DEISA Newsletter

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The 4th DEISA training session was held at the Finnish IT center for science CSC

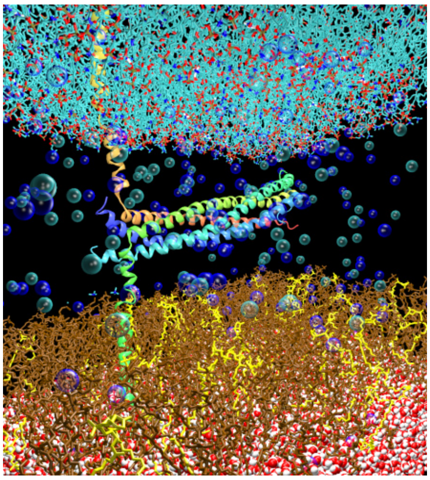
The 4th DEISA training session was held at the Finnish IT center for science CSC, in Espoo, Finland on May 30–June 1, 2007. Scientists from all European countries and members of industrial organizations involved in high performance computing were invited to attend.

The purpose of the training was to enable fast development of user skills and know-how needed for the efficient utilisation of the DEISA infrastructure. The first part of the training gave a global description and introduction to the usage of the DEISA infrastructure, followed by presentations of heterogeneous environments, like the new CrayXT4 at CSC and SGI at LRZ.

Friday, 1st of June, several use cases were presented. Marc Baaden from Institut de Biologie Physico-Chimique, CNRS, Paris, has simulated the interaction of a protein complex with two lipid membranes. For the simulations, the GROMACS software was used to compute molecular dynamics trajectories based on classical force fields. The use case describes membranes under tension by modeling the membrane-embedded SNARE complex. Baaden and his team modeled a protein complex that acts as a catalyst in the fusion of two cell membranes. This exceptionally complex model could not have been constructed and simulated without the distributed European computation capacity offered by DEISA.

Marc Baaden from CNRS Institut de Biologie Physico-Chimique, Paris, France.

The functional disorders of cell membranes are known to be associated with many metabolic diseases. The fusion of membrane structures, which is catalyzed by the protein complex studied by Baaden, may for example be disturbed by toxins, leading to medical conditions such as tetanus or botulism.



A schematic view of the SNARE protein complex embedded in the two membranes.

At present, cell membrane mechanisms are under intensive study in many research groups all over the world. By modeling and understanding these events, we may, in the future, be able to develop more efficacious drugs that are conveyed directly to their target site.

Marc Baaden and his team used standard molecular modeling methods in their work, but the system subject to simulation was exceptionally extensive and complex. The size of the system was 340 000 atoms, the timescale was 40.2 nanoseconds, real timescale 99 days with a total of 218 000 CPU hours from 96 processors. And yet, on the cellular scale, the area simulated was extremely small.

For more information:
http://www.baaden.ibpc.fr/projects/snaredeci/

Fifth DEISA training session in October 2007

The fifth DEISA training session will be organized at CINECA Supercomputing Centre, Bologna, Italy on October 29 - 31, 2007.

The purpose of the training is to enable fast development of user skills and know-how needed for the efficient utilisation of the DEISA infrastructure. The first part of the training will give a global description and introduction to the usage of the DEISA infrastructure. The second part of the training will be dedicated to the topic of Data treatment and Advanced Visualisation in HPC.

The registration is open at www.deisa.org/training/Bologna2007/ until October 8.

The 3rd DECI call resulted in over 60 proposals

The 3rd DEISA Extreme Computing Initiative (DECI) Call for Proposals resulted in over 60 proposals involving scientists from 13 European countries, and collaborators from North and South America, Asia and Australia.

The proposals will first be technically evaluated by the Applications Task Force, who will determine the technical requirements, the allocation of computational resources and the human resources required for the long term application enabling. The scientific evaluation of the proposals will be done by a number of National Scientific Evaluation Committees in early October, and they will provide recommendations to the Consortium on the proposals' scientific importance.

The decision on which proposals will be run as the next DECI projects will be made public in the middle of October.

DECI project: Hot and dense nuclear matter in particle physics and cosmology

Kari Rummukainen, University of Oulu, Finland
Ari Hietanen, University of Helsinki, Finland

During its initial moments, the universe was made up of extremely hot and dense matter. In these conditions, the structural elements of atomic nuclei – protons and neutrons – disintegrate and form a new, exotic state, quark-gluon plasma.

Kari Rummukainen's researcher team at the University of Oulu studies the properties of quark-gluon plasma by means of extensive computer simulations. The team has developed a theory enabling scientists to apply computer simulations for studying the properties of plasma at very high temperatures. These simulations produce much more precise data than simulations of the original physical theory of quarks and gluons, i.e. quantum chromodynamics. The team has also developed a simulation program for studying events during the initial moments of heavy ion experiments. In its work, Rummukainen's team utilized the DEISA resources at CINECA and CSC. The total CPU-time used is 125 000 processor-hours, 32 or 64 processors at a time.

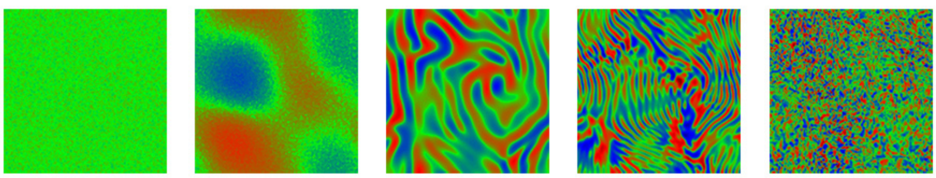
Quark-gluon plasma is studied experimentally in heavy ion collisions. In these experiments, two heavy atomic nuclei are collided together at very high energy. If the energy is great enough, the collision yields a microscopic droplet of quark-gluon plasma. An RHIC (Relativistic Heavy Ion Collider) experiment is currently under way in Brookhaven, USA, and the largest heavy ion collision experiment designed so far is being constructed in the LHC particle accelerator at CERN.

In its recent simulations, Rummukainen's team has focused on two themes: the thermodynamic properties of hot quark-gluon plasma, such as pressure and particle number fluctuations, and the stormy initial moments of heavy ion collisions when the quark-gluon plasma is just in the process of formation.

Many researcher teams all over the world are studying the thermodynamics of quark-gluon plasma by means of computer simulations. For this purpose, Rummukainen's team has developed an effective theory of quantum chromodynamics, which enables the team to use computer simulations for studying plasma properties at very high temperatures much more precisely than by simulating the original quantum chromodynamics. In particular, the effective theory is useful in making a clear distinction between the perturbative and non-perturbative elements of thermodynamic quantities, such as pressure. This distinction is very important in terms of theory: the perturbative element can – at least in principle – be calculated analytically, whereas direct computer simulations are the only means known for calculating the non-perturbative element. Some preliminary findings have already been published about the pressure of quark-gluon plasma and about fluctuations in the number of quarks.

Rummukainen's second project concentrates on the initial moments of heavy ion experiments. The collision of two nuclei with each other is immediately followed by a state of enormous energy density. This state is far from thermal equilibrium and it develops rapidly. It is not yet known for certain how this development towards thermal equilibrium takes place, but findings from heavy ion experiments indicate that it is very fast.

Rummukainen's team developed a simulation program that is suited for studying the above state of non-equilibrium. Simulations have shown that when plasma is in a state of non-equilibrium at the initial stage, it can generate a phenomenon known as plasma instability: waves that grow exponentially. According to the team's latest simulation findings, when this instability has increased sufficiently, it can push the system very rapidly towards thermal equilibrium. Plasma instability thus plays a crucial role in determining the physics of heavy ion collisions.



Plasma instability in a heavy ion collision experiment. Instability generates a rapidly growing wave in the gluon field; as it grows, the wave also moves towards shorter wavelengths. The final state has an almost complete thermal distribution. © Kari Rummukainen, University of Oulu.

CSC's DEISA connections up to par

© Jyrki Hokkanen

CSC's new Cray XT4

CSC's new supercomputer Cray XT4 was hooked up with DEISA this summer, as CSC's previous supercomputer IBMSC was phased down. At the same time, the network connections were upgraded to 10Gbps.

CSC's new Cray XT4 is the first Cray system in the DEISA environment. Consequently, most the services of DEISA have been installed to the Cray platform: GPFS, UNICORE, DESHL, etc. This update also brings about a new dimension and a significant increase in DEISA resources.

CSC's DEISA computers have been connected to the dedicated DEISA 10 Gbps network through a 10 Gbps light path provided by Nordunet and Géant2 networks. CSC's previous 1 Gbps connection to other DEISA sites was done through routers while the new 10 Gbps connection bypasses most of the routers on the way. This is reducing the delays of the TCP/IP packets and thus speeding up the data transmissions even more.