMPUTER 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
- Operating System RedHat Linux / ProPack
- Queuing System PBSPro

The SGI Altix is dedicated 50 % to Prof. S. Rosswog's group.

CLAMV SUN FIRE V880

- 8 SUN Sparc-3 processors 900 MHz
- 16 GByte RAM, shared memory

The CLAMV SUN Fire v880 is used as file and user administration server and for scientific computing. There is no general access to this machine.

CLAMV STORAGE AND DATA ANALYSIS SERVER

- 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
- SuSE Linux 10.0 Operating System

CLAMV BACKUP SERVER

- 2 AMD Athlon MP2400+ processors
- 1.0 GByte memory
- RAID system: 8 x 250 GByte
- SuSE Linux 9.3 Operating System

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

GENERAL SOFTWARE PACKAGES FOR MATHEMATICS AND ANALYSIS: IDL, Maple, Mathematica, MatLab incl: SimuLink, Curve Fitting Toolbox, Communication Toolbox, Control Toolbox, Filter Design Toolbox, Financial Toolbox, Fixed Point Toolbox, Image Processing Toolbox, Neural Network Toolbox, Optimization Toolbox, Partial Differential Equation Toolbox, Robust Toolbox, Signal Processing Toolbox, SimuLink Control Design Toolbox, Spline Toolbox, Statistics Toolbox, Symbolic Math Toolbox, System Identification Toolbox, MatLab Compiler, WaveLab, Statistical Parametric Mapping (SPM2).

SOFTWARE PACKAGES FOR VISUALIZATION: Ifrit, OpenDX, pgplot, transcode, gOpenMol, Molden, Molekel, Molmol, RasMol, Swiss PDB Viewer, VMD.

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

COMPUTATIONAL BIOLOGY AND NEUROSCIENCE MODULE: Arb, ClustalX, Emboss, Genesis, Modeller, Neuron, Statistical Parametric Mapping (SPM2, MatLab), ViennaRNA.

ELECTRICAL ENGINEERING AND COMPUTER SCIENCE MODULE: ns-2 Simulator.

GEOASTRO MODULE: GDI, GIS, GMT, Grass, iGMT, OpendTect, PetroMod, QSAS, Seismic UNIX, Tecplot.

Software locally installed on the CLAMV TeachingLab computers

COMPILER, LANGUAGES: C (GNU, Intel, Portland), C++ (GNU, Intel, Portland), Fortran (GNU, Intel, Portland), Java, Perl, Python, 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, Postgres.

EDITORS: Ed, Gvim, Jedit, Joe, Kvim, Mined, Pico, Texmacs, Vim, Xcoral, Xemacs.

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

OFFICE: OpenOffice.

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

SCIENTIFIC SOFTWARE: Basic Linear Algebra Subprograms (BLAS), Fastest Fourier Transformation in the Workd (FFTW), Feynman Diagrams (feynman), GNU Scientific Library (GSL), Grass GIS, Linear Algebra Package (Lapack), Octave, Scientific Calculator, Scilab.

WWW: Lynx, Konquerer, Mozilla, MozillaFirefox.

A.4 Seminar Schedules

Spring 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*

Fall 2005

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*

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[7]

GIS Geographic Information System

ICBM Institut fuer Chemie und Biologie des Meeres, Universitaet Oldenburg[8]

IRCCM International Research Consortium on Continental Margins[9]

JCLL Jacobs Center for Lifelong Learning[10]

NIC John von Neumann - Institute for Computing at Forschungszentrum Juelich[11]

SES School of Engineering and Science[12]

SHSS School of Humanities and Social Sciences[13]

TUC Technische Universitaet Chemnitz[14]

			Teaching Lab		Software	Cluster	SUN v880	Special Services				Remarks
			Teaching	Research				Linux	WWW, UML	Backup	Extra	
Peter Baumann	Computer Science	SES	x									
Andreas Birk	Electrical Engineering & Computer Science	SES		x								
Klaudia Brix	Biochemistry & Cell Biology	SES								x		
Marcus Brüggen	Astrophysics	SES	x	x	x	x	x					NIC
Stefano Carpin	Computer Science	SES		x	x							
Adele Diederich	Psychology	SHSS			x							
Marcelo Fernandez-Lahore	Biochemical Engineering	SES			x							
Frank Oliver Glöckner	Bioinformatics	SES	x									
Benjamin Godde	Neuroscience & Human Performance	JCLL			x							
Harald Haas	Electrical Engineering	SES		x	x							
Werner Henkel	Electrical Engineering	SES		x	x							
Claus Hilgetag	Neuroscience	SES	x	x	x							
Herbert Jäger	Electrical Engineering & Computer Science	SES			x							
Arzhang Khalili	Computational Science	SES	x									
Dietmar Knipp	Electrical Engineering	SES	x									
Michael Kohlhase	Computer Science	SES	x				x					
Hildegard Meyer-Ortmanns	Physics	SES			x	x						
Florian Müller-Plathe	Physical Chemistry	SES	x		x	x						NIC
Marcel Oliver	Mathematics	SES			x				x		Thin Client	
Bettina Olk	Psychology	SHSS			x							
Peter Oswald	Mathematics	SES	x		x							
Götz Pfander	Mathematics	SES		x	x				x	x		
Ryan M. Richards	Chemistry	SES		x	x							
Michael Rohlfing	Physics	SES	x	x	x	x						
Stephan Rosswog	Astrophysics	SES	x	x	x						SMP-Computer Installation	NIC
Angela Schäfer	Geoscience	SES	x	x	x			x			GIS - Lab	
Klaus Schömann	Sociology	JCLL			x							
Jürgen Schönwälder	Computer Science	SES			x							
Michael Stoll	Mathematics	SES			x						Thin Client	
Stefan Tautz	Physics	SES		x	x							
Vikram Unnithan	Geoscience	SES	x	x	x			x			GIS - Lab	
Joachim Vogt	Space Physics	SES	x		x	x		x				
Veit Wagner	Physics	SES		x	x							
Raymond O. Wells	Mathematics	SES						x	x			
Mathias Winterhalter	Biophysics	SES			x							
Martin Zacharias	Computational Biology	SES	x	x	x	x		x				
Bertalan Zieger	Space Physics	SES			x	x						

Table 5: CLAMV usage in 2005.

A.7 CLAMV People

Table 5 provides an overview on how and by whom CLAMV resourses were used in the year 2005.

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

[7] http://www.awi-bremerhaven.de
[8] http://www.icbm.de
[9] http://www.irccm.de
[10] http://www.iu-bremen.de/schools/jacobs
[11] http://www.fz-juelich.de/nic/index-e.html
[12] http://www.iu-bremen.de/schools/ses
[13] http://www.iu-bremen.de/schools/shss
[14] http://www.tu-chemnitz.de

Index