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

## Summary

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 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 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. CLAMV also contributes to the *International Research Consortium on Continental Margins (IRCCM)* by providing administational support, software, and hardware to this collaboration of institutions from academia and industry. Within the IRCCM, IUB aims at a leading role in the fields of data management and modeling.

## Scientific projects

Research groups from a variety of different fields are making use of CLAMV resources or are preparing to do so in the nearest future, e.g., Applied Mathematics, Astrophysics, Biochemistry, Chemical and Biological Physics, Computational Biology, Computational Materials Science, Computational Science, Computer Science, Condensed-Matter Physics, Geoscience, Mathematical Psychology, Neuroscience, Statistical Physics. The projects are described in the CLAMV Activity Report 2002/2003.

### **Involvement** in teaching

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 courses in, e.g., Bioinformatics and Computational Biology, Computational Chemistry and Biochemistry, Computer Science, Electrical Engineering, Mathematics, Geosciences and Astrophysics, a University Studies Course, a number of guided research projects, and the training for the International Collegiate Programming Contest.

#### 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.