DEISA Newsletter

DISTRIBUTED EUROPEAN INFRASTRUCTURE FOR SUPERCOMPUTING APPLICATIONS

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Distributed European Infrastructure for Supercomputing Applications

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Computational challenges discussed at the DEISA Symposium

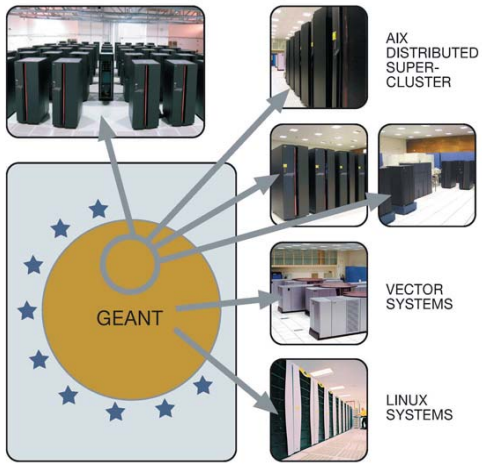
The first DEISA Symposium was held in early May, in Paris. Close to 200 people participated to this event and to the discussion on perspectives in High Performance Computing. A wide overview of the major computational challenges in all relevant areas of science and technology were given by leading computational scientists. This issue of the DEISA Newsletter is dedicated to the results of the first symposium. This newsletter contains synopsis of each scientific talk together with the link to the complete presentations available at www.deisa.org/symposium.

The symposium was the first of a series that will take place every year in April - May in different locations in Europe. The purpose is to maintain an annual DEISA event dedicated to the discussion of the scientific and strategic challenges in the area of High Performance Computing, and to assess the impact of the DEISA research infrastructure on computational science in Europe.

DEISA Extreme Computing Initiative well in progress

DEISA Extreme Computing Initiative (DECI) dealing with leading "flagship" applications is well in progress. Over 50 proposals have been received during the first call for proposals in April and May 2005 (closure date May 30). Currently proposals are assessed through national evaluation committees. Deployment of the applications in DEISA will start in early autumn 2005.

These leading, ground breaking applications must deal with complex, demanding, innovative simulations that would not be possible without the DEISA supercomputing Grid, and which will benefit from the exceptional resources from the consortium. Projects of this kind will be chosen on the basis of innovation potential, scientific excellence and relevance criteria.



The DEISA supercomputing Grid

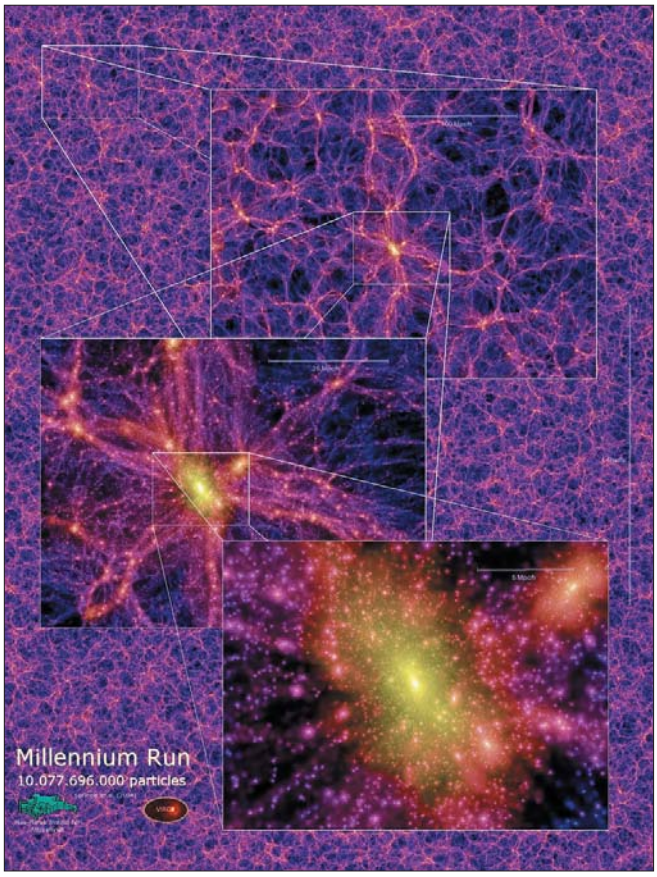
Computing the universe

Presentation by Prof. Carlos Frenk, Institute for Computational Cosmology, Physics Department, Durham University, UK

Prof. Carlos Frenk, from the Institute for Computational Cosmology, Physics Department, Durham University, UK, gave a fascinating and colourful talk, described the current state-of-the-art in simulating the evolution of the universe.

Prof Frenk described how there gas been enormous advances in recent years in the understanding of the origin and subsequent evolution of the Universe. New data have determined that, very soon after the Big Bang, the early universe had small irregularities in the distribution of the density of matter. The evolution of galaxies is erratic and unstable and, as a result, calculating their formation paths and present-day properties requires large and expensive simulations, starting from this irregular distribution of matter, and including processes associated with dark matter and gas.

Prof. Frenk went to on to describe what is now recognised to be the worlds largest computer simulation of the universe, the so-called Millennium Run, using 10 billion particles. This simulation was performed by the Virgo consortium, an international group of astrophysicists from the UK, Germany, Canada and the USA, who are early users of the DEISA computing infrastructure. The Millennium Run utilised the principal supercomputer at the Max Planck Society's Supercomputing Centre in Garching, Germany for more than a month and the technical details were published in the June 2 issue of Nature.



The picture shows a projected density field for a 15 Mpc/h thick slice of the redshift z=0 output. The overlaid panels zoom in by factors of 4 in each case, enlarging the regions indicated by the white squares. Yardsticks are included as well. Copyright of the Virgo Consortium.

Computer simulations in nanotechnology and biology

Presentation by Prof. Michele PARRINELLO, ETH Zürich, Switzerland

Prof. Michele Parrinello from the Department of Chemistry and Applied Biosciences ETH, USI Campus, Lugano, Switzerland, first gave compelling reasons for the need for computer simulations in chemical, physical, and biological processes: simulations help to interpret experimental data, replace costly or impossible experiments - in short, they act like a virtual microscope. He then explained the widely-used classical molecular dynamics (MD) method and its shortcomings, e.g., it cannot describe chemical reactions and electronic properties. In contrast, quantum-mechanical (QM) ab initio methods overcome these shortcomings, they are without fitting-parameters, and they provide high accuracy and great predictive power, but they are computationally very demanding. Combining the best of both methods leads to ab initio MD (e.g., the program CPMD), which, for instance, allows viewing enzymes at work on an atomic scale.

Despite these improvements, challenges remain: bigger systems, longer simulated times, and better simulations. To overcome these limitations, a new program for computer simulations has been developed by Prof. Parrinello et. al.: CP2K (Car-Parrinello 2000: freely downloadable at http://cp2k.berlios.de). Amongst other improvements, it contains the new QUICKSTEP code, which augments CPMD's plane wave approach with a Gaussian basis set to speed up computations. For further speedup one has to overcome the O(N3) scaling (N denotes the number of electrons) of QM codes; Prof. Parrinello suggests using field theoretical methods and parallel computing to obtain a much more favorable O(N) scaling behavior.

While ab initio MD allows simulation times of up to 10ps, classical MD reaches time scales of approximately 10ns ± still far too short to investigate many interesting processes, e.g., protein folding, phase transitions, nucleation, etc., which happen on time scales of minutes or even hours.These macroscopic processes involve activated events, i.e., moving from one basin of the complicated free energy hypersurface into another. To speed up these transitions, Prof. Parrinello floods the energy valleys with small, artificial Gaussian potentials,

thus quickly driving the simulation out of local minima, into uncharted regions of configurational space. This can be further sped up by using several independent simulations, which chart different portions of the free energy hypersurface.

Prof. Parrinello illustrated his theoretical ideas with many beautiful examples, from DNA to enzymes, to liquid metallic silicon, and back to systems as common as freezing water. Simulation results have been substantiated through comparisons with experimental data and generally show a high degree of agreement.

Simulating confined high temperature plasmas

Presentation by Prof. Karl Lackner Max Planck Institut fur Plasmaphysic, Euratom Association, Garching, Germany

Prof. Karl Lackner from the Max Planck Institute for Plasma Physics in Garching, Germany, outlined the key importance of supercomputing simulations for the progress towards designing and preparing the building of fusion devices. He explained that magnetically confined high temperature plasmas, such as of interest for thermonuclear fusion are subject to temperature and density gradient-driven microturbulence, (potentially) macroscopic (MHD) instabilities, and instabilities driven by suprathermal particles, like produced by the nuclear reactions. A high degree of complexity is introduced since the magnetized plasma is highly anisotropic, for many applications a kinetic description in a 5-d phase space is required. The involved time and space scales cover a broad range, and can partly not be separated as the scale of turbulent eddies can approach the gradient length. Prof. Lackner described the main three state-of-the-art computational approaches used which presently are still separated areas:

1) Kinetic and fluid-type turbulence simulations, aiming at an understanding of the observed anomalous energy and particle transport),

2) Nonlinear magnetohydrodynamic stability calculations, determining the operating limits of devices, but also simulate the action of external feedback interventions

3) Interaction of the suprathermal particles with macroscopic instabilities which can lead to loss of a fraction of them out of the confinement system before they have transmitted their energy to the thermal plasma.

According to Prof Lackner, the ultimate goal is the „numerical tokamak or stellarator“, where microscopic turbulence simulations cover simultaneously the whole plasma region. Predictions of these and other models shall satisfy the necessary accuracy requirements making them useful for engineering type applications as the layout of experimental and commercial power plants.

The complete presentations are available at www.deisa.org/symposium

Predicting phase behavior and molecular organizations - some computational grand challenges from soft materials

Presentation by Prof. Claudio ZANNONI, Dipartimento di Chimica Fisica e Inorganica, Università di Bologna, Italy

Liquid Crystals (LC) are self organizing molecular systems of great importance in applied materials research for their unique combination of anisotropic dielectric, optical and mechanical properties and for their applications, e.g. in electro-optical displays and in nanodevices. From the point of view of basic research, LC assume the role of prototypes' in computational materials research for the development of multi-scale techniques ranging from molecular to macroscopic length-scales The discovery of new liquid crystals or more generally of new soft materials with specifically tailored functional features increasingly relies on establishing a link between molecular features and macroscopic properties. This does not just require calculating single molecule observables, but rather determining properties of the materials at various temperatures and working conditions. This implies that very demanding computer simulations are required, and in turn critically depends on the availability of massive computer resources.

In his presentation Prof. Zannoni showed some state of the art examples of problems emerging from the liquid crystal field involving simulations at different space resolutions, highlighting the problems and making some estimates of the resources required: In particular he discussed the prediction of transition temperatures for a nematic liquid crystal essentially from scratch, using atomistic simulations. He showed that this task judged impossible until a few years ago, is now starting to be feasible. He also examined the feasibility of simulating working devices, like displays, using molecular resolution models rather than continuum approaches.

Computational challenges in the extraction, prediction and organization of protein interaction networks

Presentation by Prof. Alfonso VALENCIA, Protein Design Group National Center for Biotechnology, CNB-CSIC and Instituto Nacional de Bioinformatica, INB Cantoblanco, Madrid E-28049, Spain

The fast introduction of High Throughput technologies in Molecular Biology has created new opportunities for the global analysis of cellular systems, which can now be described in terms of the relations between their basic components. The group of Prof. Valencia is interested in the study of these protein interaction networks derived from experimental and computational approaches, as well as in the extraction of the corresponding information directly from their textual repositories (information extraction technology). For reviews see (Pazos Valencia, Curr. Op. Struc. Biol. 2003, Hoffmann et al., Sciencie STKE 2005). With all this information very interesting progress has been made in the understanding of the general physical and biological properties of these networks in terms of hierarchical organization, clustering of functions and detection of functional modules. In his presentation Prof. Valencia illustrated the activity in this area, which brings together physics, computational and experimental biology with the work that his group in modelling biodegradation networks (Pazos et al., EMBO Repor. 2003).

The fundamental scientific problems posses by the study of molecular systems in terms of networks are intimately associated to the technical problems of organizing, computing and distributing all this information. At the national

level a network of bioinformatics labs ('Spanish bioinformatics institute' www.inab.org) has been organized, which in collaboration with the recently created 'Barcelona Supercomputing Center' www.bsc.org.es, has established methodologies related with web and database connectivity that will be able to handle the information generated by our genomics research community. This national effort is complementary to the ongoing European integration efforts in the context of development of computational methods for genome annotation (Biosapiens NoE, www.biosapiens.info) and adaptation of GRID resources for the work in genomics (the recently started EMBRACE NoE).

Frontier simulations for the climate of the 21st century

Presentation by Prof. Jean-Claude ANDRE, CERFACS, Toulouse, France

Anthropogenic climate change raises a number of societal and scientific questions. Even though there is no doubt that climate change is coming, it remains to quantitatively estimate its precise time-frame as well as the level of perturbations for the main parameters which control the habitability of the planet (temperature, precipitation, extreme events etc.). This requires simulating the complete "Earth System" on very fine spatial grids (ideally of the order of a kilometer), for durations of a few centuries, and with simulations repeated very many times in order to be able to estimate the probability of occurrence of each scenario. In the presentation examples of such frontier simulations were given, with corresponding requirements for computing systems (computers and networks).

Lattice quantum chromodynamics and the impact of supercomputing on theoretical particle physics

Presentation by Prof. Thomas LIPPERT, Forschungszentum Julich, Germany

In the last decade supercomputing has become an indispensable tool to simulate quantum chromodynamics (in short, QCD), the fundamental theory of strong interactions. The theoretical foundation and interpretation of future experiments in particle and nuclear physics will strongly rely on such simulations, using the world's fastest supercomputers. QCD is a theory that describes the forces between quarks as mediated by gluons. The theory is simulated on a discretized 4-dimensional space-time lattice using Monte Carlo algorithms.

Today, the grand challenge is to include the so called chiral quarks on the lattice that behave according to the fundamental chiral symmetry of nature. Within the next five years, lattice QCD physicists in Europe need at least a hundred sustained Teraflop/s dedicated supercomputing power in order to be competitive with US and Japanese groups.

The complete presentations are available at www.deisa.org/symposium