

HPC Users Conference 2009

Preface

The High Performance Computing Center in Poznań was created in 1993. The first Cray machine was delivered by the end of the year with a peak performance of 0,5 Gflops and 0,5 GB of operational memory. This was the starting point of several scientific grants at Poznań universities, which used the HPC technology at that time. The first idea was to build a metacomputer consisting of various architectures. Later on, Poznań Supercomputing and Networking Center was equipped with vector, SMP (Shared Memory Multi-Processor), MPP (Massively Parallel Processing) and nowadays with PC clusters. The cluster systems have been dominating the IT market since 2002, when the performance of these systems was high enough to start HTC (High Throughput Computing). In addition, clusters equipped with low latency networks have been able to run MPI jobs with very good efficiency. The price-performance ratio has also been higher than for the bigger but also more expensive MPP or SMP systems.

Several projects focused on building European e-Infrastructure for grids (distributed PC clusters) and HPC environments have been started. A big infrastructure-related grid projects were initiated by DataGrid, later EGEE/EGEE-II and EGEE-III projects, which established in 2009 a non-profit organization called EGI (European Grid Initiative) synchronizing the work of national grid initiatives (PL-GRID in Poland coordinated by Cyfronet with active engagement of PSNC). At the same time, another organization called PRACE AISBL (Partnership for Advanced Computing in Europe), which aims to build a European infrastructure of HPC systems with Tier-0 sites of Pflops peak performance and connected with Tier-1 sites (national and regional HPC centers), was established. PSNC is one of the funding members of PRACE AISBL.

The European Strategy Forum for Research Infrastructures (ESFRI) has identified High Performance Computing as a strategic priority for Europe¹. Scientists and engineers must be provided with access to capability computers of leadership-class to remain competitive internationally and to maintain or regain leadership. Supercomputers are an indispensable tool to solve the most challenging problems through simulations. HET, the High Performance Computing for Europe task force, developed the fundamental concepts to create a true pan-European Research Infrastructure named Partnership for Advanced Computing in Europe or PRACE for short. The PRACE activity was recognized by the Ministry of Science and Higher Education and located on the Polish roadmap of scientific projects of high importance.

¹ European Roadmap for Research Infrastructures – Report 2006

The infrastructure-related activities of PSNC are aiming to build a local environment which allows users to use clusters and SMP systems, i.e. the best architecture for the application. In the meantime, PSNC has become a center which supports not only Poznań but also other academic communities in Poland and worldwide (HEP – High Energy Physics in CERN and several other virtual organizations like BioChem, VOCE – Central Europe VO). In 2009, PSNC delivered about 9 billion cpu hours, where 2.5 billionhours were used by VOs.

The support is given to many scientific disciplines: physics, chemistry, biology, bioinformatics, engineering and computing science, and includes direct contact with the end users who require help on running or installation new software, trainings and optimization of new applications or those moved from one system to another.

The users who received a grant project for certain grid or HPC resources in PSNC are obliged to deliver an annual report with a list of results, including a list of publications. The HPC Users Conference in 2009 was focusing on applications developed with help of PSNC computing resources. Our wish is to continue this interesting event on an annual basis. The 1-day seminar was organized in conjunction with the i3 Conference of the Pionier consortium entitled “i3: internet – infrastructures – innovations – Science in the face of the digital society”.

The selected list of papers have been published in this CMST issue. The first paper describes a Genomic Virtual Laboratory (GVL) which was developed for automate analysis of data retrieved from a microarray experiment (by B. Cegielska et al.). The system was implemented for R Bioconductor-based analysis of results obtained in the study on human acute myeloid leukemia (AML). The second article presents a molecular perspective review of biochemical role of nucleobases modified by oxidative stress (by Piotr Cysewski).

The third paper presents a model of anisotropic solids (by A. Glema et al.). The fundamental achievement is that the constitutive relation includes a description of anisotropy of metal microstructure. Such approach gives qualitatively and quantitatively new results compared with the existing models, because it is possible to trace the directions of softening and predict a damage path in process time.

The fourth paper describes two complementary calculation methods used in phononic crystal studies: the finite difference time domain (FDTD) method and the plain wave method (PWM) by P. Nowak and M. Krawczyk.

The fifth article entitled “Flexibility of Dicer Studied by Implicit Solvent Molecular Dynamics Simulations” (J. Sarzyńska et al.) is a joint effort of two groups coming from the biochemistry area and computing scientists.

The last paper presents an analysis of numerical investigations on the flow with heat transfer in rotating cavity performed by DNS (Direct Numerical Simulation) and LES (Large Eddy Simulation).

The papers published in this issue reflect a variety of applications running on PSNC resources. The nature of the applications requires various computing resources and data access. Some of them are optimized in distributed environments of thin nodes connected with high speed networks. Others will require SMP machines with many processors and shared memory access. If the input data are very large, we need to consider a data intensive computation approach with very fast repositories connected to computing resources. These discussions and analyses will be the focus of the next HPC Users Conference in 2010.

We would like to thank all the authors for their contribution to this CMST journal. We hope the effort we have made is valuable for the users of our data center and the readers of the journal.

The Editors

Tomasz Łodygowski
Norbert Meyer
Jan Węglarz