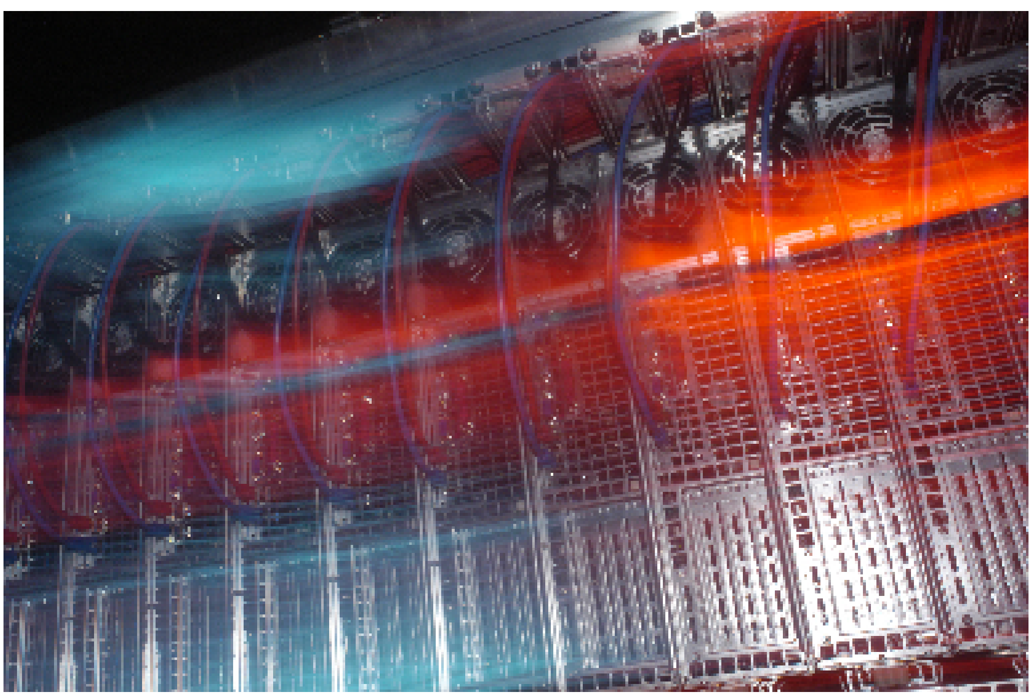
International University Bremen (IUB)
Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV)
www.clamv.iu-bremen.de

CLAMV Activity Report 2004

Compiled by the CLAMV Seminar and Editorial Committee

Achim Gelessus, Marcel Oliver, Michael Rohlfing, Joachim Vogt



Contents

1 Introduction

This is the second activity report of the *Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV)*. Founded in April 2002, CLAMV has grown from 12 initial members to a group that now includes about 35 faculty, a systems manager, associated postdoctoral researchers and graduate students. The CLAMV is the umbrella and support initiative for all computationally oriented disciplines at 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 platforms.

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 detail the CLAMV activities in the year 2004, with particular emphasis on research projects in scientific computing (section 2), involvement in teaching (section 3), the CLAMV seminar (section 4), and service and consulting (section 5).

The CLAMV Activity Report 2004 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 have been served in the year 2004.

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

The main CLAMV computing facilities are (1) a Linux cluster with 40 dual processors connected through Ethernet, (2) an 8-processor shared memory compute server of type SUN Fire v880 which is used for scientific computing, file service and user administration, and (3) a computer teaching lab for advanced undergraduate and graduate teaching consisting of 30 visualization workstations distributed over four rooms in the building Research I. The CLAMV Systems Manager also manages two additional Linux clusters with 32 and 24 dual processors, connected by fast Ethernet and Myrinet. In the near future a 24-processor shared memory machine is planned to be purchased and integrated into CLAMV.

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 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 three 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 position of the CLAMV Systems Manager formally resides 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 Outlook

At the time of writing of this report, the CLAMV enters its fourth year of existence. 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 community is still growing and the number of requested services will increase. With the existing personnel (Systems Manager and student assistants), we expect considerable difficulties to meet the growing demand. Further professional support is needed for scientists developing their own software to make efficient use of human and computer resources at IUB. We therefore strongly suggest to establish the position of an additional *CLAMV Systems Administrator* to ensure smooth continuing development of the computationally oriented disciplines at IUB.

2 Scientific Projects

CLAMV resources play an essential role for a large number of scientific projects carried out at IUB. Corresponding to CLAMV's designation, these projects includes data analysis, numerical modeling, and data visualization. Naturally, numerical modeling is by far the most resource-consuming task, calling for highly efficient and powerful hardware infrastructure. Data analysis and visualization, on the other hand, is less comsuming in terms of hardware but rather asks for advanced software and for personal consulting by experts, both of which is provided by CLAMV, as well.

The following faculty members and research groups are making use of CLAMV resources or are preparing to do so in the nearest future.

Current projects (see Sec. 2.2):

Project scientist(s)	Field	Page
A. Birk, M. Rooker	EECS	7
K. Brix et al.	BCCB	8
M. Brüggen	Astrophysics	9
H. Haas et al.	Electrical Engineering	11
C. Hilgetag, M. Kaiser	Neuroscience	13
M. Hoeft	Astrophysics	14
H. Jaeger	Computational Science	15
P. Ludes	Mass Communication	16
H. Meyer-Ortmanns et al.	Physics	17
F. Mueller-Plathe et al.	Physical Chemistry	20
B. Olk	Psychology	23
R. Richards, A. Kraynov	Chemistry	25
M. Rohlfing, N.-P. Wang	Physics	26
S. Rosswog	Astrophysics	29
J. Schmidt, J. Vogt, M. Brüggen	Solar physics	31
M. Stoll	Mathematics	32
V. Unnithan et al.	Geoscience	32
M. Zacharias	Computational Biology	35
B. Zieger, J. Vogt	Space Physics	36

Additional future projects (see Sec. 2.3):

Project scientist(s)	Field	Page
P. Baumann	Computer Science	40
C. Doose	Chemistry	41
M. Fernandez-Lahore	Downstream-Processing	41
B. Godde, C. Voelcker-Rehage	Neuroscience	42

2.1 Hardware, Software, and Support Provided by CLAMV

CLAMV provides two main machines designed for scientific projects (cf. Sec. A.2), i.e. a 80-processor Linux-operated PC cluster and a 8-node Sun Fire Compute Server. In addition, a number of PC's located in the Teaching Laboratories are also used for scientific projects during off-hours. Furthermore, two additional multi-processor Linux-operated PC clusters, that are dedicated to two of IUB's research groups (Prof. F. Müller-Plathe and Prof. M. Zacharias), have been installed by experts from CLAMV.

Numerous use is made of the software provided by CLAMV. In addition to various work tools like compilers, debuggers, and numerical/technical libraries, several scientific software packages have turned out to be very important. These include IDL, VMD, Mathematica, Matlab, and Gaussian.

Hardware and Software are maintained by CLAMV personnel, in particular by Dr. Achim Gelessus, thus providing a sound basis for the smooth running of the computer equipment and forming a vital part of the research carried out at IUB.

2.2 Selected Current Projects

Among the scientific projects that have been carried out so far, a representative selection is described below in a detailed manner.

2.2.1 Robot team simulations

Prof. Dr. Andreas Birk (Electrical Engineering & Computer Science)

In challenging environments where the risk of loss of a robot is high, robot teams are a natural choice. In many applications like for example rescue missions there are two crucial tasks for the robots. First, they have to efficiently and exhaustively explore the environment. Second, they must keep up a network connection to the base-station to transmit data to ensure timely arrival and secure storage of vital information. When using wireless media, it is necessary to use robots from the team as relay stations for this purpose. Simulations investigating a novel algorithm to solve this problem have been partially been run on the CLAMV teaching computers as part of the PhD research of Martijn Rooker.

PUBLICATIONS

Martijn Rooker and Andreas Birk, "Combining Exploration and Ad-Hoc Networking in RoboCup Rescue", in: RoboCup 2004: Robot Soccer World Cup VIII (Lecture Notes in Artificial Intelligence (LNAI), Springer, 2005).

Martijn Rooker and Andreas Birk, "Communicative Exploration in Dangerous Environments", in: Second International Workshop on Advances in Service Robotics (ASER'04) (2004).

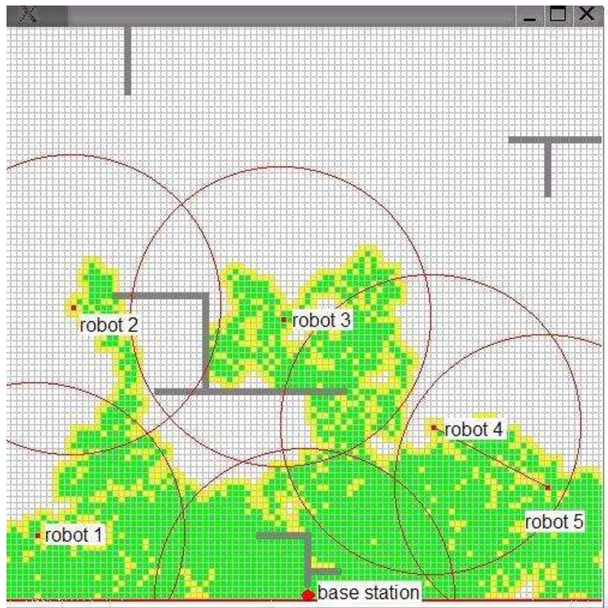


Figure 1: Robot team simulations (A. Birk)

2.2.2 Trafficking of Proteases

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

We analyze the biological significance of proteinases for the function of epithelial organs. Our research focuses on the group of lysosomal cysteine cathepsins and their roles in intestine, skin and thyroid. Recently, we have shown that cathepsins B, K, and L are vital for liberation of thyroid hormones in the extracellular space of thyroid follicles [Brix, 2004a]. These findings were explained by the regulated secretion of the enzymes from their internal stores into the extracellular compartment. Similarly, migrating keratinocytes secrete the lysosomal cysteine cathepsin B to enable remodeling of extracellular matrix constituents for proper regeneration during wound healing [Büth et al., 2004]. For a more detailed understanding of the underlying transport phenomena, we plan to study the trafficking of cysteine cathepsins within various epithelial cells through tagging with green fluorescent protein (GFP). We have now generated several vectors encoding chimeric proteins of cathepsins B and L with GFP. After expression of the chimeras, their transport can be studied in living cells. Because cells are 3-dimensional, we plan to trace the trafficking of cathepsin-GFP-containing vesicles within the volume of a cell by analysis of consecutive sections taken with a confocal laser scanning microscope in a semi-automated fashion, and at different time intervals. The use of CLAMV-resources and the interaction with CLAMV-members will be important for the further progress of this research project on the cell biology of proteinases [for review, see Brix, 2004b].

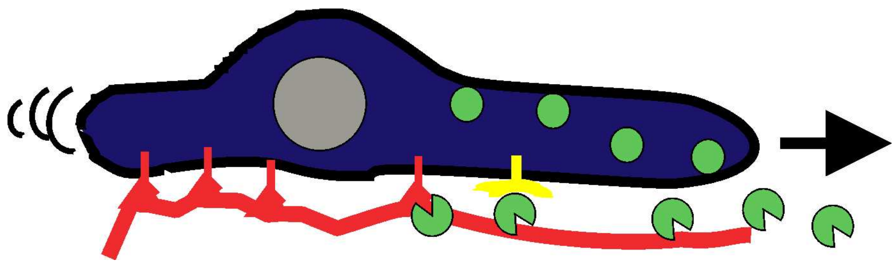


Figure 2: Migrating keratinocytes secrete lysosomal cathepsin B (green) to enable remodeling of extracellular matrix constituents (red). (K. Brix)

GROUP MEMBERS (AS OF 31/12/04)

Prof. Dr. Klaudia Brix, Heiko Büth, Silvia Jordans, Kristina Mayer, Dr. Ulf Meyer-Grahle, Hong Qu, Meike Völkner, Brit Wolters.

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

PUBLICATIONS

Brix, K. (2004a). Thyroid Cysteine Proteinases. New Transport Pathways to Liberate Thyroxine. Bioforum Europe 1/2004, 24-25.

Brix, K. (2004b). Chapter 05: Lysosomal Proteases: Revival of the Sleeping Beauty. In: Lysosomes, edited by Paul Saftig, Eurekah.com. Landes Bioscience. http://www.eurekah.com/abstract.php?chapid=2255&bookid=129&catid=15

Büth, H., B. Wolters, B. Hartwig, R. Meier-Bornheim, H. Veith, M. Hansen, C.P. Sommerhoff, N. Schaschke, W. Machleidt, N.E. Fusenig, P. Boukamp, and K. Brix (2004). HaCaT keratinocytes secrete lysosomal cysteine proteinases during migration. Eur. J. Cell Biol. 83, 781-795.

2.2.3 Simulations of Galaxy Clusters

Prof. Dr. Marcus Brüggen (Astrophysics)

Clusters of galaxies are pervaded by large amounts of dilute gas which accounts for most of the baryonic mass in the cluster. This gas has got temperatures above 10^7 K and is thus hotter than the centre of the Sun. This so-called intracluster medium (or ICM) radiates X-rays, mainly through thermal bremsstrahlung, and has been observed extensively with X-ray satellites such as *Chandra* or XMM-*Newton*.

One of the most topical issues in extragalactic astronomy is the long-standing problem of cooling flows in clusters of galaxies. These cooling flows should arise if the

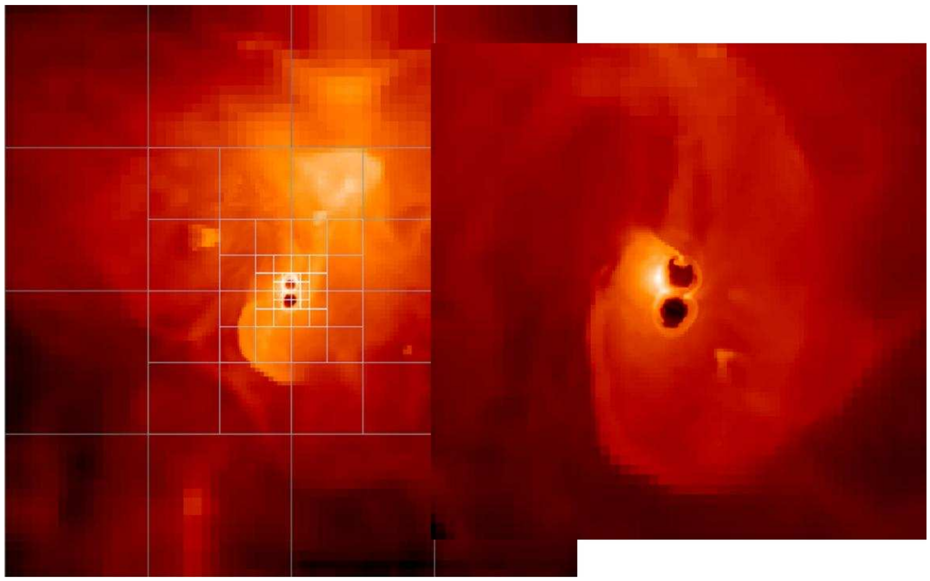


Figure 3: Block boundaries in a slice displaying the gas density at a time of 70 Myrs after the start of AGN activity. (M. Brüggen)

central cooling time of the ICM is much shorter than the age of the universe. Then the gas in the cluster is expected to collapse catastrophically on a short timescale. The original idea for maintaining the overall cluster stability was to postulate that a certain amount of gas decouples from the flow and does not contribute to the cooling of the remaining gas. This model would deposit up to 1000 $M_\odot$ yr^{-1} in mass in the centre of the cluster. This has been found to be inconsistent with recent *Chandra* and XMM-*Newton* observations. Meanwhile, *Chandra* observations have revealed a number of clusters with X-ray cavities created by the relativistic gas ejected by active galactic nuclei (AGN). These cavities are believed to heat the ICM and to prevent it from collapsing.

The main outstanding issue in this picture is *how* the AGN heating proceeds. In principle, strong shocks generated by AGN outbursts can dissipate and heat the ICM. However, imaging observations of cooling flow cores rule this mode of heating out. Recent *Chandra* observations of two well-known clusters, the Perseus cluster [1] and the Virgo cluster (Forman et al. 2004), suggest that viscous dissipation of sound waves and weak shocks could be an important source of heat. Further support for the idea that viscosity may play an important role in the ICM comes from a recent study of density profiles in clusters (Hansen & Stadel 2003). In addition to viscosity, thermal conductivity should also strongly contribute to wave dissipation. Thermal conduction could damp the sound waves *more quickly* than viscosity because thermal conductivity is dominantly produced by electrons while viscosity is mediated by ions. Because

[1] This discovery, that motivates our work, received a lot of publicity in the media and was covered by BBC, CNN, The New Your Times, The Washington Post, Discovery Channel and many others.

electrons move faster than the ions, the conductive dissipation rate exceeds the viscous one by a factor ~ 10 under simplified assumption that waves are linear and that the gas has constant density and pressure and gravity can be neglected.

We performed our simulations in three dimensions in Cartesian geometry using the adaptive mesh refinement code FLASH (version 2.4). The FLASH code was developed by the Department of Energy-supported ASCI/Alliance Center for Astrophysical Thermonuclear Flashes at the University of Chicago. FLASH is a modular block-structured AMR code, parallelised using the Message Passing Interface (MPI) library. It solves the Riemann problem on a Cartesian grid using the Piecewise-Parabolic Method (PPM). It uses a criterion based on the dimensionless second derivative of a fluid variable to refine or derefine the grid. Collsisionless matter, i.e. stars and dark matter, were represented by particles that interact gravitationally with each other and the gas. Our initial models were extracted from cosmological SPH simulations and typically included around 700,000 dark matter and star particles. We modified the FLASH code to include the effects of viscous dissipation in the energy and momentum equations.

Our primary aim was to study the effects of conductivity on, both, wave dissipation and the global heat transfer in clusters. We investigated how inclusion of thermal conductivity affects wave dispersion and spatial distribution of heat in the cluster. We found that the spatial distribution of heat from wave dissipation can heat the cluster in a quasi-stable fashion. We also simulated the observational signatures of dispersing waves, such as their detectability in X-ray cluster maps. We investigated if detection of dissipating waves can place constraints of the level of thermal conductivity in the intracluster gas. These simulations were performed in collaboration with the University of Colorado and were published in Ruszkowski, Brüggen & Begelman (2004) and Brüggen, Ruszkowski & Hallman (2005).

Fig. 3 shows the block boundaries in a slice displaying the gas density at a time of 70 Myrs after the start of AGN activity. At this stage the bubble has not yet achieved pressure equilibrium with its surroundings and is still expanding nearly spherically into the ambient medium. The bubbles are nearly spherical and do not look dissimilar from the bubbles observed in the Perseus cluster and other clusters. As a result of its rapid inflation, it has produced a weak shock wave that has started to travel outwards from the bubbles and which is clearly visible in the density plot. Fig. 3 also shows that the cluster is quite dynamic, as it shows significant substructure such as clumps and shock fronts.

2.2.4 Cellular and Wireless Communications

Prof. Dr. Harald Haas, Dr. Peter Omiyi, Hrishikesh Venkataraman, Raed Mesleh, and Shameem Chaudhury (Electrical Engineering)

The overarching goal of our research is to improve wireless and cellular systems with respect to radio frequency spectrum usage, i.e. system capacity in bits per second per Hertz per cell [bit/s/Hz/cell] for a given radio frequency spectrum. The capacity limits are given by Shannon, and current practical systems operate far off the Shannon

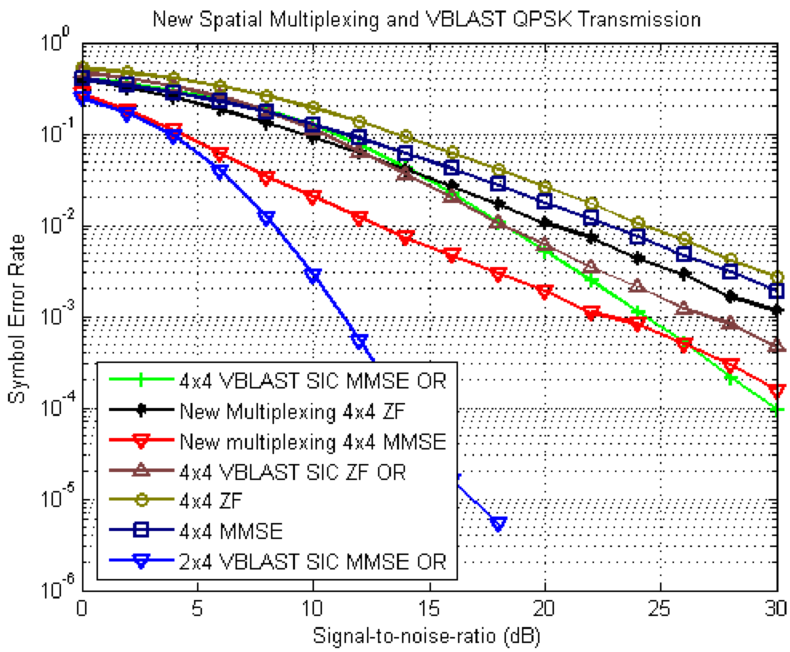


Figure 4: The bit-error performance of a new data multiplexing technique for multiple antenna transmission is compared against state-of-the-art solutions. (H. Haas et al.)

bound. This primarily is caused by multi-path propagation of the radiated electromagnetic waves. In addition, for complexity reasons, the functionality of wireless and in particular cellular systems is broken down into several so called protocol layers where each layer is composed of a number of fundamental building blocks, e.g. the physical layer is composed of data encoding, modulation, antenna steering, data detection, data decoding, etc.. The optimisation of these building blocks with respect to the overall system performance requires the modeling and simulation of wireless and cellular communication systems.

GRANTS

DFG Ha 3570/1-1: DCA Algorithms and MAC Protocols for COFDM Based Cellular Ad-Hoc Systems Using Carrier Sensing Time Division Multiple Access

DFG Ha 3570/2-1: Dynamic Spectrum Sharing for Asymmetric Services in UMTS Using a Hybrid Ad-Hoc and Cellular Approach

PUBLICATIONS

P. Omiyi and H. Haas, ”Improving Time-Slot Allocation in 4th Generation OFDM/TDMA TDD Radio Access Networks With Innovative Channel-Sensing”, in *Proceedings of the International Conference on Communications* (ICC'04, Paris, France, IEEE, June 20–24 2004), vol. 6, pp. 3133 – 3137.

P. Omiyi and H. Haas, ”Maximising Spectral Efficiency in 4th Generation OFDM/TDMA TDD Hybrid Cellular Mobile/Ad-Hoc Wireless Communications”, in *Pro-*

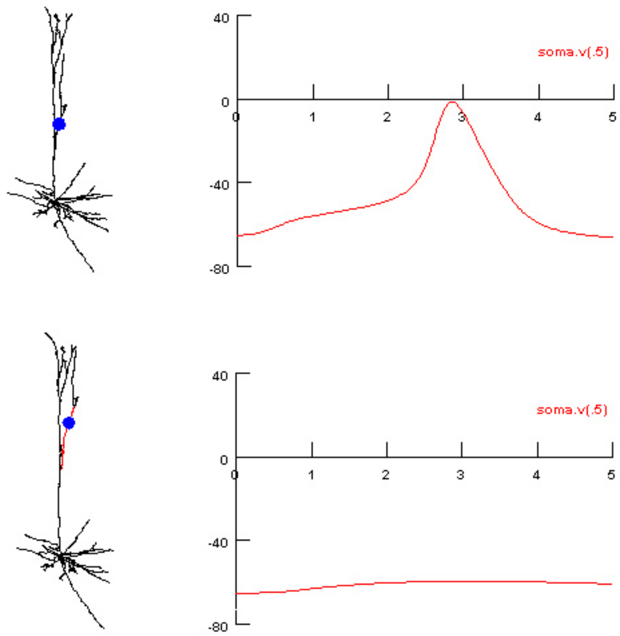


Figure 5: Impact of neuronal morphology on action potential generation. Simulations were performed in the modeling software NEURON. Cells were stimulated with the same current at the dendritic segment indicated by a dot, and resulting potentials were recorded at the soma. (Top left) Model pyramidal neuron provided by the NEURON software package (Bottom left) Model neuron with elongated apical dendritic segments. (Top and bottom right) Resulting somatic potentials. Due to the greater attenuation of dendritic potentials over the longer segments in the stretched neuron, action potentials were no longer elicited. Picture credits: L. Hurst (C. Hilgetag)

ceedings of the IEEE Vehicular Technology Conference (VTC 2004-Spring, Milan, Italy: IEEE, May 17–19 2004), p. 5

2.2.5 Computational Neuroscience

Prof. Dr. Claus Hilgetag (Neuroscience)

We used the Sun workstation for calculating edge betweenness (a measure of the importance of connections in a network) in the US power grid network. For these computations a large memory space (64bit-architecture) was required. This year, we plan the simulation of disease spreading in various large-scale networks, for which we might once again use the powerful hardware of the workstation.

SELECTED PUBLICATIONS

Kaiser, M and Hilgetag, CC, Spatial Growth of Real-world Networks, Phys Rev E 69

(2004) 036103.

Kaiser, M and Hilgetag, CC, Modelling the Development of Cortical Systems Networks, NeuroComputing 58-60 (2004) 297-302.

Kaiser, M and Hilgetag, CC, Edge Vulnerability in Neural and Metabolic Networks. Biol Cybernetics 90 (2004) 311 - 317.

Hilgetag, CC and Kaiser, M: Clustered Organisation of Cortical Connectivity, Neuroinformatics, 2 (2004) 353-360.

Sporns, O, Chialvo, D, Kaiser, M and Hilgetag, CC: Organization, Development and Function of Complex Brain Networks, Trends in Cognitive Sciences 8 (2004) 418-425.

2.2.6 Cosmological Structure Formation

Dr. Matthias Hoeft (Astrophysics)

The formation and evolution of galaxies is presently one of the most intensively studied topics topics in astrophysics. For instance, the tremendous efforts of the Sloan Digital Sky Survey results in a huge catalog of galaxies. Up to now several hundred thousand galaxies have been spectroscopically observed. On the basis of this statistically representative sample a bimodal distribution in galactic properties has been discovered: the most massive, i.e. elliptical, galaxies are mostly red while smaller galaxies, i.e spirals and dwarf, tend to be blue. This suggest that massive galaxies in the universe have evolved at earlier times than their less massive counterparts. This is in some sense contrary to the hierarchical structure formation scenario established for the underling dark matter evolution: small structures from earlier than larger ones. Hence, the challenge for numerical studies of structure formation is to explain those galactic properties.

We study the evolution of galaxies in different environments. Up to now we have focused in particular on the formation of dwarf galaxies in cosmological void regions. This have allowed us to identify the impact of the cosmic UV-background radiation.Presently we have two major goals: improving sub-grid model which are necessary to describe star formation and feedback and extending the simulations to more dense galactic environments. The work is done mainly in cooperation with Gustavo Yepes (Universidad Autonoma de Madrid), Stefan Gottlöber (Astrophysikalisches Institut Potsdam) und Volker Springel (Max Planck Institut für Astrophysik, Garching bei München).

We study also the impact to the hot gas in clusters (intra-cluster medium, ICM) of galaxies coming from the central active galactic nuclei (AGN), residing in most of the massive clusters. The large amount of emitted highly relativistic plasma stirs the ICM, heats it for example by emitting sound waves by bubble expansion, and is most likely finally mixed to the ICM. In contrast to these spectacular observational findings, numerical models still have to be improved to reach a quantitative agreement. Up to now we have studied especially the self-regulation of the AGN by its feedback in 1D models. This model should be in a heuristic manner incorporated into 3D simulations. This work is mainly done in cooperation with Marcus Büggen.

GRANTS

The work is supported by the Spanish Ministry of Science and Technology within the 'Plan Nacional de Astronomia y Astrofisica (AYA2003-07468)' under the grant *Estudio de la formación y evolución de galaxias y de las estructuras que forman en un contexto cosmológico mediante simulaciones hidrodinámicas*

USING CLAMV RESOURCES

Carrying out competitive numerical simulations needs the use of massive-parallel computing resources. We use the highly scalable code Gadget. The new Clamv resource of a Myrinet-Linux cluster is well suited to run medium-sized simulations. They are in particlar necessary to explore the parameter-space and to test different models and their implementation. These studies provide essential scientific insight itself. They are also indispensable in order to prepare production runs on national supercomputer centers, e.g. at the John-von-Neumann Institute for Computing.

PUBLICATIONS

M.Hoeft, G, Yepes, S. Gottlöber, and V. Springel, *Dwarf galaxies in voids: Suppressing star formation with photo-heating*, MNRAS, submitted, astro-ph/0501304

M. Hoeft, *Galaxy formation in voids*, Proceedings of 'Baryons in Dark Matter Halos', Editors: R. Dettmar, U. Klein, P. Salucci

M. Hoeft and M. Brüggen, *Feedback in Active Galactic Nucleus Heating of Galaxy Clusters*, ApJ 617 (2004) 896

M. Hoeft and M. Brüggen, *Heating of the ICM due to fossil plasma*, 'X-Ray and Radio Connections', Santa Fe

M. Hoeft, M. Brüggen, and G.Yepes, *Radio relics in a cosmological cluster merger simulation*, MNRAS 347 (2004) 389

2.2.7 Machine Learning and Nonlinear Stochastic Systems Modelling

Prof. Dr. Herbert Jaeger (Computational Science)

In a joint venture between IUB and the Fraunhofer Institute for Autonomous Intelligent Systems (AIS) in Sankt Augustin, a project group of three Fraunhofer researchers worked on the IUB campus (Dr. Mathias Bode, Stéphane Beauregard, Paul Gemin), continuing from the previous year. In October 2005 the group was dissolved after having established a co-operation with an SME (Planet GmbH, www.planet.de) who develop systems for automated recognition of handwritten address fields. This co-operation will fully unfold in 2005.

The project group used a novel method for learning nonlinear dynamical systems from observation data, Echo State Networks (ESNs). ESNs have been developed by Dr. Jaeger at AIS before he came to IUB. The technique is based on artificial

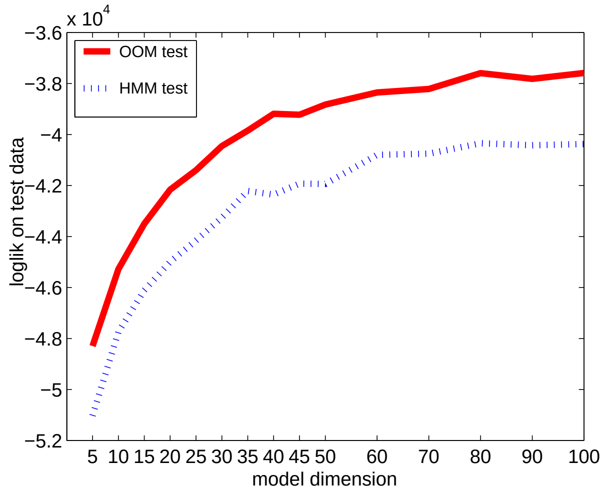


Figure 6: Test performance of the HMM and OOM models of different sizes obtained on an English text (Mark Twain's short story "The 1,000,000 Pound Note"). (H. Jaeger)

neural networks and enables engineers to obtain highly precise nonlinear system models by a computationally cheap and simple method. See http://www.faculty.iu-bremen.de/hjaeger/esn_research.html for more information on ESNs.

Activities of this project group were mostly carried out using the MATLAB installation at CLAMV, which thereby represented a central infrastructure component for the group's work.

Another strand of research of Dr. Jaeger's concerns observable operator models (OOMs), a novel technique for predicting random symbol sequences, such as English texts, preprocessed speech signals, or amino acid sequences. In a student project, a comparative study of OOMs vs. the more widely known hidden Markov models was carried out using again the MATLAB installation at CLAMV. Because a large number of datasets were analyzed, the computational capacity of CLAMV was essential. Fig. 6 shows an exemplary finding, demonstrating that OOMs significantly outperform HMMs on a difficult dataset.

In 2005, the MATLAB installation on CLAMV and the MATLAB software administered by CLAMV will be relied on to carry out ESN computations within the co-operation with Planet GmbH. In addition, it will again be needed for various student projects both on ESNs and OOMs.

2.2.8 Semi-Automatic Picture Retrieval

Prof. Dr. Peter Ludes (Mass Communication)

In the spring semester 2004 Prof. Peter Ludes (IUB/SHSS) and Prof. Otthein Herzog (Universitt Bremen/Technologiezentrum Informatik TZI) gave a USC "Olympic Key

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

This server has also been used by members of our research project on key visuals, which cooperates with universities in Brazil, China, Germany and the USA and was honored by the Ernst A.C. Lange prize for innovative cooperation between universities in Bremen. The upcoming detailed analysis of annual TV reviews from four countries needs a reliable server environment, provided by the CLAMV.

2.2.9 Monte Carlo Simulations in Statistical Physics

Prof. Dr. Hildegard Meyer-Ortmanns (Physics)

1. Observable effects of the QCD transition in heavy-ion collisions

(in collaboration with B. Berg and A. Velytsky, Florida State University, Tallahassee)

Relativistic heavy-ion collisions are performed at large colliders at CERN (the European Center for Nuclear Research in Geneva), or at BNL (the Brookhaven National Laboratory) at Stony Brook (US). Heavy ions such as lead or gold are smashed together at relativistic energies to create for a very short instant of time (of the order of some 10^{-23} sec) an extremely hot fireball in a rather exotic state of matter. These experiments are sometimes called little-bang experiments to emphasize the analogy to the big-bang at the earliest instants of time of our universe. About 10^{-6} sec after the big-bang the universe was still so hot that the state of matter could be described by a plasma of quarks and gluons. It is therefore challenging to study the question of which signatures may be visible in little-bang experiments from the transition to this exotic state, and back to "ordinary" matter. A simulation of the phase transition in QCD with SU(3)-gauge fields and quarks would be rather time-consuming for realistic quark-mass values, not to say that it is practically impossible. For the purpose of our interest it is instructive to study the conversion dynamics in a related spin model, the so-called three-state Potts model in three dimensions with three-component state vectors at each lattice site. The spins are exposed to an external magnetic field to mimic the effect of quark masses. We used Glauber dynamics to study the phase conversion for different speeds of the cooling and heating processes. From our hysteresis measurements we find a dynamics dominated by spinodal decomposition. A quench in temperature leads to competing domains in the vacuum. There is evidence that these effects survive even the case of a smooth crossover phenomenon (which is more likely to happen in real experiments than a true phase transition).

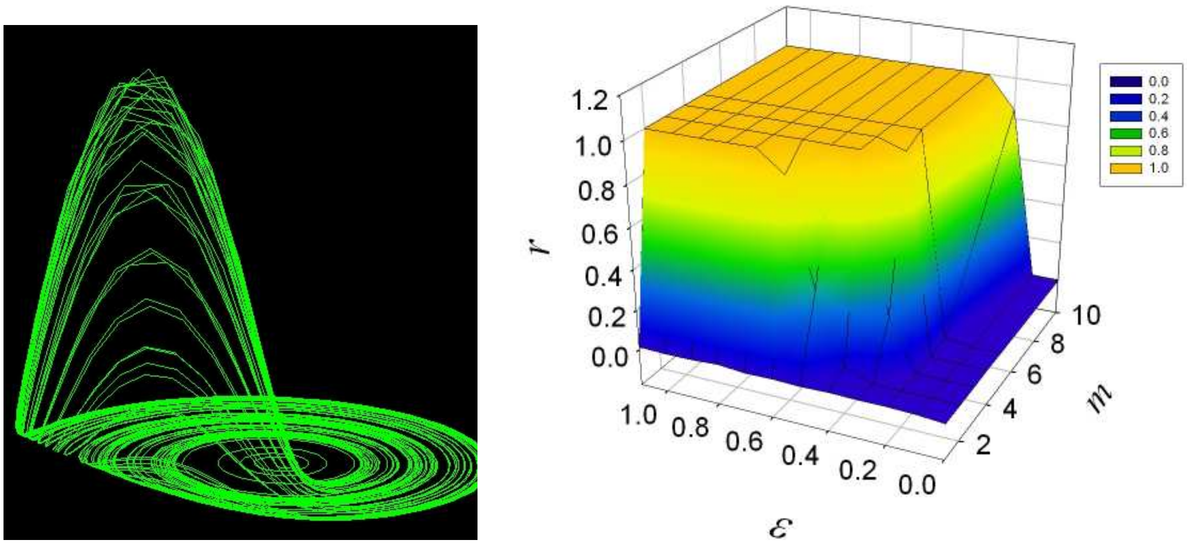


Figure 7: Left panel: Typical trajectory of one Rössler oscillator in phase space. Right panel: Order parameter r as a function of coupling strength and topology parameter m. (H. Meyer-Ortmanns et al.)

COMPUTATIONAL ASPECTS

The Monte-Carlo simulations were performed on three-dimensional space-grids with three-component vectors assigned to their nodes. The grid size was varied between 103 to 1203. Further parameters are the temperature, the speed of varying the temperature in a given interval, and the strength of the external magnetic field. As observables we measured structure functions for about ten momenta as well as the size of the largest clusters as a function of time, where ”time” refers to the number of Monte-Carlo sweeps. All these measurements were repeated for various combinations of the parameters (i.e., size, temperature, external field).

2. SYNCHRONIZATION OF CHAOTIC OSCILLATORS ON SCALE-FREE NETWORKS

(in collaboration with S.-H.Yook, IUB)

Synchronization phenomena are ubiquitous in nature, ranging from flashing fireflies in the Australian forests , clapping of hands in social systems, to unwanted synchronization between nerve and muscle cells in Parkinson's disease. When synchronization of dynamical systems was modeled on regular geometries, it turned out that even chaotic systems are able to synchronize under certain conditions on the coupling strength. A prototype for such chaotic systems are Rössler oscillators. In our simulations we simulated Rössler oscillators on scale-free Barabasi Albert networks. Scale-free networks have neither a regular nor a random geometry, but a scale-free degree distribution of edges which explains their name. This type seems to be realized in many natural systems. Therefore it is quite interesting to study the synchronization properties of an interacting system of chaotic oscillators on this geometry. As it turns out in our work, synchronization is facilitated by loops and shortcuts, but impossible on a tree-like geometry, independently of the coupling strength.

COMPUTATIONAL ASPECTS

The Rössler oscillators are described as three-component vectors in phase-space. The number of nodes in the network was varied between N=50 to N=500, typically it was chosen as 200. The number of edges m, attached to a newly generated node in the growth algorithm of the network, was chosen between 1 and 10. For the integration of the coupled, ordinary differential equations we used a fourth-order Runge-Kutta algorithm with step-size up to 10^{-3}. As indicators for the state of the system we measured different order parameters as a function of the coupling strength and the topology parameter m. One of these order parameters is shown in Fig. 7. Currently we are summarizing these results to submit them for publication. Since the system size is usually one of the important control parameters in simulations of network dynamics, the simulations are CPU-time consuming in general.

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. In 2005 my collaborators (one post-doc, one PhD-student, and one Humboldt fellow) will need the CLAMV-facilities. I also expect three students for guided research, who are interested in simulating certain aspects of population dynamics. They will need CLAMV-facilities for restricted periods of time (of the order of three months each).

TECHNICAL DETAILS

To 1: On the muscle cluster we used 8 CPUs (i.e. 4 nodes) in sustained manner. One run took typically several weeks. Since jobs survived for 5 days, we submitted jobs in batch of 8 for 5 days and restarted them. Each job needed of the order of 10 MB memory. From the software we used the Portland group compiler, which is the best one we have tested so far, and the portable batch system.

To 2: The muscle cluster was also used for the numerical integration of the system of nonlinear oscillators to study their synchronization. In order to reduce the computing time, we divided the entire calculation into parts that could be implemented by a set of serial codes. We used the Intel C/C++ compiler to generate these serial codes. Each code required around three days of CPU time. We submitted up to 50 processes to the batch scheduler.

GRANTS

One PhD-student is supported by a DFG (Deutsche Forschungsgemeinschaft)-grant since June 2004. Parts of his PhD-thesis are also numerical simulations of dynamical processes on networks. In June 2005 I expect a Humboldt-fellow from China (University of Shanghai), who graduated in Computer Science and will join our group for one year, working on networks. His contributions will be almost exclusively numerical work. Since the Humboldt foundation expects the support of computer facilities from the host university (IUB in his case), he will extensively need the facilities of CLAMV.

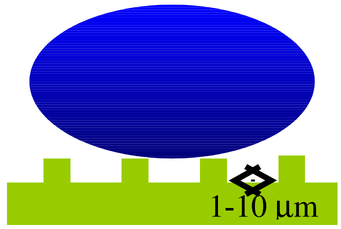


Figure 8: The Lotus effect, schematic. (F. Müller-Plathe)

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2.2.10 Computational Materials Science

Prof. Dr. Florian Müller-Plathe (Physical Chemistry)

THE NANO-LOTUS EFFECT: SURFACES BETTER THAN IN NATURE?

The Lotus flower grows in the mud. Yet, its leaves are always clean. This feature has earned the Lotus flower the status of a sacred plant in India, in ancient Egypt and Greece. How does the Lotus, and many other plants, avoid wetness, dirt and parasites? The answer lies in an ingenious combination of surface physics and chemistry. Its effect is that water drops do not attach to the leave's surface, but they roll off. In doing so, they take dirt, dust and even microorganisms with them, so every rain shower cleanses the Lotus leave. This extreme water-repellency is called superhydrophobicity.

The Lotus' first ingredient is a surface structure of micrometer size. It makes water drops stay away from the surface proper. The water drop is held together by the enormous surface tension of liquid water and it rests only on the tips of the micron-sized surface structures (Fig. 8). This, however, would not work without the second ingredient, the chemistry of the materials, which form the surface structure. They are themselves already very hydrophobic. Plants use waxes composed of very long chain fatty acids, which assemble into micrometer-size crystallites.

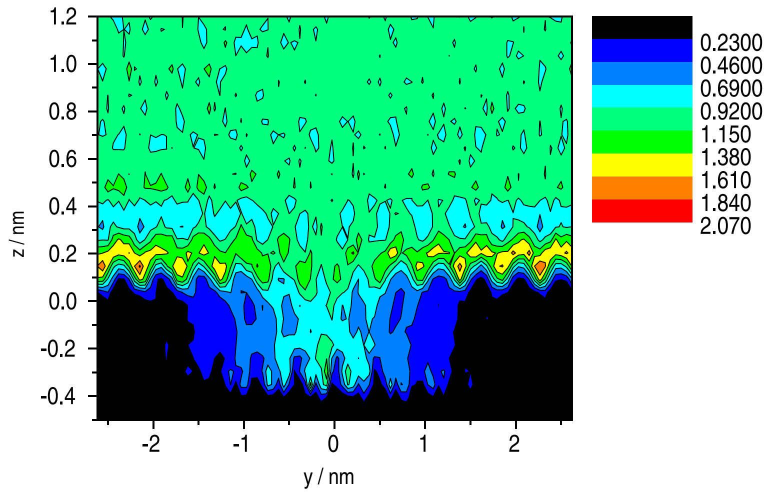

Figure 9: The density of water (g/cm^3) is lower in and around a nanohole in the surface of an alkane crystal (black). This is indicative of an increased hydrophobicity in these regions. (F. Müller-Plathe)

There are continuing attempts to use the Lotus effect, or superhydrophobic coatings in general, also for technical surfaces. Paints, surface coatings and special glasses are already available for several applications. They all make use of the Lotus' two ingredients: microstructuring and a hydrophobic base chemical. Of these, microstructuring is well under control, the hydrophobic chemistry is not. Micron-sized powders are easily made in a variety of ways; of hydrophobic chemical moieties there are essentially only two: large alkyl (CHx) and perfluoroalkyl (CFx) groups. The plants use CHx. CFx is better but also more expensive and environmentally problematic. With the limited choice in chemistry, what can be done to further improve the inherent hydrophobicity of a surface? One route is nanostructuring, i.e. providing a surface roughness on the nanometer scale in addition to the structure on the micrometer scale. The idea behind this is that vacuum is the most hydrophobic "material", and if parts of the surface are replaced by vacuum the surface will be more water-repellent. A vacuum portion of the surface can be realized by putting nanometer-size holes, grooves or pits into an otherwise flat surface. This nanostructure has to coexist with the microstructure of the Lotus effect. So far, the speculation.

Creating surfaces with nanometer-size indentations or protrusions from hydrophobic alkane or perfluoroalkane-based compounds is experimentally difficult. Therefore, this is where Computational Chemistry comes into play. Using molecular dynamics (MD) simulations, we have investigated in the computer if and how different surface nanostructures improve the hydrophobicity of alkane and perfluoroalkane materials. This can be done without having to synthetise or prepare any surface in the lab.

As a model for a hydrophobic material, we have used a section from an alkane (C20H42) crystal. Into this surface we made well-defined indentations of various shapes by suitably shortening selected alkane chains. The surfaces are put in contact with a liquid water phase of several thousand molecules. The hydrophobicity of different surfaces is then compared using a variety of indicators. One of them is the water density. Figure 2 shows it near a circular hole along a plane, which cuts vertically through surface and hole. It is evident that the water density in the hole, especially near the sidewalls, is lower than either in the bulk or near the unindented surface. Thus, water is trying to avoid the hole; the hole is water-repellent, and more so than a smooth hydrophobic surface. This finding can be quantified by comparing the number of residual water-surface contacts or the interfacial free energies for different structures. The result, however, is unchanged: Putting a nanostructured, rather than a flat, surface on a hydrophobic material makes it more hydrophobic.

The success of the Lotus effect on the micron-scale can therefore be repeated on the nanoscale: Surface structure on both scales increases the hydrophobicity of an already hydrophobic material. One may call this a nano-Lotus effect. One has to keep in mind, though, that the physics on both scales is quite different. The governing interaction for the (micrometer)-Lotus effect is the macroscopic surface tension of water, which makes it pull away from a pointed surface structure. The reason for the nano-Lotus effect is molecular: The hydrophobic hydration is more difficult for structured surfaces, and the water density near the structures is lower, but not zero.

We have characterized the hydrophobicity for circular holes as well as trenches and protrusions of different sizes. As a result we were able to suggest optimized structures for synthesis. The work has also been extended to other hydrophobic materials (C20F42), and the results are very similar.

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2. "Molecular Dynamics Simulations of Cellulose Oligomers: Conformational Analysis", S. Queyroy, F. Müller-Plathe, and D. Brown, Macromol. Theory Sim. 13, 427-440 (2004).

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7. ”Coarse-Graining in Polymer Simulations”, S. Girard and F. Müller-Plathe, in: M. Karttunen, I. Vattulainen and A. Lukkarinen (Eds.) Novel Methods in Soft Matter Simulations, Lecture Notes in Physics 640, 327-356 (Springer, Heidelberg, 2004).

8. ”Wie verhaken Polymerketten?”, F. Müller-Plathe, Nachr. Chem. 52, 409 (2004).

9. ”Uni privat: Chemie an der International University Bremen”, F. Müller-Plathe, Nachr. Chem. 52, 636-637 (2004).

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USE OF CLAMV

We are not using the CLAMV machines for our research. However, as our group’s Linux cluster is technically very similar to the CLAMV cluster, it is administered by Dr. Achim Gelessus, too. And we are most grateful for the excellent support! In addition, CLAMV machines and rooms are used for teaching the 3rd-year course Computational Chemistry and Biochemistry. A site licence of Gaussian03 for teaching and research is maintained by the CLAMV.

GROUP MEMBERS (AS OF 31/12/04)

Prof. Dr. Florian Müller-Plathe, Dr. Giuseppe Milano, Dr. Welchy Cavalcanti, Dr. Volker Weiß, Sandeep Pal, Konstantin Tarmyshov, Enrico Lussetti, Meimei Zhang.

Dr. Sylvain Goudeau left the group in November 2004 for a position at the CNRS in Toulouse, France.

FUNDING 2004

BASF AG, Rhodia SA, BMBF Kompetenzzentrum ”Werkstoffsimulation”, DFG (5 grants), Humboldt-Stiftung, Fonds der Chemischen Industrie, John-von-Neumann Centre Jülich (computer time)

2.2.11 Reflexive and Volitional Attention

Prof. Dr. Bettina Olk (Psychology)

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

We are currently preparing a series of experiments that will investigate the interaction between reflexive and volitional attention in the healthy and injured brain. We are using MATLAB for the presentation of the displays and data recording. Young and elderly healthy participants as well as participants who have suffered a stroke will be included in the experiments. The studies will allow us to shed light on normal and abnormal attention processes.

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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

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DECODING OF GAZE DIRECTION

The direction of eye gaze is an important element of social communication. Gaze direction allows effective nonverbal communication about potentially rewarding or dangerous stimuli. Moreover, the direction of eye gaze triggers reflexive attention shifts in the observer and can be used voluntarily or involuntarily to direct attention and gaze of others towards certain objects or people as well as to express someone's intentions. Gaze processing is present very early on in life, underlining its importance to human communication and behaviour. But how do we determine where someone is looking and importantly, what is the nature of this process? We are setting up a series of experiments that will investigate the role of geometric and of luminance cues that are thought to be crucial for the determination of gaze direction. MATLAB will be used for the presentation of the displays and data recording.

SELECTED RELEVANT PUBLICATIONS

Olk, B., Jassal, M., Symons, L.A. and Kingstone, A. (2005). Judging gaze direction depends on how you look at it. Journal of Cognitive Neuroscience, Suppl. S.

Symons, L. A., Olk, B., Jassal, M., Chung, V., & Kingstone, A. (2004). The brightness of a looker's iris is not important in determining direction of gaze [Abstract]. Journal of Vision, 4(8), 911a, http://journalofvision.org/4/8/911/, doi:10.1167/4.8.911.

Olk, B., Symons L.A., Hammad, S., Jassal, M. and Kingstone, A. (2004). Judging gaze: more than just black and white. Journal of Cognitive Neuroscience, C 147 Suppl. S.

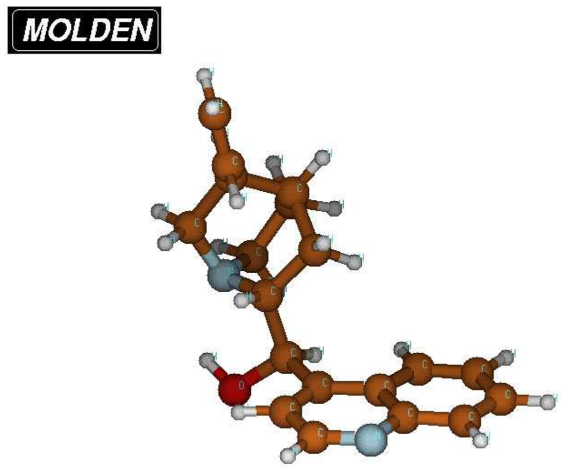

Figure 10: Vibration of the cinchonidine. (R. Richards et al.)

2.2.12 Geometry of Adsorbed Chiral Ligands on Nanoscale Pt and Ru Particles

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

Nanoscale catalysts are attractive because of their high surface areas, enhanced chemical reactivity and the potential for tailoring their composition (alloys, core/shell). However, the determination of the geometry of adsorbed chiral organic ligands for example in the case of cinchonidine (Fig. 10 is crucial to the understanding of the mechanisms of enantioselective reactions occurring at modified metal surfaces. Although such methods as attenuated total reflection (ATR)IR and reflection-absorption infrared spectroscopy (RAIRS) have provided valuable information about these conformations for thin films and extended metallic surfaces, diffuse reflectance IR (DRIFTS) is more appropriate for the study of finely divided powders such as nanoscale metal particles. For analysis of DRIFTS spectra of adsorbed compounds we need to compare it with calculated and reference spectra. Moreover, it is desirable to be able to attribute every signal in the infrared spectrum to an orientation of a transition dipole moment of a vibration. Because of the adsorption selection rule, only vibrations with transition dipoles orientated along the normal (Fig. 11 of a metal surface are present in the IR spectrum of the adsorbed molecules. In particular, optimization of the molecular geometry and calculation of the corresponding IR spectrum for the free molecule has proven to be an invaluable aid in these studies. These calculations have been performed on the CLAMV of IUB.

COMPUTATIONAL METHODS AND TECHNICAL DETAILS

Geometry optimization and calculation of IR spectra of our compounds; cinchonidine, quiphos and benzene, quinoline, and phenazine were carried out using the Gaussian 03 program. Density functional theory (DTF) calculations were performed using the B3PW91 and RB3LYP methods and LANL2DZ, 6-311 and others basis sets. Calculations were performed by using one CPU for one task and take from one to 15 days depending on molecular complexity and computational method. Vibrations were visualized by MOLDEN software.

2.2.13 Dynamics of Excited Electronic States

Prof. Dr. Michael Rohlfing and Dr. Neng-Ping Wang (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 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.

FEMTOSECOND DYNAMICS

Excitations often happen via states that are not eigenstates of the electronic structure, thus giving rise to state propagation in time which typically happens on a femtosecond time scale. Two prominent examples are resonant charge transfer processes (e.g.,

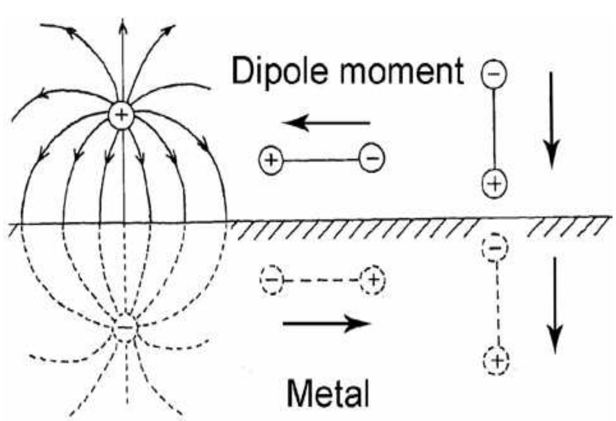

Figure 11: Adsorption selection rule. (R. Richards et al.)

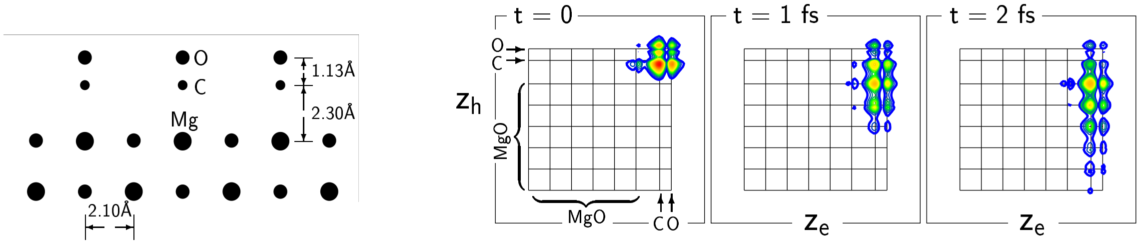

Figure 12: Left panel: Geometry of the CO:MgO(001)-(1×1) adsorption system. Right panel: Vertical electron-holr correlation function of the singlet excitation of CO:MgO(001)-(1×1) (starting with $|^1\Pi\rangle$) at increasing time. z_h (z_e) indicates the vertical position of the excited hole (electron). The horizontal and vertical lines indicate the z position of the atoms of the CO molecule (at the right and top of each panel), as well as the atomic layers of the 6-layer substrate slab (at the left and bottom). (M. Rohlfing et al.)

from an adsorbate to the substrate) and decay mechanisms due to the finite lifetime of electronic states resulting from electron-electron interaction.

By evaluating the time propagation for excited electronic states (either for single quasi-particles or for coupled electron-hole states), the dynamics of charge carriers, resonant charge transfer, etc. is addressed. This step is easily done within MBPT, just taking the MBPT Hamiltonian as time propagator. Essentially, it requires to solve the time-dependent Schrödinger equation, starting from an initial state.

As an example, Fig. 12 displays the spatiotemporal evolution of an electron-hole excitation ($^1\Pi$) of carbon monoxide (CO). The time propagation results from the quantum-mechanical coupling of the molecular state to the electronic degrees of freedom of the magnesium oxide (MgO) substrate. The state, which is not an eigenstate of the coupled system, separates into a hole (which is transferred into the substrate) and an electron (which remains on the molecule). The separation occurs within a few femtoseconds, which is considered extremely fast concerning the insulator nature of the subsrate.

Adsorption of organic molecules on metal substrates

Motivated by vast amounts of experimental data obtained on IUB's experimental physics groups, we have started to investigate the structure of organic adsorbates on metals, in particular of PTCDA on Ag(111). Using density functional theory, we were able to show that two-fold binding mechanisms occur (see the cross section shown in the left panel of Fig. 13). On the one hand, significant cvalent bonding occurs between the substrate and the center of the molecule, as is obvious from the enhancement of valence-charge density in that part. On the other hand, strong electrostatic interaction exists between the oxygen atoms at the corner of the molecule and the underlying Ag atoms, leading to significant polarization and electric dipoles. These electrostatic interactions cause a strong deformation of the (originally flat) nmolecule, bending the

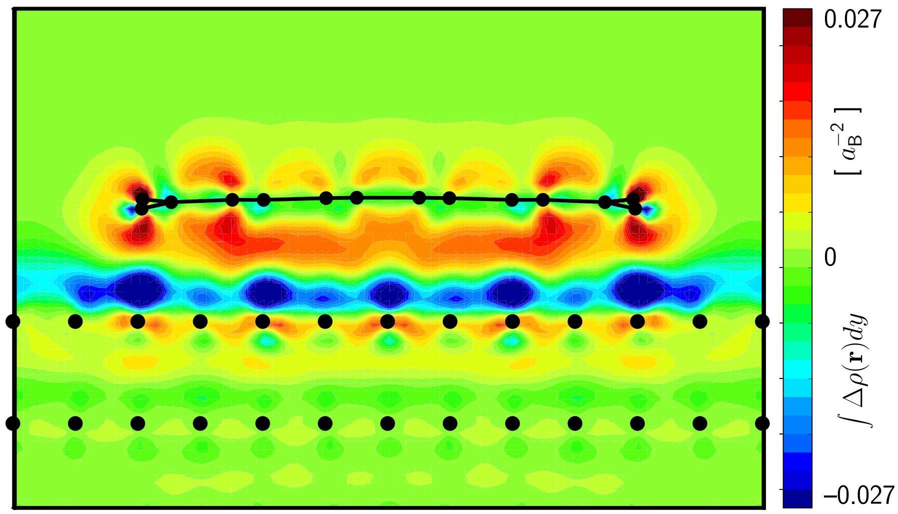

Figure 13: Change of the electronic charge density due to adsorption of a PTCDA molecule on Ag(111) (blue = reduction, red = enhancement of electrons). Charge accumulates below the molecule, accompanied by polarization of the Ag surface layer and by charge re-distribution at the oxygen atoms at the ends of the molecule. (M. Rohlfing et al.)

corner oxygens down by about 0.2 Å.

Grants

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

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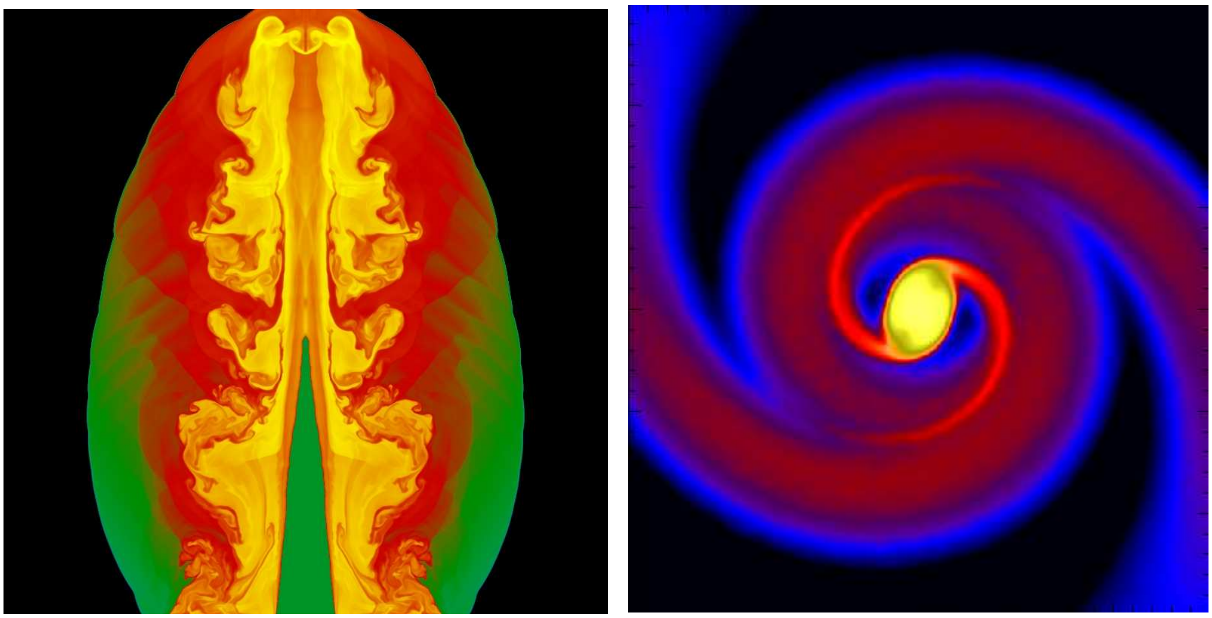

Figure 14: 2D-simulation of a relativistic, astrophysical jet, and 3D-simulation of a coalescence of two neutron stars. (S. Rosswog)

2.2.14 Encounters of Compact Binary Systems

Prof. Dr. Stephan Rosswog (Astrophysics)

Essentially every star ends up its life as a compact stellar object, either as a White Dwarf, a Neutron Star, or a stellar mass Black Hole. As most stars are gravitationally bound in binary systems, there is a fair fraction of such systems that contain compact stellar objects. Among them are systems where *both* components are compact components.

To date, several of these exotic systems are known, and one of them, the binary pulsar PSR 1913+16, has been studied in much detail for three decades. Its orbit decays under the action of gravitational wave emission and this orbital decay agrees to date with the predictions from general relativity to better than 0.2 %. The final coalescence of this system in around 10^8 years is an inescapable consequence.

Mergers of binary systems with either two neutron stars or a neutron star and a stellar mass black hole are extremely interesting systems as they are the prime targets of the ground-based gravitational wave detectors that will be in operation in the very near future. In addition, the coalescence of such a binary system has long been identified as a potential site for a class of cosmological explosions, the so-called gamma-ray bursts. Moreover, the disruption of a neutron star in such an event yields very promising conditions to form the heaviest elements in the universe.

COMPUTATIONAL APPROACH

The focus of the last few month has been on encounters of stellar mass black holes

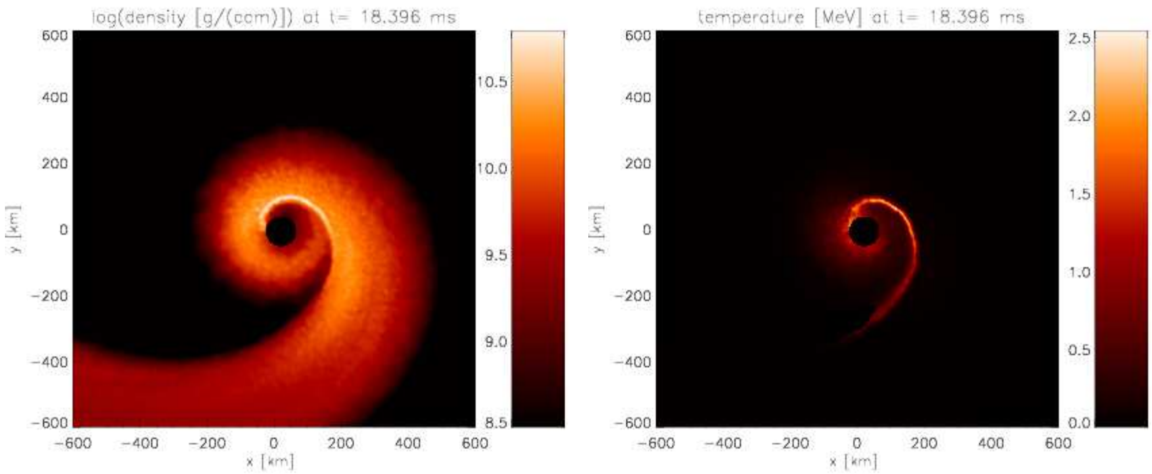

Figure 15: Disruption of a 1.4 $M_\odot$ neutron star by a 14 $M_\odot$ black hole. The self-interaction of the neutron star debris leads to the spiral shock that is clearly visible in both density (left) and temperature (right). (S. Rosswog)

with neutron stars.

Such a coalescence is an intrinsically three dimensional process and several branches of physics play a vital role. Therefore, (semi-)analytical models are only of restricted use and it has to be resorted to a fully three-dimensional numerical modeling. The equations of hydrodynamics have to be solved, threedimensional (strong-field) self-gravity has to be taken into account, and the neutron star matter has to be modeled using a temperature-dependent, nuclear equation of state. At the encountered temperatures the weak interaction time scales are comparable to the dynamical time scales, therefore β-equilibrium cannot be assumed. It is this non-equilibrium that drives the main neutrino processes via electron and positron captures onto free nucleons. The above requirements are met by the relativistic mean-field equation of state that we use in our simulations. Coupled with the hydrodynamics and this equation of state is a detailed, multi-flavour neutrino treatment that takes the effects of the neutrino opacity into account (opposite to most environments where the neutrino mean free path is for practical purposes essentially infinite, the neutrino mean free path in the debris of a compact merger remnant covers the whole range from a few centimeters (neutrino diffusion) to the completely transparent regime; for neutrino emission calculations and the subsequent annihilation processes this opacity-dependent emission is vital).

All these effects are integrated into a parallelised computer model that is currently run at the Höchstleistungsrechenzentrum Jülich. The current generation of calculations is unprecedented in both input physics and numerical resolution. One of the main conclusions of our recent work is that non-spinning, Schwarzschild black holes are not able to launch a cosmological gamma-ray burst explosion. Black hole spinning close to their maximum spin rate, however, may well be.

The access to the machines of the CLAMV has been vital for the code development work and the subsequent analysis and visualisations of the simulations.

In 2004 I have successfully applied for a HBFG grant that will pay for one half of the 24 processor shared-memory supercomputer that will be purchased in early 2005. 50 % of its capacity will be available for CLAMV-users. Most of my future simulations will be performed on this machine.

PUBLICATIONS

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S.Rosswog, R. Speith, G.A. Wynn, *Accretion dynamics in neutron star black hole binaries*, Monthly Notices of the Royal Astronomical Society, 351, 1121 (2004)

2.2.15 Synthetic Radiograms from CME Simulations

Dr. Joachim Schmidt, Prof. Dr. Joachim Vogt, and Prof. Dr. Marcus Brueggen (Solar Physics)

Coronal Mass Ejections (CMEs) are generally considered as being major transient events at the Sun that carry away huge amounts of solar material (up to $10^{1}6\,\mathrm{g}$) at large velocities (between 100 and 2000 km/s). These eruptions are essential for the transport of mass and momentum from the Sun into interplanetary space, and they can cause major geomagnetic disturbances if they hit the Earth. Since CMEs constitute a moving bulk of material, they are usually preceded by a shockwave that can accelerate charged particles like free electrons through Fermi acceleration. Such electrons can excite Langmuir waves in the solar wind plasma which in turn emit radio waves when they are dissipated by scattering mechanisms. Therefore, observations of radio waves in the meter-band are ideal diagnostics to monitor moving shock waves in the solar corona between about 1 to 2.3 solar radii that are driven by CMEs. Radio emissions may also be caused by magnetic reconnection in solar flares, gyrating ions within the core of the CME, or the compression of localized radio sources in the solar corona.

CME associated radio emissions fall into the detectable range (10–240 MHz) of a large-scale radio telescope called LOFAR, funded mainly by Dutch agencies. LOFAR is supposed to become operational in about three years, and IUB will act as a core institution in the German LOFAR consortium. The antenna array will consist of a large number of ground stations with several hundred dipole antennas each, and is expected to yield a high spatial resolution of up to 2 arc seconds. LOFAR will be steerable throughout the entire solar disc and its surrounding coronal plasma to provide high-resolution radio images of the Sun and, in particular, of CME-type eruptions.

In order to prepare LOFAR observations of CMEs and to guide the interpretation of the resulting radio maps, we are planning to run MHD simulations in two and three spatial dimensions. The simulation codes yield spatial and temporal distributions of macroscopic variables like density, bulk velocity, pressure, and magnetic field which have to be convoluted with radio emission intensity functions to produce synthetic radiograms. As a starting point we plan to model CME associated radio bursts of types II and III by identifying and tracing the acceleration regions of electrons, namely, magnetic reconnection sites and CME driven shockwaves. The accelerated electrons serve as a free energy source for plasma emissions at frequencies that will be detectable with the LOFAR facility.

2.2.16 Proving Nonexistence of Rational Points on Curves

Prof. Dr. Michael Stoll (Mathematics)

In 2004, I have used a lttle bit above 20 hours of CPU time on the 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 aim of the computations was to prove that certain algebraic curves of genus 2, given by an equation of the form

$$C : y^2 = f(x)$$

with f a squarefree polynomial of degree 6, do not have rational points (i.e., the equation above does not have any solution in rational numbers). The method used is based on a suitable embedding of the curve C into its Jacobian variety J (an abelian variety of dimension 2). The group $J(\mathbb{Q})$ of rational points on J had been computed previously; this knowledge was used to compute necessary conditions for points in $J(\mathbb{Q})$ to be in the image of $C(\mathbb{Q})$, the set of rational points on C. The conditions are obtained by comparing the image of the "mod-p" points on C with the image of $J(\mathbb{Q})$ in the "mod p" points of J, for many prime numbers p. In the end one hopes to obtain a contradiction, proving that $C(\mathbb{Q})$ is empty. The computations are time- and space-consuming (there is a combinatorial explosion effect). Several of the teacing lab machines were used to work on different curves in general. In the end, the computations were successful for all curves where the group $J(\mathbb{Q})$ has free abelian rank 2.

A paper reporting on the method used and on the results of the computation is in preparation.

2.2.17 International Research Consortium on Continental Margins (IRCCM)

Prof. Dr. Vikram Unnithan, Dr. Angela Schäfer, and Jakob Hauschild (Geoscience)

The CLAMV has provided invaluable support to the IRCCM's modelling research and aided the development of the GIS lab.

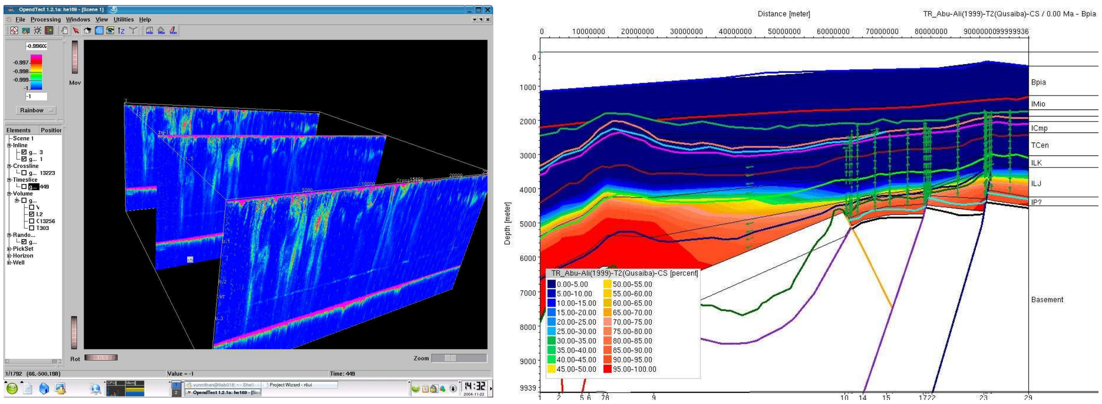

Figure 16: Left: Visualisation of parametric echosounder data showing of seafloor gas seepage in the North Sea. Right: Depth profile showing results from Petroleum System's Modelling of the Norwegian Margin. Green arrows indicate the direction of hydrocarbon migration while the colours represent hydrocarbon generation maturity. (V. Unnithan et al.)

Modelling

The modelling efforts in 2004 have focused on understanding the role and influence of heat budgets on fluid transport. Heat is one of the primary driving forces for fluid flow in the subsurface. In addition this will provide mathematical modelling and numerical simulations are also being carried out within the framework of an ongoing Master thesis to understand gas hydrate stability fields and methane concentrations within the shallow subsurface. Testing of the results and models obtained is being performed on a reconnaissance scale on the Irish continental margin where ideal conditions exist for the development of gas hydrates. The shallow part deals with various issues related to non-linear wave propagation in the subsurface. High-resolution parametric echosounders use this parametric effect to provide detailed images of the shallow subsurface. The physics, mathematics, experimental and numerical simulation of this parametric effect is an integral part of an ongoing PhD thesis work. Schlumberger have granted IUB a free Charisma university license (industry standard seismic interpretation software). This software is currently being installed and will provide additional techniques for seismic interpretation, visualization and modelling of fluid flow. 3D seismic data from the Kristin Field has been requested from NPD and StatOil. 3D geological process modelling is being performed with the advanced PetroMod Software. Currently post doc research on the shallow part (upper 500 m of the seabed) deals with gas hydrates and hydrofracturing models on the Cascadian Margin, while the deep part focuses on the hydrocarbon play systems on the Voring Plateau, Norwegian Margin. Seismic data from the Kristin field will be used for this purpose. Results from these modelling efforts are to be presented to StatOil for further analysis and discussion.

Data Analysis, GIS and Visualisation Laboratory

The spatial and temporal analysis of data is critical for understanding continental margin processes. Geographic Information System (GIS) is a broad field that deals with the analysis, processing and visualization of geoscience related data. To fulfill this need within the IRCCM, a GIS and enhanced visualization laboratory has been set-up in IUB with the help of the CLAMV. This laboratory is equipped with specialized high performance pc's linked to the IUB and partner Linux clusters providing access to a large pool of computing infrastructure. In addition, industry-standard software such as ArcGIS and Open Source tools provide a wide range of tools to analyse data currently being gathered by the partners from sites on the Norwegian Margin, North Sea, Irish Continental Margin.

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 at IUB with IRC and CLAMV help. In order to visualize the gathered datasets, advanced visualization techniques are currently implemented. These include the immersive, real- and virtual 3D visualization using stereo image enhancement and projection. Acquisition of specialist software such as Fledermaus provides the user the ability to be immersed into the data volume.

Seabed observatories that provide online, real-time access to instruments generate a large volume of data. The storage and archiving of this large data volume needs a comprehensive and integrated data management strategy flexible enough to meet the changing demands of users, technology and digital standards. IRCCM is developing a system based on MarineXML (eXtended Markup Language). Data from instruments 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. Since most large relational databases deal with geo-coded vector data, a new concept has been developed for integrating image or raster data. IRCCM partners along with the SME Rasdaman have submitted a proposal to ESA (European Space Agency) for supporting the development of a raster (image) relational database. This technology will be able to store and access a very large (10 Terabyte or more) raster relational database quickly and efficiently. It will also provide users with the functionality to process and visualize data on the fly.

INFRASTRUCTURE

Hardware acquired within the framework of CLAMV and IRCCM includes three high-end visualisation pc's equipped with dual monitors. The pc's along an internet map server forms part of the CLAMV - StatOil - IRCCM GIS and visualisation lab. The lab is physically hosted in R3, room 96. Funding for the above mentioned hardware was provided by IRCCM.

In terms of software, over 1 million euro (commercial value) of software was installed by the CLAMV in the GIS Lab. 25 classroom licenses of ArcGIS, ArcIMS and ArcSDE provide the main GIS software. 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 and Charisma. IUB has been granted a special university license worth 500.000 euro for Charisma. 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. This software is used for modelling oil and gas accumulations and migration through time. PetroMod has been installed on the CLAMV teaching labs. Additionally several graduate students are being trained in the GIS lab. Their current guided research projects help to establish a broad data base on geoscientific data focused on IRCCM activity sites.

WORKSHOPS

The CLAMV helped organise and host a two-day workshop on “Advanced Petroleum Systems Modelling” in May 2004. This workshop provided scientists from various Northern German geoscience institutes hands-on experience with the Petroleum System’s Modeling Software - PetroMod.

GRANTS

For the forthcoming year, funds will be available from the IRCCM budget for various research projects and acquisition of hardware.

2.2.18 Computer Simulation of Biomolecules

Prof. Dr. Martin Zacharias (Computational Biology)

Our main research focus is on computer simulation of biomolecular association and conformational flexibility. Our goal is to better understand structure formation of biomolecules and the mechanism of ligand-receptor association. The prediction of putative ligand binding geometries and binding sites on a biomolecule is of tremendous importance for the design of new drugs that can bind and interfere with the function of biomolecules. A particular focus of our research is on better accounting for flexibility of binding partners during docking simulations. We use extensively the Master and Muscle Linux Cluster as well as the teaching lab computer resources of CLAMV. During 2004 we have completed the development of a new ligand-receptor docking approach that allows to efficiently account for receptor flexibility employing pre-calculated soft degrees of conformational freedom [1]. In addition, work on a new potential scaling approach for docking and protein modelling has been finished [2,3]. During the three months visit of Karine Bastard from Paris another extension of our protein-protein docking approach ATTRACT [4] has been developed based on a multiple copy representation of mobile parts of a protein molecule [5]. A systematic conformational search method for nucleic acids has been developed that in part also used CLAMV resources [6].

Within the last year we investigated in a collaborative effort with the group of Prof. W. Nau (IUB Chemistry) the dynamics of end-to-end contact formation of small peptides in aqueous solution. Goal of this research project is to study in atomic detail the pathway of contact formation and to understand its sequence dependence using the molecular dynamics simulation method. A significant part of the simulations have been performed on CLAMV teaching lab computers and on the Master cluster. One paper on this work has been published [7] another has been submitted. Collaborative simulation work with S. Springer (IUB) [8] and J. Engels (Uni-Frankfurt) [9] also involved in part CLAMV computers.

PUBLICATIONS

[1] Zacharias M. 2004. Rapid Protein-ligand docking including soft degrees of freedom from molecular dynamics simulations to account for protein flexibility: FK506 binding to FKBP binding protein as an example. Proteins 54:759-767.

[2] Riemann N., and M. Zacharias. 2004. Reversible scaling of dihedral angle barriers during molecular dynamics to improve structure prediction of cyclic peptides and protein loops". J. Peptide Res. 63:354-364.

[3] Riemann N., and M. Zacharias. 2005. Refinement of protein cores and protein-peptide interfaces using a potential scaling approach. Prot. Engineering, submitted.

[4] Zacharias M. 2003. Protein-protein docking with a reduced protein model accounting for side-chain flexibility. Protein Science 12:1271-1282.

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[6] Villescas, G., and M. Zacharias. 2004. Efficient search approaches on energy minima for structure prediction of nucleic acid motifs. J. Biomol. Struct. Dyn. 22:355-364.

[7] Roccatano, D. W. Nau, and M. Zacharias. 2004. Structural and dynamical properties of CAGQW peptide in water: A molecular dynamics simulation study using different force fields. J. Phys. Chem. 108:18734-18742.

[8] Zacharias, M., and S. Springer. 2004. Conformational flexibility of the MHC class I ?1-?2 domain in peptide bound and free states: A molecular dynamics simulation study. Biophys. J., 87:2203-2214.

[9] Zacharias, M., and J. W. Engels. 2004. Influence of a fluorobenzene nucleobase analogue on the conformational flexibility of RNA studied by molecular dynamics simulations. Nucleic Acids Res. 32:6304-6311.

2.2.19 Magnetohydrodynamic Simulations of Paleomagnetospheres and Numerical Simulations of Magnetosphere-Ionosphere Coupling

Bertalan Zieger, Ph.D., and Prof. Dr. Joachim Vogt (Space Physics)

The Michigan BATS-R-US 3D magnetohydrodynamic (MHD) code has been used to simulate different kinds of dipolar and quadrupolar paleomagnetospheres. The code currently runs on parallel computing platforms like the CLAMV Linux Cluster and the CLAMV SUN Fire v880. However, simulations with enhanced resolution must be run on the CLAMV Linux Cluster because of the large memory requirement.

We carried out simulations of the so-called equatorial dipolar paleomagnetosphere, where the Earth's internal dipole moment is perpendicular to the rotation axis. With such a dipole field orientation, the dipole tilt in GSM coordinates changes, due to the Earth's rotation, from zero through 360 degrees in the course of the day, resulting in an extremely dynamic magnetosphere on the diurnal timescale. We calculated steady state solutions with different dipole tilts in order to represent the paleomagnetosphere at different times of the day. We described the regular diurnal variation of the geomagnetic field-line configuration and the topology of large-scale magnetospheric current systems, like the Chapman-Ferraro currents and the tail current sheet. Fig. 17 demonstrates the diurnal variation of the magnetic field configuration of an equatorial dipolar paleomagnetosphere, assuming a regular Parker spiral interplanetary magnetic field (IMF) in the away sector. Furthermore, we investigated the effect of the IMF orientation on the solar wind-magnetosphere coupling in case of pole-on magnetospheric configurations, where the dipole axis is aligned with the Sun-Earth line. These simulation results were published in the Journal of Geophysical Research [Zieger et al., 2004].

We simulated different types of quadrupolar paleomagnetospheres as well, varying the orientation of the internal magnetic field, the IMF orientation, and the quadrupole shape parameter controlling the topology of the internal field. Zero IMF conditions were used as reference cases. We studied the magnetopause currents and the cross-tail current systems in quadrupolar paleomagnetospheres, which are much more complicated than the current systems in a simple dipolar paleomagnetosphere. The cross-tail currents in paleomagnetospheres with neutral line quadrupoles are depicted in Fig. 18 for different IMF conditions. IMF orientations with nonzero component perpendicular to the solar wind flow were found to have a much stronger effect on the global magnetospheric configuration than a purely parallel or antiparallel IMF. A comprehensive study of quadrupolar paleomagnetospheres has been published recently in the Journal of Geophysical Research [Vogt et al., 2004].

Making use of the ionospheric module of the BATS-R-US MHD code, we studied the magnetosphere-ionosphere (M-I) coupling in axial dipolar paleomagnetospheres. We simulated the change of the ionospheric transpolar potential and the corresponding field-aligned currents (FAC) in the function of the dipole moment, the ionospheric height-integrated Pedersen conductance, and the IMF Bz component, respectively. The numerical simulations fairly well reproduced the saturation of the transpolar potential predicted by the analytical Hill model and confirmed by recent observations. After validating our simulation results, we gave estimates of the transpolar potential and the total region 1 FAC in paleomagnetospheres with strongly reduced dipole moments. Our simulation results fit reasonably well to the corresponding theoretical curves of the Hill model, though the simulations show a somewhat steeper drop of the transpolar potential with decreasing dipole moment. A perfect fit cannot be expected anyway, as the Hill model is only a simplified model of M-I coupling, replacing the region 1 FAC system with two circular current loops in the Y-Z plane in GSM coordinates and neglecting the influence of region 2 FACs. The MHD simulations, on the other hand, simulate region 1 FACs in a self-consistent way in three dimensions. Therefore we deem our predictions of paleomagnetospheric transpolar potentials and

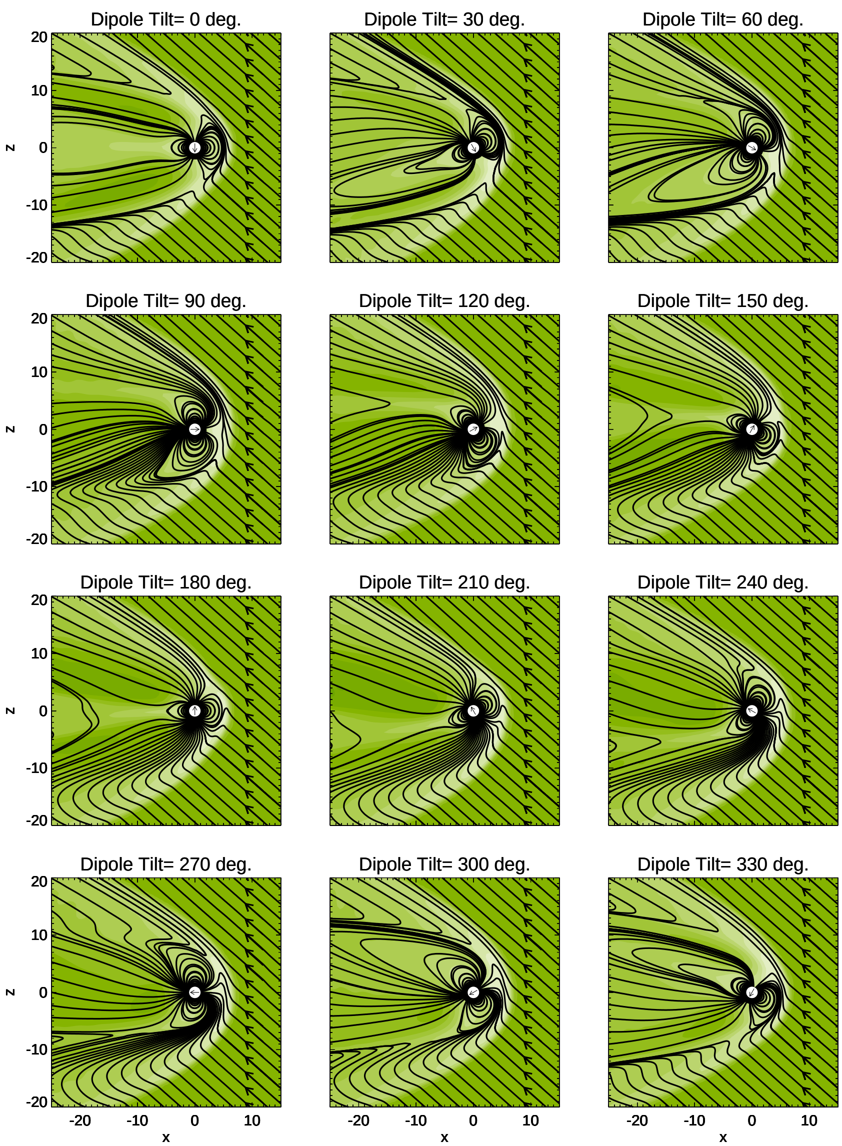

Figure 17: Diurnal variation of the magnetic field configuration and pressure in the equatorial plane of an equatorial dipolar paleomagnetosphere. (B. Zieger, J. Vogt)

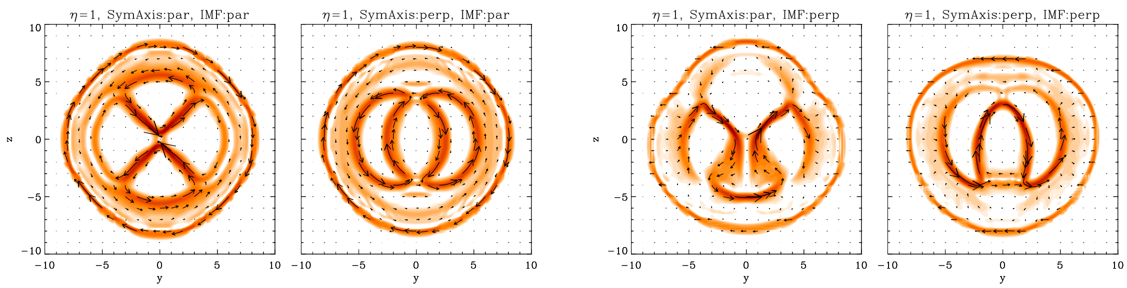

Figure 18: Tail currents projected onto the plane $x = -4R_E$ for paleomagnetospheres with neutral line quadrupoles. Left panel: both IMF (interplanetary magnetic field) and quadrupole neutral line parallel to the solar wind flow. Second panel: IMF parallel, neutral line perpendicular. Third panel: IMF perpendicular, neutral line parallel. Right panel: both IMF and neutral perpendicular to the solar wind flow. (B. Zieger, J. Vogt)

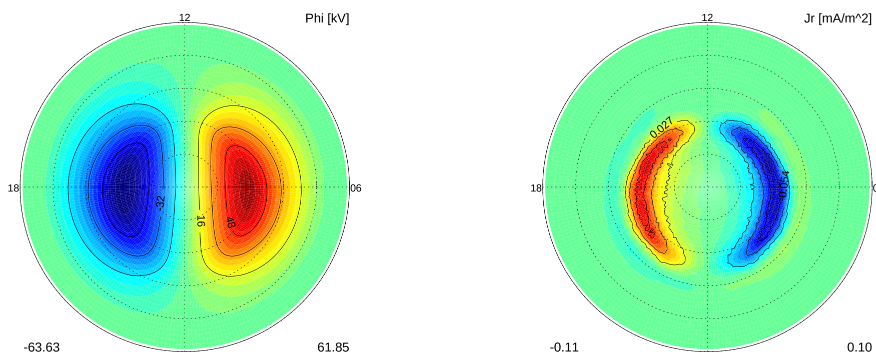

Figure 19: Ionospheric potential pattern (left) and the corresponding field aligned currents (right) for an axial dipolar paleomagnetosphere with a normalized dipole moment of 0.5. (B. Zieger, J. Vogt)

region 1 FACs more reliable. Fig. 19 shows the ionospheric electric potential pattern and the corresponding region 1 and region 2 FACs for an axial dipolar paleomagnetosphere with a dipole moment reduced to one half of the present value. We presented these results at the COSPAR 2004 meeting, and a paper on this topic is in press [Zieger et al., 2005].

Future plans

In addition to further MHD simulations of paleomagnetospheres and exoplanetary magnetospheres, we are planning to install and run the Energetic Particle Orbits in Paleomagnetospheres (EPOP) simulation code on the CLAMV computers. The code has been developed at the TU Braunschweig in cooperation with IUB. Particle simulations generally require a lot of CPU time but the code can be easily parallelized. Therefore we are expecting to use the parallel computing resources of CLAMV more extensively.

GRANTS

DFG Vo 855/1-2 (2002–2004) and DFG Vo 855/1-3 (2004–2006): Studies of paleomagnetospheric processes

PUBLICATIONS

Zieger, B., J. Vogt, K.-H. Glassmeier, and T. I. Gombosi: *Magnetohydrodynamic Simulation of an Equatorial Dipolar Paleomagnetosphere*, Journal of Geophysical Research, 109, A07205, 2004

Vogt, J., B. Zieger, A. Stadelmann, K.-H. Glassmeier, T. I. Gombosi, K. C. Hansen, and A. J. Ridley: *MHD Simulations of Quadrupolar Paleomagnetospheres*, Journal of Geophysical Research, 109, A12221, 2004

Zieger, B., J. Vogt, A. J. Ridley, and K.-H. Glassmeier: *A Parametric Study of Magnetosphere-Ionosphere Coupling in the Paleomagnetosphere*, Advances in Space Research, in print, 2005

2.3 Additional Future Projects

CLAMV has become an essential part of research at IUB, and its importance is expected to further develop in the nearest future. All current projects (see above) are expected to continue using CLAMV ressources. Furthermore, several other projects are about to enter a phase of computer-based analysis and simulation using CLAMV hardware and software. Nearly all of these current and future projects are financially supported by third-party grants for postdoctoral and PhD positions, embedding CLAMV and IUB in a sceintific environment on a national and international scale.

Among the planned projects, a number of examples are discussed here.

2.3.1 Real-Time Web Services for Multi-Terabyte Raster Archives

Prof. Dr. Peter Baumann (Computer Science)

A planned activity starting early 2005 is to set up a large-scale database for combined earth observation, oceanographic, and geophysical data. Initiated by Vikram Unnitham and Peter Baumann, who both have joined IUB in fall 2004, this Web-accessible database will be part of the IRCCM (www.irccm.de) data center which is being established at IUB. Hosting multi-Terabyte raster objects such as 2-D satellite imagery, 2-D / 3-D bathymetric data, and 3-D seismic data from the sea bottom, this will form a worldwide unique gathering of multidimensional raster data. Results will be presented to the geo Web services standardization body, OpenGIS Consortium, by Peter Baumann who is active member on behalf of IUB. Further, this database will act as a test vehicle for further research and as a proof of concept for forthcoming transdisciplinary geo / computer science research proposals. A first joint proposal already has been submitted to ESA by the end of 2004.

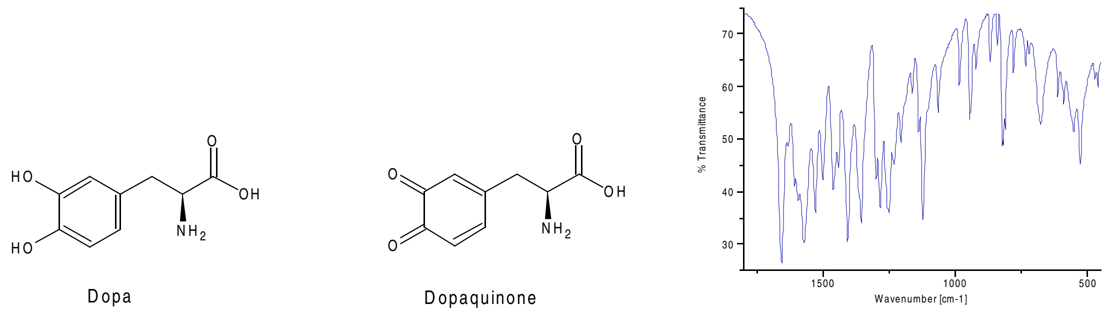

Figure 20: Left panel: Structure of Dopa and Dopaquinone. Right panel: IR spectrum (fingerprint region) of Dopa. (C. Doose)

2.3.2 Molecular Structure and Vibrations of the Amino Acid 3,4-Dihydroxyphenyl Alanine

Dr. Caren Doose (Chemistry)

Both amino acids 3,4-dihydroxyphenyl alanine (Dopa) and its oxidation product Dopaquinone are thought to play an essential role in the adhesion of mussel glue proteins on different surfaces. In order to investigate the molecular interactions underlying the adhesion processes in the group of Dr. Doose in cooperation with Prof. Tautz surface analytical techniques are implemented, as e.g. High-Resolution Electron Energy Loss Spectroscopy (HREELS). The interpretation of the obtained spectra requires the identification of the specific vibrational modes of the molecule. This is done by means of computational methods supported by CLAMV resources.

Calculations of the molecular structure and of molecular vibrations of Dopa and Dopaquinone in its acid form as shown in Fig. 20 have been performed with Gaussian03. The neutral acid form however is only present in the gaseous phase. In the solid state the zwitterionic (-NH_3^+/-COO^-) form of the amino acid is favored, stabilized by intermolecular interactions unaccounted for by Gaussian03. In order to include this charge separation, the molecular structure of Dopa has been optimized with SIESTA 1.2.25 starting from the experimentally obtained crystal structure. Hence, both the molecule in the crystal as well as the isolated molecule have been calculated. Based on these data, the dynamic matrices of the molecules were determined. The extraction of the available information about specific vibrational frequencies of the molecules is currently being performed.

2.3.3 Neural Networks in Biochemical Engineering Unit Operations

Prof. Dr. Marcelo Fernandez-Lahore (Downstream Processing)

The downstream processing laboratory at IUB is generating data on the performance of several "integrated" technologies for the recovery and purification of biotechnological products. Preferred operation are adsorption processes, which are able to selectively capture the targeted species for crude biological feedstock e.g. fermentation liquors even in the presence of suspended cellular matter. Optimization and simulation of the adsorption behavior in such technological systems require appropriate modeling strategies. Surrogate modeling will be attempted employing artificial neural networks. Raw data describing underlying phenomena (e.g., flow mixing, mass transfer limitations, equilibrium adsorption) will be processed so as to yield adimentional groups or described by simplified mathematical expressions. These relationships will be set as inputs in the neural networks. Theoretical results will be confronted with experimental findings at the laboratory and pilot scales.

2.3.4 Analysis of Brain Slice Images from fMRI Measurements

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

Recent studies suggest that aerobic fitness training improves cognitive performance capabilities. Mechanisms might be increased brain vascularization (e.g. density of capillaries) and survival and growth of existing or development of new neurons and/or synapses. We will use fMRI to investigate cerebral blood flow and stimulus or task-related hemodynamic activity in the aged brain. Physiological parameters like heart rate, blood pressure and oxygen consumption will also be recorded. We then plan to apply an aerobic fitness-training program to elderly subjects and to investigate its effect on sensory and cognitive performance and on brain hemodynamics.

Each single fMRI measurement results in a number of two-dimensional brain slice images which have to be aligned to each other and to an anatomical reference, motion corrected, temporally and spatially filtered, and statistically analyzed to achieve a three-dimensional reconstruction of brain activity over time and under different conditions. For this time and memory consuming data preprocessing and analysis we plan to use Matlab software (provided by the CLAMV) and SPM2 (a free software package running within the Matlab workspace and made available by the Wellcome Department of Imaging Neuroscience, London, UK).

3 Teaching

The CLAMV is primarily designed as a computational laboratory for graduate and faculty research, however, its resources have been used extensively also for undergraduate teaching and research. In the years 2002 and 2003 all undergraduate hands-on computer instruction was conducted in the CLAMV teaching lab. In January 2004 a second computer facility was installed for undergraduate courses, namely, a single lecture hall equipped with 40 workplaces (thin clients). This computer lecture hall (CLH, also called 'CS Lecture Hall' or 'Undergraduate Teaching Lab') is complementary to the CLAMV Computer Teaching Lab (CTL, also called 'Graduate Teaching Lab') in the sense that the CLH is designed for large courses in computer science and related fields whereas the CLAMV CTL hosts smaller (graduate and advanced undergraduate) courses, guided research projects, and research groups.

3.1 Undergraduate Programs

In 2004, 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.

The courses which made use of the CLAMV CTL are listed in tables 1 (spring 2004) and 2 (fall 2004). In the following, we give examples of special uses of the CLAMV as a teaching facility.

The BICB experience

Contributed by Frank-Oliver Glöckner

In the emerging field of Bioinformatics and Computational Biology (BICB) lab courses in CLAMV are essential for practical "hands on" education of the students. In each semester the students assemble in the CLAMV lab two times a week to get basic skills in programming, molecule modelling and sequence analysis. The BICB lab courses are taught by Martin Zacharias and Frank Oliver Glckner, Professors for Computational Biology and Bioinformatics, respectively. In 2004 a genome server has been integrated in the CLAMV system to support enhanced sequence- and genome analysis and phylogenetic reconstructions. The new server is equipped with two Xeon 2.8 GHz processors and 4 GB of main memory and is running with SuSE-Linux Professional as operating system. Specific command line software tools like BLAST, signal peptide, transmembrane helices and transfer RNA prediction are installed for batch processing of DNA and protein sequences. Furthermore the two software suites GenDB and ARB are available. GenDB[2] is an open source software system for genome annotation de-

[2] www.cebitec.uni-bielefeld.de/groups/brf/software/

Courses	Instructors
Advanced Bioinformatics	M. Zacharias, F.O. Glöckner
Graphics and Visualization	H. Kenn
NatSciLab Mathematics	P. Bangert
Computational Chemistry	F. Müller-Plathe
Computational Neuroscience	C. Hilgetag
Computational Fluid Dynamics	A. Khalili
NatSciLab GeoAstro	M. Brüggen
Database and Internet	M. Kohlhase

Table 1: Spring semester 2004 courses that made use of the CLAMV CTL facility.

veloped by the University Bielefeld. It is able to run all kinds of similarity and pattern based tools for assigning potential functions to predicted genes. All data are stored in the relational database system MySQL for data mining and graphical visualisation. Search and retrieval of specific data can be done via an API (applications programmer interface). For the students CLAMV is a perfect environment to get the principles to process large amounts of sequence data as well as to store and retrieve them.

The second software suite now available is ARB. ARB[3] (latin: arbor, tree) is a comprehensive software package for phylogeny which had primarily been developed for ribosomal RNA (rRNA) data, but can be used for any kind of sequence data. The rational behind the program design was to arrange a database of sequences and any other additional information according to the phylogenetic relationships of the corresponding organisms. This phylogenetic tree can be visualized on the screen and be used for walking through the database by mouse click. ARB integrates all kinds of distance matrix, parsimony and maximum likelihood based phylogenetic reconstruction programs under a common graphical user interface (GUI). Access to the data via a database management system as well as an enhanced sequence editor and probe design functions are also implemented. The students are able to import their own sequences, align them and reconstruct phylogenetic trees with different methods. ARB is a good model to illustrate students how large software systems are created, maintained and improved by the scientific community over years.

Linear Algebra for High-Performance Computing

Contributed by Jakob Hauschild

The lecture "Linear Algebra for High Performance Computing", taught by Prof. W. Hiller (AWI) and Prof. M. Oliver in the fall semester 2004, was attended by eight undergraduate students (fifth semester Computational Science). The course covered several aspects of large scale problems in numerical linear algebra. After introductory lessons on computer architectures, parallel programming paradigms and

[3] www.arb-home.de

Courses	Instructors
Computational Logic Lab	M. Kohlhase
Lab, Field and Data Analysis II	J. Vogt, S. Rosswog
NatSciLab GeoAstro	M. Brüggen
Advanced Bioinformatics	M. Zacharias, F.O. Glöckner
Computational Chemistry	F. Müller-Plathe
Computational Physics	M. Rohlfing
Numerical Methods	P. Oswald
Scientific Computing	W. Hiller
Time Series Analysis	J. Freund
NatSciLab Numerical Software	P. Bangert

Table 2: Fall semester 2004 courses that made use of the CLAMV CTL facility.

basic subroutines for vector and matrix operations, this knowledge was applied to iterative solvers for linear systems and eigenvalue problems, fast Fourier transforms and multigrid methods.

Tutorial sessions in the CLAMV Teaching Lab supplemented the lecture with exercises on the Hockney and Ping-Pong benchmarks, studying the concepts of the OpenMP and the MPI standard. Finally the students presented a detailed evaluation of parts of the HPC challenge benchmark[4] on the 24-processor Linux Cluster III. Access to this cluster was exceptionally given to the small group of students during a period of low processor load and caused minor interference with research activities.

Psychology Lab Course II

Contributed by Bettina Olk

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

Undergraduate Research

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, we look at the guided research project carried out by Peter Dabrowski who majored in Geosciences and Astrophysics. The

[4]http://icl.cs.utk.edu/hpcc/

student was supposed to come up with error estimates for the electrical current density determined from magnetometer measurements of ESA's multi-spacecraft mission Cluster-II. On the CLAMV computers he simulated satellite orbits in various model magnetic fields to find out how the errors depend on the inhomogeneity length scales of the magnetic field. He finally tested and confirmed analytical error formulas.

3.2 Graduate Programs

With the start of several new graduate programs in Fall 2004, computationally oriented graduate research began to require significantly more CLAMV resources than before. Many of these research projects are implictly covered in the contributions to section 2. In 2005 we expect this activity to grow further so that in the forthcoming CLAMV Activity Report a separate subsection will probably devoted to teaching and research within the graduate courses.

3.3 Workshops and Other Activities

Like in 2003, the Training for the International Collegiate Programming Contest was again held in the CLAMV Computer Teaching Lab. This activity was already described in the CLAMV Activity Report 2002/2003.

The CLAMV Computer Teaching Lab hosted two workshops in 2004, namely, a workshop on the geological basin modeling software *PetroMod* and on the visualization software package *IDL*. The workshops are described in section 2 (PetroMod) and section 5 (IDL).

4 CLAMV Seminar

The CLAMV seminar is the weekly research seminar of the CLAMV. It aims at creating a community of IUB computational scientists and researchers from adjacent disciplines by

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

The seminar always draws a diverse audience of faculty, post-doctoral researchers, and graduate students; many talks are also attended by a good number of undergraduates. CLAMV talks have already initiated or strengthened informal discussion among IUB faculty from different disciplines—at least some of them have the potential to develop into active collaborations with subsequent publications or grant applications.

In 2004, guests from industry were invited in addition to the regular presentations of internal speakers. Furthermore, the proportion of technical talks increased in order to broaden the appeal of the seminar. A detailed seminar schedule can be found in Appendix A.4.

5 Service and Consulting

The CLAMV services can be subdivided into three categories.

Basic services: This term refers to all services commonly used for research and teaching. Examples are the TeachingLab including user administration and maintenance of (scientific) software packages.

Advanced services: This term refers to all services which are mainly or even exclusively used for research. Examples are the facilities for parallel computing and storage.

Off-campus services: This term refers to all cooperations with external partners. Examples are the cooperation within the BremHLR and the access to high performance computing centers.

5.1 Basic Services

The CLAMV teaching lab consists of 30 Linux PCs which are spread over 4 class rooms in building Research I. The teaching lab computers are fully connected to the internet and are equipped with a nVidia graphics adapter with 3D acceleration for visualization projects. The administration of the user accounts (more than 500 in December 2004) is done on a SUN v880 server. A thorough discussion of the CLAMV account is given in the CLAMV primer (Achim Gelessus, 30. November 2004)[5] .

In January 2004 the undergraduate lecture hall in building Research I was taken into service by IRC and CLAMV. The user administration has been incorporated into the CLAMV user administration for providing an identical user environment (user login, home account) on the CLAMV teaching lab and the undergraduate lecture hall computers. The hardware maintenance of the undergraduate lecture hall is now done by the IRC.

CLAMV provides the IUB community with software which is essential for the daily work in an scientific environment. This concerns commercial software as well as free software including the required license management. The focus of the software installations is on the Linux operating system but other operating systems like SUN Solaris, Microsoft Windows and Apple MAC OS are also partially supported. For an easier handling the scientific Linux software is subdivided into 4 categories (modules), i.e.:

- Computational Chemistry,
- Computational Biology and Neuroscience,
- Electrical Engineering and Computer Science,
- Geoscience and Astrophysics.

More information about the CLAMV software installations and how to use them can

[5] http://www.clamv.iu-bremen.de/CLAMV/Publications/CLAMV-Primer.pdf

Figure 21: IDL Workshop in CLAMV Seminar Room on 9 December 2004.

be found in the CLAMV primer[6].

CLAMV runs a software download page[7] where frequently requested Windows software can be found.

In December 2004 CLAMV organized a technical workshop for the program IDL. Participants got an overview about the features of IDL and also had the chance to discuss user specific topics with trained personnel from the German IDL distributor (Creaso GmbH, Gilching), see figure 21.

5.2 Advanced Services

Currently there are 3 Linux computer clusters on the IUB campus. The clusters are equipped with different communication interfaces covering the range from low communcation rates (100 MBit/s Ethernet, 'embarassing parallel') up to 2 GBit/s Myrinet. In summer 2004 two clusters were extended with additional computing nodes and storage space. Now the total theoretical peak performance of the 3 clusters sums up to a little bit more than 1 TFlop/s.

In summer 2004 the GIS lab (Geographic Information System) in building Research III was opened. It consists of several computers with advanced visualization hardware (dual-head graphics adapters) and software for geoscience and statistical analysis. The GIS lab is intended to be used for geoscience projects, scientific visualization and large scale data analysis.

[6] http://www.clamv.iu-bremen.de/CLAMV/Publications/CLAMV-Primer.pdf
[7] http://www.clamv.iu-bremen.de/CLAMV/downloads.html

CLAMV runs 1 small server as storage area for scientific data. The storage computer is fully integrated into the CLAMV Linux environment and can also be accessed from a Windows system via a Samba connection. The CLAMV storage computer is also used for data transfers (FTP server) between members of the IRCCM (International Research Consortium on Continental Margins[8]. Furthermore, the CLAMV storage computer is used as backup device by several groups (K. Brix, G. Pfander).

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

CLAMV runs two computers with UML (User Mode Linux). An UML system makes it possible to run several independent Linux systems on the same physical platform. Currently UMLs are used for WWW presentations. The following WWW presentations run on an UML system:

- CLAMV[9],
- Mathematics[10],
- IRCCM[11],
- Alumni Database[12],
- Events4[13].

5.3 Off-campus Services

IUB is represented through CLAMV in the BrenHLR (Competence Center of High Performance Computing Bremen). The BremHLR partners (Alfred Wegener Institute, University Bremen and IUB) have agreed on to give mutual access to their parallel computer platforms for evaluation purposes. This agreement enables each BremHLR partner to get access to a great variety of different hardware platforms. Furthermore BremHLR is used to discuss hardware and software issues related to scientific and high performance computing.

Highly computer intensive projects are carried at the national computer centers. In 2004 computer resources at the NIC (John von Neumann - Institute for Computing at Forschungszentrum Juelich[14] have been requested by the following groups:

- F. Mueller-Plathe, Computational Chemistry, Parallel and Vector Computer

[8] http://www.irccm.de
[9] http://www.clamv.iu-bremen.de
[10] http://www.math.iu-bremen.de
[11] http://www.irccm.de
[12] http://world.iu-bremen.de
[13] http://www.events4.de
[14] http://www.fz-juelich.de/nic/index-e.html

- M. Brueggen, Astrophysics, Parallel Computer
- S. Rosswog, Astrophysics, Parallel Computer

The other national computer centers (HLRS (High Performance Computing Center Stuttgart[15], LRZ (Leibniz Computing Center Muenchen[16]) have not been used so far.

5.4 Future Projects

In the first half of 2005 a SGI Altix Bx2 parallel computer will be installed at IUB. It has a theoretical peak performance of more than 150 GFlop/s, 96 GByte shared memory and more than 4 TByte disk space. The Altix computer will probably fully operational in April 2005. 50% of the computer resources are reserved for the astrophysics group of S. Rosswog while the remaining 50% are available to the CLAMV community. The new parallel computer fills the gap in the provision concept that IUB offers the whole range from weakly coupled cluster systems up to shared memory systems for parallel computing. Beside projects in astrophysics the parallel computer will be used for projects in geoscience, nanoscience and computational biology, chemistry and physics.

The user administration will be integrated into the IUB-wide file server and user administration which is based on LDAP (Lightweight Directory Access Protocol)[17]. This project is expected to extremely simplify user administration. After a successful trial period the user administration will be completely removed from the currently used SUN v880 server. The SUN v880 server will be reconfigured and will become usable for scientific projects. Examples are visualization and data analysis requiring requiring more than 4 GByte and the 'European Connexions' (ECNX) project by M. Kohlhase which was described in detail in the previous CLAMV Activitiy Report[18].

There have been several requests for large data storage areas with up to 10 TByte or more. This is of particular interest for reasearch groups working with simulation data at a large scale or with high resolution images. CLAMV will deal with the question how to handle this issue.

The GIS lab will be equipped with a 3D visualization system (GeoWall). It is intended for visualization projects of geophysical data but it can also be used for visualization projects in other areas like molecular science. Furthermore the ongoing projects in the GIS lab mainly in the framework of the IRCCM activities require more software installations.

It is very likely that more research groups will request an integration of their UNIX/Linux computers into the CLAMV environment. This makes it necessary to work out a general strategy which also tackles questions like backup of local disk space and cost sharing for hardware, software and personnel.

[15] http://www.hlrs.de
[16] http://www.lrz-muenchen.de
[17] http://www.openldap.org
[18] http://www.clamv.iu-bremen.de/CLAMV/publications.html

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: Ronny Wells, assisted by Sibylle Haas.

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

Executive Director: 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.

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) Holger Kenn (left IUB in June 2004), and (2) the IRC Chief Technology Officer Torge Schmidt.

CLAMV committees

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

Scientific Computing Committee (SCC): Michael Rohlfing (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), Patrick Bangert, 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): Marcel Oliver (Chair), Achim Gelessus, Michael Rohlfing, Joachim Vogt.

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 Teaching Lab

The CLAMV Teaching Lab (CTL, also called Graduate Teaching Lab) consists of four class rooms which are equipped with altogether 30 Linux PCs. The CLAMV Teaching Lab is intended to be used by smaller groups especially for graduate teaching. The hardware is also suited for couses in computer graphics and (scientific) visualization.

Technical specifications

- 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 8.2 Operating System

CLAMV SUN Fire v880

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.

Technical specifications

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

CLAMV Linux Cluster I

The CLAMV Linux Cluster I is used for projects in scientific computing at IUB. There is no general access to this machine.

Technical specifications

- 40 compute nodes

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

CLAMV Linux Cluster II (dedicated to the computational chemistry group)

The CLAMV Linux Cluster II is used for projects within the computational chemistry group at IUB. There is no general access to this machine.

Technical specifications

- 32 compute nodes
- 2 Intel Pentium Xeon 2.80 GHz (node 1 - 16), 3.20 GHz (node 17 -32) processors per node
- 1.0 GByte (node 1 - 30), 4.0 GByte (node 31, 32) RAM per node
- RAID System 8 * 160 GByte
- 1000 MBit Ethernet interconnect
- Operating System RedHat Linux
- Queuing System PBS

CLAMV Linux Cluster III (dedicated to the computational biology group)

The CLAMV Linux Cluster III is used for projects within the computational biology group at IUB (66.6 general access to this machine.

Technical specifications

- 24 compute nodes
- 2 Intel Pentium Xeon 2.80 GHz processors per node
- 1.0 GByte RAM per node
- RAID System 8 * 160 GByte
- Myrinet 2000 interconnect
- Operating System RedHat Linux
- Queuing System PBS

CLAMV Storage Server

CLAMV runs a PC-server for storage purposes. There is no general access to this machine.

Technical specifications

- 2 AMD Athlon MP2400+ processors
- 1.0 GByte RAM
- RAID System 8 * 250 GByte
- 1000 MBit Ethernet
- Samba Server
- SuSE Linux 9.1 Operating System

CLAMV GIS Lab

The CLAMV GIS Lab is used for projects in geoscience. Currently there 3 dual boot PCs with an high-end graphic adapter. A 3D visualization system (GeoWall) will be installed soon. There is no general access to these machines.

Technical specifications:

- Intel Xeon processor 3.2 GHz
- 2.0 GByte RAM
- 80 GByte SATA harddisk
- 1000 MBit Ethernet
- Matrox Parhelia-512 / nVidia Quadro4 980 graphic adapter
- SuSE Linux 9.1 Operating System / Windows 2000

Special purpose systems

In addition CLAMV runs several special purpose machines for User Mode Linux, and backup. There is no general access to these machines.

Computer equipment for work groups

In some cases CLAMV also runs the computer equipment for work groups. Usually standard PCs with SuSE Linux operating system are used. For simulation and visualization projects in space physics a 64-bit Linux server has been set up. There is no general access to these machines.

Technical specifications

- 2 AMD Opteron processors 1.6 GHz
- 8.0 GByte RAM
- 500 GByte harddisk
- 1000 MBit Ethernet
- nVidia GeForce FX 5200 graphic adapter
- Operating System SuSE 64-bit 9.0 Linux

A.3 Software

Software on the central server

General software packages for mathematics and analysis: IDL, Maple, Mathematica, MatLab incl.: SimuLink, Communication Toolbox, Control Toolbox, Filter Design Toolbox, Financial Toolbox, Image Toolbox, Neural Network Toolbox, Optimization Toolbox, Robust Toolbox, Statistics Toolbox, Symbolic Toolbox, MatLab Compiler, WaveLab, Statistical Parametric Mapping (SPM2)

Software for visualization: Ifrit, OpenDX, pgplot, transcode

Software for molecular science: Gaussian03, gOpenMol, Jmol, Molden, Molekel, Molmol, RasMol, Swiss PDB Viewer, VMD, YASP

Software for Bioinformatics: Arb, ClustalX, Emboss, Modeller, ViennaRNA

Software for Geoscience and Astrophysics: GDI, GMT, Grass GIS, iGMT, OpendTect, PetroMod, QSAS, Seismic Unix, Tecplot

Software locally installed on the CLAMV Teaching Lab computers

Compiler, Languages: C, C++, Fortran, 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), Graphical interface to gdb (kdbg), Revision Control System (RCS)

Databases: MySQL

Editors: Emacs, Joe, Lyx, Pico, TeXmacs, Vi

Graphics: Gimp, Chemtool, Xfig, Xv, Gnuplot, Povray, Xmgrace

Office: OpenOffice

Publishing: Acroread, Bibview, Gv, Tetex (Latex)

Scientific Software: Basic Linear Algebra Subprograms (BLAS), Fastest Fourier Transformation in the World (FFTW), Feynman Diagrams (feynman), GNU Scientific Library (GSL), Linear Algebra Package (Lapack), Octave, Scientific Calculator (calctool), Scilab.

A.4 Seminar Schedules

Spring 2004

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

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

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

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

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

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

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

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

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

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

Fall 2004

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

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

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

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

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

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

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

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

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

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

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

07/12/2004 Onno Bokhove (Twente University), *TBA*

A.5 Abbreviations

AWI Alfred-Wegener Institut, Bremerhaven[19]

GIS Geographic Information System

ICBM Institut fuer Chemie und Biologie des Meeres, Universitaet Oldenburg[20]

IRCCM International Research Consortium on Continental Margins[21]

JCLL Jacobs Center for Lifelong Learning[22]

NIC John von Neumann - Institute for Computing at Forschungszentrum Juelich[23]

SES School of Engineering and Science[24]

SHSS School of Humanities and Social Sciences[25]

TUC Technische Universitaet Chemnitz[26]

A.6 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.

[19] http://www.awi-bremerhaven.de
[20] http://www.icbm.de
[21] http://www.irccm.de
[22] http://www.iu-bremen.de/schools/jacobs
[23] http://www.fz-juelich.de/nic/index-e.html
[24] http://www.iu-bremen.de/schools/ses
[25] http://www.iu-bremen.de/schools/shss
[26] http://www.tu-chemnitz.de

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.7 CLAMV people

Table 3 provides an overview on how and by whom CLAMV resourses were used in the year 2004.

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

			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							
Jan Freund		ICBM	x									
Frank Oliver Glöckner	Bioinformatics	SES	x									
Harald Haas	Electrical Engineering	SES		x	x							
Werner Henkel	Electrical Engineering	SES		x	x							
Claus Hilgetag	Neuroscience	SES	x	x	x							
Wolfgang Hiller		AWI	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					
Peter Ludes	Mass Communication	SHSS		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 Procurement	NIC
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	Physics	SES	x		x	x		x				
Veit Wagner	Physics	SES		x	x							
Raymond O. Wells	Mathematics	SES						x	x			
Martin Zacharias	Computational Biology	SES	x	x	x	x		x				
Additional CLAMV Usage for research in 2005												
Peter Baumann	Computer Science	SES										
Klaudia Brix	Biochemistry & Cell Biology	SES										
Benjamin Godde	Neuroscience & Human Performance	JCLL										
Ulrich Kleinekathöfer		TUC										Cooperation with A. Materny, IUB

Table 3: CLAMV usage in 2004.

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