

## **Abstracts**

### ***Paolo Malfetti and Hermann Lederer***

#### ***DEISA Overview***

The talk gives a DEISA overview from the technical perspective, discussing

- what is DEISA (its objectives and services),
- how much DEISA can be considered mature,
- the technologies used by DEISA and
- their integrated vision.

The talk then gives an overview of the user, project and application related aspects of DEISA. The role and achievements of the scientific Joint Research Activities for early adopters of the distributed HPC infrastructure are shown. Details of the DEISA Extreme Computing Initiative DECI are presented, together with its support through the Applications Task Force of leading European experts in high performance and distributed computing. The pioneering work of DEISA for an integrated European HPC infrastructure is outlined, and an outlook is given.

### ***Thomas Eickermann***

#### ***PRACE Overview***

Supercomputers are indispensable tools to solve the most challenging problems through simulations. To remain internationally competitive, European scientists and engineers must be provided access to leadership class supercomputers systems. PRACE, the Partnership for Advanced Computing in Europe, has been founded in April 2007 with the goal to create a persistent pan-European HPC service and infrastructure, provided by several tier-0 HPC centres. PRACE will enter close collaborations with national and regional HPC centres, scientific user groups and the European IT industry to advance and shape the European HPC ecosystem.

In the framework of a two year project funded by the European Commission, PRACE prepares for the implementation of the infrastructure in 2009/2010 by defining and setting up a legal and organisational structure involving all stakeholders to ensure adequate funding, coordinated procurements, efficient use, and fair access.

In parallel, PRACE will prepare the deployment of Petaflop/s systems in 2009/2010. Prototype systems will be procured and evaluated, scientific libraries and codes from major scientific user communities will be ported and scaled to the Petaflop/s range. A permanent process of technology evaluation for future

Multi-Petaflop/s systems will be initiated. The development of new technologies and components will be influenced through collaborations with the European IT-industry.

The presentation gives an overview over the goals and current status of the project.

## ***Marian Garcia Vidondo***

### ***GEANT2: Networking Services for the Research Community***

GEANT2 is an advance Pan-European network that collaborates with all of the European National Research Networks to deliver state-of-the-art networking services to thousands of research and education establishments across Europe.

The GEANT2 consortium delivers a wide variety of network services for demanding applications such as grid supercomputers and radio telescope infrastructures. These services include the advanced IP services, wavelength solutions and multi domain monitoring services.

## ***Alistair Dunlop***

### ***OMII-Europe - Enabling Grid Interoperability***

Abstract: OMII-Europe is an EU funded project that has championed, developed and implemented standards for grid middleware over the past 2 years to further the goal of creating a federated architecture of heterogeneous grid systems. The project has made advances in unifying security for different grid middleware systems and has produced a number of key, standards-compliant services for the major grid middleware distributions enabling users to seamlessly work across multiple resource infrastructures even if they employ different grid middleware. This talk will present results from this project and describe how these outputs are facilitating new scientific research.

## ***Ed Seidel***

### ***Petascale Computing Initiatives and Issues***

Petascale computing is upon us, with numerous initiatives around the world poised to deploy machines exceeding 1PF sustained performance in a few short years. I will review the promise of these efforts, as well as the challenges facing the community, focusing on programs in the US that are already underway.

**Alasdair R. Kellie**

## **NCAR & Climate Plans**

NCAR is a National Science Foundation (NSF) Federally Funded Research and Development Center (FFRDC) and plays a key strategic role in serving as a “commons” for atmospheric and related sciences. NCAR was founded in 1960 and plays a critical role in providing high-end computing facilities, leadership in developing community models, and data curation and stewardship for the research community.

This talk will provide a glimpse of NCAR and the reach of its computational facilities and look at some of the elements that NCAR plans for the next round of IPCC (AR5) simulations what are some of the challenges or research tasks for longer-term next generation Climate Models or Earth System Models.

Many individuals across NCAR have provided input to this talk, including Peter Gent, chair of the Scientific steering Committee of CCSM, Gerald Meehl, Senior Scientist at NCAR, Rich Loft Director of Technology development CISL, Marianna Vertenstein chair of the CCSM Software Engineering group

**Xavier Daura**

## **Simulation of Protein Dynamics in Vaccine Research**

High throughput cloning and expression of large sets of genomic ORFs has become a preferred industrial strategy for genome-wide searches of new vaccine candidates. For invasive infections in particular, the aim is to find proteins eliciting antibodies capable of binding to the bacterial cell surface and, through interaction with the complement system, effectively kill the bacteria. However, current data accumulating from reverse vaccinology studies (targeting of possible vaccine candidates starting from genomic information) shows that only a small fraction of surface-exposed proteins appears to elicit antibodies with bactericidal activity. Our group is coordinating a project (BacAbs[1]) which is attempting the implementation of a multidisciplinary approach for the discovery of structural requirements for viable (bactericidal) vaccine candidates and developing bioinformatics tools to predict compliance with such requirements. To this end, a systematic analysis of sequence, structure, dynamics and interactions of selected protein targets is undertaken using model systems such as serogroup-B *Neisseria meningitidis*, a pathogen causing septicemia and meningitis for which no effective vaccine exists. In my talk, I will present the BacAbs project and discuss the analysis of antigen and epitope dynamics, probed by molecular-dynamics simulation and enabled by DEISA.

[1] Project supported by funding under the Sixth Research Framework Programme of the European Union (<http://www.bacabs.org>)

***Karsten Reuter***

### ***Molecular Switches at Metal Surfaces***

In view of the rapidly advancing miniaturization in microelectronics and sensing, molecules are envisioned as fundamental building blocks in a future “molecular nanotechnology”. Since controlled switching between defined states is a crucial basis component for storage and logic, molecules offering this functionality (e.g. through externally stimulated changes between conformational isomers) attain a central importance. Considering contacting and defined integration into a larger framework, it is more precisely the molecular function when the molecule is stabilized at a solid surface that is of key interest. Within this context, the large-scale density-functional theory calculations enabled by this DEISA project have provided unprecedented atomic-scale insight into the structural and electronic properties of the prototypical molecular switch azobenzene adsorbed at coinage metal surfaces. Particularly for copper, the computations reveal an interaction that is far more complex than the anticipated weak physisorption, with the final bonding resulting from quite different interactions of different molecular moieties with the solid surface. The trend understanding emerging from the study of Cu, Ag and Au surfaces clearly identifies Ag as a preferred system where a controlled reversible switching should be possible.

***Jukka A. Heikkinen***

### ***Plasma turbulence and flows at conditions of transport transients***

Transport barriers appear to be necessary in enhancing plasma performance in magnetized fusion. Simulation of development of such barriers is challenging and is presently considered by first principles within gyrokinetic plasma theory using both continuum and particle methods. Both of these methods require significant HPC resources in practical applications.

Particle simulation methods are discussed in the context of resolving sheared poloidal flows in the turbulent tokamak plasmas. Reynolds stress and neoclassical effects are considered and analysed for experimental small and medium sized configurations. A so called full  $f$  gyrokinetic simulation method is described and it is shown how both neoclassical and turbulent mechanisms in sheared flow generation and related turbulence suppression can be studied with this scheme.

**Lucas Visscher,**

### ***Simulating the Photodissociation of Tri-iodide***

The triiodide ion ( $I_3^-$ ) has a very interesting electronic structure by being one of the few closed-shell negative ions that has excited electronic states below its electron detachment threshold. This feature leads to a complex photodissociation process that is still not fully understood due to the many different pathways that need to be considered. This makes  $I_3^-$  an ideal benchmark system for studies of reaction dynamics with ultrashort laser pulses. The TRIPOD project aims at developing a fully theoretical counterpart to such experimental studies by providing a complementary picture of this complicated reaction.

This is possible by performing wavepacket simulations on an accurate set of potential surfaces that describe both the region around the equilibrium structure for the ground state and the dissociation limits for all states of interest. With the facilities provided within the DEISA environment we were able to construct a high quality map of the surfaces including spin-orbit coupling, scalar relativistic and electronic correlation effects. This map can be used in future theoretical work on this benchmark reaction.

**Sascha Husa,**

### ***Gravitational Wave Signals from Black Hole Coalescence***

The last three years have seen a phase transition in the field of numerical relativity, where the Einstein equations are solved numerically in order to study phenomena such as the collision of black holes and neutron stars, and the gravitational wave signals emitted in such violent astrophysical events.

This talk reviews the motivation for research on the numerical modeling of black hole collisions as part of a large international effort to detect gravitational waves and establish a new field of research "gravitational wave astronomy", summarizes the status of the field and the computational techniques and requirements, and highlights some recent astrophysical results.

**Stefano Corni,**

### ***Protein-Surface-Interactions mediated by Water***

Recent combinatorial biotechnologies have shown that the molecular recognition capability of proteins can be specifically oriented toward inorganic surfaces. However,

at present the principles regulating protein-surface interactions are poorly understood. What features of the surface and of the proteins determine which protein is able to bind to a given surface and how? In addition, the exact role of water in the process of protein-surface interaction is unknown. The comprehension of such mechanisms would foster several technological applications based on the rational design of protein/surface interactions, ranging from biomaterials to nanobioelectronics.

The aim of our work is to elucidate the mechanisms of interaction between a surface and a protein, including the role played by water. In particular, we have chosen to focus on the interaction of a polypeptide with one of the experimentally most studied surfaces, namely Au(111), for which from the theoretical view-point very little is understood and even the wetting behavior without the protein has not been studied yet via *ab initio* molecular dynamics (AIMD). Contrary to classical MD, AIMD calculates the forces in the system from quantum mechanics first principles, and does not need empirical physical parameters as input. We have performed AIMD simulations (at finite temperature) on a system that is composed of an Au(111) slab and an anti-parallel sheet of poly-Serine (a natural amino acid occurring in experimental gold-binding peptides), immersed in explicit water molecules and replicated by 3D periodic boundary conditions. AIMD is computationally very expensive, and the calculations have been performed in the framework of the DECI project PSI-Wat (“*Ab initio* simulations of Protein Surface Interactions mediated by *Water*”)

The results of our simulations show the mechanisms of interaction between the three components of the system, i.e., between water and gold, poly-Serine and gold, and poly-Serine and water. In particular, analogies and differences in the behavior with respect to gold of water and the related side-chain of the Serine (hydroxyl group, OH) could be identified. Remarkably, some of the found mechanisms were not known before, and requires AIMD for a correct description.

## **Speaker Biographies**

### ***Stefano Corni***

Dr. Stefano Corni is a research staff member at INFN-CNR National Research Centre on nanoStructures and bioSystems at Surfaces (INFN-CNR) S3 in Modena, where he is coordinating a working group on simulations of protein-surface interactions in the framework of the European FP6 New and Emerging Science and Technology (NEST) project PROSURF (Computational Toolkit for Protein Surface Docking). He has experience in *ab initio* and classical calculations on structures and properties of molecules in solution, biomolecules and solid state structures.

## ***Xavier Daura***

Dr. Xavier Daura was awarded his Ph.D. degree from Autonomous University of Barcelona (UAB), Barcelona, Spain in 1996 and joined the Laboratory of Physical Chemistry, Swiss Federal Institute of Technology (ETH), Zurich, Switzerland where he performed research on computational modelling and simulation of biomolecular systems under the direction of Prof. Wilfred van Gunsteren. In 2002 he was appointed Research Professor by the Catalan Institution for Research and Advanced Studies (ICREA) and took this position to the Institute of Biotechnology and Biomedicine (IBB) of UAB, where he leads the group for Computational Biology. Since 2005 he is, in addition to ICREA Research Professor, Associate Professor at UAB and Vice-Director of IBB. Dr. Xavier Daura has established himself as a well-known scientist in the field of biomolecular modelling and simulation. His studies focus, primarily, on the mechanisms of polypeptide folding and aggregation and protein-ligand recognition. Dr. Xavier Daura has published over 50 papers, with an *h*-index of 22. He is currently leading a European Consortium on vaccine research funded by the European Commission's FP6.

## ***Alistair Dunlop***

Dr Alistair Dunlop is project director for the OMII-Europe project and was instrumental in bringing together the major middleware developers required to ensure its success. Prior to this he was director of the OMII in the UK. Alistair has worked internationally in both academia and commercial companies including a previous position as IT director for a major UK company. He holds a PhD in Computer Science from the University of Southampton and undergraduate degrees in Computer Science from the University of the Witwatersrand in South Africa.

## ***Thomas Eickermann***

Since he finished his PhD in Physics at the University of Düsseldorf in 1994, Thomas Eickermann is working at the Research Centre Jülich. After some years in system administration and metacomputing, he became head of the communication systems division in 2002. Currently Thomas is the project manager of PRACE.

## ***Jukka Heikkinen***

Jukka A. Heikkinen (Dr.Tech, technical physics, Helsinki University of Technology, 1987) is a senior research scientist in the Fusion Physics and Plasma Technology group at VTT. His current research interests include kinetic plasma modelling, radio frequency heating and diagnostics in plasmas.

## ***Sascha Husa***

Research interests: numerical solution of the Einstein equations, black hole physics, gravitational waves.

Born 1967 in Vienna, Austria.

PhD from University of Vienna 1998 (work on initial data in general relativity), supervisor Prof. Beig.

1998 - 2000 Postdoc at the University of Pittsburgh

2000 - 2005 Junior scientist, Max Planck Institute for Gravitational Physics/Albert Einstein Institute in Potsdam

2005 - 2006 Postdoc at the University of Jena

2006 Habilitation in Theoretical Physics, University of Jena

2006 - 2007 Lecturer at the University of Jena

2007 - VESF fellow of the European Gravitational Observatory (EGO) at the Max Planck Institute for Gravitational Physics/Albert Einstein Institute in Potsdam

## ***Alasdair R. Kellie***

Mr. Kellie graduated from the University of Manitoba (Canada) in Science and did his postgraduate work for a MSc. at the University of Alberta in Edmonton. Mr. Kellie spent more than 30 years with Environment Canada's Meteorological Services of Canada (MSC), the last 14 as a Senior Executive in various divisions and the last 7 years with responsibilities for managing the supercomputer and telecommunications centre located at the Canadian Meteorological Centre, in Dorval Quebec outside Montreal. Primary in this responsibility was operating the largest NEC supercomputer complex outside of Japan. In his last year with MSC, Mr. Kellie served as the Director General of the Canadian Meteorological Center.

Mr. Kellie's experience covers all aspects of the Weather Forecasting operations and Climate Research activities of MSC. He has served as Director of the Weather Services Program in Toronto as well as establishing a Development Division in Montreal for exploiting the numerical weather prediction program run by MSC. Mr. Kellie was responsible to lead Canada's weather services in preparing for the year 2000 and organized a \$25m project involving more than 360 staff

Mr. Kellie has been prominent in the international arena, representing Canada at the United Nations Agency, the World Meteorological Organization working group committees for data management, observations, telecommunications and most recently serving as Chair of the Working Group on Data Processing.

Mr. Kellie is currently an NCAR Associate Director where he directs of the Computational and Information Systems Laboratory of the National Center for Atmospheric Research and held this post for the last 9 years. Under Mr. Kellie, NCAR has transitioned from parallel vector supercomputing environment to scalar clusters and

increased available sustained computing resources 186 fold.

Currently serves on IBM's Deep Computing Advisory Board and their eServer Advisory Board. Most recently appointed to Battlespace Environment Institute Board of Directors. A board overseeing the migration of existing DoD Climate Weather Ocean, Air Quality Models and Space weather applications to the Earth System Modeling Framework. Previously a member of Canada's High Performance Computer Network Board of Directors. Co-chair of the WMO Expert Team on future Weather Information System and Data Collection Data Provision Centers

### ***Hermann Lederer***

Dr. Hermann LEDERER is head of application support at Garching Computing Centre (RZG) of the Max Planck Society. He received a diploma in physics from the University of Munich and a PhD in Natural Sciences from the Technical University of Munich. After a post-doc position at Max Planck Institute of Biochemistry with research stays at Institut Laue-Langevin, Risoe National Laboratory and DESY, he took a position at RZG. After a group leader position for workstations and applications, he became head of the high performance applications group and project manager at RZG for supercomputing projects of the Max Planck Society. In the EU FP6 DEISA project he is leader of the Applications Task Force and leader for the Joint Research Activities in Materials Science and in Plasma Physics.

### ***Jane Nicholson***

Jane Nicholson is Head of Research Infrastructure and International Affairs at the Engineering and Physical Sciences Research Council. Amongst a range of responsibilities, Jane represents the UK on the PRACE Management Board and leads the team which procures and manages the investment by the Research Councils in the UK National high performance computing services. Two national services are currently supported, HECToR and HPCx, and both are part of the DEISA activities. The Engineering and Physical Sciences Research Council (EPSRC) is the UK's main agency for funding research in engineering and the physical sciences. The EPSRC invests around £740 million a year in research and postgraduate training, to help the nation handle the next generation of technological change. The areas covered range from information technology to structural engineering, and mathematics to materials science. This research forms the basis for future economic development in the UK and improvements for everyone's health, lifestyle and culture. EPSRC also actively promotes public awareness of science and engineering. EPSRC works alongside other Research Councils with responsibility for other areas of research. The Research Councils work collectively on issues of common concern via Research Councils UK.

## ***Paolo Malfetti***

Mr. Paolo Malfetti is head of Technology Management Sector inside the CINECA Systems and Technology Department. He received his laurea degree in 1995 from the University of Bologna. He joined CINECA High Performance Computing Sector in 1996 as “weather forecast junior programmer”. In the EU FP6 DEISA and eDEISA projects he is leader of the service activity 3 named “Resource Management and middleware”. Inside DEISA 2 he will lead the service activity on “Technology development”.

## ***Karsten Reuter***

Karsten Reuter did his undergraduate and graduate studies in physics at the Universities of Erlangen-Nürnberg (Germany), York (UK), Madrid (Spain) and Milwaukee (USA), and obtained his doctoral degree in 1998. After postdoctoral stays at the Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin and the FOM-Institut for Atomic and Molecular Physics in Amsterdam, he heads an Independent Junior Research Group at the Fritz-Haber-Institut since 2005, combined with the position of a Privatdozent at the Free University of Berlin. Karsten’s research interests center on a multiscale modeling of materials properties and functions, in particular on linking predictive-quality quantum-mechanical electronic structure calculations with more coarse-grained statistical models.

## ***Ed Seidel***

Edward Seidel is a physicist recognized worldwide for his work on numerical relativity and black holes, as well as in high-performance and grid computing. In 2003, LSU recruited Seidel to lead its investment in the Governor's Information Technology Initiative, and he became director of LSU's newly formed Center for Computation & Technology. Seidel also is the Floating Point Systems Professor in LSU's Departments of Physics & Astronomy and Computer Science. In addition to leading the CCT, he helped initiate, and is presently the chief scientist for, the \$40M Louisiana Optical Network Initiative.

Seidel earned his Ph.D. from Yale University in relativistic astrophysics. Prior to becoming CCT director, Seidel was a professor at the Max-Planck-Institute for Gravitational Physics (Albert-Einstein-Institute, or AEI) in Germany from 1996-2003. There, Seidel founded and led AEI's numerical relativity and e-science groups, which became leading forces worldwide in solving Einstein's equations using large-scale computers, and in distributed and grid computing. He still maintains a strong affiliation with AEI. LSU and the AEI numerical relativity and computational science groups still work very closely together.

He also was a senior research scientist at the National Center for Supercomputing Applications and associate professor in the Physics Department at the University of Illinois, Urbana-Champaign.

Seidel's Awards:

2008 Internet 2 Board of Trustees, Discipline Researcher Representative

2007 Fellow of the American Physical Society

2006 Recipient, Sidney Fernbach Award

2004 Rising Star of the Year, Louisiana Governor's Technology Awards

2001 Gordon Bell Prize

1998 Heinz-Billing-Preis of the Max-Planck-Gesellschaft

Winner of various HPC Challenge awards at SC98, SC01 and SC02.

### ***Marian Garcia Vidondo***

Marian Garcia Vidondo finished her masters degree in Telecommunication Engineering in 1999 at the Public University of Navarra (Spain). In April 2000 she became part of the DANTE team, working in projects such as the 'GEANT-IPv6' project focused in deploying native IPv6 in the GEANT network. Since July 2007 Marian occupies the position of Chief Operations Officer. She is responsible for the operations of GEANT2 and for providing IP services and point-to-point Ethernet circuits to interconnect European NRENs. Marian works together with Internet2 and Esnet in the definition of global operations for such services.

### ***Lucas Visscher***

#### Positions

7-2003 - present Associate Professor Vrije Universiteit Amsterdam

1-1998 - 6-2003 Assistant Professor Vrije Universiteit Amsterdam

5-1996 - 12-1997 Postdoc Odense Universitet, Denmark

4-1995 - 2-1996 Postdoc Rijks Universiteit Groningen

3-1994 - 3-1995 Postdoc NASA Ames, USA

8-1993 - 1-1994 Postdoc Rijks Universiteit Groningen

#### Thesis

Title Relativity and Electron Correlation in Chemistry

Promotor Prof Dr W. C. Nieuwpoort

University Rijks Universiteit Groningen

Date 10-9-1993

Judicium cum laude

## Awards

2006 Dirac medal (WATOC)

2005 Vici grant (NWO)

1996 Clemens Roothaan award (KNCV)

1996 Marie Curie fellowship (EU)

1994 National Research Council Associate (USA)