2013-14 Severo Ochoa
Research Seminar
Lectures at BSC

Book of Abstracts

GOBIERNO DE ESPAÑA
MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

BSC Barcelona Supercomputing Center
Centro Nacional de Supercomputación

EXCELENCIA SEVERO OCHOA

2013-14 Severo Ochoa Research Seminar Lectures at BSC

Book of Abstracts

Acknowledgements

The BSC Education & Training team gratefully acknowledges all the experts contributing to this Book of Abstracts participating in the Severo Ochoa Research Seminar Lectures at BSC held during 2013 and 2014, the Summer Schools and the 1st BSC Doctoral Symposium and thanks the attendees for joining in.

BSC Education & Training team
education@bsc.es

CONTENTS

SEVERO OCHOA RESEARCH SEMINAR LECTURES AT BSC

Opening Session [Sep 27, 2013]

Opening by Josep Casanovas (BSC Severo Ochoa Programme Coordinator)

Josep introduced the main aims of the Research Seminar Lectures in the context of the Severo Ochoa Programme. Also thanked the lecturers and attendees for their cooperation, explained the importance of the Severo Ochoa Seminar Lectures and provided an overview on some of the issues to be tackled by the world leading scientists that will give the different lectures during the whole seminar cycle.

Lecture by Mariano Vazquez (CASE Dept. at BSC)

Understanding Cerebral Aneurysms through HPC-based Computational Modeling

Abstract

This talk addresses the use of HPC-based simulation tools in understanding cerebral aneurysms. In particular, coupled CFD and Solid Mechanics simulations could help to assess the risk of rupture. The tools are FeFlo for CFD and Alya for the solid mechanics problem. The work flow starts with acquiring images for several patients, which are used next to create a CFD

simulation scenario. Then, the mean values of pressure and strains are transferred to Alya solver as boundary conditions for a 3D solid mesh created by extrusion of the surface fluid mesh. Mechanical and material properties are modulated according to some criteria and the inner stress analysed.

Short Bio

Since 2005, MV is research group leader at the Computer Applications in Science and Engineering (CASE) Department of the Barcelona Supercomputing Center – Centro Nacional de Supercomputación de España (BSC-CNS). He leads the High Performance Computational Mechanics Group. His group's main task is to develop Computational Mechanics tools adapted to run efficiently in large-scale parallel computers. This involves Physical modelling, Mathematical algorithms and code development and optimization, all with the strong constraint of efficient use of parallel resources. This multidisciplinary group is composed by 10-15 researchers including post-docs, PhD students and programming engineers. MV is one of the three main architects of the Alya System, the in-house

HPCM tool. His main lines of research are on Computational Mechanics and HPC, with a strong focus in Biomechanics. In particular, all the computational aspects of Cardiac Computational Modelling (partially financed by the Severo Ochoa Program), Respiratory System or Hemodynamics (aneurisms).

Severo Ochoa Mobility Grant - Visitor: Juan R. Cebral, Professor at the Center for Computational Fluid Dynamics, College of Science, George Mason University, in Fairfax, Virginia, USA visited BSC to work with the CASE Dept.

[Oct 25, 2013] Lecture by Ramon Goñi (Life Sciences Dept. at BSC)

Receptor Sampling with Dpedmd for Virtual Screening

Abstract

The genetic profile of patients directly affects their reaction against medication: sometimes in a positive manner (increasing the therapeutic effect), sometimes in a negative manner (increasing toxic side effects, or simply deactivating a drug response). Apparently trivial variations in the genome have a demonstrated impact in different aspects of drug therapy, among them a decrease of drug effect on receptors (Stingl et al. CPT 2010), which open a significant uncertainty on the impact of a given drug when applied to the population level. Experimental evaluation of the connection between genotype and pharmacological response is a priori possible, but its cost is prohibitive, forcing the use of in silico approaches (Alvarez, J. C. J. C. Curr. Opin. Chem. Biol. 2004), which need to be improved and extended to tackle the formidable problem coming from world-wide genotyping

initiatives. We aim to improve the screen of large collection of libraries developing an in silico platform that combines the classical structure-based and ligand-based approach. The platform increase the performance of predictions integrating determination of molecular receptor flexibility using computational modeling approaches, amongst which molecular dynamics (MD) and) and coarse grained dpED/MD simulations.

Short Bio

Dr. Ramon Goñi holds a PhD in Biotechnology from the University of Barcelona (UB, 2008). He graduated in Computer Science from the Universitat Politècnica de Catalunya (UPC, 2002). He joined the Institute de Recerca Biomèdica de Barcelona (2004-2007) where he participated in several research projects like the study of anti-gene therapies, the development of gene-predictors or the study of the physical properties of genomic DNA. In 2007 he joined the sales and marketing department of the bioinformatics company Integromics (2007-2009). He led the development genomics data analysis solutions for Pharma/Biotech industry. In 2009 he joined the BSC as Senior Researcher and Project Manager of Technology Transfer projects. He taught bioinformatics in the University of Barcelona (UB, 2010) and in the Universitat de Vic (UVIC, 2005-2007).computational aspects of Cardiac Computational Modelling (partially financed by the Severo Ochoa Program), Respiratory System or Hemodynamics (aneurisms).

Severo Ochoa Mobility Grant – Outgoing visit: Ramon Goñi visited the University of Nottingham, UK to collaborate on topics linked with a SO Personalized Medicine application research and development.

[Oct 25, 2013] Lecture by Ruth Arís (CASE Department at BSC)

Analysis of Mechanical Parameters Using End-Diastolic Measurements

Abstract

Cardiac modelling is a powerful tool for a comprehensive understanding of cardiac function. Since the late nineteenth century, many models have been proposed to describe and predict mechanical function of the heart. Mathematical models provide a quantitative description of the mechanical activity of the myocardium and they can help to interpret experimental data or cardiac mechanisms. The creation of a finite element model of the heart based on cardiac data obtained from images, using the most recent advances in this field, is useful to validate theories or predict clinical results. For example, they can be a platform to test new techniques, such as drug interactions for arrhythmia. Since cardiac biomechanics requires the definition of myocardial parameters in the simulation, data assimilation is often employed to characterise electromechanical properties of the heart, which most of the times are not accessible through clinical technology directly. Then, measurements can be combined with the mathematical model to predict the

evolution of the system. With this purpose, data assimilation is a useful tool to estimate the state variables, parameters or initial conditions of the model. Then, material values in the nonlinear cardiac mechanics model, such as myocardial stiffness, can be determined with data assimilation. This work will give the cardiac simulator a method to optimize the mechanical parameters and fit the model to real cases.

Short Bio

Ruth Arís was born in Barcelona. He holds an MSc in Physics from Universitat de Barcelona. She has worked as associate professor at Universitat de Barcelona and Universitat Politècnica de Catalunya. Since 2007, Ruth Arís is working at the Computer Applications in Science and Engineering (CASE) Department of the Barcelona Supercomputing Center (BSC). She is PhD student, developing a Large Scale Computational Model in the Ventricular Myocardium at the High Performance Computational Mechanics Group (HPCM). The Cardiac Computational Mechanics tool involves Physical modelling, Mathematical algorithms, code development and optimization, all adapted to run efficiently in large-scale parallel computers. Alya System is the in-house HPCM tool. His main lines are on Computational Mechanics and HPC, with a strong focus in Biomechanics. In particular, the computational aspects of Cardiac Computational Modelling, which are partially financed by the Severo Ochoa Program.

Severo Ochoa Mobility Grant – Outgoing visit: Recently, Ruth Arís visited the Biomedical Engineering Department at King's College, London (KCL).

[Oct 25, 2013] Lecture by Oriol Jorba (Earth Sciences Dept. at BSC)

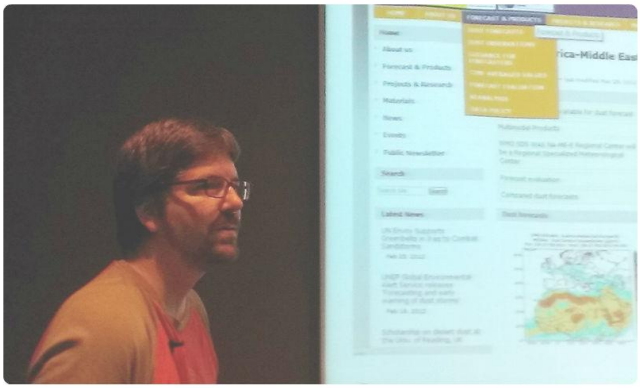
The multiscale NMMB/BSC Chemical Transport Model: developments of inlined aerosol and gas chemistry processes

Abstract

The Earth Sciences Department of the Barcelona Supercomputing Center (BSC) is working on the development of a chemical weather forecasting system based on the NCEP/NMMB multiscale meteorological model. In collaboration with the National Centers for Environmental Prediction (NOAA/NCEP/EMC), the NASA Goddard Institute for Space Studies (NASA/GISS), and the University of California Irvine (UCI), the group is implementing aerosol and gas chemistry inlined within the NMMB model. In the framework of the Severo-Ochoa research program, the group is extending the range of applicability of the NMMB/BSC-CTM from high-resolution regional to global scales, and for short-term to long-term modeling scenarios.

This talk will overview the status of development of the system, the efforts done on the evaluation of the different modules, and its application as a research forecast tool. NMMB/BSC-CTM is providing mineral dust forecasts with its regional configuration for the Northern Africa-Middle East-Europe (NA-ME-E) Node of the Sand and Dust Strom Warning Advisory and Assessment System (SDS-WAS) of the World Meteorological Organization (WMO). Complementing the mineral dust processes, a multi-component aerosol module is under development. Results on the evaluation of different sea-salt emission schemes will be shown. Furthermore, gas and aerosol chemistry is under evaluation at both global and regional scales. In this

sense, the NMMB/BSC-CTM is contributing to the AQMEII-Phase2 initiative on on-line air quality model intercomparison.



Short Bio

Born in 1975 in Barcelona (Spain), Industrial Engineer (Technical University of Catalonia -UPC-, Barcelona, Spain, 1999); Diploma of Advanced Studies in Environmental Engineering(Technical University of Catalonia -UPC-, Barcelona, Spain, 2002); Ph.D. in Environmental Engineering (Technical University of Catalonia -UPC-, Barcelona, Spain, 2005). His research activities and interests have included high resolution mesoscale meteorology and air quality, development of online meteorology-chemistry models, boundary layer studies, chemical mechanisms and environmental impact assessment. In 2005, he was enrolled as researcher at the Earth Sciences Department of the Barcelona Supercomputing Center, and in 2008 moved to the Atmospheric Modelling Group Manager position at BSC.

He held a research position at the University of California Irvine (USA) in 2011, and at the NASA Goddard Institute for Space Studies (USA) in 2013. He has co-authored 30 papers in international scientific journals and over 80 communications to international conferences. He has participated in several Spanish and European projects of the FP5 and FP7 Framework Programme (e.g., EARLINET, ACCENT, IS-ENES, FIELD-AC, IS-ENES2). He has been the principal investigator of the Spanish research project CGL2008-02818, and coordinates the development of the multiscale chemical weather forecasting system NMMB/BSC-CTM. He is member of the management committee of 2 European COST Actions (ES1002, ES1004) as a Spanish representative, and of the Scientific Committee of the International Technical Meeting on Air Pollution Modelling and its Application. He has acted as reviewer of several international journals (Atmospheric Environment, Atmospheric Research; Geoscientific Model Development; Tethys; Water, Air and Soil Pollution).

Severo Ochoa Mobility Grant – Outgoing visit: Oriol Jorba visited the National Center for Environmental Prediction, University of California Irvine, USA.

[Nov 15, 2013] Lecture by Nick Schutgens, (Atmospheric, Oceanic and Planetary Physics Department at the University of Oxford)

Known and unknown unknowns in aerosol modelling

Abstract

Atmospheric aerosols (small airborne particles) present an exciting scientific puzzle: they come in a variety of shapes and species and interact in complicated ways with eachother and the rest of the climate system. Consequently, it is challenging both to observe and model them. Yet aerosols affect the planet in many important ways: they modify the amount of global warming due to greenhouse gases, they represent a health hazard for humans and a nutrient source for the biosphere. This talk will consist of two parts: an introduction to aerosol science and an overview of work on uncertainties in aerosol modelling.

Short Bio

He is a member of the Climate Processes Group in the sub department of Atmospheric, Oceanic and Planetary Physics. He has a PhD in astrophysics from Utrecht University in the Netherlands, but has since then worked in atmospheric science. Initially his interest was in remote sensing (trace gases, clouds) but in the past 8 years he has worked on aerosol

modelling and data assimilation. Currently he is working on structural and parametric uncertainties in aerosol models.

Severo Ochoa Mobility Grant - Visitor: Nick Schutgens visited BSC.

[Dec 15, 2013] Lecture by Dieter Kranzlmüller, (Ludwig-Maximilians-Universität München, Germany, Member of the Board of Directors of Leibniz-Rechenzentrum)

Extreme Scaling on SuperMUC

Abstract

The HPC System SuperMUC at the Leibniz Supercomputing Centre (LRZ) in Garching near Munich is one of the most powerful computing systems of the world. Its performance of up to 3 Petaflop/s is provided by more than 155,000 cores, using a complex structure of thin and fat islands and an Infiniband interconnect. While the x86-compatible cores allow portability with smaller systems, the full performance is only achievable with scalable algorithms. At the same time, power consumption and energy restrictions apply. All this requires novel approaches in programming and dedicated training and support of the users. An example is the recent extreme scaling workshop taking place at LRZ, where users were rovoked to use as many cores as possible for their applications. The observations and results from the workshop provide an interesting insight

into the state-of-the-art of scalable applications today and some of these results and interesting findings will be presented during the talk.

Short Bio

Dieter Kranzlmüller is full professor of computer science at the Ludwig-Maximilians-University (LMU) Munich and member of the board of the Leibniz Supercomputing Centre (LRZ) of the Bavarian Academy of Sciences and Humanities. He has worked in parallel computing and computer graphics since 1993, with a special focus on parallel programming and debugging, cluster and especially grid computing. He has participated in several national and international research projects, has been acting as reviewer and international expert for several countries and research programs, and has co-authored more than 150 scientific papers in journals, and conference proceedings.

At present, he serves as Strategic Director for EGI_DS, the European Grid Initiative Design Study and as Area Director Applications of the Open Grid Forum (OGF). Before his recent move to Munich, he has been deputy head of GUP, the Institute of Graphics and Parallel Processing at the Johannes Kepler University Linz, Project Director of EGI_DS, appointed national representative of Austria in the EU e-Infrastructures Reflection Group (eIRG), and member of the Austrian Grid Executive Board.

[Jan 14, 2014] Lecture by Martin Schulz (Lawrence Livermore National Laboratory)

Performance Analysis Techniques for the Exascale Co-Design Process

Abstract

Reaching exascale will require substantial advances at all levels of the computational ecosystem: the hardware, the OS, the runtime system, algorithms, as well as the applications themselves. Further, we need to work on these aspects together - individual solutions limited to single layers won't provide the necessary benefits. Following this idea, a wide range of efforts focus on the idea of Co-Design for exascale, including three dedicated Exascale Co-Design centres initiated by the US Department of Energy. A central aspect in any of these Co-Design efforts are techniques to measure, track and analyse a wide range of performance metrics, incl. execution time, memory system behaviour, power consumption and the resiliency to faults.

Short Bio

Dr. Martin Schulz is a Computer Scientist at the Center for Applied

Scientific Computing (CASC) at Lawrence Livermore National Laboratory (LLNL). He earned his Doctorate in Computer Science in 2001 from the Technische Universität München (Munich, Germany) and also holds a Master of Science in Computer Science from the University of Illinois at Urbana Champaign. He has published over 160 peer-reviewed papers. He is the PI for the Office of Science X-Stack project "Performance Insights for Programmers and Exascale Runtimes" (PIPER) and for the ASC/CCE project on Open|SpeedShop. Further, he is the chair of the MPI forum, the standardization body for the Message Passing Interface, and is involved in the DOE/Office of Science Exascale Co-Design Centres CESAR and ExMatEx, as well as the Exascale OS centre ARGO.

[Jan 24, 2014] Lecture by Young Shi (CASFEDS Centre, Chinese Academy of Sciences and University of Omaha)

Multi-objective Optimisation and Big Data

Abstract

At present, Big Data becomes reality that no one can ignore. Big Data is our environment whenever we need to make a decision. Big Data is a buzz word that makes everyone understand how important it is. Big Data shows a big opportunity for academia, industry and government. Big Data then is a big challenge for all parties. This talk will discuss some fundamental issues of Big Data problems, such as data heterogeneity vs. decision heterogeneity, data stream research and data-driven decision management. The talk will focus on various approaches based on optimization and intelligent knowledge. The optimization techniques include multiple criteria linear programming and multiple criteria quadratic programming. The intelligent knowledge is the research beyond

traditional data mining. Furthermore, this talk will provide a number of real-life Bid Data Applications. In the conclusion, the talk suggests a number of open research problems in Data Science, which is a growing field beyond Big Data.

Short Bio

Yong Shi is a Senior Member of IEEE, the Executive Deputy Director, Chinese Academy of Sciences Research Center on Fictitious Economy & Data Science. He has been the Charles W. and Margre H. Durham Distinguished Professor of Information Technology, College of Information Science and Technology, Peter Kiewit Institute, University of Nebraska, USA 1999-2004. Dr. Shi's research interests include business intelligence, data mining, and multiple criteria decision making. He has published more than 20 books, over 200 papers in various journals and numerous conferences/proceedings papers. He is the Editor-in-Chief of International Journal of Information Technology and Decision Making (SCI), and a member of Editorial Board for a number of academic journals. Dr. Shi has received many distinguished awards including the Georg Cantor Award of the International Society on Multiple Criteria Decision Making (MCDM), 2009; Fudan Prize of Distinguished Contribution in Management, Fudan Premium Fund of Management, China, 2009; Outstanding Young Scientist Award, National Natural Science Foundation of China, 2001; and Speaker of Distinguished Visitors Program (DVP) for 1997-2000, IEEE Computer Society. He has consulted or worked on business projects for a number of international companies in data mining and knowledge management.

[Feb 28, 2014] Lecture by Janko Strassburg (Computer Science Department at BSC)

HPC simulation using xSim – The Extreme-scale Simulator

Abstract

The Extreme-scale Simulator (xSim) is an HPC performance investigation toolkit developed at the Oak Ridge National Laboratory (ORNL). It allows for hardware and software co-design and to model behaviour of HPC applications. Native HPC applications can be executed in a controlled environment with millions of concurrent execution threads. MPI applications can be simulated on a much smaller system in a highly oversubscribed fashion. To achieve these simulations the development of xSim traded off scalability and simulation performance against simulation accuracy. Performance data can be extracted based on a processor and a network model with an appropriate simulation. The simulator supports user-level failure mitigation (ULFM) extensions at the simulated MPI layer and permits injection of MPI process failures to aid development and debugging of resilient fault tolerant applications. Examples on selected applications will be presented and applicability discussed.

Short Bio

Janko Strassburg is a PhD student in Computational Science. His research interests are in the areas of High Performance Computing, Network Centered Computations, Scalable and Fault-Tolerand Algorithms and Accelerator Architectures. His current work is focusing on Monte Carlo algorithms that are applied in the fields of Linear Algebra and Computational Finance. He is studying for his PhD at the University of Reading, UK and is currently working as a researcher at the Barcelona Supercomputing Center.

Severo Ochoa Mobility Grant – Outgoing visit: Janko Strassburg visited the Oak Ridge National Laboratory.

[Mar 18, 2014] Lecture by Paolo Faraboschi (HP Labs)

The Perfect Storm

Short Bio

Paolo is a Distinguished Technologist in the Exascale Computing Lab. He has been with HP Labs since 1994. His current research area is in low-power servers.

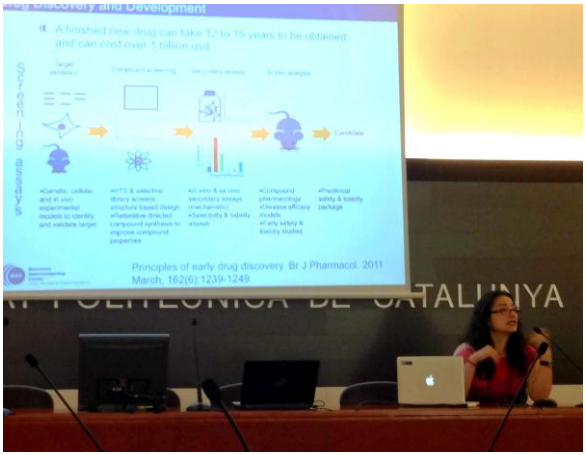
From 2004 to 2010, Paolo led a research group in Barcelona, Spain. The focus of the group was on system-level simulation and modelling of compute fabrics for next-generation computing systems. The COTSon simulator was released as open source in January 2010. From 1995 to 2003 he was the technical lead of the "Custom-Fit Processors" Project at HP Labs Cambridge (MA). In that role, he was the principal architect of the instruction set architecture of the Lx/ST200 family of VLIW embedded processor cores (developed as a partnership between HP Labs and STMicroelectronics). Paolo holds a Ph.D in EECS (1993) and an M.S. (Laurea) in Electrical Engineering (1989) from the University of Genoa (Italy).

[May 9, 2014] Lecture by Jazmín Aguado Sierra (CASE Department at BSC)

An In-silico framework for Cardiac Drug Testing: From Genes, to function, to human heart physiopathology

Abstract

The current and future work towards building an insilico drug-testing framework for high throughput screening of the electro-mechanic effect of drugs at the tissue and organ level using a multi-scale, multi physics, massively parallel program, called Alya, will be explained. With close collaboration of a highly recognized experimental cardiology laboratory, the



expertise on multi-physics, HPC simulations and the supercomputing power of Marenostrum, the new tools for cardiac safety drug testing are being build.

Short Bio

Biomedical Engineer from Universidad Iberoamericana, México City, México. PhD on Bioengineering on Mathematical models of Blood flow in Arteries, including Coronary Arteries, from Imperial College London, UK. PostDoctoral studies at the Cardiac Mechanics Research Group, Bioengineering Department, University of California, San Diego, USA.

Severo Ochoa Mobility Grant – Outgoing visit: Jazmín Aguado visited the Masonic Medical Research Laboratory.

[May 9, 2014] Lecture by Suwipa Saen-Oon (Life Sciences Dept. at BSC)

Exploring mechanistic details in enzyme catalysis through mutiscale hybrid QM/MM simulations

Abstract

The origin of many diseases responsible for the death of many thousands of people in the world reside in the malfunctioning of certain proteins.

Enzymes are proteins that catalyze all chemical reactions necessary for life. Understanding the principles of mechanistic details in enzymatic reaction is crucial as it is a foundamental and important for further development in drug design, drug metabolism, overcoming drug resistance as well as enzyme

engineering. During the past decades, hybrid quantum mechanical/molecular mechanical (QM/MM) simulations have demonstrated its abilities and accomplishments to elucidate the enzymatic catalytic reaction mechanisms at an electronic and atomic level. This talk will present an application of hybrid QM/MM method in studying the reaction mechanism in enzyme Plasmodium falciparum Phosphoethanolamine Methyltransferase, an attractive target for anti-malarial drug development.

Short Bio

Suwipa Saen-Oon received her PhD in Computational Chemistry (October-2003) from Kasetsart University (Thailand). She spent her post-doctoral research training at Chulalongkorn University (Thailand), Emory University (Atlanta) and Albert Einstein College of Medicine (New York). She is currently a researcher with Prof. Victor Guallar at the Barcelona Supercomputing Center. Her research interests involve computer simulations of chemical reactions and dynamics in enzymes as well as electron transfer process in proteins.

Severo Ochoa Mobility Grant – Outgoing visit: Suwipa Saen-Oon visited the school of Chemistry, University of Bristol , United Kingdom. The visit was to collaborate on topics linked with a SO Personalized Medicine application research and development.

[June 4, 2014] Lecture by Ross C. Walker (Associate Professor, San Diego Supercomputer Center & Department of Chemistry and Biochemistry, University of California San Diego)

Lights, Computer, Action: GPU Accelerated Molecular Dynamics, from Enzyme Activation to Membrane Dynamics

Abstract

This talk will focus on the impact that GPUs have had on Molecular Dynamics (MD) Simulations. In particular it will highlight the massive performance improvements that GPUs have brought to MD simulations with AMBER. Individual desktops with NVIDIA Kepler based GPUs can routinely provide simulation rates (for a 25,000 atom simulation) exceeding 130ns/day per GPU. A single desktop is now able to provide aggregate performance exceeding half a microsecond a day. Employing various tricks for longer time steps and constrained degrees of freedom and performance can exceed microseconds per day. Meanwhile replica exchange approaches to accelerating convergence enable hundreds of GPUs to be employed in parallel. The GPU revolution has transformed the MD landscape. No longer is access to supercomputer resources required to routinely access microsecond timescales and beyond. The world of MD research is now flat, with all researchers, young and old, rich and poor being able to run simulations that previously were restricted to those privileged enough to have routine access to supercomputers. Further, recent focus on algorithmic improvements aimed at accelerating the rate at which phase space is sampled has transformed things further. A recent success, which will be highlighted here, has been the reproduction and extension of key results from the DE Shaw 1 millisecond Anton MD simulation of BPTI (Science, Vol. 330 no. 6002 pp. 341-346) with just 5

days of dihedral boosted AMD sampling on a single GPU workstation, (Pierce L, Walker R.C. et al. JCTC, 2012, p5092). These results show that with careful algorithm design it is possible to obtain sampling of rare biologically relevant events that occur on the millisecond timescale using just a single $500 GTX680 Graphics Card and a desktop workstation.

Short Bio

Ross Walker is an Assistant Research Professor at the San Diego Supercomputer Center, an Adjunct Assistant Professor in the Departments of Chemistry and Biochemistry at the University of California, San Diego and an NVIDIA CUDA Fellow. He runs the Walker Molecular Dynamics Lab in San Diego where he leads a team that develops advanced techniques for Molecular Dynamics Simulations supporting simulations aimed at improved drug and biocatalyst design. He is a key developer of the Molecular Dynamics engine

AMBER and has hosted numerous international workshops on Molecular Dynamics. His work includes improved Quantum Mechanical, Molecular Mechanical models, development of new force fields for simulation of lipid membranes and the development of a GPU accelerated version of the AMBER Molecular Dynamics engine PMEMD.

[June 5, 2014] Lecture by Raul Cetto (Department of Otorhinolaryngology and Head and Neck Surgery, Imperial College Healthcare Department of Aeronautical Engineering, Imperial College London).

Assessment of Form and Function in the Large Airways

Abstract

The overall objectives of the research are to investigate the geometry of the large airways and the influence this exerts on patterns of airflow and functional performance. Two specific regions are considered: the nasal (upper) airways and the segment of the lower airways from larynx to carina. The nasal airways present a highly complex geometry, displaying a large degree of inter and intra subject variability. The nasal airways not only perform essential air conditioning physiological functions (heat and water exchange and primary filtration) but also house the olfactory receptors. Here a major clinical interest is in relating morphology to physiological function with the aim of providing better information for clinical assessment. In the large airways, the interest of this investigation is tracheal malformations and their effect on flow limitation.

The research seeks first of all to gather the necessary data, which is presently lacking, and secondly to apply analysis to characterise the salient geometric features and their influence on flow and particle delivery. The tasks of characterising the features and modelling the effects of flow and

particle deposition are primarily computational, although we have validated these models using rapid prototype physical models for experimental studies.

Currently our decision to intervene surgically and our methods of interpreting surgical outcomes rely on subjective measures. Computational Fluid Dynamics (CFD) techniques and geometrical analysis tools of medical imaging can provide quantitative outcome measures to guide our decisions and the means to quantify our results.

Topical drug administration into the nasal cavity has become a widely prescribed form of delivering medications such as intranasal steroids for the treatment of sinonasal inflammatory, allergic, and infectious disorders. Topical nasal medication targets.

[June 6, 2014] Lecture by Toyotaro Suzumura (IBM Research, University College Dublin and Tokyo Institute of Technology).

Big Data Processing in Large-Scale Network Analysis and Billion-Scale Social Simulation

Abstract

Graphs will be a prominent computational workload in the Exascale era. Large graph analysis is a dilemma faced by programmers in various domains such as scientific applications, biology, national security, business analytics, and so forth. In this talk we present our research project called ScaleGraph which is an open-source X10 library for massive graph analytics targeting large scale graph analysis scenarios.

Next, we introduce other effort that pursue the ultimate performance of large-scale graph analytics in the Graph500 benchmark recently paid attention by the Supercomputing

community as one of the important big data benchmarks. We have developed a scalable and high-performance implementation of BFS (Breadth First Search) for large distributed
environments based on 2D partitioning and other methods such as communication compression and vertex sorting. Our optimized implementation can handle BFS of a large graph with Scale 35 (34.3 billion vertices and 549.7 billion edges) with 462.25 Giga TEPS (Traversed Edges Per Second) while using 1366 nodes and 16,392 CPU cores. The talk will also cover more recent activities and the trend in this area.
We finally will introduce a platform for billion-scale social simulations. Towards the contribution to the human society, global economy, ecology, the analysis of human brain characteristics and our daily life, the research in multi-agent simulation is entering into the era of simulating billion-scale agents. Although prior arts tackle distributed agent simulation platform to achieve this goal, it is not sufficient to simulation billion-scale agent behaviors. Based on this observation, we introduce our work for building such an infrastructure platform that handles billion-scale agent simulation platform.

Short Bio

Toyotaro Suzumura received his Ph.D. in Computer Science from Tokyo Institute of Technology in 2004 mainly focusing on Grid computing and highly distributed systems mainly supervised by Prof. Satoshi Matsuoka. He published top-tier international conferences such as ACM/IEEE Supercomputing and IPDPS during his Ph.D, and also spent part of his Ph.D. research activities in San Diego Supercomputing Center, eXtreme Scale Computing led by Prof. Dennis Gannon, and Innovation Computing

Laboratory led by Prof. Jack Dongarra. He joined IBM Research - Tokyo in 2004 and had involved with several projects such as high performance XML processing, the PHP scripting language, stream computing, the X10 programming language and so forth. Since 2010, he has started to develop an X10-based billion-scale agent simulation platform on highly distributed systems and its application to large-scale traffic simulation. He has also explored billion-scale large scale analytics and been leading an open source graph library called ScaleGraph (http://www.scalegraph.org) and also continuously achieves 3rd or 4th place in the big graph processing competition called Graph500. He also had taken a role of a visiting associate professor at the Graduate School of Information Science and Engineering of Tokyo Institute of Technology since April 2009 for almost 5 years and supervised 16 students including 3 Ph.D. students. Since April, 2013, He also serves as a visiting associate professor at University College Dublin, Ireland. He has published 50 reviewed paper for international conferences and workshops, 41 domestic conferences, and 12 international patents. He is now a co-principal investigator for two Japanese government projects called "JST CREST" by leading both large-scale graph analytics and billion-scale agent simulation towards exa-scale computing environment.

[June 20, 2014] Lecture by Enza Di Tomaso (Earth Sciences Dept. at BSC)

How to ingest measurements into a computer simulation: data assimilation enhancement of an atmospheric model

Abstract

This talk describes the outcome of my visit to the Atmospheric, Oceanic and Planetary Physics department of the University of Oxford in UK, sponsored by the Severo Ochoa mobility programme. The major result of the collaboration with the local host has been the enhancement of an atmospheric model maintained by the Earth Sciences department, the NMMB/BSC Chemical Transport Model, with a data assimilation tool, i.e. a tool able to ingest measurements into a computer simulation of a real system.

She will give a brief introduction to the specific implementation of an ensemble Kalman filter that we have coupled with our atmospheric model, and show how we use it for aerosol data assimilation in order to aid the forecast of aerosol concentrations in the atmosphere. The specific type of ensemble Kalman filter that we use is particularly suited to high performance computing applications and is able to improve the forecast of our model.

The assimilation of measurements into atmospheric models combines many concepts from mathematical, physical and computing areas of

research, and might therefore be of interest to BSC scientists from a variety of backgrounds.

Short Bio

Enza Di Tomaso has a degree in Physics from the University of Bologna in Italy and a PhD in Engineering Mathematics from the University of Bristol in UK. She has worked as lecturer at the University of Bristol before moving to the field of atmospheric science, initially working for the Italian Research Council on the retrieval of precipitation from satellite observations, and subsequently working at the European Centre for Medium-Range Weather Forecasts in Reading, UK, on exploiting satellite observations for Numerical Weather Prediction. Recently, at BSC, she has expanded her interest to atmospheric chemistry and in particular to aerosol data assimilation.

Severo Ochoa Mobility Grant – Outgoing visit: Enza Di Tomaso visited the Department of Physics, University of Oxford.

Closing Session [July 7, 2014]

[July 7, 2014] Lecture by Yale Patt (The University of Texas at Austin).

Parallelism: a serious goal or a silly mantra (And what else is needed for the microprocessor of 2024)

Abstract

In this talk, I want to reflect on two things: (1) the enormous promotion of parallelism, often by those who are clueless as to what it is or why it could be such a good idea, and (2) the transformation hierarchy, heralded with practically no fanfare at all, but just may contain a few silver bullets.

The hoopla over parallelism comes naturally from the existence of multicore, which is the simplest result of the continuing increase in transistor count (Moore's Law). Unfortunately, that increase comes with problems, and I humbly suggest the transformation hierarchy may help solve some of them. If there is time I hope to show examples of some of the work we are doing that will benefit from moving the run-time system from the operating system to where it belongs.

Short Bio

Yale Patt is Professor of Electrical and Computer Engineering and the Ernest Cockrell, Jr. Centennial Chair in Engineering at The University of Texas at Austin. He enjoys equally teaching freshmen, teaching graduate students, and directing the research of nine PhD students in high performance computer implementation. He has, for more than 40 years, combined an active research program with extensive consulting and a

strong commitment to teaching. The focus of his research is generally five to ten years beyond what industry provides at that point in time. His rationale has always been that he does not do revenue shipments, preferring to produce knowledge that will be useful to future revenue shipments and, more importantly, graduates who will design those future products.

In 1965, Yale Patt introduced the WOS module, the first complex logic gate implemented on a single piece of silicon ["A complex logic module for the synthesis of combinatorial switching circuits," Proceedings of the 1967 Spring Joint Computer Conference, Atlantic City, April, 1967]. In 1984, he (and his students Wen-mei Hwu, Steve Melvin, and Mike Shebanow) introduced HPS, a high performance microarchitecture that exploits instruction level parallelism by combining wide-issue (fetching and issuing multiple instructions each cycle), aggressive dynamic branch prediction, dynamic scheduling, out-of-order execution, and checkpoint in-order retirement (enabling precise exceptions). The first two papers describing this work, "HPS, A New Microarchitecture: Rationale and Introduction" and "Critical Issues Regarding HPS, A High Performance Microarchitecture," were presented at Micro-18, and published in the Proceedings of the 18th Microprogramming Workshop, Asilomar, CA, December, 1985. In 1991 he (and his student Tse-Yu Yeh) introduced the Two-Level Branch Predictor, which provided much greater accuracy than was available before that. The paper, "Two-Level Adaptive Branch Prediction," was presented at Micro-24, and published in the Proceedings of the 24th International Symposium and workshop on Microarchitecture, Albuquerque, November, 1991.

Today, Yale Patt works on problems for the microprocessors of the year 2018, when technology promises each chip will contain more than 30 billion

transistors. His research focuses on breaking the abstraction layers that separate the problem statement in natural language from the circuits that execute the program. Some of his current projects include (1) ACMP, a heterogeneous multi-core microprocessor, where many of the cores are reconfigurable either for high-performance ILP or for high-throughput, (2) improving the interface between the processor core and the DRAMs, (3) GPUs for non graphics processing, (4) effective prefetching in a multi-core environment, and (5) more effective use of the run-time system for performance. Much as he enjoys research, Professor Patt's first love is teaching. The focus of his teaching has always been on understanding the fundamentals. At Michigan, he overhauled the introductory computer organization course, the intensive computer design course, and (with his former colleague Kevin Compton) the first required computing course for undergraduate EE, CS, and CE majors. Their motivated bottom-up approach is the subject of the textbook, "Introduction to Computing Systems, From Bits and Gates to C and Beyond," McGraw-Hill, 2001, ISBN: 0-07-237690-2, which he co-authored with his former PhD student Sanjay Patel, who is now a tenured Professor at the University of Illinois, Urbana-Champaign. The 2nd edition was published in 2004, ISBN 0-07-246750-9, and the 3rd edition is in progress. He has also taught more than 5000 engineers in industry, -- in ACM/IEEE conference tutorials and in short courses at company sites.

Yale Patt earned his BS at Northeastern University and his MS and PhD at Stanford University, all in electrical engineering. He received the 1995 IEEE Emannuel R. Piore Medal "for contributions to computer architecture leading to commercially viable high performance microprocessors," the 1996 IEEE/ACM Eckert-Mauchly Award "for important contributions to

instruction level paralelism and superscalar processor design," and the 1999 IEEE Wallace W. McDowell Award "for your impact on the high performance microprocessor industry via a combination of important contributions to both engineering and education." In 2005, he received the IEEE Computer Society Charles Babbage Award "for fundamental contributions to high performance processor design." In 2011, he was selected as the inaugural recipient of the annual IEEE B. Ramakrishna Rau Award "for significant contributions and inspiring leadership in the microarchitecture community with respect to teaching, mentoring, research, and service." In 2013, he received the IEEE Computer Society Harry H. Goode Award "for nearly half a century of significant contributions to information processing, including microarchitecture insights, a breakaway textbook, and mentoring future leaders." He is a Fellow of both the IEEE and the ACM, and a member of the National Academy of Engineering.

For his teaching, he has received several awards, most notably the ACM Karl V. Karlstrom Outstanding Educator Award for 2000. He was inducted in

2011 into The University of Texas Academy of Distinguished Teachers, a body charged with advising the President of the University in matters of undergraduate education. He also received the 2002 Texas Excellence Teaching Award for the College of Engineering at The University of Texas at Austin. Also, the 2002 Dad's Centennial Fellowship for his commitment to teaching freshmen. At Michigan, he was named Outstanding Professor of the Year by the Michigan Chapter of Eta Kappa Nu in 1992. He received the Teaching Excellence Award of the EECS Department at Michigan in 1995 and the College of Engineering of Michigan in 1996. In 1998, he was named an Arthur F. Thurnau professor at Michigan for his commitment to undergraduate education. In 1999 (for the academic year 1998-1999), and again in 2001 (for the academic year 2000-2001), he was named the National ACM Lectureship Program's Outstanding Lecturer of the Year.

[July 3, 2014] Lecture by Monica Zoppè (Inst. of Clinical Physiology, National Research Council, Pisa)

Summer lecture: BioBlender: 3D Computer Graphics for Structural Biology

Abstract

Recent advances in highly performant investigation methods contribute to obtain information about cells, from molecules to tissues, acros 4 orders of magnitude: from cell shape and composition to atomic structure of macromolecules. Our aim is to integrate available information about biomolecules activities and present them in an intuitive, animated form (www.scivis.it). The cellular environment and its components are recreated in Blender, a free, open-source, 3D modelling, animation and rendering package.

We focused on atomic scale visualization and developed BioBlender (www.bioblender.eu), a package dedicated to biological work, that comprise two major features: elaboration of proteins' motions using the game engine and the simultaneous visualization of physico-chemical features on molecular surface.

Blender's Game Engine is used to calculate protein motions by interpolating between different conformations according to specific rules. Transition between NMR collections or different X-rays structures of the same protein are obtained, as physically plausible sequence of intermediate conformations that are the basis for the subsequent visual elaboration.

A new visual, photo-realistic code, is introduced for MLP visualization: a range of optical features, from dull-rough-dark surfaces for hydrophilic areas to shiny-smooth-clear for lipophilic.

EP is represented as animated line particles that flow along field lines, from positive to negative, proportional to the total charge of the protein.

BioBlender is a new and fast system to calculate conformational changes of proteins between known conformations. It also includes a novel code for their intuitive representation, which contributes to gain insight into the function of molecules by drawing viewer's attention to the most active regions of the protein. A more direct visualization can result in an increased understanding of biological activities.

Severo Ochoa Mobility Grant - Visitor: Monica visited the BSC to work with the CASE Dept.

[July 24, 2014] Lecture by Emmanel Jeannot (Senior research scientist, LaBRi laboratory at INRIA-Bordeaux)

Summer lecture: Topology-aware placement and load-balancing

Abstract

Current generation of NUMA nodes clusters feature multicore and many core processors. Programming such architectures efficiently is a challenge because numerous hardware characteristics have to be taken into account, especially the memory hierarchy. One appealing idea to improve the performance of parallel applications is to decrease their communication costs by matching the communication pattern to the underlying hardware architecture. In this task we detail the algorithm and techniques proposed to achieve such a result. First, we gather both the communication pattern information and the hardware details. Then we compute a relevant reordering of the various process ranks of the application. Finally, those new ranks are used to reduce the communication costs of the application. To show the relevance of this approach we have:

1) compared the placement to standard MPI ones (round-robin)

2) developed two load balancers for Charm++ that take into account topology and communication aspects depending on the fact that the

application is compute-bound or communication-bound
3) implement it in a batch scheduler (SLURM) to improve the election of the nodes for a given application.

Severo Ochoa Mobility Grant - Visitor: Monica visited the BSC to work with the CASE Dept.

[Sept 25, 2014] Lecture by Scott A. Klasky

(Oak Ridge National Laboratory and Georgia Tech University, University of Tennessee Knoxville, North Carolina State University)

Summer lecture: Co-design for Next-Generation Extreme Scale Data Processing

Abstract

As we move closer to extreme scale computing, applications face numerous challenges that must be addressed before they can deliver breakthrough science. Data processing is one of the major challenges many of the applications are facing at the extreme scale. The ORNL team in this area has led efforts to create a new paradigm for data management on HPC platforms, which utilizes a Service Oriented Architecture to combine data-in-transit techniques with extreme performance I/O, and "in situ" data processing. This talk will present the evolution of this vision, from its inception to assembling a collaborative team, to breakthrough science delivered using the associated software platform. In

addition to over 60 publications over the last three years, the ORNL software stack has gained widespread adoption in the HPC community, and is being used in over one billion hours on the Oak Ridge Leadership Computing Facility. One of the main focus areas here is in co-designing the next generation version of our system, based on our system, ADIOS, https://www.olcf.ornl.gov/center-projects/adios/, which focuses on hybrid approaches to deliver breakthrough science.

Short Bio

Scott A. Klasky is a distinguished scientist and the group leader for Scientific Data in the Computer Science and Mathematics Research Division at the Oak Ridge National Laboratory. His leadership in big data and high performance computing work resulted in ADIOS, which recently run a R&D 100 award, which recognizes and celebrates the top 100 technology products of the year in the USA. Dr. Klasky holds a Ph.D. in Physics from the University of Texas at Austin 199 4and has previously worked at the University of Texas at Austin, Syracuse University, and the Princeton Plasma Physics Laboratory. Dr. Klasky is a co-author on over 180 papers in the field of relativity, fusion, and high performance computing.

SUMMER SCHOOLS

[June 2 to 6, 2014] AMBER Workshop 2014

A number of workshops that teach Molecular Dynamics via practical introduction to the AMBER Molecular Dynamics Software have been taught over the years by Ross C. Walker and Adrian E. Roitberg assisted by other members of the AMBER development team.

Recent workshops include:
Recife, Pernambuco, Brazil. 2013
Imperial College, London, UK. 2012
IRB-BSC, Barcelona, Spain. 2011
University of Dusseldorf, Germany. 2010
Sultan Qaboos University, Muscat, Oman, 2010
UC Merced, California, USA, 2009
University of Westminster, London, UK, 2009
Imperial College London, UK, 2008
University of Bergen, Norway, 2008

Scope

The duration of the meeting is 5 days, from 2nd of June to 6th. Typically there will be lectures 3 hours per day, and hands-on tutorials, about 5 hours per day. The content of the Workshop will include:

- Molecular Dynamics with Amber
- Using VMD to visualize AMBER
- Dealing with non-standard residues
- Building protein-ligand complexes

- Statistical Mechanics for Free Energy Calculations
- MM/PBSA calculations
- Calculating relative binding free energies for protein/carbohydrate complexes
- Enhanced sampling techniques
- Maximizing Performance (Parallel Execution and NVIDIA GPU Acceleration)
- Umbrella sampling simulations
- Analyzing Simulations
- Introduction to QM/MM Calculations
- Lipid Simulations with AMBER

Target group

The target audience is graduate students and postdocs as well as a few faculty interested in learning about Molecular Dynamics techniques. The course is designed to introduce Molecular Dynamics techniques from an introductory perspective but will progress quickly. Some experience with the Linux operating system is essential but experience with AMBER or other molecular dynamics packages is not required.

Sponsors

The workshop was supported by NVIDIA and the BSC Severo Ochoa Center of Excellence program. NVIDIA research explores challenging topics on the frontiers of visual, parallel, and mobile computing. NVIDIA supports advances in the field of physical simulation through collaboration with academic and industrial research institutions, and disseminate results in technical conferences, journals, and other academic venues.

Organizing Committee

The organising committee was composed by:

Ross C. Walker (University of California San Diego, USA)
Adrian E. Roitberg (University of Florida, USA)
Dwight McGee Jr. (University of Florida, USA)
Pablo D Dans (IRB Barcelona)
Federica Battistini (IRB Barcelona)
Modesto Orozco (Univ. Barcelona, INB, IRB, BSC, Spain)
Ramon Goñi (BSC, Spain)

[June 9 to 20, 2014] 2nd E2SCMS
SECOND EUROPEAN EARTH SYSTEM AND CLIMATE MODELING SCHOOL

The school is launched by the European Network for Earth System modelling (ENES) with support of the FP7 project IS-ENES2 (http://is.enes.org). The Barcelona Supercomputing Center (BSC, Spain) will host the school, which merges two very successful summer schools: the Earth System Modelling School by MPI for Meteorology (MPI-M, http://issmes.enes.org) and the Climate Modelling Summer School of the British National Centre for Atmospheric Science (NCAS). Three European models - HAD-GEM, MPI-ESM and EC-Earth - will be employed at the 2nd E2SCMS.

Background

Earth System and Climate Models are complex mathematical tools developed to improve our understanding of the natural environment around us. These scientifically and computationally advanced models and methods allow scientists to investigate the behaviour of climate processes and phenomena on a wide range of temporal and spatial scales. Models help scientists to assess the impact of human activities on the Earth system through climate scenario projections. Simulation results are used for societal and economic decision-making, from public weather forecasting, to resource management and natural disaster risk analysis. The comparison of models and multi model ensembles help to decrease model uncertainty and foster understanding of the climate system.

Scope

The school is offering the unique opportunity to study and compare the behaviour of the three models for the same climate problem sets. The school combines a series of lectures and discussions with practical modelling and data processing exercises, and will include the interpretation and presentation of simulation results. Attendance of international experts in Earth system and climate modelling will ensure an advanced and stimulating learning environment for participants. The preliminary course schedule is available on the E2SCMS web pages, http://schools.enes.org.

Target group

Early career scientists (advanced PhD candidates, Postdoctoral scientists and scientific programmers affiliated to European research institutions) with a strong background in mathematics, advanced computation and in the Earth system sciences are invited to apply. The competitive selection procedure will account for academic interests and excellence.

Sponsors

The workshop was supported by the IS-ENES2 project (Infrastructure for the European Network of Earth System Modelling) of the FP7 and the BSC Severo Ochoa Center of Excellence program.

Organizing Committee

The organising committee was composed by:
British National Centre for Atmospheric Science (NCAS)
Max Plank Institute for Meteorology's (MPI-M)
Earth Sciences Department of the BSC

1st BSC Doctoral Symposium [May 27 & 28, 2014]

Scope

The goal of the symposium was two-fold: first we aimed at providing a framework to share research results of the thesis that are being developed by PhD students at BSC; and second, we offered training sessions on topics and skills that will be useful to hem as future researchers and professionals.

The symposium has been conceived in the framework of the Severo Ochoa Program at BSC, following the project aims regarding the talent development and knowledge sharing. Taking that into account, the symposium provides an interactive forum for PhD students considering both the ones just beginning their research and the others who have progressed far enough to share some results.

Target group

Advanced PhD candidates, and early career scientists.

Sponsors

The workshop was supported by the Severo Ochoa Program at BSC.

Organizing Committee

Education and training team at BSC with the support of the BSC directors, PhD advisors, group leaders and department directors.

1st BSC Doctoral Symposium Book of Abstracts

Download the book of abstracts at www.bsc.es/doctoral-symposium-2014

Programme

First Day 27th May 2014		
9.30h	Welcome Address by Mateo Valero, BSC Director	
9.45h	Talk on 10 things you shouldn't do in a presentation	Invited Speaker: *Fernando Cucchietti,* BSC
10.45h	Poster Session and coffee	*Mercè Planas*, LS *Milos Panic*, CS *Nikola Rajovic*, CS *Lluis Gifré*, CS *Marc Guevara*, ES
11.30h	Cancer genomics at BSC	*Santiago González*, LS
12:00h	Atomic Dataflow Model	*Vladimir Gajinov*, CS
12:30h	Air Quality Impacts of Electric Vehicles in Barcelona	*Albert Soret*, ES
13:00h	CODOMs: Protecting Software with Code-centric Memory Domains	*Lluis Vilanova*, CS
13.30h	Lunch Break	
14.30h	PELE applications	*Israel Cabeza de Vaca*, LS
15:00h	Techniques for Improving the Performance of Software Transactional Memory	*Srđjan Stipić, CS*
15:30h	Coffee Break	
15:45h	Modelling volcanic ash dispersal and its impacts on civil aviation	*Chiara Scaini, CASE*
16:15h	Supporting Scatter/Gather Tasks in Manycore Architectures	*Tassadaq Hussain*, CS
16:45h	1st day closing remarks	
17:00h	Adjourn	

Acronyms of the BSC departments
CASE: Computer Applications in Sience and Engineering
CS: Computer Sciences
ES: Earth Sciences
LS: Life Sciences

Second Day 28th May 2014		
9.15h	Talk on The legal protection of computer programs	Invited Speaker: *Carles Comes*, ZBM Patents & Trademarks
11:15h	Poster Session and coffee	*Karthikeyan Palavedu*, CS *Alvaro Villalba*, CS *Roger Hernandez*, CS *Víctor Valverde*, ES *Vincenzo Obiso*, ES
12:00h	A new empirical approach to energy functions for protein-protein interactions	*Iain Moal*, LS
12:30h	Evaluation of the on-line NMMB/BSC-CTM model gas-phase results on the European domain for 2010 in the framework of the AQMEII-Phase2 project	*Alba Badia*, ES
13:00h	Per-task Energy Measuring and Accounting in the Multicore Era	*Qixiao Liu*, CS
13.30h	Lunch Break	
14.30h	Development and optimization of high-performance computational tools for protein-protein docking	*Brian Jimenez*, LS
15:00h	Source-level compiler analyses for OmpSs	*Sara Royuela*, CS
15:30h	Coffee Break	
15:45h	A CASE study	*Beatriz Eguzkitza*, CASE
16:15h	Hybrid and Resilient Monte Carlo Methods for Matrix based Linear Algebra Problems	*Janko Strassburg*, CS
16:45h	Closing remarks	
17:00h	Adjourn	

Acronyms of the BSC departments
CASE: Computer Applications in Sience and Engineering
CS: Computer Sciences
ES: Earth Sciences
LS: Life Sciences

Edited by Montserrat González F.
BSC Education & Training team
education@bsc.es
5th August, 2014
Barcelona (Spain)

GOBIERNO
DE ESPAÑA

MINISTERIO
DE ECONOMÍA
Y COMPETITIVIDAD

Barcelona
Supercomputing
Center
Centro Nacional de Supercomputación

EXCELENCIA
SEVERO
OCHOA