International University Bremen (IUB)

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

CLAMV Activity Report 2002/2003

Compiled by the CLAMV Seminar and Editorial Committee

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1 Introduction

The *Computational Laboratory for Analysis, Modeling, and Visualization (CLAMV)* is the umbrella and support initiative for all computationally oriented disciplines at IUB. Founded in April 2002, it has grown from 12 initial members to a group that includes more than 25 faculty, a systems manager, associated postdoctoral researchers and graduate students. Its hardware and software infrastructure now serves large parts of the IUB community.

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.

This report first provides an overview about the CLAMV community, available resources, and CLAMV's interaction with other university bodies and institutions outside IUB. It then details the CLAMV activities in the years 2002 and 2003, 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 2002/2003 was compiled by the CLAMV Seminar and Editorial Committee, and approved at the CLAMV Spring Assembly on March 23, 2004.

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 250 students and more than 50 scientists have been served in the years 2002 and 2003.

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 be included in 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 16 dual processors each, 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, 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 two student assistants.

1.3 Cooperation

The primary university body that CLAMV interacts with is the *Information Resource Center (IRC)*. CLAMV complements the general information services provided by the IRC in well-defined and specific areas, namely, graduate teaching and computationally oriented research. The 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

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 should host smaller (graduate and advanced undergraduate) courses, guided research projects, and research groups.

A prime example of how CLAMV serves new faculty members is the case of Stephan Rosswog who joined IUB in fall 2003 and needs a multi-processor shared-memory machine to pursue his research. CLAMV personnel and associated faculty are helping in obtaining offers from different vendors, in writing applications to third-party funding institutions, and in testing different hardware platforms. This way efficient use can be made of IUB resources and third-party money.

To conclude the introduction, CLAMV serves a large community at IUB and provides a broad spectrum of resources. CLAMV engages in computationally oriented research and teaching and is open to the whole university. Since the community is growing and the number of services is increasing, the CLAMV Systems Manager will need more help in the near future than can be provided by student assistants. We strongly suggest that in the next year of operation a second full-time position for systems administration should be assigned to CLAMV. In this context, a person with a solid background in scientific software development would be preferred.

2 Scientific projects

CLAMV resources play an essential role for a large number of scientific projects carried out at IUB. Corresponding with 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 consuming in terms of hardware but rather asks for advanced software and for personal consulting by experts, areas which are also both provided by CLAMV.

The following research groups are making use of CLAMV resources or are preparing to do so in the nearest future:

Current projects:

M. Brüggen	Astrophysics
A. Diederich	Mathematical Psychology
M. Hoeft	Astrophysics
U. Kleinekathoefer	Chemical and Biological Physics
H. Meyer-Ortmanns	Statistical Physics
F. Müller-Plathe	Computational Materials Science
M. Oliver	Mathematics
J. Vogt	Geophysics
M. Zacharias	Computational Biology

Additional future projects:

K. Brix	Biochemistry
C. Hilgetag	Neuroscience
H. Jaeger	Computational Science
M. Kohlhase	Computer Science
M. Rohlfing	Condensed-Matter Physics
S. Rosswog	Astrophysics

2.1 Hardware, Software, and Support provided by CLAMV

CLAMV provides two main machines designed for scientific projects (cf. Sec. A.2), i.e. an 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.

Frequent 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 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 Metal Enrichment of the Intra-Cluster Medium

Dr. Marcus Brueggen, Professor of Astrophysics

Clusters of galaxies are massive enough to be considered representative samples of the Universe and to retain all the heavy elements synthesized in their constituent stars. Over the recent years, great progress has been made in the area of galaxy evolution. This was facilitated by the wealth of new high spatial and spectral resolution observations from space (HST, XMM-Newton, Chandra); by large increases in sensitivity from ground-based 10m-class telescopes (VLT, Keck, Subaru, Gemini, etc.); by the availability of deep or/and large radio surveys (VLA, HIPASS) and by similar increases in the computing power available for running numerical simulations. However, one critical aspect of galaxy evolution that remains to be understood is the transformation and recycling of the gaseous and stellar material both within and outside of galaxies: gas consumed by star formation and subsequently ejected by supernovae or superwinds into the inter-galactic medium (IGM); injection in the IGM of metal-enriched material via Active Galactic Nuclei (AGN)-driven jets; material ejected from galaxies through interactions and mergers; and gas stripped from galaxies by the ram-pressure of the intracluster medium (ICM). Numerical simulations can now follow in detail the evolution of the gaseous medium in galaxies through these violent events.

At the same time, our knowledge of the IGM has improved dramatically:

i) The nature of the Intra-Cluster Medium, the hot plasma in which most of the metals reside, can now be constrained more tightly through X-ray observations by Chandra and XMM. These observations have revolutionized our understanding of the cooling/heating processes in the ICM, and allow us to measure its elemental abundances with unprecedented precision.

ii) The intergalactic medium at high redshift is investigated using absorption lines detected in high-resolution spectra of background Quasi-Stellar Objects (QSOs). Besides Hydrogen and Helium, also heavy elements such as Carbon, Silicon and Oxygen have been found. The distribution of heavy elements in the IGM is not uniform but depends on the local density (Schaye et al. 2003). This suggests that metals ejected by galaxies only travel a limited distance from their source. In the vicinity of the Virgo Supercluster enriched Lyman alpha clouds have been studied in detail and it has been concluded that the enrichment took place by unbound galactic winds caused

by type II supernovae. Moreover, no time evolution of the metal enrichment has been found which points to a relatively early 'pollution phase'.

iii) In the local Universe, molecules in low-density gas clouds are observed well outside the galactic disks through absorption against background UV sources. The first metallicity measurements of the high-velocity clouds in the Local Group were obtained by this method. Strangely enough, no pristine hydrogen clouds, devoid of any heavy elements, have yet been found, either locally or at high redshift.

All observations suggest a wide-spread "pollution" of the intergalactic medium by galaxy ejecta, even at high redshifts. Various models of galaxy mass-loss via dynamical processes or superwinds have attempted to account for these observations, but they still disagree on the efficiency of the IGM enrichment mechanisms and on the nature of the progenitors.

It is likely that a large fraction of the material liberated by galaxies during their evolution may fall back into the galaxies. This is in agreement with numerical experiments which predict the re-accretion of tidal debris as well as gas stripped by ram-pressure. This reservoir of expelled material can be recycled in their progenitors, fueling star-formation episodes with a time-delay depending on how far into the IGM the gas clouds had been injected. On the other hand, there is now observational evidence that galactic material may be recycled in the space between galaxies, forming a new generation of objects.

Topics to be addressed:

In the present project we study the fate of galaxy material, from its liberation by galaxies, its journey into the IGM, to its final recycling in and outside galaxies.

The abundances of several elements in the ICM have been measured quite accurately, and steep abundances gradients near the centres of the clusters have been detected (Finoguenov et al. 2000; White 2000; De Grandi and Molendi 2001). These spectroscopic studies have constrained the spatial distribution of various elements. Since the abundances and the distribution of heavy elements in the IGM are sensitive to the processes of hierarchical clustering, cosmological simulations are useful to understand the impact of the hierarchical build-up of structure on the chemical enrichment of the IGM (Cora, White & Springel 2003, in prep.).

The role of dynamical removal and wind ejection of metals from galaxies and pregalactic outflows was investigated using numerical simulations (Aguirre et al. 2001; Tamura et al. 2001). The effects of the environment on stellar winds, the contribution of dwarf galaxies and ellipticals to the enrichment of the IGM via stellar winds, and the interaction between the relativistic plasma from the Active Galactic Nuclei (AGN) and the IGM have been discussed by several groups (Murakami & Babul 1999; Ferrara & Tolstoy 2000; Pettini et al, 2001; Silich & Tenorio-Tagle 2000; Churazov et al. 2001; Conselice et al. 2001; Rejkuba et al. 2002).

In this ongoing project we perform a series of simulations to investigate the dynamics of galactic winds at different epochs of the universe and the role of these winds on the metal enrichment of the IGM.

Studies of quasar absorption lines show that the low-density IGM at z=3 is enriched by metals. The enrichment may have occurred in an early generation of Population III stars at redshifts > 10, by protogalaxies at intermediate redshifts or by large galaxies at redshifts between 6 and 3. One of our aims is to shed some light onto which one of these scenarios is the prime source of metals in the IGM. For this purpose we intend to make 3D simulations of supernova-induced winds that are blown out of the gravitational well of their host galaxy. With the expertise in adaptive grid codes, we will be able to resolve the IGM form cluster scales down to the inner regions of galaxies. We will introduce into the code microphysics, such as realistic radiative cooling and photoionisation.

The grid-based simulations will be performed with the FLASH code, which is a parallel, adaptive-mesh code that is designed to simulate compressible flows. It uses a Riemann solver and can also be used to solve the MHD equations. Importantly, it solves the relevant equations in comoving coordinates and can thus be used to simulate the IGM over cosmologically significant lengths of time. Moreover, we intend to compute quasar absorption spectra along lines of sight through the wind-blown bubbles and will compare the artificial spectra to the observed spectra. Here, we rely on expertise that is derived from a close collaboration with Dr. Theuns (Durham) and Dr. Schaye (Princeton).

2.2.2 Mathematical models to account for phenomena in human behavior

Dr. Adele Diederich, Professor of Psychology

The research is concerned with the study of information processing in various psychological contexts, in particular, sensory processes in perception and higher cognitive processes in decision-making. The approach includes both the development of theories and models and their testing by experiment and empirical observation.

Information processing in sensation & perception. Perceptual processes are typically investigated within one modality only. Triggered by recent physiological findings (e.g., multisensory neurons in various brain structures) multisensory research has caught interest of cognitive psychologists as well. We have studied the interaction of different modalities (vision, audition, touch) in space and in time with experiments using elementary stimuli and measuring manual response times and saccadic eye movements. We developed quantitative psychological models for the behavioral results taking into account results from neurophysiological studies of the lower brain structures.

Decision making projects. Multi-Attribute Decision Field Theory (MDFT) is a theory developed for multiattribute (binary) decision problems which takes into account both the dynamic and stochastic nature of decision making. Its goal is to describe the motivational and cognitive mechanisms that guide the deliberation process in decisions under uncertainty. MDFT provides an explanation for why preferences waver over time and suggests a mechanism for predicting how long it takes to come up with a decision. Observed data are reaction time and relative frequencies.

Model developments are based on stochastic processes (such as Poisson counter models, diffusion processes, in particular the Wiener and Ornstein-Uhlenbeck process), extreme value models, and Bayesian models. The quantitative predictions of the diffusion processes are calculated using Markov chain approximation (utilizing the sparse matrix function of MATLAB). Models are fitted to data by using optimization procedures such as the OPTMUM toolbox of MATLAB.

Grants

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

2. International Graduate School for Neurosensory Science and Systems (DFG), see `http://www.physik.uni-oldenburg.de/Docs/medi/projects/eurogk/index.html`

Selected Publications

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Diederich, A., & Busemeyer, J.R. (2003) Simple Matrix Methods for Analyzing Diffusion Models of Choice Probability, Choice Response Time and Simple Response Time. *Journal of Mathematical Psychology*, 47, 3, 304–322.

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2.2.3 Cosmological structure formation

Dr. Matthias Hoeft

Scientific aims

On largest scales in the universe the distribution of galaxies is governed by the underlying dark matter. The latter interacts only gravitationally, therefore the distribution of galaxies can be simulated without sub-resolution scale processes. It has been shown that a good agreement with observations is obtained in a cold dark matter model. However, observations are based on the distribution of the luminous matter. Therefore, modeling the structure formation must also incorporate basic hydrodynamical processes. We model especially the formation of the intra-cluster medium (ICM) and

the formation of rather isolated galaxy in underdense regions in the cosmos, so-called voids.

The ICM is a very hot, X-ray emitting, diluted plasma which fills the interspace between galaxies in clusters of those. Basically the temperature of the ICM depends on the potential well of the cluster, i.e. the mass of the cluster. However, merging between clusters increases also the temperature of the ICM. Moreover recent X-ray and radio observations have revealed a huge number of non-relaxed structures, e.g. cold fronts, associated with mergers. Numerical simulation allow to interpret those structures and allow to derive, e.g., the associated velocities of the merger itself.

On the other hand we are interested in modeling the galaxy formation especially in the dependence of integral galactic properties, i.e. luminosity, morphology and color, on environmental effects. Galactic surveys like Sloan Digital Sky Survey will give in very near future the distribution of galaxies in cosmological volumes. By means of already released data it has been shown that the color of galaxies depends on the local density. We will be able to provide an interpretation of those observations using the simulations of the structure formation including prescriptions for the star formation.

Numerical method

The gravitational interactions may be computed by a tree scheme. This is a suitable method for the considered problems since intrinsically the spatial resolution depends on the local density. We use the Message-Passing Interface (MPI) based, public code Gadget, which provides beside the solver for gravity also a treatment of the basic hydrodynamical processes. The latter are calculated according to smoothed-particle hydrodynamics. In addition radiative cooling for a primordial chemical composition and heating by the UV-background has to be incorporated. This allows to estimate the amount of cold gas in dark matter halos which is able to form stars. Moreover, a simple model for star formation is necessary, since the feedback from stars may inhibit further cooling in halos.

Cooperation and grants

This project is carried out mainly in cooperation with Gustavo Yepes (Universidad Autonoma de Madrid) and Stefan Gottlöber (Astrophysikalisches Institut Potsdam). The work is based on previous investigations of cosmological structure formation with pure dark matter physics. Methods for generating initial mass distributions, especially with local refinement, in concordance with the Cosmic Microwave Background, for identifying halos and driving their physical properties, and for determining the merger history of individual halos has been carried out. More recently the treatment of the gas component, with cooling and star formation has been investigated.

The project is supported by the Spanish Ministry of Science and Technology within the ”Programa Nacional de Astronomy y Astrofisica” under the grant ‘Study of galaxy and cluster formation and evolution and of the Large Scale Structure in the Universe’.

Using CLAMV resources

Carrying out competitive numerical simulations needs the use of massive-parallel computing resources. Using the highly scalable code Gadget, the CLAMV Linux-

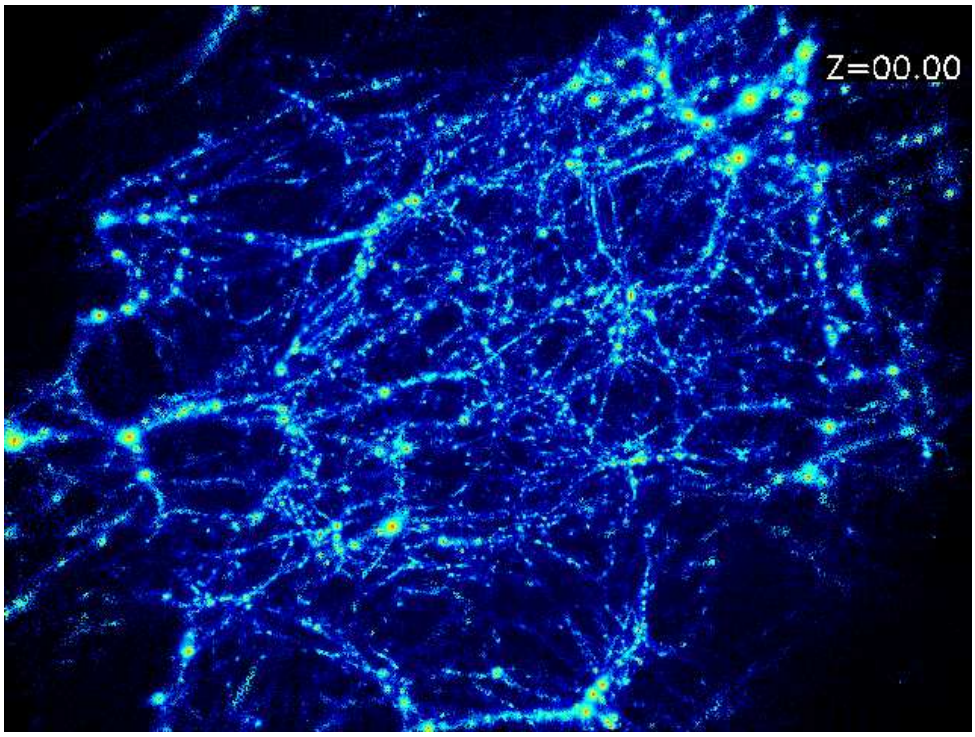

Figure 1: The 'cosmic web'. The density distribution in a refined area in a cosmological simulation at redshift $z = 0$. The huge amount of dense knots, 'halos', becomes apparent. It is still an open question if all those small dark matter halos are also hosts of galaxies.

clusters allow to run preparation simulations and medium-sized production runs. A limitation arises since calculating the gravitational interaction needs inescapably, even with a tree code, a considerable amount of communication between the different nodes. Therefore, the degree of parallization is restricted due to the network communication speed. We use also the CLAMV resources to prepare production runs on national supercomputing centers. For this purpose the local massive-parallel computing resources are essential. We are grateful for the excellent support of the CLAMV system manager, Dr. Achim Gelessus, in installing software and during the runs of the simulations.

2.2.4 Classical and quantum dynamics in molecular systems

Dr. habil. Ulrich Kleinekathöfer

The research projects performed using CLAMV resources are within the area of chemical and biological physics, both on a classical as well as quantum mechanical level. A first project concerned method development for molecular quantum dynamics. For the description of dynamical effects in quantum mechanical systems on ultra-short time

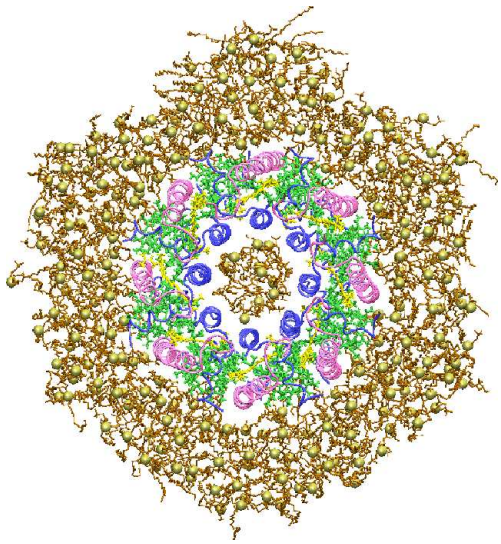

Figure 2: Top view of the light-harvesting LH-II octameric complex of *Rhodospirillum molischianum* embedded into a lipid bilayer that fits into a hexagonal unit cell.

scales memory effects play an important role. We proposed two new approaches which are based on a time-local scheme and a partial time-ordering prescription. The proposed theories as well as the method by Meier and Tannor based on a time-nonlocal scheme employ a numerical decomposition of the spectral density. For the example of the damped harmonic oscillator these non-Markovian theories were compared among each other, to Markovian approaches neglecting the memory effect and to path integral calculations. Some of the non-Markovian theories mentioned above treat the time dependence in the system Hamiltonians nonperturbatively. To test these new methods for longer time-scales and a broader parameter the Muscle cluster of CLAMV was used. This was also the case for the test of analytical path integral calculation of curve-crossing dynamics. Although the evaluation of the analytical results could be performed using MATHEMATICA several time-consuming calculations using other benchmark algorithms had to be performed.

In a second project a method for stochastic unraveling of general time-local quantum master equations (QMEs) was proposed. The proposed kind of jump algorithm allows a numerically efficient treatment of QMEs which are not in Lindblad form, i.e. are not positive semidefinite by definition. The unraveling can be achieved by allowing for trajectories with negative weights. Such a property is necessary, e.g. to unravel the Redfield QME and to treat various related problems with high numerical efficiency. The method was successfully tested on the damped harmonic oscillator and on electron transfer models including one and two reaction coordinates. The obtained results were compared to those from a direct propagation of the reduced density matrix as well as from the standard quantum jump method. This new algorithm is easily parallelized and for the benchmark calculations the Muscle cluster was used.

In a further more applied project the time dependence of the anisotropy of fluores-

cence in the B850 ring of the purple bacterium *Rhodopseudomonas acidophila* was calculated using the reduced density matrix formalism. The influence of static and dynamic disorder was taken into account simultaneously. Extending earlier calculations within the Markovian Redfield theory which were based on a perturbative treatment of the exciton-phonon coupling, the focus of the present work was on memory effects within the exciton dynamics. The inclusion of the memory effects make the algorithm quite CPU-time consuming and together with the required orientational and statistical sampling this project relied heavily on the CLAMV Linux cluster.

Another numerical very demanding project in the area of computational biology concerned the synthesis of ATP. The F_1 unit of ATPase has three-fold symmetry and consists of three noncatalytic α and three catalytic β-subunits. The β-subunits furnish the binding sites where ADP is transformed into ATP. We have investigated the properties of isolated β-subunits as a step towards explaining the function of the integral F_1 unit. The β-subunits exist in different conformations at any moment of the F_1 unit reaction cycle. This project is still in progress.

Publications

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2.2.5 Spinodal Decomposition in Phase Transitions Out-Of-Equilibrium

Dr. Hildegard Meyer-Ortmanns, Professor of Physics

Scientific Background

My work together with Bernd Berg, Alexander Velytsky (both at Florida State University, Tallahassee) and Urs Heller (SCRI, Tallahassee) deals with applications of statistical physics to the phase structure of particle physics. To cut a long story short, imagine that you throw a hot piece of iron (with disordered spins) into ice, or, even simpler, cold water into a hot hole in the volcanic ground (say of some hundred degrees Kelvin). This is called a quench. A quench amounts indeed to some kind of shock for a piece

of matter, suddenly being exposed to an environment, in which it normally would be in a quite different state. The quench is reflected in specific dynamical signatures during the relaxation to the appropriate state. A kind of quench may be also relevant for relativistic heavy-ion collisions at CERN (the European Center for Nuclear Research in Geneva), where heavy ions from gold, lead or other elements are smashed together with such high energies that their protons and neutrons dissolve most likely into their basic elementary constituents, the quarks and gluons, at least for a very short instant of time (about some 10^{-23} sec). This exotic state of matter was probably realized in the early universe up to 10^{-6} sec after the big-bang. Roughly speaking, our work was about possible signatures of a rapid crossover from the quark-gluon-plasma phase to the hadronic ("normal") phase of matter. Differently from most other approaches, we implemented more realistic off-equilibrium conditions, in particular conditions resembling a quench. Cold water, thrown into a hot hole in the ground – after some delay – suddenly comes back as a vapor fountain. We speculate that the effect of a kind of quench in heavy-ion collisions is an increased gluon-production that should be observable. The work amounts to extensive Monte Carlo calculations, partially performed on the Muscle-Cluster of CLAMV at IUB, partially at the Florida State University.

Computational Aspects

The dynamics of heavy-ion collisions is governed by quantum chromodynamics (QCD), the theory of strong interactions. It can be shown, however, that the phase structure of QCD is very similar to the phase structure of a much simpler model, the so-called Z(3) Potts model in three dimensions, exposed to an external magnetic field. This is a model with spins on a space-grid in three dimensions with ferromagnetic interaction, with each spin variable taking one of three integer values. The magnetic field mimics the effect of finite quark masses in QCD, while the integer-valued spins replace the gauge fields, represented by SU(3) matrices in QCD. This may indicate already the enormous computational reduction as compared to the original model. In the first part of our work we simplify the model even further to Potts models in two dimensions in order to test our numerical methods. The number of states q at a given lattice site is no longer restricted to three (as in Z(3)), but varies between the different models from q=2 to 10, because the phase conversion mechanism is known to depend on that value of q via the order of the phase transition. The lattice size varies from 40x40 to 100x100 sites (in steps of 20) in order to control finite size artifacts. We measure certain observables, which are sensitive to the conversion mechanism, via Monte Carlo calculations. In order to simulate different speeds of the phase conversion, ranging from adiabatic conversion to a quench, we choose Glauber dynamics. The temperature is varied from an initial value over a certain interval across the transition temperature in steps of different size (depending on the speed) and backwards to the initial temperature. For each temperature value the whole lattice is updated in one Monte Carlo sweep. During the loop in temperature one observes a hysteresis in certain observables like the energy. Each measuring point on the hysteresis loop that is finally stored amounts to an average over at least 640 hysteresis cycles. This average is needed for obtaining a reliable statistics. In summary, the parameters are the lattice size, the number of states at a given site, the speed for varying the tem-

perature, the number of hysteresis cycles. Their variation explains why the project is CPU-time consuming. As a result we find spinodal decomposition as the dominating conversion mechanism in these Potts models even in situations where one would expect nucleation in adiabatic cooling or heating across the phase transition temperature. Spinodal decomposition as signaled by an explosive growth of low-momentum modes has to be translated into the corresponding phenomenon in particle physics, which we expect to be an increased gluon-production. Work in the three-dimensional Z(3)-Potts model is ongoing and will be finished probably in summer 2004.

Technical Details

On the muscle cluster we use 8 CPUs (i.e. 4 nodes) in sustained manner. One run takes typically several weeks. Since jobs survive for 5 days, we submit jobs in batch of 8 for 5 days and restart them. Each job needs of the order of 10 MB memory. From the software we use the Portland group compiler, which is the best one we have tested so far, and the portable batch system.

Future Projects

My main focus, currently and in the near future, is statistical physics of networks with applications in biology and information science. In 2004 I expect two Ph.D.students, 1 Post-doc and a Humboldt fellow (not yet confirmed), who will perform numerical simulations of such networks. Each of them will need disc space and CPU-time somewhat less or comparable to the project described above.

Grant Proposals

As host at IUB I have supported an application for a Humboldt-fellowship, submitted in January 2004. If the fellowship will be awarded in summer 2004, the fellow would need support from CLAMV in using the computer facilities for extensive numerical simulations, of comparable size in disc space and CPU-time to the running project. A grant from DFG (Deutsche Forschungsgemeinschaft) was awarded in the end of 2003 for a Ph.D. position on Network Analysis (see below).

Publications

B.A. Berg, U. Heller, H. Meyer-Ortmanns, and A. Velytsky, Dynamics of phase transitions with hysteresis measurements I, hep-lat/0309130, Phys.Rev.D , in press

B.A. Berg, U. Heller, H. Meyer-Ortmanns, and A. Velytsky, Spinodal decomposition and the Deconfining Phase Transition, hep-lat/0308032, to be published in Nucl. Phys. B (Proc. Suppl.) 2003 B.A. Berg, H. Meyer-Ortmanns, and A. Velytsky, Dynamics of phase transitions with hysteresis measurements II, in preparation

2.2.6 Computational Materials Science

Dr. Florian Müller-Plathe, Professor of Physical Chemistry

Systematic coarse graining of polymer models

Polymers are an important class of man-made materials. Their uses range from the simple plastic cup to the latest functional nanocomposite. Polymers have attracted

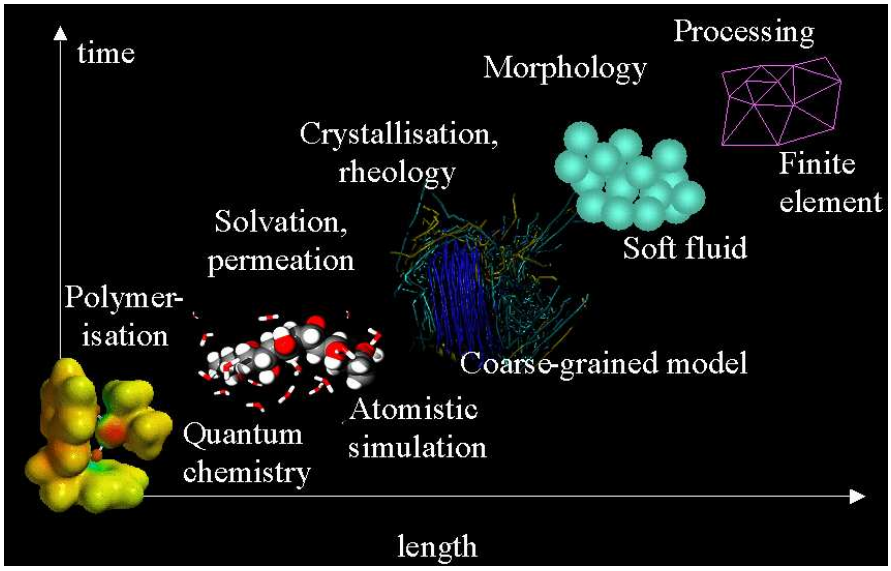

Figure 3: Many methods exist for simulating polymers at various individual length and time scales. The challenge is to combine them.

the interest of theoretical physicists and computational chemists for many years. Particularly intriguing is the presence of so many length and time scales and their influence on various materials properties. For example, the permeation of oxygen into a drug in a blister pack is controlled by the very local packing of the polymer chains of the packaging. Their length is relatively unimportant. The elementary time scale of the permeation process is of the order of nanoseconds. In contrast, the viscosity of a polymer melt is determined by the speed with which entire polymer chains slide past each other, which may take milliseconds. It depends heavily on the size of the polymer: Doubling the chain length leads to a viscosity increase by a factor of 10. We focus on mesoscale models, as we want the best of the two worlds: Polymer models which are simple enough so that realistically large polymer samples can be simulated for realistically long times, but detailed enough, so they capture the behaviour of real polymers and distinguish between, say, polyethylene and polystyrene, or between cellulose and collagen. We have developed a rigorous and robust statistical-mechanical scheme to make a mesoscale model match the properties of a more detailed model of the same polymer. In this way, an accurate atomistic model can be used to obtain reference properties. The mesoscale model is then adjusted until it reproduces these properties exactly. A part of our development is also a numerical method, which automates the generation of mesoscale models from parent atomistic models. An example is shown in Fig. 4. The coarse-graining method has been shown to work well for a variety of synthetic and biopolymers, for solutions as well as melt. It generates trustable mesoscopic models, which in spite of their simplicity still capture the features of the polymer they are meant to represent. These are mainly structural and thermodynamic properties. Established variants of the method are routinely used in

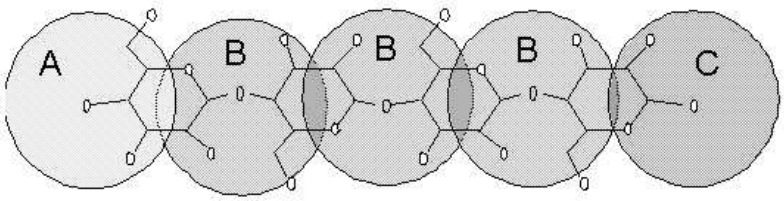

Figure 4: Coarse graining generates an accurate mesoscopic polymer model, the spheres, by matching their structure to that of the underlying atomistic model, the chemical structure. The example shows cellulose, a biopolymer: For every repeat unit of cellulose (21 atoms), one sphere is introduced. This reduces the complexity of the model by 21 and the computer time requirement roughly by a factor of 5000.

the group to generate models to study problems of technological interest: Inorganic fillers in Nylon, the morphology of polystyrene/polyisoprene blends, stabilization of catalytic nanoparticles by poly(vinyl alcohol). Without our mesoscale models, such problems would not be amenable to computational investigation. At the same time the method is being further developed to generate polymer models, which reproduce not only structure and thermodynamic properties of the parent atomistic model, but also viscoelastic properties of the material.

Reverse Non-equilibrium Molecular Dynamics

We develop methods to calculate transport properties in materials: for example diffusion coefficients, thermal conductivities, shear viscosities, Soret coefficients. In the framework of linear-response theory they are given as

$$J = -\lambda \nabla X \tag{1}$$

Here, ∇X is the gradient of some intensive state variable X (temperature, concentration, etc.), J is the flux of a conserved extensive quantity (heat, mass, etc.) caused by this gradient, and the proportionality constant λ is the corresponding transport coefficient. The traditional way to calculate the transport coefficient by non-equilibrium molecular dynamics (and in experiment) is to set up the gradient ∇X in the system, measure the resulting flux J in steady state and divide one by the other. We have found a way of reversing the approach: We drive the flux through the system and measure the resulting gradient. This has certain technical advantages over the traditional methods, such as robustness and fast convergence, as well as physical advantages: the algorithm conserves the total energy and can be run without external thermostatting. The method has been successfully applied to low-molecular-weight liquids. Presently, we are extending it to polymeric materials.

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 group of faculty from physics, chemistry and bioinformatics is jointly acquiring a site licence of Gaussian03 for teaching and research, the master version is to be maintained by the CLAMV.

Group Members (as of 31/12/03)

Prof. Dr. Florian Müller-Plathe, Dr. Giuseppe Milano, Dr, Sylvain Goudeau, Dr. Welchy Cavalcanti, Sandeep Pal, Konstantin Tarmyshov, Enrico Lussetti, Meimei Zhang, Kai Kohlhoff. Dr. Lus de Souza left the group in 2003 for a position with the Brazilian Central Bank.

Grants

Alexander-von-Humboldt Foundation, BASF, BMBF (Centre of Excellence for Materials Simulation), DFG (Schwerpunkt 1155 Molecular Modelling and Simulation in Chemical Engineering), Fonds der Chemischen Industrie, International University Bremen, John-von-Neumann Institut für Computing, Rhodia SA.

Publications:

F. Müller-Plathe, "Scale-hopping in Computer Simulations of Polymers", Soft Materials, 1, 1-31 (2003).

S. Girard, F. Müller-Plathe, "Molecular Dynamics Simulation of Liquid Tetrahydrofurane: On the Uniqueness of Force Fields", Mol. Phys., 101, 779-787 (2003).

D. Reith, M. Pütz, F. Müller-Plathe, "Deriving Effective Mesoscale Potentials from Atomistic Simulations ", J. Comp. Chem., 24, 1624-1636 (2003).

P. Bordat, J. Sacristan, D. Reith, S. Girard, A. Glättli F. Müller-Plathe, "An Improved Dimethyl Sulfoxide Force Field for Molecular Dynamics Simulations", Chem. Phys. Lett., 374, 201-205 (2003).

P. Bordat, F. Affouard, M. Deschamps, F. Müller-Plathe, "The Breakdown of the Stokes-Einstein Relation in Supercooled Binary Liquids", J. Phys. Condens. Mat., 15, 5397-5407 (2003).

M. Doxastakis, D.N. Theodorou, G. Fytas, F. Kremer, R. Faller, F. Müller-Plathe, and N. Hadjichristidis, "Chain and local dynamics of polyisoprene as probed by experiments and computer simulations", J. Chem. Phys., 119, 6883-6894 (2003).

2.2.7 Generalized Magnus and Fer expansions

Dr. Marcel Oliver, Professor of Mathematics

In many dynamical systems the equations of motion impose implicit constraints: Provided the initial state satisfies some special condition, the motion will never depart from it. However, if standard numerical algorithms are used to approximate the solution, these constraints constraints are usually not preserved, resulting in instabilities

or unphysical states. Therefore, there is need to either find structure preserving numerical methods, or explicitly impose the relevant constraints.

One class of structure preserving methods are called Magnus and Fer integrators, which apply to linear, non-autonomous differential equations on Lie groups. In addition to preserving the Lie-group structure under discretization, it turns out that these methods also fare extremely well for general highly oscillatory problems, and are thus relevant for a large class of applications including molecular dynamics simulations, and eigenvalue problems that arise in the linear stability theory for partial differential equations and in mathematical physics.

Each method is based on a particular solution ansatz, and there are in principle a large number of different approaches that could be pursued. The goal of this ongoing project is to isolate methods that are specifically suitable for efficient adaptive step size control.

This research requires manipulation of asymptotic expansions involving a large number of terms. The computations are therefore automatically performed by *Mathematica* on CLAMV machines. *Mathematica* is also used to auto-generate the code for the complete integration scheme, and runs simple test cases fast enough for experimental study of the schemes.

2.2.8 Magnetohydrodynamic Simulations of Paleomagnetospheres and Exomagnetospheres

Dr. Joachim Vogt, Professor of Physics, and Bertalan Zieger, Ph.D.

The Earth is embedded in a magnetic cavity called the magnetosphere which shields our planet from high-energetic particles of solar and cosmic origin. The magnetosphere results from the interaction of the solar wind (a magnetized plasma of solar origin) with the geomagnetic field generated in the Earth's outer core. Paleomagnetic records have shown that the geomagnetic field changed dramatically during Earth's history which in turn should have had strong effects on the structure and the shielding efficiency of the magnetosphere.

At IUB the paleomagnetosphere is studied by means of large-scale magnetohydrodynamic (MHD) simulations. We use the simulation code BATS-R-US developed at the University of Michigan which solves the full set of three-dimensional MHD equations in a self-adaptive numerical grid. The code runs on a number of parallel computing platforms like the CLAMV Linux Cluster and the CLAMV SUN Fire v880. Steady-state simulations usually take only a few hours of CPU time whereas fully time-dependent runs are computationally much more expensive. The project is funded by the DFG and embedded in the Priority Programme "Geomagnetic variations". The simulation results are used by working groups at partner institutions (U Osnabrück, U Bremen, TU Braunschweig) in order to quantify the effects of changing particle fluxes on the upper and middle atmosphere.

The present-day geomagnetic field is dominated by its dipolar part but during geomagnetic polarity transitions higher-order multipoles can become important. Figure 5

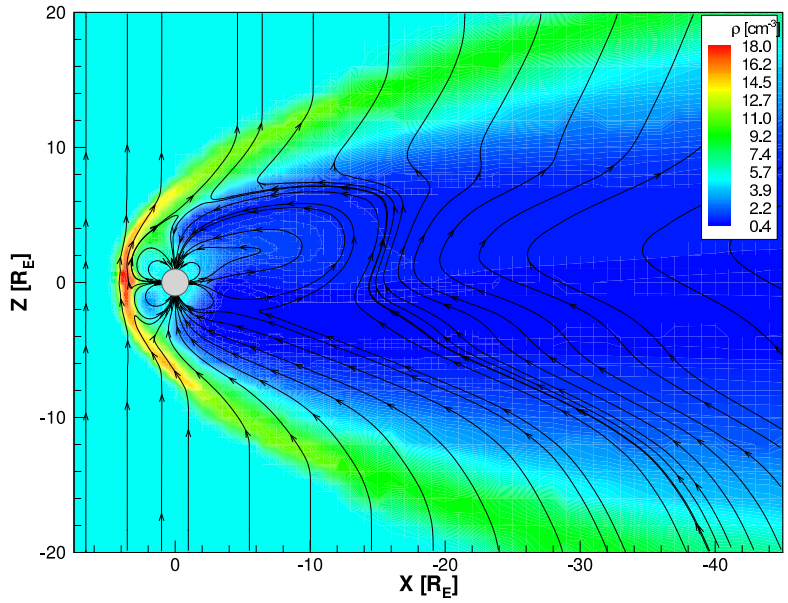

Figure 5: MHD simulation of a quadrupolar paleomagnetosphere. Explanations see text.

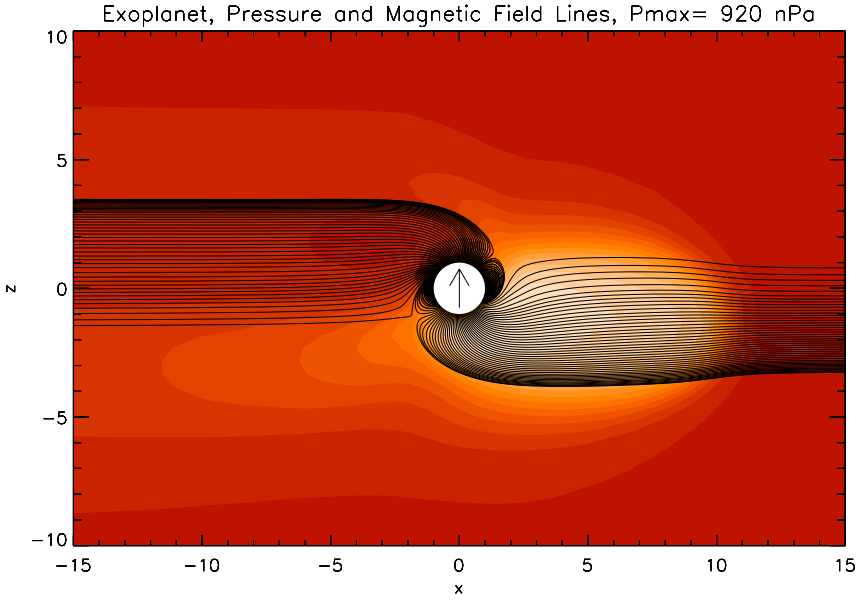

Figure 6: Magnetosphere of a Jupiter-type exoplanet that is exposed to a strong radial interplanetary magnetic field. Explanations see text.

shows the magnetospheric configuration for an axisymmetric quadrupolar core field. At the dayside magnetospheric boundary in the southern hemisphere the geomagnetic field lines reconnect with the interplanetary magnetic field (IMF) and allow solar wind plasma to enter the magnetosphere. In such a paleomagnetosphere almost all IMF orientations lead to some sort of field line reconnection processes and magnetospheric activity whereas in the present-day dipolar magnetosphere only southward IMF conditions yield significant reconnection rates. Therefore, during geomagnetic polarity transitions the magnetosphere is expected to be more affected by solar activity than today.

Another type of 'exotic' magnetospheres are exomagnetospheres. A large number of so-called exoplanets, i.e., planets around distant stars, have been detected in the past few years. They are typically of the size of Jupiter but orbit around the central star at a much smaller radial distance where the interplanetary magnetic field is expected to be almost radial. Figure 6 shows the simulation of such an exomagnetosphere for a tidally locked exoplanet. The stellar magnetic field lines have access to almost one full hemisphere of the planet. The pressure distribution is asymmetric with respect to the ecliptic plane which means that magnetic pressure plays a much more important role than in the Earth's magnetosphere.

Grants

DFG VO 855/1-2
Applicants: J. Vogt and K.-H. Glassmeier
Title: Studies of paleomagnetospheric processes

Publications

J. Vogt, B. Zieger, A. Stadelmann, K.-H. Glassmeier, T. Gombosi, K.C. Hansen, and A. Ridley, MHD simulations of quadrupolar paleomagnetospheres, submitted to J. Geophys. Res., 2003.

B. Zieger, J. Vogt, K.-H. Glassmeier, and T. Gombosi, Magnetohydrodynamic simulation of an equatorial dipolar paleomagnetosphere, submitted to J. Geophys. Res., 2004.

2.2.9 Computer simulation of biomolecules

Dr. Martin Zacharias, Professor of 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 major drawback of most existing computational methods is the neglect of receptor flexibility during docking. During 2003 we have developed a new ligand-receptor docking approach that allows to efficiently account for receptor flexibility employing pre-calculated soft degrees of conformational freedom. Focus of

another research area is to improve protein structure modelling based on sequence similarity to proteins with known structure. Improving the accuracy of structural modelling of proteins is of central importance to use such structural models in drug design. In the last year we developed a new molecular dynamics potential scaling method to improve protein loop prediction and work on a similar scheme to improve side chain prediction is in progress. The CLAMV teaching lab computers were used in part to systematically test these approaches on model systems [1,2]. Within the last year we started a collaborative effort with the group of Prof. W. Nau (IUB Chemistry) to investigate the dynamics of end-to-end contact formation of small peptides in aqueous solution. The group of Prof. W. Nau uses the fluorescence quenching method to study the conformational dynamics of peptides experimentally. Understanding the conformational dynamics of peptides allows to better understand the mechanism of protein folding in particular the initial events of forming folding nucleation sites along a protein sequence. 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. In addition, this work allows to directly compare and check the performance of various force fields and simulation conditions to accurately reproduce experimental results on the dynamics of peptides. Publications of this work are in progress (Roccatano et al., in prep.). A significant part of the simulations have been performed on CLAMV teaching lab computers.

Publications

M. Zacharias, "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, in press (2004).

N. Riemann, M. Zacharias, "Reversible scaling of dihedral angle barriers during molecular dynamics to improve structure prediction of cyclic peptides and protein loops", J. Peptide Res. in press (2004).

2.3 Outlook

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 Proteinases and thyroid function

Dr. Klaudia Brix, Professor of Cell Biology:

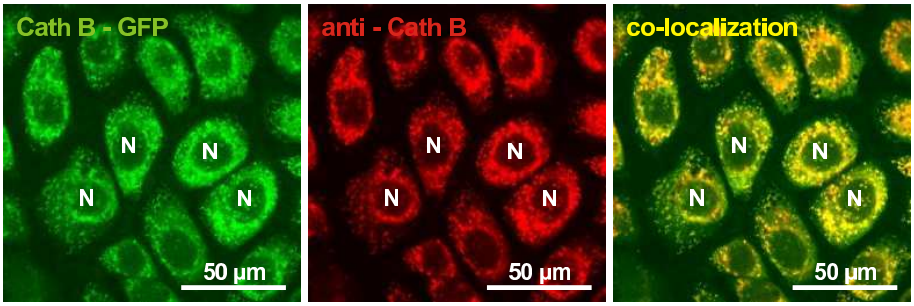

Figure 7: Cathepsin-trafficking in thyroid epithelial cells: cathepsin B tagged with the reporter green fluorescent protein (green) is transported in an identical fashion as the endogenous cathepsin B (red) as is obvious from the yellow color indicating co-localization of both.

The research group of Prof. Brix is interested in the analysis of the biological significance of proteinases for the function of the thyroid gland. We were able to show that the secretion of cathepsins B, K, and L is essential in order to allow the thyroid gland to fulfill its tasks, because the enzymes help to liberate thyroxine by proteolytic cleavage of its precursor molecule [Friedrichs et al., 2003]. Thyroid hormones are needed for proper development and growth of vertebrates as well as for thermoregulation and for the control of metabolic pathways of the adults. The thyroid hormone-liberating enzymes are sorted into transport vesicles which travel from the central regions of the cells towards their periphery to enable secretion of the cathepsins. The trafficking of cathepsins within thyroid epithelial cells can be visualized through the use of green fluorescent protein (GFP) of the jellyfish. Our research group engineered chimeric proteins in which the cathepsins are tagged with the reporter protein GFP [Linke et al., 2002]. The tagged cathepsins (green) were transported in the identical fashion as the endogenous cathepsins (red) as is obvious from Fig. 7, in which yellow indicates co-localization of both. In addition to the analysis of the trafficking of cathepsin-GFP chimeras, we would like to study the transport of mutated variants of the cathepsins. For this purpose, we are currently expressing cathepsins from tumor cells and cathepsins with an active site mutation, i.e. which are proteolytically inactive, in thyroid epithelial cells. The analysis of the transport of the various GFP-tagged proteins needs to be done within 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. The event of cathepsin secretion lasts for about 30 min, hence, different time intervals need to be analysed. As a long-term perspective, we aim to compare the trafficking of different cathepsins at the same time and within the same cell. This part of the project might have the potential to explain the significance of the enormous redundancy of cathepsins [see also Brix, 2004, in press]. Certainly, the interaction with members of the CLAMV and the use of CLAMV-resources will be most beneficial for the rapid progress of this research project in which we need to

combine computational biology with cell biology.

Literature:

Brix, K. (2004). Lysosomal Proteases: Revival of the Sleeping Beauty. In: Lysosomes, P. Saftig (Ed.), Landes Bioscience, in press.

Friedrichs, B., C. Tepel, Th. Reinheckel, J. Deussing, K. von Figura, V. Herzog, Ch. Peters, P. Saftig, and K. Brix (2003). Thyroid functions of mouse cathepsins B, K, and L. J. Clin. Invest. 111, 1733-1745.

Linke, M., V. Herzog, and K. Brix (2002). Trafficking of lysosomal cathepsin B - green fluorescent protein to the surface of thyroid epithelial cells involves the endosomal/lysosomal compartment. J. Cell Sci. 115, 4877-4889.

2.3.2 Organizational Principles of Network Robustness

Claus Hilgetag, Ph.D., Professor of Neuroscience, and Marcus Kaiser

In our research we seek to compare different kinds of real-world networks (e.g., transportation routes, power grid, Internet, biological networks) and identify the patterns that make many of them surprisingly robust towards damage of removing network nodes or connections. Furthermore, we test structural measures to predict the actual damage. In order to assess the impact of damage on the network, the increase of the average shortest paths in the network (an all-pairs shortest paths calculation) is performed. In addition to measuring the length of paths, we also want to know which edges are frequently part of the shortest paths. We plan to use the CLAMV for such computations, as we are investigating large networks with more than 10.000 nodes. Their representation in memory, including the memory for the shortest paths of each pair of nodes, is above the 4 GB memory limit for personal computers. We, therefore, plan to use the 16 GB SUN workstation in the CLAMV for our calculations.

2.3.3 Machine Learning and Nonlinear Stochastic Systems Modelling

Dr. Herbert Jaeger, Professor of Electrical Engineering and Computer Science

In a joint venture between IUB and the Fraunhofer Institute for Autonomous Intelligent Systems (AIS) in Sankt Augustin, a group of three Fraunhofer researchers settled on the IUB campus (Dr. Mathias Bode, Stephane Beauregard, Paul Gemin). Their mission is to acquire industry contracts in the field of nonlinear signal processing and control and at the same time giving IUB students the opportunity to participate in industrial applications of modern engineering methods.

The group uses 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. This technique is based on using artificial neural networks and for the first time enables engineers to obtain highly precise nonlinear system models by a computationally cheap and simple method. The modeling precision achievable with ESNs often surpasses the previous state of the art by orders of magnitude.

See http://www.ais.fraunhofer.de/INDY/echo_net_research.html for more information on ESNs.

Equipped with this new method, the Fraunhofer team at IUB sets out to find industry partners for joint application projects. A contract with an SME in the field of automated recognition of handwritten address fields has been secured. Negotiations are under way for the following projects:

- Prediction of instabilities in hot plasma
- Short-term power prediction for windmill power plants
- Quality control in assembly lines
- High-precision position control for printing cylinders in
- high-throughput printing machines

Research and development related to these projects is mostly carried out using the software installation at CLAMV, which thereby represents a central infrastructure component for the group's work.

2.3.4 Establishing a Competence Center for "European Connexions" at IUB

Dr. Michael Kohlhase, Professor of Computer Science

"European Connexions" (ECNX) is an initiative by the IRC, interested faculty, and academic affairs at IUB to establish an European competence center for the Connexions system (CNX; see http://cnx.rice.edu) from Rice university and deploy it to the benefit of our students here at IUB. The idea is to employ the Connexions system as a well-established technology basis and community driven workgroup solution and extend it by semantic markup and cognitively driven methods developed in Europe. This extension is a logical continuation of the CNX project and is welcomed by Rice university, which will cooperate with us in the endeavor. Concretely, we plan a version of the CNX system which is based on the OMDoc representation format (http://www.mathweb.org developed by Michael Kohlhase at IUB) and which incorporates modules from the OMDoc-based ActiveMath system (http://www.activemath.org developed at DFKI Saarbrücken).

We envision that combined platform will provide our students with user-adaptive, self-paced learning experience (ultimately empowering the students in the academic learning situation), and the university with data about the student's progress (the user model, which is collected by the system by measuring user interactions). Such data could ultimately be integrated into the IUB admissions process or be used as a means to offer specialized crash courses for our student body of diverse cultural and educational background. Importantly, it would give the university hard data to measure and scientifically refine academic curricula, rather than relying on anecdotal evidence.

Of course, this vision needs both fundamental research about system design, knowledge representation, user modeling, etc. and an infrastructure for the deployment and support on the IUB campus. This will be the role of the "European Connexions Competence Center" (ECCC@IUB). We envision an entity that is hosted collaboratively by the IRC (contributing expertise of and supporting the deployment side) and ClamV (for the research effort).

There are various attempts to secure external funding for the ECNX initiative; in particular proposals to the DFG and to the EU 6^{th} framework. However the time seems ripe to start with the establishment of the ECCC center now to take advantage of the impetus after the first public release of the CONNEXIONS system and build up the practical know-how and support structures. An already-established center would greatly increase the credibility of the funding efforts.

In the following, we will detail the goals of the ECCC and a plan for an initial setup of the center.

Setting up the ECCC

The goals of the ECCC are

1. to deploy an advanced platform for computer-supported learning at IUB (the ECNX system),
2. to support faculty in course content creation and sharing
3. to foster a community of authors, instructors, learners, and reviewers of course materials
4. to engage in research on computer-supported learning and user modeling technologies and to develop the platform further.

Initial Work plan

We see three phases in the establishment, which we envision to be six months duration each.

Phase 1: Setup, Training, Outreach (Spring '04) In the first phase the ECCC will concentrate on getting the CONNEXIONS and ACTIVEMATH system running at IUB, and to make them interoperable at a system level. The fusion of these systems will become the prototype ECNX system. There are long-standing cooperations with the CONNEXIONS and ACTIVEMATH projects that will facilitate this process. The CONNEXIONS system is open source software, and IUB is in the process of signing a cooperation agreement with DFKI Saarbrücken, which will give it access to the source code under similar conditions.

During this phase, the ECCC staff will accumulate know-how and operational experience with the systems, disseminate the existing technology to the faculty and try to entice them to start experimenting with existing CONNEXIONS or ACTIVEMATH content or create new course content. There are faculty on campus who have experience with

this from Rice or DFKI. The research assistants will work closely with the early authors, introduce them to the necessary tools and even transform existing materials into the necessary formats.

Phase 2: Exemplary Deployment (Fall '04)

In the second phase, we plan exemplary deployment of the ECNX system in selected courses. Likely candidates are course materials prepared by early adopters among the faculty in phase 1 or existing course modules, e.g. the digital signal processing (DSP) materials from CONNEXIONS or the statistics course from ACTIVEMATH.

Phase 3: Deployment and Evaluation (2005)

In the third phase the deployment of the ECNX system will be extended beyond pilot usage. First full courses will be supported by the system, and learning effectiveness will be evaluated in controlled experiments. The data collected in the second phase will be used to refine the content and develop first tacit suggestions for curricula.

Organization and Staff

The competence center will initially be staffed by a research-programmer/system administrator together with 4 to 8 research assistants (students at 12h per week). The research programmer is a staff-level position, and will be responsible for running and deploying the systems, systems interoperability, routine maintenance and programming the necessary system extensions. The main responsibilities of the research assistants will be to support faculty in creating and maintaining course materials (4 students in phase 1) and support students in their interaction with the system (additional 4 students starting in phases 2 and 3).

The ECCC will be organized and led in its day-to-day operation by Michael Kohlhase with Ronny Wells, Tom Hochstettler, Torge Schmidt, and Diann Rusch-Feja as consultants on policy matters.

Hardware, Rooms, and Consumables

The ECCC will need office space for the research programmer and the research assistants in close proximity to either the IRC, ClamV or Michael Kohlhase's office in order to foster teamwork and ensure efficient communication and collaboration. The center will initially need three desktop computers for the research programmer and the research assistants (two can share a work space). The center will initially not need a dedicated server, since ClamV has offered computing and storage resources. Depending on the system load in phase 3, additional hardware may have to be procured.

2.3.5 Electronic Structure of Condensed Matter

Dr. Michael Rohlfing, Professor of Physics

The focus of this work is on excited electronic states in condensed matter. Such states and their spectra play a key role in understanding optical properties, for optoelectronic mechanisms, charge-transfer processes, femtosecond dynamics, and more. Of particular interest are systems that are characterized by quantum-mechanical states

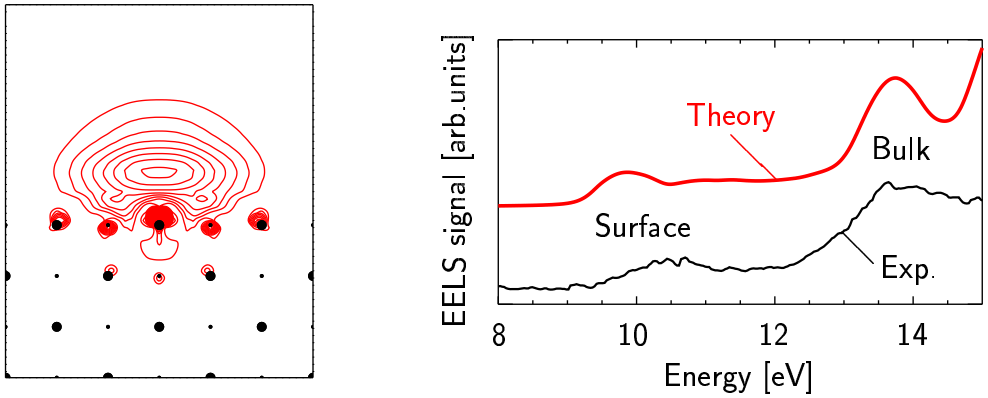

Figure 8: Left panel: Cross section of the image-state wave function at the LiF(001)-(1x1) surface, attracted to a hole at the central fluorine atom in the surface layer. The dots indicate the atomic structure (Li and F atoms) of the outermost four atomic layers. Right panel: Calculated electron-energy loss spectrum of the LiF(001)-(1x1) surface in comparison with experimental data (Mabuchi 1988). The peak labelled "Surface" near 10 eV originates from the image state.

on the length scale of the atomic bond. The properties of such nanostructured materials go far beyond those of the extended solid. A microscopic theory is required which takes the single atom and its orbitals as the smallest unit. In addition, electronic states and their spectra are significantly affected by electronic exchange and correlation effects. The evaluation of such many-body effects for a real system (crystals, molecules, surfaces, polymers, and others) requires highly demanding numerical computation.

As one example, we discuss image potential states on crystal surfaces, that can be considered as a prominent example of electronic correlation effects. A so-called "image potential" occurs when a free electron in vacuum approaches the surface of a crystal to within a few nanometers. In this case, a positive "image charge" is induced inside the crystal to which the external electron is attracted. It has long been suggested that the electron could be trapped in the potential resulting from this attraction, leading to "image states" that qualitatively resemble the spectrum of a hydrogen atom. Such states are indeed observed on some metal surfaces, but it was not clear so far whether this concept also holds for other materials. Recent experiments like electron energy loss spectroscopy on insulators and two-photon-photoemission measurements on semiconductor surfaces indicate that image states may be relevant for such materials, as well.

In the present study we show that image states indeed occur on insulator surfaces, in particular on the LiF(001)-(1x1) surface. Since the image-potential attraction is a complicated quantum-mechanical many-body correlation effect, a highly advanced computational investigation was necessary to address this issue. Based on several hundred basis functions, correlation between several thousand electronic states must

be considered. This allows us to identify the image state (see left panel of Fig. 1) and to reveal its role in elementary excitations of the surface. The image state and the related electronic excitations lead to a characteristic surface peak in the electron energy loss spectrum near 10 eV (see right panel of Fig. 8) in accordance with experimental data (Mabuchi 1988).

Future projects will include, among others, the photodissociation of surfaces and molecules, excited-state femtosecond dynamics, the adsorption of organic molecules on metal substrates, and the discussion of Stokes shifts in polymers and molecules. This involves both the efficient performance of existing computer programs on powerful platforms, as well as the development of new and advanced codes for further problems. The CLAMV hardware resources will play a crucial role in this progress.

Grants

DFG RO 1318/4-2
Title: Excited states of adsorbed molecules on semiconductor and insulator surfaces

Publication

M. Rohlfing, N.P. Wang, P. Krüger, and J. Pollmann, "Image States and Excitons at Insulator Surfaces with Negative Electron Affinity", Physical Review Letters **91**, 256802 (2003).

2.3.6 Compact stellar object collision

Dr. Stephan Rosswog, Professor of Astrophysics

The key purpose of this project is the simulation of compact stellar object collision within particle hydrodynamics. Focusing on objects like white dwarfs, neutron stars, and black holes, the interest is both on the hydrodynamical aspects and on the appropriate modelling of the microphysics (e.g. nuclear equation of state, neutrino emission, nuclear burning processes).

3 Undergraduate Teaching

3.1 Overview

Although the CLAMV is primarily designated for graduate and faculty research, its resources have been used extensively for undergraduate teaching and research. In fact, until the new Undergraduate Teaching Lab in the Research I Lecture Hall was operational, all undergraduate classes involving hands-on computer instruction where conducted in the CLAMV teaching lab.

In 2003, the CLAMV teaching lab (i.e. the teaching lab Linux PCs as well as network and file server for license management and file storage), were used by the following courses.

- First year natural science laboratory modules (6 modules Computer Science, 4 modules Mathematics, 1 module Geosciences and Astrophysics).
- Second year laboratory courses in Electrical Engineering, Computer Science, Bioinformatics and Computational Biology, Computational Chemistry and Biochemistry, Geosciences and Astrophysics.
- The University Studies Course "Mathematics and Democracy" described in Section 3.2.
- Guided research projects, see Section 3.3.
- Training for the International Collegiate Programming Contest, see Section 3.4.

The CLAMV continues to play an active role in undergraduate teaching and research. While the larger courses have moved to the Undergraduate Teaching Lab which, for the first time, provides adequate space for the large first and second year lab sessions in Computer Science, the CLAMV teaching lab is used for many smaller classes that run in parallel and were previously competing for the same limited space.

In the following, we give examples of special uses of the CLAMV as a teaching facility.

3.2 USC Mathematics & Democracy

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

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

Figure 9: USC Mathematics and Democracy on May 25, 2003: Members of the coverage group studying the latest projection of the Bremen state elections in the CLAMV teaching lab.

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

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

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

The project was a tremendous success: in contrast to the official projections of the major German television stations ARD and ZDF, the IUB project used data from only half as many precincts (66 compared to 150) and was conducted entirely by students with no previous experience in election projection. Still, the IUB projection was accu-

rate within a variation of just one seat compared to the official end result. The web site received about 800 hits on election night alone and several newspaper articles have appeared covering the project.

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

3.3 Undergraduate Research

Several 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. The participants include

Vlad Lazar "Isolating Filament Channels in Magnetograms" using IDL and C++. Supervisor: Patrick Bangert.

Milko Krastev "Braid Reduction using Simulated Annealing" using Java server to run simulations remotely on CLAMV machines. Supervisor: Patrick Bangert.

Vinod Devanathan "N-body simulations of open galaxy clusters" using IDL on the CLAMV. Supervisor: Stephan Rosswog.

Peter Dabrowski "Analysis of magnetic and electric field data from the multi-spacecraft mission Cluster-II" using IDL, and teaching lab PCs for data storage and analysis. Supervisor: Joachim Vogt.

3.4 International Collegiate Programming Contest (ICPC)

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

The contest is structured as follows. The organizers post a set of problems on a web site and an evaluation server is started. Participants have to solve problems and submit the source code to the evaluation server, which will compile and run the program over a set of undisclosed test cases. Only when the program correctly answers all the test cases the problem is considered solved and the team is given credit. Typically, a contest runs for 5 hours in which 8 problems have to be solved.

Figure 10: CLAMV on the move: The IUB team on the way to the International Collegiate Programming Contest in Lund, Sweden.

On September 27, 2003, the local IUB contest was held in the CLAMV teaching lab, in order to select the best two teams for the regional competition. Although the competition took place on a Saturday evening starting at 19.00, about 20 students participated. The contest was won by Mathias Goerner, Michael Thon, and Andreas Pfeil. As the second place resulted in a draw, CLAMV hosted a second local contest the following Saturday. This second contest was won by the students Vlad Vicol, Dan Popovici and Ioan Sucan. The two winning teams, together with their coach, Dr. Stefano Carpin, went to the Northern Europe regional competition, which took place at the Lund Institute of Technology, Sweden, on November 23, 2003. The IUB teams ranked on positions 16 and 26 out of more than 50 teams. As all students involved where keenly interested, IUB will participate in 2004 as well.

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.

From September 2002 until the Fall Semester 2003, the CLAMV seminar has primarily focused on the first two aspects: Out of a total of 31 scientific talks, we had 8 external and 23 internal speakers; in addition, two of the sessions were devoted to an overview on the CLAMV infrastructure by the systems manager and the presentation of the newly established curriculum for the Bachelor in Computational Science to our undergraduates. A detailed seminar schedule can be found in Appendix A.4.

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.

For 2004, the first guests from industry have been invited, and the proportion of technical talks will increase in order to broaden the appeal of the seminar. In addition, it is expected that the CLAMV seminar will, sooner rather than later, feature outstanding research contributions from IUB graduate students and possibly even undergraduate students.

At the time of writing, in its fourth semester running, the CLAMV seminar has established itself as one of the main interdisciplinary seminars at IUB, as well as the focal point of Computational Science.

5 Service and consulting

CLAMV supports research and education in all computer oriented disciplines with a wide variety of services. The necessary management and consulting tasks are the domain of the *CLAMV Systems Manager*, who receives additional help from currently two student assistants.

5.1 Software management

Most academic software products of broader interest to the IUB community are purchased, installed and maintained by the CLAMV. This includes, in particular, license negotiations, license management, and the implementation of access regulations. Even in cases of specialist academic software, the CLAMV systems manager helps at all stages of procurement, installation and maintenance.

The following major commercial packages are currently available and maintained on a pair of redundant servers; a full list of available software is contained in Appendix A.3.

General software packages for analysis, numerics, and visualization: IDL, Mathematica, MatLab (including several toolboxes)

Software for molecular science: Gaussian03, rasmol, VMD, ...

Software for Bioinformatics: Emboss, Modeller, ...

Software for Geoscience and Astrophysics: PetroMod, Tecplot

Most of these packages are available for both research and education; in some cases, however, license conditions restrict the domain of usage.

Access is provided via the network or through the CLAMV teaching lab—a set of 30 well-equipped Linux workstations with a fully configured desktop and software development environment (including compiler, debugger, editors, parallel environment, scientific libraries, and databases).

5.2 Administration of HPC environments

CLAMV provides access to high performance computer (HPC) equipment in three ways. First, researchers use CLAMV resources, or contribute with their grant and start-up funds directly to resources that are fully integrated with the CLAMV. Second, the CLAMV systems manager has assisted with setting up local HPC equipment. In some cases, the entire system administration is done through CLAMV.

In each case, CLAMV creates an “economy of scale” that allows researchers to use idle time on remote machines or, vice versa, have others use idle time on their hardware. Moreover, administration can be substantially simplified by a centralized setup, which is developed and maintained jointly with the IRC.

The third way of accessing high performance computing environments is through off-campus partners such as the BremHLR and the HLRN. The CLAMV is involved in negotiating cooperation agreements and assists local users with gaining access to these facilities.

5.3 Strategic planning

Currently, the most crucial strategic planning activity is early stage consulting in the procurement of HPC equipment for IUB working groups. The aim is to identify hardware and software solutions that not only provide good performance for the task at hand, but also fit well into the existing computer environment and its medium term development.

The CLAMV systems manager helps surveying the market, and contacts and invites vendors for presentations of their products. Examples of current activities are the procurement of a 24-processor shared memory server for astrophysical simulations, and of a new computer cluster with distributed memory for bioinformatics.

In addition, the CLAMV advises on products on the workstation level, for example the evaluation of the 64-bit technology (on AMD opteron processors). The CLAMV is also involved in all IRC activities which relate its mission, for example the recent reorganization of the IUB campus network and the procurement of a campus-wide file server for home accounts, web presentations, and disk space for scientific projects.

5.4 User support and service

The CLAMV also provides a number of services, in close cooperation with the IRC, that are not directly related to high performance scientific computing.

End user support, primarily related to CLAMV software and hardware, complementing the services of the IRC.

User Mode Linux, a way of setting up virtual servers on existing hardware for small-scale projects, in particular web servers, on which project members can have root access without security implication for the network at large. Several IUB websites currently run as UML virtual machines on CLAMV hardware. A joint project to making UMLs part of the IRC services is planned.

Desktop Thin Clients as low-cost, low-noise desktops which use the teaching lab PCs as their compute backend. Two such clients are currently in use within the Mathematics group, and there is a lot of potential for future expansion.

Account service and backup for the Undergraduate Teaching Lab; moreover, CLAMV machines frequently serve as compute backends for the Undergraduate Teaching Lab thin clients.

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 (until June 2003: Nani Clow).

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 (10-12/2002: Matthias Mittler, 1-7/2003: Michael Koehne).

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, 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): Marcus Brueggen (Chair), Adele Diederich, Hildegard Meyer-Ortmanns, Goetz Pfander, Achim Gelessus.

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

- 16 compute nodes
- 2 Intel Pentium Xeon 2.80 GHz processors per node
- 1.0 GByte RAM per node
- 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. There is no general access to this machine.

Technical specifications

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

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
- 4.0 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 analysis and visualization: IDL, Mathematica, MathWorks products: MatLab, SimuLink, Communication Toolbox, Control Toolbox, Image Toolbox, Signal Toolbox, Symbolic Toolbox, MatLab Compiler.

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

Software for Bioinformatics: ClustalX, Emboss, Modeller, ViennaRNA

Software for Geoscience and Astrophysics: PetroMod, 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 Past Seminar Schedules

Fall 2002

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

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

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

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

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

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

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

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

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

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

Spring 2003

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

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

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

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

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

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

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

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

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

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

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

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

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

Fall 2003

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

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

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

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

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

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

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

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

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

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