John von Neumann Institute for Computing

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published in

NIC Symposium 2006 ,
G. Münster, D. Wolf, M. Kremer (Editors),
John von Neumann Institute for Computing, Jülich,
NIC Series, Vol. **32**, ISBN 3-00-017351-X, pp. 1-2, 2006.

http://www.fz-juelich.de/nic-series/volume32

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Thomas Lippert

Central Institute for Applied Mathematics, John von Neumann Institute for Computing (NIC)
Research Center Jülich, 52425 Jülich, Germany
Department C, Bergische Universität Wuppertal, 42097 Wuppertal, Germany
E-mail: th.lippert@fz-juelich.de

With the foundation of the John von Neumann Institute for Computing (NIC) in 1987, the former "Höchstleistungsrechenzentrum HLRZ" and first National German Supercomputing Centre, the NIC contractors—at that time the Forschungszentrum Jülich (FZJ), the German Electron Synchrotron (DESY) and the once National Research Centre for Information Technology (GMD)—decided to fund topical research groups working in selected fields of computational science.

Currently, FZJ operates the research group "Computational Biology and Biophysics". The group succeeds the former research group "Complex Systems", which acted at the interface between biology and physics, and was led by Prof. Peter Graßberger. After Graßberger's retirement, the Computational Biology and Biophysics group started in July 2005 under Prof. Ulrich Hansmann. At Zeuthen, DESY supports the research group "Elementary Particle Physics" which is led by Dr. Karl Jansen. In 2006, the "Gesellschaft für Schwerionenforschung, GSI" in Darmstadt will join the NIC with the intention to establish a new research group in the field of "Computational Hadron Physics".

The staff positions for the Computational Biology and Biophysics group at FZJ comprise the group head, six researchers and two Ph.D. students. At NIC-DESY/Zeuthen in addition to the head again six researchers and two Ph.D. students are assigned to the group. Both groups complement their teams by several third party funded positions. It is a distinctive feature of the NIC research groups that their leading persons are recruited for three years with the option for prolongation to six years. The candidate must be a professor with a permanent position at a University or research institute. This policy guarantees a high flexibility for re-orientation of research towards new developments.

The mission of the NIC groups is to carry out excellent, internationally recognized research in topical fields of the computational sciences, including life sciences, by means of supercomputers of highest performance, state-of-the-art data processing capabilities and fastest connections to Grids and the Web. The objective of the groups is to act both as cores and as hubs for the establishment of novel fields in computational science, and to foster novel developments in these fields, thus generating highest visibility of the computational science activities of the NIC.

Furthermore, the NIC research groups concentrate on the development of new methods and algorithms. The Complex Systems group, for example, has introduced a highly cited approach for sequential sampling, the "Pruned Enriched Rosenbluth Method" (PERM), a depth first algorithm including importance sampling and re-sampling. To mention an important application, PERM is most efficient for the simulation of low energy configurations of lattice heteropolymers. The Elementary Particle Physics group has substantially boosted the simulation efficiency of light dynamical fermions by exploiting several techniques as

twisted mass fermions and combinations of algorithmic improvements including Hasenbusch preconditioning. One should remark that the group in the past has paved the way for the polynomial HMC scheme, now a standard technique which has led to the Rational Hybrid Monte Carlo method. RHMC is used for instance by the QCDSF group, which is led by Prof. Schierholz, a member of the NIC research group, to simulate very small quark masses. The Computational Biology and Biophysics group has contributed with the SMMP algorithm, now a freely available simulation package for protein folding which is widely used. The group is continuing the development of the "generalized ensemble approach" with the goal to predict the structure of stable domains in proteins with finally up to 200 residues.

A third major activity of the NIC research groups is to act as pilot users and driving forces in the development of novel computing technologies. In the past, DESYs Elementary Particle Physics group was a forerunner in the usage of the Italian APE100 system and was involved in the joint construction of APEmille and apeNEXT. Today, the NIC scientists are among the first to utilize and to develop algorithms for the 45 Teraflop/s Blue Gene /L leadership-class system installed at NIC-Jülich in January 2006.

In the future, the NIC research groups will play a major role in the realization of the integrated Helmholtz supercomputing concept. The research groups are foreseen to act as the scientific focal points in simulation laboratories, created for the respective fields. Following an open model, the simulation labs will be jointly operated by the NIC support teams at the Central Institute for Applied Mathematics (ZAM) at FZJ and by members of the scientific communities, maintaining a web portal for dissemination of best practice and providing Grid based access to algorithms, optimized code elements, simulation data and other data bases.

The NIC research groups are an essential element of NIC's strategy towards a European supercomputing centre. Their deep integration in existing pan-European research communities became evident at the workshops for the preparation of the European scientific case for supercomputer infrastructures in Barcelona (11/2005) and Cadarache (2/2006).

In the coming years, the NIC will continue this successful research model and intends to establish further groups. The NIC as a virtual computational science institute will be expanded in order to meet the continuously growing importance of supercomputing, computational methods and algorithms for computational science and engineering.

The next three contributions will give an overview of the activities of the NIC research groups, starting with the Complex Systems groups, led until June 2005 by Prof. Peter Graßberger, followed by the new Computational Biology and Biophysics group, led by Prof. Ulrich Hansmann since July 2005, and finally presenting the Elementary Particle Physics group of Dr. Karl Jansen.