Distributed European Infrastructure for Supercomputing Applications

DEISA SYMPOSIUM

PERSPECTIVES ON HIGH PERFORMANCE COMPUTING

on 4 – 5 May 2006 in Palazzo Re Enzo, Bologna, Italy

PROGRAM

Thursday, May 4

Session 1, Chairman: Claudio ZANNONI, UNIBO, Italy

13.30 Welcome by CINECA
DEISA Perspectives, Victor ALESSANDRINI
14.00 Chasing the Flames: The Challenge of Modeling Thermonuclear Supernova in 3D, Wolfgang HILLEBRANDT
14.40 End-to-end simulations of the Planck-LFI space mission, Fabio PASIAN
15.20 Computing wall turbulence at experimental Reynolds Numbers, Sergio HOYAS
16.00 Break

Session 2, Chairman: Axel BERG, SARA, the Netherlands

16.30 Large scale computation for materials and life sciences using DEISA, Peter COVENEY
17.10 The Quest for Solving QCD: Light Quarks with Twisted Mass Fermions, Karl JANSEN
17.50 Use of ensemble climate simulations to detect variations in extreme event statistics, Henk A. DIJKSTRA
18.30 End of the day
19.00 Cocktail reception

Friday, May 5

Session 3, Chairman: Hugh PILCHER-CLAYTON, EPSRC, the United Kingdom

9.00 EU e-Infrasructure plans for FP7 – The discussion on a new European Supercomputing policy, Kyriakos BAXEVANIDIS
9.35 EGEE – A Large-Scale Production Grid Infrastructure, Neil GEDDES
10.10 NASA Supercomputing: Impact on Present and Future NASA Missions, Walt BROOKS
10.45 Break

Session 4, Chairman: Mario LANZARINI, CINECA, Italy

11.00 Cray XT3 on the US TeraGrid, Michael LEVINE
11.45 JuBL - Blue Gene/L System – in Jülich, Klaus WOLKERSDORFER
12.20 Closing
13.00 Lunch

Abstracts

Chasing the Flames: The Challenge of Modeling Thermonuclear Supernovae in 3D

W. HILLEBRANDT
MPI für Astrophysik, Garching, Germany)

We present, compare and discuss results of three-dimensional hydrodynamic simulations of the thermonuclear burning phase in (Type Ia) supernova explosions performed on IBM Regatta system at the Rechenzentrum Garching and the HPCx at the Edinburgh Parallel Computing Centre. Our emphasis is on the validation of the underlying numerical model, i.e., large-eddy simulations (LES) of the turbulent flows and a level-set description of the flame front, as well as on the investigation of the influence of the initial conditions, such as the flame geometry inside the white dwarf star at the onset of the thermonuclear explosion, and its density and chemical composition on the outcome of the simulations. Moreover we investigate whether the obtained results of such 'parameter-free' models are in agreement or in conflict with observational constraints, such as the amount of radioactive nickel produced and explosion energy. We find that our models predict most properties within their observed ranges, provided resolution of the numerical simulations is sufficiently high to justify the LES approach.

End-to-end simulation of the Planck-LFI mission

Fabio PASIAN
INAF Information Systems Unit and Osservatorio Astronomico, Trieste, Italy

Planck is the third generation space mission for the mapping and the analysis of the microwave sky: its unprecedented combination of sky and frequency coverage, accuracy, stability and sensitivity is designed to achieve the most efficient detection of the Cosmic Microwave Background (CMB) in both temperature and polarisation. In order to achieve the ambitious goals of the mission, unanimously acknowledged by the scientific community to be of the highest importance, data processing of extreme accuracy is needed.

The supercomputing framework provided by DEISA is being used to simulate several times the whole mission of Planck's LFI instrument, on the basis of different scientific and instrumental hypotheses, and to reduce, calibrate and analyse the simulated data down to the production of the final products of the mission, in order to evaluate the impact of possible LFI instrumental effects on the quality of the scientific results, and consequently to refine appropriately the data processing algorithms.

Computing wall turbulence at experimental Reynolds numbers

Sergio HOYAS
Computational Fluid Dynamics Laboratory, Universidad Politécnica de Madrid, School of Aeronautics, Madrid

Using direct numerical simulation (DNS) of turbulent channels at higher Reynolds number (Re_τ=2000) and in larger computational domains than those available up to now, we study the dynamics of the turbulent logarithmic layer, and the interaction between the large scales of wall turbulence away from the wall, and the small scales near it.

The problem is not just of scientific interest. Wall-bounded turbulence is the interface between the ambient fluid, water or air, and moving vehicles, and between flows and pipes and channels. The large scales, for example, play an important role in the dispersion of chemical agents in the atmosphere, and more than half of the friction drag in vehicles resides in the near-wall and intermediate layers. The hopes of controlling and alleviating all these phenomena pass through the understanding of their dynamics.

The main objective of the simulation was to run enough time to get statistically converged properties of the flow. From previous experience this requires about 10 washouts (250 h/U in the present case, where h is the channel half-thickness and U the centreline velocity). This was a very costly initiative. It ran for about 6.000.000 CPU-Hours on 2048 processors during the pre-production phase of the MareNostrum supercomputer at the Barcelona Supercomputing Center. We obtain also 800.000 CPU-Hours, needed for run two washouts more and complete our study, assigned through a DEISA project.

The Quest for Solving QCD: Light Quarks with Twisted Mass Fermions

Karl JANSEN
John von Neumann-Institute for Computing, Zeuthen

The strong interactions of elementary particles are described theoretically in the framework of Quantum Chromodynamics (QCD). The solution of QCD is an outstanding problem in modern particle physics. The most promising way is given by numerical simulations using Monte Carlo Methods, in which the space-time continuum is replaced by a lattice. We shall demonstrate that since the invention of this approach by K. Wilson the conceptual, algorithmic and computer developments have progressed so much that today realistic simulations of lattice-QCD become possible, bringing us close to a, at least, numerical solution of QCD.

Ensemble Simulations of Extreme Weather Events

Henk A. DIJKSTRA
Department of Physics and Astronomy, Utrecht University, The Netherlands

It is still very poorly known how extremes in precipitation and temperature over Europe will change under a warmer future climate. To analyse changes in extreme event statistics, we are performing large-member ensemble simulations with state-of-the-art climate models. An integration interval of 140 year (1940–2080) is chosen in each of these simulations. Up to the year 2000, observed forcing fields are specified and after the year 2000, one of the Intergovernmental Panel on Climate Change (IPCC) emission scenarios for greenhouse gases (the SRES A1B scenario) is used. Currently, the ESSENCE (Ensemble SimulationS of Extreme weather events under Nonlinear Climate changE) project is carried out on the NEC-SX8 at HLRS (Stuttgart) within the DEISA-DECI initiative. I plan to present first results of the analysis of these simulations (if available at the time of the workshop), and will focus on the changes in specific extreme events and the changes in the behavior of the North Atlantic Oscillation (associated with the strength of the mid latitude jetstream) and El Nino. Results will also be compared with those of an earlier large-member ensemble simulation project which was carried out in 2003. The data sets of these ensemble simulations are unique sources of information for many climate researchers.

EU e-Infrasructure plans for FP7 – The discussion on a new European Supercomputing policy

Kyriakos BAXEVANIDIS
European Commission

Recent advances in Europe in the area of grid-based e-Infrastructures resulted in the creation of world class, production quality, and pan-European coverage research infrastructures, notably DEISA (in the area of supercomputing) and EGEE (in the area of cluster-computing). It is highlighted that both DEISA and EGEE are strongly driven by the needs and the deployment efforts of important scientific user-communities. The above developments reflect relevant political level commitments by the EU Member States and the European Commission as the area of ICT-infrastructures is considered key for the European economy.

It is this important role of ICT that calls for the continuous upgrade and advancement of the e-Infrastructures in a way that these infrastructures continuously provide, on the one hand, the best service – on a world scale – to the European

researchers and that these represent, on the other, investments of maximum efficiency for the funding agencies.

Pertinent discussions in the context of the preparations of the 7th European Research Framework (FP7) point strongly to the need for Europe to enhance its efforts on continuously advancing its e-Infrastructures and to include a new supercomputing policy and activity as a central part of its FP7 e-Infrastructure plans. The current position of the e-Infrastructures, the status of the preparations for FP7, and the developments around a new European supercomputing policy are discussed in this presentation.

EGEE – A Large-Scale Production Grid Infrastructure

Neil GEDDES
EGEE project

EGEE is a pan European project to deploy and operate a production grid infrastructure in support of science. The project began in April 2004 and has now just entered a second phase which will run through to 2008. I will give a brief overview of the EGEE project, covering the project history, current status and future plans. I will focus on the operational aspects of the pan European Grid infrastructure deployed by EGEE and the applications which currently make use of this infrastructure. To conclude I will summarise current developments towards a sustainable European Grid infrastructure beyond EGEE.

Walter Brooks
NASA, NAS Division

In November of 2004 NASA deployed an SGI Altix system, named Columbia that has ranked in the top four computers in the world over the last 18 months. This talk will summarize the impact on NASA science and engineering as well as the changes that have occurred in NASA's use of this computer. As with all large computers 18 months into a systems life the team is already considering the follow on systems. In addition the challenges of keeping the system in balance from a storage and networking standpoint will be discussed. Finally recent work in NASA astrophysics will be used as an example of the impact these large systems are having on science and engineering.

Cray XT3 on the US TeraGrid

Michael LEVINE
Pittsburgh Supercomputing Center

Cray XT3/Red Storm massively parallel computer systems are now in production at a large number of sites being used for a wide range of scientifically and technically important applications. The largest of these systems is growing beyond 10,000 nodes and plans exist for more and larger systems of this design. The roadmap for XT3 and successor systems extends well into the petaflops domain. We will summarize the XT3 system design and review its successful production deployment at the Pittsburgh Supercomputing Center as part of the US/NSF TeraGrid including application range, performance and scaling.

JuBL – Blue Gene/L System – in Jülich

K. WOLKERSDORFER
Forschungzentrum Jülich

In summer 2005, JuBL (Juelich Blue Gene/L), an IBM Blue Gene system, was installed at the Research Center Juelich (FZJ) as the first of its kind in Germany. The system is suited for high scaling applications and has major advantages regarding power comsumption, footprint and price/performance ratio. As the first results of the applications were very promising, FZJ decided to extend the configuration to 16384 processors. This system was installed in January 2006 and reached a peak performance of 46 TeraFlop/s. In the presentation the architecture of the system is described as well as first experiences administrating the system. Also some performance results of selected applications will be presented.

Speakers

BAXEVANIDIS, Kyriakos

Kyriakos Baxevanidis is the Deputy Head of the Research Infrastructures Unit, DG INFSO of the European Commission. The Unit supports the provision of computer and communications infrastructures of the highest quality and performance to Europe's researchers, namely by establishing a high-capacity and high-speed communications network for all researchers in Europe (GÉANT) and specific high performance Grid-enabled advanced infrastructures (e.g. EGEE and DEISA), exploiting the benefits of a strong co-ordination between the Research Infrastructures and the Information Society Technologies (IST) Programmes of the Commission, and an enlarged co-operation with corresponding national and international initiatives. Mr. Baxevanidis has particular involvement in the Grid related efforts of the Unit and in the shaping, implementation and further evolution of the EU e-Infrastructure concept. He previously served in the areas of Services Engineering, Communications Management and Security of IST and of previous EU-RTD programmes. Before joining the Commission, he worked for several years in Siemens in the field of telecommunication systems as an engineer and leader of a development group.

He holds degrees from the Aristotle University of Greece and from Carnegie-Mellon University, US.

BROOKS, Walter

As chief of the NASA Advanced Supercomputing (NAS) Division, Walt Brooks oversees the entire gamut of high performance computing work done within the division, and is working to transform the vision, mission, and direction for NAS.

His focus on building collaborative relationships with other NASA groups, industry partners, and colleagues at universities and other government agencies reflects his dedication to making NAS a national resource for expertise in distributed heterogeneous computing. Brooks' history at NASA Ames began in 1977. During his early career he led groups that simulated and designed space science missions such as Infrared Astronomical Satellite (IRAS), Space InfraRed Astronomy (SOFIA). In 1993 he was selected to lead the Space Station redesign management team. He served as both Assistant Director of Aerophysics for Ames and Chief of the Information Systems Programs and Projects Division before becoming acting NAS Division Chief in summer 1995. Brooks later worked as senior scientist for the Research Institute for Advanced Computer Science Center (RIACS), where he represented Ames in NASA's Earth Science technology Enterprise at Goddard Space Flight Center. In this role, he developed strategy roadmaps for developing advanced information systems technology. Brooks received a doctorate in physics from Stevens Institute of Technology, performing research for his thesis at Brookhaven National Laboratory. He earned a master's degree from the Stanford Graduate School of Business in 1991.

DIJKSTRA, Henk A.

Henk A. Dijkstra is Full Professor for Physical Oceanography at the Institute of Marine and Atmospheric research Utrecht (IMAU) at the Department of Physics and Astronomy of Utrecht University, the Netherlands. After graduating in applied mathematics at the University of Groningen in 1984, he worked on his Ph.D. in Groningen on a Spacelab experiment and on Marangoni convection under microgravity conditions. He continued this research in chemical engineering at Cornell University. In 1990 he started working on physical oceanography at Utrecht University. His main research interests are in the stability of ocean currents and physics of low-frequency variability of the climate system. He became member of the Royal Dutch Academy of Sciences and Arts in 2002 and was awarded the Lewis Fry Richardson Medal from the European Geosciences Union in 2005. He has published over 100 scientific papers and the book "Nonlinear Physical Oceanography" (Springer, 2e edition in 2005).

HILLEBRANDT, Wolfgang

Born on 25th February, 1944, in Rerik (Mecklenburg). Study of physics and mathematics, doctorate Cologne Univ. (1973), habilitation in physics Darmstadt Technical Univ. (1977), Scientific Member at the Institute for Astrophysics in the Max Planck Institute for Physics and Astrophysics (since 1985), "Honorar professor" (part-time prof.) Munich Technical Univ. (1990), Director and Scientific Member at the Max Planck Institute for Astrophysics since 1997). Research Fields: Theoretical astrophysics, Nuclear and particle astrophysics, Stellar structure and evolution, Computational fluid dynamics

HOYAS, Sergio

Sergio Hoyas hold a Juan de La Cierva postdoctoral fellowship at the Computational Fluid Dynamics Laboratory, Universidad Politécnica de Madrid, School of Aeronautics, Madrid. He received his doctoral degree in applied mathematics in 2003 at Universidad Complutense de Madrid.

LEVINE, Michael

Michael Levine is Professor of Physics at Carnegie Mellon University, specializing in theoretical particle physics. He is also a founder and Co-Scientific Director of the Pittsburgh Supercomputing Center (PSC). He is the author of numerous papers in computational, theoretical, and particle physics. His physics research over the last few years has been in high order quantum electrodynamics. His earlier work in Physics includes a series of papers applying symbolic computation methods and computational systems devised by him, to fundamental problems in electrodynamics done in collaboration with Professor Ralph Roskies. Professor Levine initiated Carnegie Mellon's degree program in Computational Physics and continues to teach courses in that program. In 1984, together with Ralph Roskies and James Kasdorf of Westinghouse Electric Company, he wrote the proposal to the National Science Foundation for what was eventually to become the PSC. As Scientific Director at PSC, he continues to oversee operations, plan its future course, and concern himself with its scientific impact. He also serves as the Associate Provost for Scientific Computing for Carnegie Mellon University.

JANSEN, Karl

Karl Jansen is the leader of the research group Particle Physics at the John von Neumann Institute of Computing hosted by DESY, Zeuthen. He worked on various aspects in the field of Lattice Gauge Theory ranging from algorithms and spin models to high performance simulations of Quantum Chromodynamics. He is heading a large European collaboration as well as the association of German Lattice Physicists. He has been a member of several international evaluation boards. Recently he became chair of an international lattice data grid network.

WOLKERSDORFER, Klaus

Klaus Wolkersdorfer is head of the High-Performance-Systems (HPS) division of the Central Institute of Applied Mathematics (ZAM) within the Research Center Jülich (FZJ). He is responsible for integrating the wide range of FZJ's supercomputers into a production environment. Among them are currently JuBL (Blue Gene/L with 46 TeraFlops Peak Performance) and JUMP (p690+ Cluster with 9 TF). Through the John von Neumann Institute for Computing (NIC) Jülich provides HPC resources to Europe-wide community of researchers. Prior to his current position Klaus led several projects dealing with large computer systems. His research areas are performance optimisation and tuning of large systems. He obtained a masters degree of mathematics and computer science at the University of Erlangen and worked on structured programming and programming languages. He participated in IBM's World Trade Postdoctoral Program for one year at the IBM Thomas J. Watson Research Center from where he moved to the operating system division in ZAM (which he is now leading).