DEISA Symposium – May 9-10 2005

Palais des Congrès, Porte Maillot, PARIS, FRANCE

Perspectives in High Performance Computing

Program

Monday, May 9, 2005

Session 1. Chairman: Marco LANZARINI, CINECA, Italy

13:30 Opening of the Symposium
Marco LANZARINI

13:40 " Frontier simulations for the climate of the 21st century"
J.C. ANDRE

14:20 " Computer simulations in nano-technologies and biology",
Michele PARRINELLO

15:00 " Computational challenges in the extraction, prediction and organization of protein interaction networks"
Alfonso VALENCIA

15:40 " Simulating confined high temperature plasmas"
Karl LACKNER

16:20 Break

Session 2. Chairman: Hugh PILCHER-CLAYTON, EPSRC, UK

17:00 "Technology trends in high performance computing"
Michael LEVINE

17:40 "The future of high end and Grid computing"
Edward SEIDEL

18:20 "DEISA: towards cooperative extreme computing in Europe"
Victor ALESSANDRINI

19:00 Cocktail reception

Tuesday, May 10, 2005

Session 3. Chairman: Stefan HEINZEL, Max Planck Institute, Germany

9:00 "TeraGrid: successes and functionalities from a user's perspective"
Ralph ROSKIES

9:40 "Computing the Universe"
Carlos FRENK

10:20 Break

10:40 "Predicting phase behaviour and molecular organization: some computational challenges from soft materials"
Claudio ZANNONI

11:20 "Lattice Quantum Chromodynamics and the impact of supercomputing on theoretical particle physics"
Thomas LIPPERT

12:00 Closing the Symposium
Stefan HEINZEL

ABSTRACTS

Session 1: May 9, 2005 at 13:30 hs

FRONTIER SIMULATIONS FOR THE CLIMATE OF THE 21st CENTURY

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 …). This requires simulating the complete "Earth System" on very fine spatial grids (ideally of the order of a kilometre), 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. Examples will be given of such frontier simulations, with corresponding requirements for computing systems (computers and networks).

COMPUTER SIMULATIONS IN NANOTECHNOLOGY AND BIOLOGY

Michele PARRINELLO

We shall briefly review the scope and role of molecular dynamics simulations in nanosciences and biology. We shall underline present limitations and outline our strategy overcome them. We shall show that due to recent progress a number of previously insoluble problems can be tackled. A number of examples from nanotechnology and biology will be presented.

COMPUTATIONAL CHALLENGES IN THE EXTRACTION, PREDICTION AND ORGANIZATION OF PROTEIN INTERACTION NETWORKS

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. My group 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 this networks in terms of hierarchical organization, clustering of functions and detection of functional modules. I will illustrate the activity in this area, which brings together physics, computational and experimental biology with the work that my 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 we have organized a network of bioinformatics labs ('Spanish bioinformatics institute' www.inab.org) that, 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).

SIMULATING CONFINED HIGH TEMPERATURE PLASMAS
Karl Lackner
Max Planck Institut fur Plasmaphysic, Euratom Association, Garching, Germany

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. The magnetized plasma is highly anisotropic, and requires for many applications a kinetic description in a 5-d phase space. 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.

We describe the state of art in the presently still separated areas of (1) kinetic and fluid-type turbulence simulations (aiming at an understanding of the observed anomalous energy and particle transport), (2) the nonlinear magnetohydrodynamic stability calculations (determining the operating limits of devices, but also simulate the action of external feedback interventions) and (3) the 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). Ultimate goal is the "numerical tokamak or stellarator", where microscopic turbulence simulations cover simultaneously the whole plasma region, and where the predictions of these and other models satisfy accuracy requirements making them useful for engineering type applications (layout of experimental and commercial power plants).

Session 2: May 9, 2005 at 17:00 hs

THE FUTURE OF HIGH END AND GRID COMPUTING
Edward SEIDEL
Center for Computation and Technology, Louisiana State University, USA

As the complexity and computational demands of scientific and engineering applications continue to increase, and as explosions of data overwhelm our ability to store, move, manage, and analyze it, computing, network, grid, and collaborative technologies are rapidly evolving to support new applications. I will give an overview of current and future trends in high end computing and cyberinfrastructure tools for these applications. I will also describe programs emerging in the USA from various federal and state agencies, and review recent recommendations made by the US Presidential Information Technology Advisory Committee (PITAC) and others on what is needed to support next generation computational sciences.

DEISA: TOWARDS COOPERATIVE EXTREME COMPUTING IN EUROPE
Victor ALESSANDRINI
IDRIS, CNRS, France

The purpose of DEISA research infrastructure is to contribute to enable Europe's terascale science by the integration of Europe's most powerful supercomputing resources. After a short introduction on the project strategies and the current status of the infrastructure, we will discuss the ongoing actions and initiatives that are directly focused on the support to leading, ground breaking computational science.

Session 3: May 10, 2005 at 9:00 hs

TERAGRID: SUCCESSES AND FUNCTIONALITIES FROM A USER'S PERPECTIVE
Ralph ROSKIES, Scientific Director, Pittsburgh Supercomputing Center

We will begin by briefly describing the TeraGrid, its partners, resources and goals. Then we will give several examples of scientific successes that the TeraGrid has enabled, describing which features of the Teragrid played a role in these successes. We will conclude by outlining, from the user's perspective, which functionalities currently exist and which we are working to implement.

COMPUTING THE UNIVERSE
Carlos Frenk
Institute for Computational Cosmology, Physics Department, Durham University, UK

There have been enormous advances in recent years in understanding the origin and evolution of the cosmic large scale structure. New data have pinned down the ``initial conditions'' for structure growth: small density irregularities imprinted very soon after the Big Bang. Galaxies are strongly non-linear objects and, as a result, calculating their formation paths and present-day properties requires direct simulation, starting from these initial conditions and including processes associated with dark matter and gas. I will review recent progress in calculating the evolution of galaxies and the cosmic large-scale structure.

PREDICTING PHASE BEHAVIOR AND MOLECULAR ORGANIZATIONS. SOME COMPUTATIONAL GRAND CHALLENGES FROM SOFT MATERIALS
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 the talk we shall show 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 we shall discuss the prediction of transition temperatures for a nematic liquid crystal essentially from scratch, using atomistic simulations. We shall show that this task judged impossible until a few years ago, is now starting to be feasible.We shall also examine the feasibility of simulating working devices, like displays, using molecular resolution models rather than continuum approaches.

LATTICE QUANTUM CHROMODYNAMICS AND THE IMPACT OF SUPERCOMPUTING ON THEORETICAL PARTICLE PHYSICS

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 q 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.

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THE SPEAKERS

ALESSANDRINI, Victor

Born in Argentina. PhD in Theoretical Physics from University of La Plata, Argentina. Visiting Scientist at Lawrence Radiation Laboratory, Berkeley, USA and CERN Theory Division in the late 60's and early 70's. Professor of Theoretical Physics at the University of Paris from 1976 until 2002. Research Director at CNRS since 2002. Director if IDRIS supercomputing centre since 1993. Coordinator and acting director of the DEISA Research Infrastructure Project.
Scientific interests: quantum field theory and statistical mechanics; numerical parallel algorithms and advanced computer simulation techniques.

ANDRE, Jean-Claude

Director of CERFACS, European Centre for Research and Advanced Training in Scientific Computing (since 1995). Formerly Head of Research at Météo-France
Corresponding Member of the French Academy of Sciences.
Member of the French Academy of Technology.
Research themes: Theory of turbulence, numerical modelling of the atmospheric boundary layer and of the upper ocean, climate modelling.

FRENK, Carlos

Carlos Frenk is the Ogden Professor of Fundamental Physics and Director of the Institute of Computational Cosmology at Durham University. He has contributed to the development of the ``Cold dark matter'' theory of cosmogony since its inception in the early 1980s and has helped pioneer the use of computer simulations in cosmology. He has written over 200 scientific papers and is one of the most cited authors in Space Sciences. He was elected a Fellow of the Royal Society in 2004.

LACKNER, Karl

Karl Lackner holds a Ph.D. obtained in 1966 at the University of Innsbruck, and is currently co-Director of the Divition of Tokamak Physics at the Max Planck Institute for Plasma Physics (IPP). He has a long carrier in the area of Plasma Physics. In 2002 he was Leader of the European Fusion Development Agreement (EFDA) (on leave of absence from IPP), with overall responsibility for EU ITER contributions, JET, and the EU Technology Programme. Member of several evaluation boards and standing advisory committees of US and European Experiments and Institutions.

Scientific interests: since 1966: computational plasma physics (initially plasma accelerators, later space physics, since 1972 fusion oriented, including for a brief period also inertial fusion); plasma equilibria and macroscopic stability, plasma physics of the plasma –boundary interaction zone („also called divertor physics"). Since 1978 leading a (continuously growing) team of theoreticians working on all sub-topics of high-temperature plasma physics (turbulent transport, MHD stability, plasma heating, plasma boundary physics), including involvement in design of experiments.

LIPPERT, Thomas

Prof. Dr. Dr. Thomas Lippert received his diploma in Theoretical Particle Physics in 1987 from the University of Würzburg. He completed Ph.D.theses at Wuppertal University on simulations of lattice quantum chromodynamics and at Groningen University in the field of parallel computing with systolic algorithms. He is director of the Central Institute for Applied Mathematics at the Research Centre Juelich, member of the board of directors of the German national supercomputing centre John von Neumann Institute for Computing (NIC), and he holds the chair for Computational Theoretical Physics at the University of Wuppertal. His research interests include lattice gauge theories, quantum computing, numerical and parallel algorithms, and cluster computing.

PARRINELLO, Michele

Michele Parrinello is Professor in Computational Science at ETH Zürich. Together with Roberto Car he has introduced the ab-initio molecular dynamics method, which he is still developing and applying. His scientific interests include the study of complex chemical reactions, hydrogen bonded systems, catalysis and materials science in particular systems under pressure. He is also known for the Parrinello-Rahman method of molecular dynamics which allows the study of crystalline phase transitions under constant pressure. Prior to moving to Lugano in 2003, he was Director at the CSCS Manno, Director at the Max-Planck-Institute for Solid State Research in Stuttgart and he was at the IBM Zurich Research Laboratory. He also was full professor at SISSA, Trieste, Italy.
Born in Messina, Italy, he obtained his degree in physics in 1968 from Bologna, Italy. For his research he has been awarded numerous prizes. He is member of several academies, among which The Royal Society.

ROSKIES, Ralph

Roskies is Professor of Physics at the University of Pittsburgh and a founder and Co-Scientific Director of the Pittsburgh Supercomputing Center (PSC). He is the author of over 60 papers in theoretical elementary particle physics. As PSC Scientific Director, Roskies oversees operations, plans its future course, and concerns himself with its scientific impact. He maintains close ties to leading computational scientists in the US. He has served as advisor to and as reviewer of a large number of U.S. and international supercomputing centers. The PSC has been a national leader in providing the highest capability computing to the US national research community. It has pioneered developments in file systems, heterogeneous computing, parallel algorithms and scientific visualization.

SEIDEL, Edward

Edward Seidel is a physicist recognized worldwide for his work on numerical relativity, black holes, and high-performance computing. He earned his Ph.D. from Yale University in 1988. Seidel worked at the University of Illinois and led the National Center for Supercomputing Applications Numerical Relativity group for a number of years. He was a professor at the Max-Planck-Institut fuer Gravitationsphysik (Albert-Einstein-Institute) in Golm, Germany from 1996 - 2003. Seidel is currently serving as the director of the Center for Computation & Technology at Louisiana State University and Floating Point Systems Professor of Physics and Computer Science.

VALENCIA, Alfonso

Alfonso Valencia obtained his PhD in Biochemistry at U. Autónoma Madrid. He was post-doctoral fellow at American Red Cross, Bethesda and EMBL-Heidelberg (Chris Sander's Group, 1988-1994). He is currently Research Professor at the Spanish Research Council (CSIC), Group leader of the Protein Design Group, Director of the National Institute for Bioinformatics, INB, and Senior scientist of the Centre for Astrobiology (CAB-INTA-CSIC).

His main scientific interest is associated to the use of genomics and proteomics for the study of molecular evolution and for the development of new biotechnological resources, what requires the development of Bioinformatics and Computational Biology methods. His group has contributed to the development of various bioinformatics systems, and collaborates actively with experimental biologists in the study of different molecular systems, such as Chemokine receptors, bacterial cell division proteins, and small GTPases. The scientific activity of his group includes the analysis and comparison of genomes, prediction of protein structure and function, analysis of protein interactions, and more recently the extraction of information from scientific text.

ZANNONI, Claudio

Claudio Zannoni graduated in Chemistry at the University of Bologna, IT, in 1972 and obtained his PhD in Chemical Physics from the University of Southampton, UK. In 1975 he returned to Bologna, where he is now Full Professor of Physical Chemistry (from 1987) and Head of Department (from 2004).
His current research interests include Modelling and Computer Simulations and the use of Fluorescence Depolarization, ESR, NMR, to investigate bulk and nanoconfined Liquid Crystals. He is an author of over 170 papers and has given more than 150 invited lectures on these topics.

He is at present director of the Theory and Modelling section of INSTM, the Italian National Consortium for Science and Technology of Materials and sits on its Scientific Board.
He is or has been on the Editorial Board of various Journals, including *Chem. Society Reviews* (UK), *ChemPhysChem* (DE), *Mol. Cryst. Liq. Cryst.* (USA), *Liquid Crystals* (UK), *Molec. Physics* (UK), *PCCP* (UK), *J. Fluorescence* (USA).
He is director of the International School of Liquid Crystals, Erice, IT, since 1998.
A list of publications and activities can be found at the web page http://www.fci.unibo.it/~bebo/z/index.html .