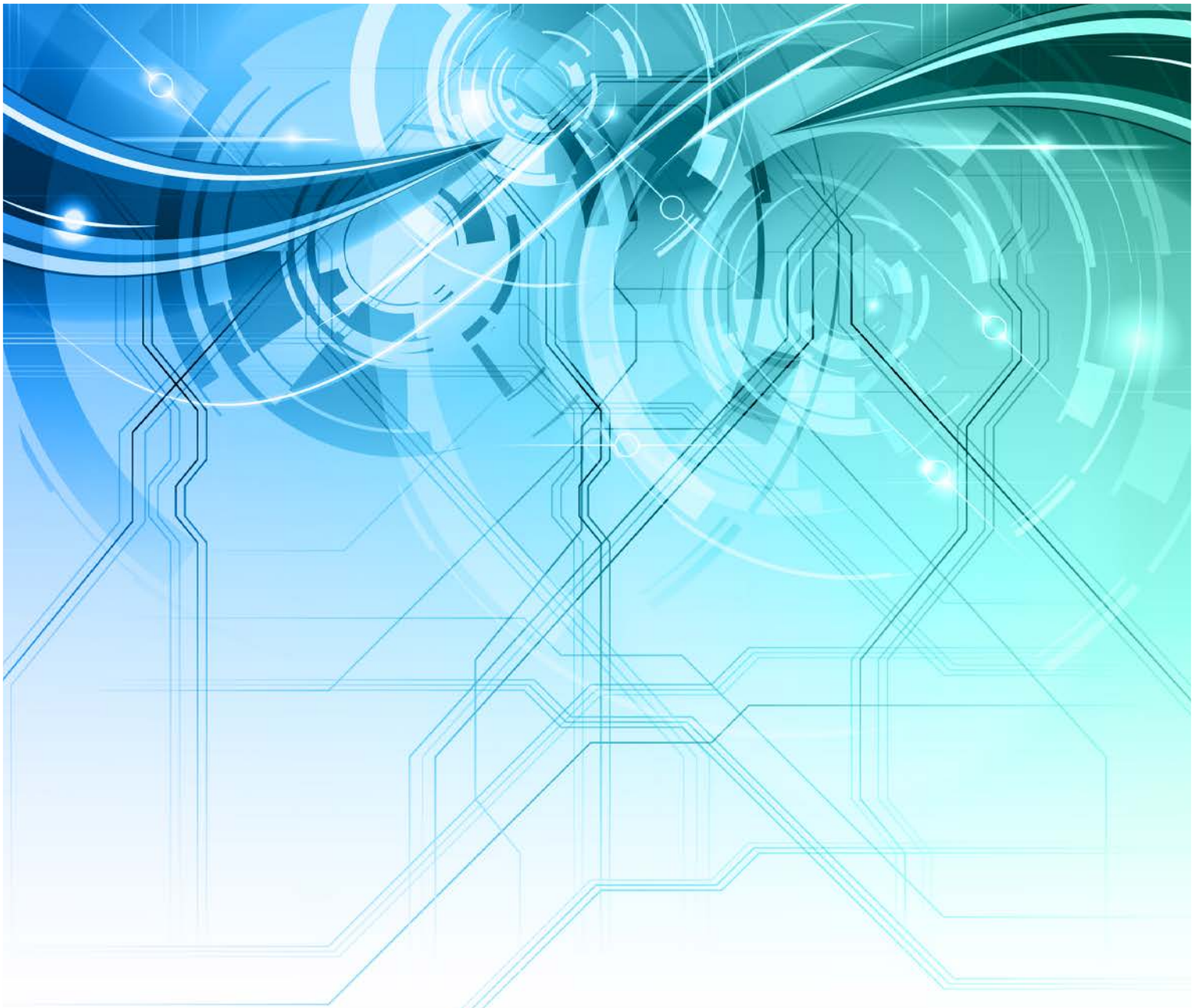

PRACE Scientific and Industrial Conference 2015

Enable Science Foster Industry

26 – 28 May 2015

PRACEdays15

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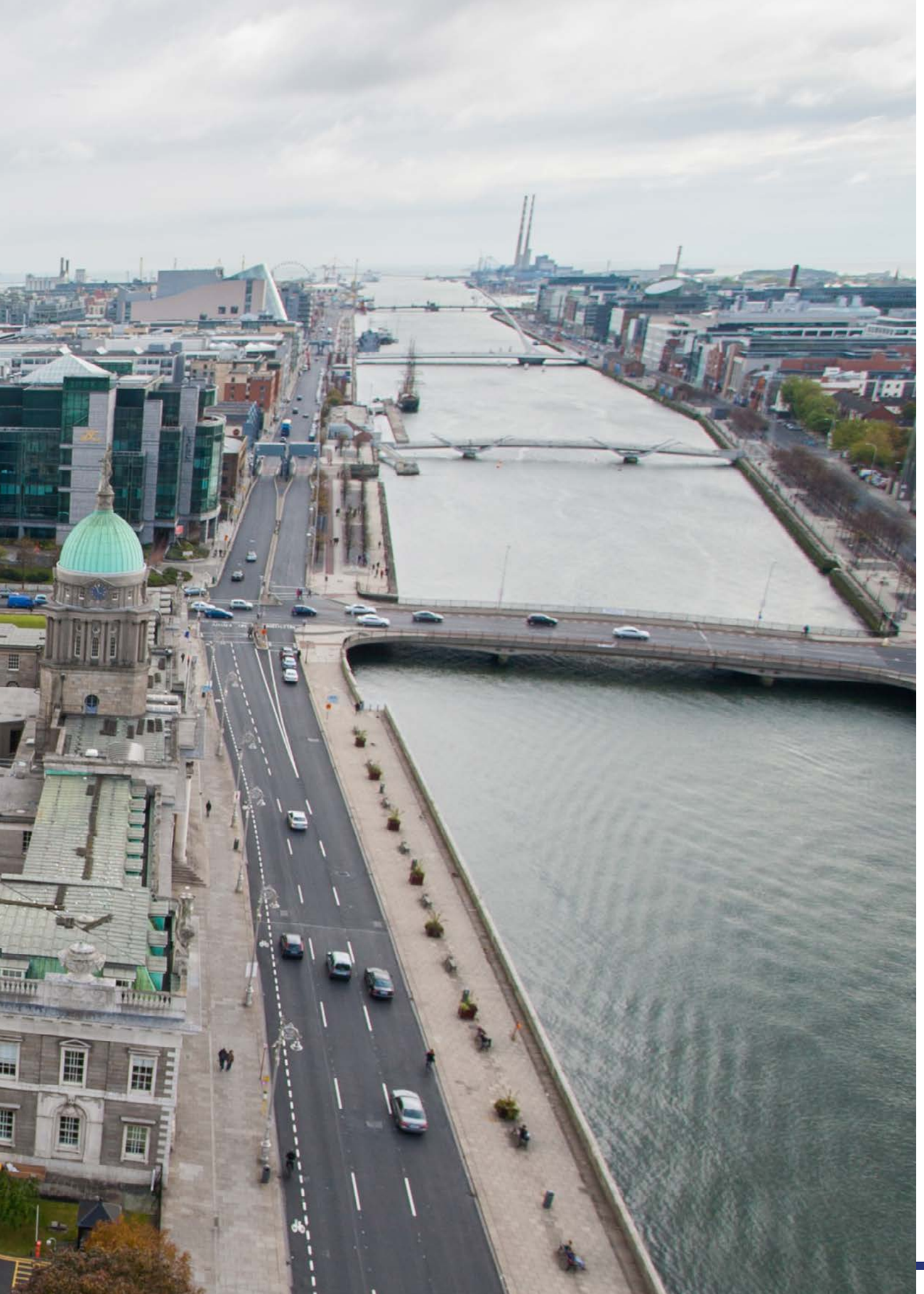


WELCOME

Dear Participant,

It is a great pleasure for us to welcome you to the PRACE Scientific and Industrial Conference 2015 - the second edition of PRACEdays – which is hosted by PRACE and the Irish Centre for High-End Computing (ICHEC) under the motto:

Enable Science Foster Industry

What better country than Ireland, the thriving digital hub of Europe and the academic home to the father of computing, George Boole, to host the PRACE Scientific and Industrial conference!

The Irish Centre for High-End Computing (ICHEC) is proud to welcome this high-level scientific and industrial conference at Dublin's world-renowned Aviva Stadium. Participants at PRACEdays15 will enjoy the unique combination of Dublin's legendary 'céad mile fáilte', as well as world-class science and research.

With two satellite events focussing on Exascale European projects and on Women in HPC, an open session of the PRACE User Forum, the bi-annual meetings of the PRACE Industrial Advisory Committee and the PRACE Scientific Steering Committee, and the EESI2 conference held back to back with the conference, PRACEdays15 has grown already beyond the expectations set in 2014.

The main conference programme is packed with high-level international keynote speakers, including a talk by RIST, Japan, and many parallel sessions dealing with different HPC topics in science and industry. We have lined-up an impressive group of speakers from Europe and beyond, who will present their advancements in HPC-supported science and engineering. The European Commission will give a plenary address on "Implementing the European Strategy on HPC" on Wednesday 27 May.

On Wednesday afternoon, you will have a choice of 6 parallel streams dedicated to various industrial and scientific topics. We recommend you try to join at least one presentation from the Industrial stream, to hear about some ground-breaking results from our host country, Ireland.

Last, but not least, on Thursday 28 May, a moderated panel will discuss the topic "Science and Industry: Partners for Innovation", coming full circle and closing the conference by referring to the motto of this edition.

A social programme including a conference dinner at the Ballsbridge Hotel will offer some entertainment and opportunities to convene and connect in a more informal setting.

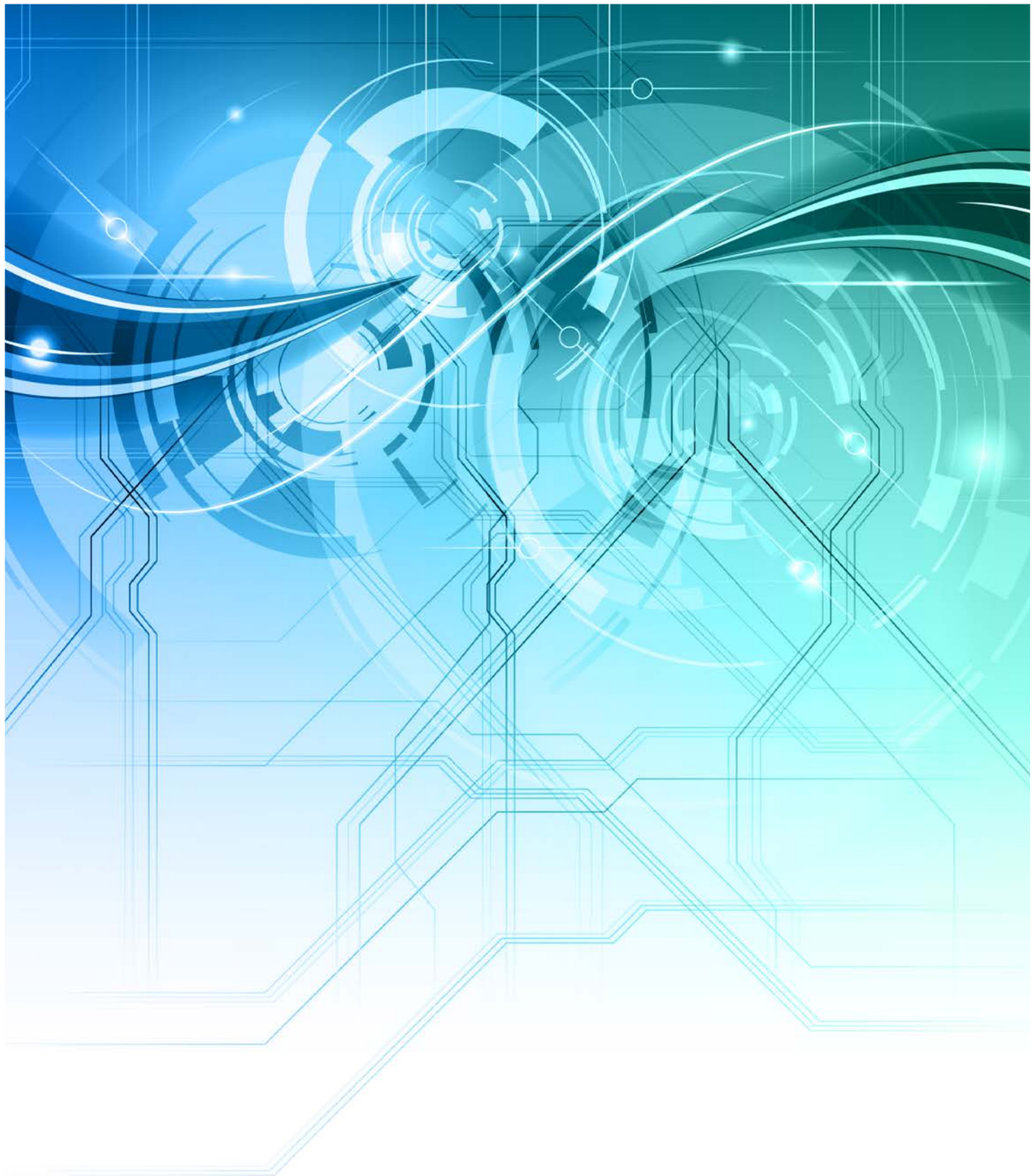
We would like to take this opportunity to thank all those who have made this event possible: the Organisation and Programme Committee, the PRACE Board of Directors, the PRACE Scientific Steering Committee, the PRACE Industrial advisory Committee, the User Forum, the team at ICHEC, and many others. We also want to thank the speakers and contributors without whom we would not have been able to offer you this complete and in-depth programme.

Wishing you a fruitful and inspiring conference!

Yours sincerely,

Sanzio Bassini
Chair of the PRACE Council

Sergi Girona
Chair of the PRACE Board of Directors



Committees

ORGANISATION & PROGRAMME COMMITTEE

Kenneth Ruud	Chair of the PRACE Scientific Steering Committee (SSC)
Dietmar Erwin	Chair of the Organisation & Programme Committee
Sergi Girona	Chair of the PRACE Board of Directors
Marjolein Oorsprong	PRACE Communications Officer
Emma Hogan	ICHEC - Local Host
Jürgen Kohler	Chair of the PRACE Industrial Advisory Committee (IAC)
Anders Rhod Gregersen	Vice-Chair of the PRACE Industrial Advisory Committee (IAC)
Koen Hillewaert	Chair of the PRACE User Forum
Gustavo Yepes	Outgoing Chair of the PRACE User Forum

SCIENTIFIC STEERING COMMITTEE

Christoph Dellago	University of Vienna
Luke Drury	Dublin Institute for Advanced Studies
Sylvie Joussaume (Chair)	CNRS/IPSL, LSCE
Richard Kenway	University of Edinburgh
Dimitri Komatitsch	LMA CNRS-MRS
Petros Koumoutsakos	ETH Zürich
Christian Lang	University of Graz
Erik Lindahl	KTH Royal Institute of Technology
Carlo Massimo Casciola	University of Rome
Antonio Navarra	CMCC
Maurizio Ottaviani	CEA Cadarache
Ignacio Pagonabarraga Mora	University of Barcelona
Olivier Pironneau	LJLL-UPMC
Simon Portegies Zwart	University of Leiden
Kenneth Ruud	University of Tromsø
Wolfgang Schröder	University of Aachen
Christof Schütte	Free University of Berlin
Luis Silva	Instituto Superior Técnico
Dominik Tildesley	EPFL
Joost VandeVondele	ETH Zürich
Claudio Zannoni	University of Bologna

PRACEdays15

From Tuesday 26 May to Thursday 28 May 2015

VENUE

Aviva Stadium, Lansdowne Road, Dublin 4, Ireland

REGISTRATION DESK

The main registration and information desk is situated at the entrance to the Aviva and will be open as follows:

Tuesday 26th May	**08:00 – 18:00**
Wednesday 27th May	**08:00 – 18:00**
Thursday 28th May	**08:00 – 13:00**

REGISTRATION QUERIES

Enquiries for the following should be made at the registration desk:

Accommodation queries & bookings

General information

Social events

Internet access

COFFEE BREAKS AND LUNCHES

Coffee breaks and lunches are all being held in the President's Terrace – adjacent to the main conference room. This is also where the conference posters will be on display

WELCOME RECEPTION

Tuesday 26 May 2015

The AVIVA Stadium Dublin

18:00 – 20:00 the AVIVA Stadium, Dublin

Included in Registration Fee

This reception will take place in the President's Terrace, and will give delegates the opportunity to browse the posters as well as connect with colleagues and friends.

CONFERENCE DINNER

Conference Dinner – Wednesday 27 May 2015 19:30 – 22:00, The Ballsbridge Hotel

This dinner is included in the registration fee.

The Ballsbridge Hotel is situated approximately 10 minute walk from the conference venue.

The map on page 07 will show you exactly where it is located.

Useful Information

TEMPERATURE

Ireland enjoys a temperate climate, with (until recently) mild winters and relatively cool summers. Mean daily temperature in May is 17 °C. Dublin enjoys reasonable sunshine and rain belts reaching the east coast are frequently light and generally clear within a few hours. However it is always wise when travelling to Ireland to pack rain gear or an umbrella.

SHOPPING

Dublin has a busy city centre shopping area around Grafton Street and Henry Street. There is a huge range of products to bring home – from traditional Irish hand-made crafts to international designer labels. Things to buy: woollen knits, tweeds, crystal, Claddagh rings, pottery, silver and music. Shopping hours are from 09.00 to 18.00 Monday to Saturday, with shops open until 20.00 on Thursdays, and many shops open from 14.00 – 18.00 on Sunday.

CURRENCY

The currency in Ireland is the Euro.

CREDIT CARDS

Major credit cards are widely accepted.

SMOKING POLICY

Under Irish law smoking is not permitted in pubs, restaurants, hotel lobbies and all enclosed public buildings.

ELECTRICITY

220 / 240 volts

Please bring a suitable adaptor for type G power sockets

TIME

From March to October, Ireland operates on GMT Greenwich Mean Time + 1.

IMPORTANT NUMBERS

Conference Organisers	+353 1 296 8688
Emergency Number	999 or 112
Taxi	+353 1 6772222
Dublin Tourist Office	+353 1 4370969

WIFI

Delegates can avail of free WiFi at the Aviva Stadium.

WiFi Name:	Stadium WiFi
Password:	No Password

Aviva Stadium

Aviva Stadium is a sports stadium located in Dublin, Ireland, with a capacity for 51,700 spectators (all seated). It is built on the site of the former Lansdowne Road stadium, which was demolished in 2007, and replacing it as home to its chief tenants: the Irish rugby union team and the Republic of Ireland football team.

The stadium, located adjacent to Lansdowne Road railway station, officially opened on 14 May 2010. The stadium is Ireland's first, and only, UEFA Elite Stadium and in 2011, it hosted the Europa League Final. It also hosted the inaugural Nations Cup, as well as the regular home fixtures of the national rugby team, national football team and some home fixtures for Leinster Rugby from August 2010 onwards.

Ballsbridge Hotel ****

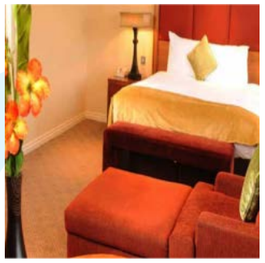
PEMBROKE ROAD, BALLSBRIDGE, DUBLIN 4

Ballsbridge Hotel is located in Dublin's most prestigious postcode and only minutes from the city centre. The rooms are designed with your comfort in mind and The Dubliner traditional pub is a popular venue for both Irish residents and hotel guests with a delicious all-day menu and live music at the weekends.
www.ballsbridgehotel.com


Clyde Court Hotel ****

LANSDOWNE ROAD, BALLSBRIDGE, DUBLIN 4

The jewel in the crown of Hotels in Ballsbridge is the 4 star Clyde Court Hotel, perfect for discerning business executives who expect the red carpet treatment at a fraction of the cost. The elegant Clyde Court Hotel is comprised of 184 fully air conditioned and spacious guest rooms in the sumptuous leafy suburb of Dublin's premier postcode - Dublin 4. Over the years, the Clyde Court Hotel Ballsbridge has been host to many famous celebrities and Heads of State including Nelson Mandela, Frank Sinatra, Madonna, Elton John, and Cher to name but a few, so you'll be in good company.
www.clydecourthotel.com

Pembroke Hotel

90 PEMBROKE ROAD, BALLSBRIDGE, DUBLIN 4

Welcome to Pembroke Townhouse where you can enjoy real Irish hospitality in this Ballsbridge hotel. Pembroke Townhouse boasts 48 COSY en-suite bedrooms equipped with all the modern conveniences that other hotels in Ballsbridge offer but with a personal touch to rival any guest house in Dublin.
www.pembroketownhouse.ie


KEYNOTE SESSIONS

Tuesday 16:00 - 18:00
President's Suite

WELCOME

SERGI GIRONA
Partnership for Advanced Computing in Europe (PRACE)

SERGI GIRONA

Sergi Girona is Chair of the Board of Directors of PRACE, as well as Director of the Operations Department of the Barcelona Supercomputing Center (BSC). He belongs to the BoD of PRACE since its creation in 2010, and currently is both its Chair and Managing Director.

He holds a PhD in Computer Science from the Technical University of Catalunya. In 2001, EASi Engineering was founded and Sergi became the Director of the company for Spain, and the R&D Director for the German headquarters.

In 2004, he joined BSC for the installation of MareNostrum in Barcelona. MareNostrum was the largest supercomputer in Europe at that time, and it maintained this position for 3 years. Sergi was responsible for the site preparation and the coordination with IBM for the system installation. Currently, he is managing the Operations group with the responsibilities for User Support and System Administration of the different HPC systems at BSC.

FOSSILS, PHYSICS AND FAST COMPUTERS UNLOCKING A VIRTUAL PAST

WILLIAM SELLERS
Faculty of Life Sciences, The University of Manchester

ABSTRACT

The past is a fascinating place. It can tell us how we came to be like we are today, and it contains a huge range of bizarre creatures that are no longer alive. However since we do not yet have a suitable time machine, all our knowledge about the distant past comes from evidence preserved in the rocks around us. The most important source of evidence is from fossils. These are the preserved remains of animals and plants and they have been collected and studied by geologists for hundreds of years. However nowadays other disciplines want to get in on the fun. Engineers, physicists and computer scientists have developed techniques that help us find out more about fossil organisms. This talk will concentrate on what we can learn from studying the mechanics of fossil organisms using high performance computers. It will demonstrate the way early humans moved and what this tells us about the origins of moderns humans. It will also show how fast and how heavy the largest dinosaurs were and what this means about the way they lived. But most importantly it will explain how we can actually answer these questions scientifically and avoid some of the guesswork and exageration that has happened in the past

WILLIAM SELLERS

William Sellers is a computational zoologist interested in the use of numerical techniques for investigating morphological, physiological and ecological factors in vertebrate evolution. He has a background in zoology and scientific industrial experience in computer modelling and image analysis. He runs the Animal Simulation Laboratory based at the University of Manchester with current external funding for two full time staff and two PhD students. In 2012, he was awarded a Japan Society for the Promotion of Science visiting fellowship to Kyoto University. He is a member of the NERC peer review panel and a member of the EPSRC grant review college. He is on the editorial board of Folia Primatologia and a fellow of the Higher Education Academy. He was Programme Director of Zoology at Manchester between 2009 and 2012. He has been reelected as a council member for the Primate Society of Great Britain for the 3rd time and recently completed a one year post as the President of the Anthropology and Archaeology Section of the British Science Association. In addition, he does considerable public engagement work including science festivals, museum days, and regular appearances on international television and radio.

His research interests are: Evolution of Vertebrate Locomotion, Ancient Pigment Preservation, Biomechanics (both laboratory and field based), and Comparative Functional Anatomy.

Dr Sellers has over 50 publications.

LISTENING TO BLACK HOLES WITH SUPER COMPUTERS

SASCHA HUSA
Relativity and Gravitation Group at the University of the Balearic Islands

ABSTRACT

One century after Einstein's theory of general relativity has revealed space and time as dynamical entities a new generation of gravitational wave detectors is starting operation, and the first detection of gravitational wave events is expected to push open a new window on the universe within the next 5 years. The experimental challenge to meet the tremendous sensitivity requirements of GW detectors is paralleled by the computational modelling challenge to accurately predict the complicated dependence of the wave signals on the masses and spins of the black holes. In this talk will report on a program to explore the gravitational wave signatures of coalescing black holes by solving the Einstein equations with high order finite difference mesh refinement methods for judiciously chosen cases, and the synthesis of analytical models from our numerical data and perturbative results. These models are already used to analyse data from gravitational wave detectors and will help to identify the first such signals ever to be observed.

SASCHA HUSA

Sascha Husa's research is focused on numerical relativity and black hole physics, more specifically the modeling of sources of gravitational waves with high-performance computing, and he is currently an associate professor at the University of the Balearic Islands in Palma de Mallorca, Spain, which he joined as assistant professor in 2008. Husa is currently co-Principal Investigator (PI) of the UIB gravitational wave effort.

Husa received his PhD from the University of Vienna (Austria) in 1998, and his habilitation in theoretical physics from the University of Jena (Germany) in 2006. He has worked as a postdoctoral research associate at the University of Vienna (1998), University of Pittsburgh (1998-2000), Max-Planck Institute for Gravitational Physics (2000-2005 and 2007-2008) and the University of Jena (2005-2007).

Husa's contributions to numerical relativity range from its mathematical foundations to binary black hole physics and the interface to gravitational wave data analysis, and he has co-authored more than 100 scientific publications, with more than 5800 citations and an h-Factor of 45.

The main focus of his recent work has been the program of "phenomenological waveform modeling", which was started in 2006 as a collaboration involving the Max Planck Institute for Gravitational Physics in Germany, the University of Jena and the University of the Balearic Islands. Taking this programme further, he is currently leading the BBHMAP project, a collaboration of about 20 scientists from Europe, India, South Africa and the USA to use the top level European supercomputing infrastructure to explore the parameter space of black hole binaries and develop analytical waveform models, and he has received a grant of 16.7 million CPU hours in the 3rd PRACE project call (2011-2012), and 37 million hours as a continuation project in the 5th PRACE Call for Proposals for Project Access call (2012-2013).

Since 2006 Husa has given several invited talks at international conferences and summer schools per year, and he has co-organized a number of meetings in the field, most recently the Numerical Relativity-data analysis meeting 2013 in Mallorca and the extended programme "Dynamics of General Relativity" at the Erwin Schrödinger Institute for Mathematical Physics in Vienna in 2011 and 2012.

HPC SIMULATION AT EDF ENABLING ENERGY CHALLENGES

ANGE CARUSO
Information Technologies Program Manager, Electricité de France R&D

ABSTRACT

An industrial utility like EDF needs to better understand the behavior of energy infrastructures like power plants (nuclear, thermal, renewable,…), electrical networks, but also energy management. The objective is to increase safety, performance, lifetime, and optimize processes. To reach these goals, it is necessary to better understand various phenomena met inside the infrastructures, for example: nuclear components (containment building, PWR vessel, steam generator, fuel rods), networks (electrical grids) or energy management (quality of electricity), in order to win margins. This is done using various numerical softwares developed at EDF R&D. The use of HPC simulation allows new approaches and new perspectives. Some applications will be shown.

ANGE CARUSO

Ange Caruso obtained his PhD in 1988, in the field of Energy Transfer and Combustion. From 1989 to 1998, he has worked in the field of CFD, developing softwares using finite elements and finite volumes methods. In 1999, he was project manager in order to numerically simulate the behavior of PWR vessels in EDF nuclear power plants, using CFD, thermal, structural mechanics and neutronics softwares. From 2001 to 2008, he was responsible for various study groups treating about subjects like nuclear accidents, thermal-hydraulics and chemical effects, mechanical behavior on nuclear components, fuel storage, and codes development. In 2008, he was Deputy Manager of Fluids Mechanics, Energy and Environment Department. Since 2012, Ange Caruso is the Information Technologies Program Manager at EDF R&D, driving projects on Advanced Simulation, Information and Communication Technologies, and Complex Systems Modeling.

COCKTAIL RECEPTION AND POSTER PRESENTATIONS

Tuesday 18.00 - 19.30
President's Terrace

PRACE invites you to network with colleagues over a cocktail and discuss the posters with the presenters. The posters will be displayed throughout the conference.

OPENING & KEYNOTES

Wednesday 27 09.00 - 10.30
President's Suite

WELCOME FROM THE LOCAL HOST

JEAN-CHRISTOPHE DESPLAT
Director of the irish Centre for High-End Computing (ICHEC)

JEAN-CHRISTOPHE DESPLAT

Jean-Christophe (JC) Desplat is Director of the Irish Centre for High-End Computing (ICHEC) since 2012. He joined ICHEC in 2005 as Technical Manager and with his expertise and guidance, ICHEC is now one of the leading technology centres in Europe and a sought-after technology partner within industry and semi-state. Prior to joining ICHEC, JC spent ten years at the Edinburgh Parallel Computing Centre (EPCC) in the UK. There, he held a number of technical and European co-ordination roles, including pioneering work leading to the original proposal to establish the Distributed European Infrastructure for Supercomputing Applications (DEISA).

JC is Honorary Professor of Computational Science at the Dublin Institute for Advanced Studies since 2008 and is Adjunct Professor at NUI Galway since 2012. He is a member of the UK EPSRC e-Infrastructure Strategic Advisory Team since 2011 and has served on a number of management and advisory bodies. These include the Digital Humanities Observatory Management Board (2008-2012), the Environmental Protection Agency (EPA) Climate Change Coordination Committee (2008-2013) and the ICT Sub-Committee of the Irish Medical Council (2011-2013).

JC is one of the original authors of the e-INIS white paper describing a vision for the establishment of a National e-Infrastructure in Ireland, and a co-investigator of the €13M Higher Education Authority (HEA) PRTLI4-funded e-INIS project. He is also the Principal Investigator for a number of awards from Science Foundation Ireland (SFI), the HEA, the Dept. of Jobs, Enterprise & Innovation, Dept. of Education & Skills, the Environmental Protection Agency (EPA) and the European Commission FP7.

OPENING ADDRESS

SANZIO BASSINI
Chair of the PRACE Council

SANZIO BASSINI

In 1981 Sanzio Bassini was responsible for the scientific computing systems installed at CINECA. In 1984 he joined the Italian Supercomputer Project that introduced the first supercomputer of this class in Italy. In 1986 he was convenor of the Operating System Committee of the Cray User Group independent conference. In 1989 was responsible for the project to migrate the Consortium production environment towards UNIX. In 1992, he was appointed Team Leader of the CINECA Supercomputing Group. From 1992 to 1996 he has been member of the EC High Performance Computing & Networking EC committee. In 1996, he was appointed CINECA High Performance System Division Manager.

From 2006 to 2009 he was CINECA Director of the System and Technology Department for the Development and Management of CINECA Information System. From 2010, through the delegation from the Italian Ministry of Education University and Research CINECA to represent Italy within the PRACE aisbl for the implementation of the European Supercomputing Research Infrastructure, he was appointed CINECA's Director of the Supercomputing Application & Innovation Department for the development of technical and scientific computing service, innovation and technology transfer activities. In his position of Technical Director since 2006 he is a member of the CINECA Consortium Technical Committee. In his career he has been project leader of many European projects funded by the DG INFSO and by the DG Research and participated in many infrastructure projects in the area of information technology, networking and supercomputing. He is Chair of PRACE Council, since 3 June 2014.

PRESENT STATUS OF RIST IN PROMOTION OF HIGH PERFORMANCE COMPUTING INFRASTRUCTURE IN JAPAN

MASAHIRO SEKI
President of RIST, Japan

ABSTRACT

High Performance Computing Infrastructure (HPCI) has been established in Japan as a platform for the integrated use of high performance computer systems including the K computer. HPCI currently integrates 12 systems to provide hierarchical capability, with the K computer as the flagship. Other supercomputers serve as the second layer systems, which play various unique roles. All the computer systems are connected via a high speed network and are operated with the same policy to realize common operational features such as single-sign-on. The mission of RIST includes: (1) call for proposals, (2) screening and awarding and (3) user support. Roughly speaking, RIST in Japan is like PRACE in Europe.

In his presentation, he will describe the evaluation process including recent results, supporting activities for shared use, promotion activities for industrial use and publication management.

MASAHIRO SEKI

Masahiro Seki is currently the president of RIST (Research Organization for Information Science and Technology). RIST has been serving as the Registered Organization to promote shared use of ther K computer since 2012. He joined RIST in 2006 as the president. He was the Director General of Naka Fusion Research Establishment of Japan Atomic Energy Research Institute (JAERI) for the period of 2003-2006. He graduated from the University of Tokyo in 1969, then joined JAREI. He received his Ph.D. from the University of Tokyo in 1982. His research field includes thermal hydraulics, plasma facing materials and components of fusion reactors. He had supervised the Japanese engineering activities for ITER, which is now under construction in France as the joint project by the 7 parties of China, EU, India, Japan, Korea, France, and USA.

COFFEE BREAK

Wednesday 10.30 - 11.00

KEYNOTES

Wednesday 11.00 - 12.30
President's Suite

TOWARDS EXASCALE: THE GROWING PAINS OF INDUSTRY STRENGTH CAE SOFTWARE

LEE MARGETTS
Research Computing Services The University of Manchester

ABSTRACT

In the Exascale community, there is some concern that commercial computer aided engineering (CAE) software will not be ready to take advantage of Exascale systems when they eventually come online. This talk will consider this issue from three perspectives: (i) Industry end users whose business will benefit from early access to Exascale computers; (ii) Independent software vendors who develop and market engineering software and (iii) Open source software initiatives led by Universities and government laboratories. Each of these stakeholders has a unique set of needs and motivational drivers that, if linked together in a simple and elegant way, can lead to the development, use and exploitation of CAE software on Exascale systems. The Lee Margetts will draw upon academic experience as leader of an open source software project and business insight through roles at NAFEMS and PRACE to set out a possible roadmap towards Exascale CAE.

LEE MARGETTS

Lee Margetts is an expert in large-scale computational engineering. He has more than 15 years experience in HPC and started his career as a consultant in the UK National HPC Service, CSAR (1998-2008). Lee currently holds various posts at the University of Manchester, is a Visiting Research Fellow at the Oxford eResearch Centre, University of Oxford and an Affiliate Research Fellow at the Colorado School of Mines, USA. He leads the open source parallel finite element analysis project ParaFEM and is author of the accompanying text book, "Programming the Finite Element Method". He is an investigator on the EU FP7 European Exascale Software Initiative and his ambition is for ParaFEM to be one of the first engineering applications with Exascale capability. Lee has a particular interest in HPC technology transfer between academia and industry, holding an MBA with distinction in International Engineering Business Management. He contributes to international activities through his roles as Chairman of the NAFEMS HPC Technical Working Group; elected member of the PRACE Industrial Advisory Committee and academic lead on EPSRC's UK-USA HPC Network.

IMPLEMENTING THE EUROPEAN STRATEGY ON HIGH PERFORMANCE COMPUTING

AUGUSTO BURGUEÑO ARJONA
European Commission, DG Communications Networks, Content and Technology

ABSTRACT

HPC is a strategic tool to transform big scientific, industrial and societal challenges into innovation and business opportunities. HPC is essential for modern scientific advances (e.g. understanding the human brain or climate change) as well as for industry to innovate in products and services. “Traditional” areas like manufacturing, oil&gas, pharmaceutical industry etc. consider HPC indispensable for innovation, but also emerging applications (like smart cities, personalized medicine, or cosmetics) benefit from the use of HPC and its convergence with Big Data and clouds. The most advanced countries in the world recognise this strategic role of HPC and have announced ambitious plans for building exascale technology and deploying state-of-the-art supercomputers in the following years.

Europe has the technological know-how and market size to play a leading role in all areas: HPC technologies and systems, services and applications. The European HPC Strategy in Horizon 2020 combines three elements in an integrated and synergetic way: (a) developing the next generations of HPC towards exascale; (b) providing access to the best facilities and services for both industry and academia; and (c) achieving excellence in applications. The Commission has taken several ambitious steps to support this strategy, such as the establishment of a contractual Public Private Partnership (PPP) on HPC. Support to the HPC Strategy is expected to continue in the future Horizon 2020 work programmes.

AUGUSTO BURGUEÑO ARJONA

Augusto Burgueño Arjona is currently Head of Unit “eInfrastructure” at European Commission Directorate General for Communications Networks, Content and Technology. His unit coordinates the implementation of the European HPC strategy as well as the deployment of European research eInfrastructures such as Géant, PRACE, EUDAT, OpenAIRE and the European Grid Initiatiave (EGI). Previously he served as Head of Unit “Finance” Directorate General for Communications Networks, Content and Technology at European Commission and Head of inter-Directorate General Task Force IT Planning Office at European Commission.

LUNCH

Wednesday 12.30 - 13.30

You are invited to join everybody for a group photo immediately before lunch.

SCIENTIFIC SESSIONS

Wednesday 13.30 - 15.30
President’s Suite

EUROPEAN RESEARCH COUNCIL PROJECTS

CHAIR: KENNETH RUUD
The Arctic University of Norway and SSC chair and Outgoing Chair of the PRACE Scientific Steering Committee (SSC)

KENNETH RUUD

Kenneth Ruud received his PhD in theoretical chemistry from the University of Oslo in 1998. He spent two years as a postdoc at the University of California, San Diego/San Diego Supercomputer Centre (USA), before moving to Tromsø (Norway) in 2001. Since 2002 he has been a professor of theoretical chemistry at the University of Tromsø - The Arctic University of Norway, and he has published more than 260 papers in the field of computational chemistry. His main research interests are in the development and application of quantum-mechanical methods for understanding the interaction between molecules and electromagnetic fields, with a particular focus on molecular spectroscopy. He holds since 2011 an ERC Starting Grant entitled “SURFSPEC - Theoretical Spectroscopy of Surfaces and Interfaces”. He is a member of the Centre of Theoretical and Computational Chemistry, a Norwegian Centre of Excellence. He has since 2010 been a member of the PRACE Scientific Steering Committee. 2011-2012 he was the Chairman of the PRACE Access Committee, and 2013-2014 the Chairman of the PRACE Scientific Steering Committee.Note: The S01 will be in slot P1.3 and S03 in P1.1 in the afternoon

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COMPUTATIONAL CHALLENGES IN SKELETAL TISSUE ENGINEERING

LIESBET GERIS
Biomechanics Research Unit, University of Liège

ABSTRACT

Tissue engineering (TE), the interdisciplinary field combining biomedical and engineering sciences in the search for functional man-made organ replacements, has key issues with the quantity and quality of the generated products. Protocols followed in the lab are mainly trial and error based, requiring a huge amount of manual interventions and lacking clear early time-point quality criteria to guide the process. As a result, these processes are very hard to scale up to industrial production levels. In many engineering sectors, in silico modeling is used as an inherent part of the R&D process. In this talk I will discuss a number of (compute intensive) examples demonstrating the contribution of in silico modeling to the bone tissue engineering process.

A first example that will be discussed is the simulation of bioreactor processes. Currently, only a limited number of online read-outs is available which can be used to monitor and control the biological processes taking place inside the bioreactor. We developed a computational model of neotissue growth inside the bioreactor that, in combination with the experimental read-outs, allow for a quantification of the processes taking place inside the bioreactor. Scaffold geometry (curvature-based growth), fluid flow (Brinkman equation) and nutrient supply were simulated to affect the growth rate of the neotissue. The model captured the experimentally observed growth patterns qualitatively and quantitatively. Additionally, the model was able to calculate the micro-environmental cues (mechanical and nutrient-related) that cells experience both at the neotissue-free flow interface and inside the neotissue.

The second example pertains to the assessment of the in vivo bone regeneration process. As normal fractures lead to successful healing in 90-95% of the cases, people in need of tissue engineering solutions often suffer from severe trauma, genetic disorders or comorbidities. One of these genetic disorders impacting the bone regeneration process is neurofibromatosis type I. Starting from an established computational model of bone

regeneration, we examined the effect of the NF1 mutation on bone fracture healing by altering the parameter values of eight key factors which describe the aberrant cellular behavior of NF1 affected cells. We show that the computational model is able to predict the formation of a non-union and captures the wide variety of non-union phenotypes observed in patients. A sensitivity analysis by "Design of Experiments" was used to identify the key contributors to the severity of the non-union.

LIESBET GERIS

Liesbet Geris is professor in Biomechanics and Computational Tissue Engineering at the Department of Aerospace and Mechanical Engineering at the university of Liège and part-time associate professor at the Department of Mechanical Engineering of the KU Leuven, Belgium. From the KU Leuven, she received her MSc degree in Mechanical Engineering in 2002 and her PhD degree in Engineering in 2007, both summa cum laude. In 2007 she worked as a postdoctoral researcher at the Centre of Mathematical Biology of Oxford University.

Her research interests encompass the mathematical modeling of bone regeneration during fracture healing, implant osseointegration and tissue engineering applications. The phenomena described in these mathematical models reach from the tissue level, over the cell level, down to the molecular level. She works in close collaboration with experimental and clinical researchers from the university hospitals Leuven, focusing on the development of mathematical models of impaired healing situations and the in silico design of novel treatment strategies. She is scientific coordinator of Prometheus, the skeletal tissue engineering division of the KU Leuven. Her research is financed by European, regional and university funding. In 2011 she was awarded an ERC starting grant to pursue her research. Liesbet Geris is the author of 43 ISI indexed journal papers, 8 book chapters and over 80 full conference proceedings and abstracts.

HPC FOR COMBUSTION INSTABILITIES IN GAS TURBINES: THE ERC INTECOCIS PROJECT IN TOULOUSE

GABRIEL STAFFELBACH
CERFACS

ABSTRACT

Combustion accounts for 80% of the worlds energy. Ever progressing trends in design and research have and continue to yield spectacular changes for turbines, cars, rocket propulsion etc.. The joint ERC project INTECOCIS coordinated by CNRS (DR14 Midi Pyrénées) and lead by two research centres, Institut de Mécanique des Fluides de Toulouse and CERFACS aims at introducing recent progress in the field of High Performance Computing (HPC) for combustion simulation into studies of Combustion Instabilities. The project integrates experimental and industrial applications to build and validate tools built to predict combustion instabilities using modern high performance computing. This presentation will highlight the recent progress of the project.

GABRIEL STAFFELBACH

Gabriel Staffelbach is a senior researcher at Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS). He has been working on numerical simulation of combustion and high performance computing since 2002 and is an active user of most HPC systems available to the scientific community. His expertise ranges from numerical simulation to computational science as well as combustion instabilities.

RUNTIME AWARE ARCHITECTURES

MATEO VALERO
Director at Barcelona Supercomputing Center (BSC)

ABSTRACT

In the last few years, the traditional ways to keep the increase of hardware performance to the rate predicted by the Moore's Law have vanished. When uni-cores were the norm, hardware design was decoupled from the software stack thanks to a well defined Instruction Set Architecture (ISA). This simple interface allowed developing applications without worrying too much about the underlying hardware, while hardware designers were able to aggressively exploit instruction-level parallelism (ILP) in superscalar processors. With the eruption of multi-cores and parallel applications, this simple interface started to leak. As a consequence, the role of decoupling again applications from the hardware was moved to the runtime system. Efficiently using the underlying hardware from this runtime without exposing its complexities to the application has been the target of very active and prolific research in the last years. Current multi-cores are designed as simple symmetric multiprocessors (SMP) on a chip. However, we believe that this is not enough to overcome all the problems that multi-cores already have to face. It is our position that the runtime has to drive the design of future multi-cores to overcome the restrictions in terms of power, memory, programmability and resilience that multi-cores have. In this talk, we introduce a first approach towards a Runtime-Aware Architecture (RAA), a massively parallel architecture designed from the runtime's perspective.

MATEO VALERO

Mateo Valero, is a professor in the Computer Architecture Department at UPC, in Barcelona. His research interests focuses on high performance architectures. He has published approximately 600 papers, has served in the organization of more than 300 International Conferences and he has given more than 400 invited talks. He is the director of the Barcelona Supercomputing Centre, the National Centre of Supercomputing in Spain.

Dr. Valero has been honoured with several awards. Among them, the Eckert-Mauchly Award, Harry Goode Award, The ACM Distinguished Service award, the "King Jaime I" in research and two Spanish National Awards on Informatics and on Engineering. He has been named Honorary Doctor by the Universities of Chalmers, Belgrade and Veracruz in Mexico and by the Spanish Universities of Las Palmas de Gran Canaria, Zaragoza and Complutense in Madrid. "Hall of the Fame" member of the IST European Program (selected as one of the 25 most influential European researchers in IT during the period 1983-2008, in Lyon, November 2008)

Professor Valero is Academic member of the Royal Spanish Academy of Engineering, of the Royal Spanish Academy of Doctors, of the Academia Europaea, and of the Academy of Sciences in Mexico, and Correspondant Academic of the Spanish Royal Academy of Science, He is a Fellow of the IEEE, Fellow of the ACM and an Intel Distinguished Research Fellow.

COFFEE BREAK

Wednesday 15.30 - 16.00

COMPUTATIONAL DYNAMICS

Wednesday 16.00 - 18.00
Room 442

CHAIR: PETROS KOUMOUTSAKOS
Computational Science Lab, ETH Zürich

PETROS KOUMOUTSAKOS

Petros Koumoutsakos holds the Chair of Computational Science at ETH Zurich. He received his Diploma (1986, National Technical University of Athens) and Master's (1987, University of Michigan, Ann Arbor) in Naval Architecture. He received a Master's (1988) and PhD in Aeronautics and Applied Mathematics (1992) from the California Institute of Technology. He was an NSF fellow in parallel computing (1992-1994, Center for Research on Parallel Computation) at the California Institute of Technology and a research associate (1994-1997) with the Center for Turbulence Research at NASA Ames/Stanford University. He was an assistant professor of Computational Fluid Dynamics (1997-2000) at ETH Zurich and the founding director of the ETH Zurich Computational Laboratory (2000-2007). He was full professor of Computational Science between 2000-2011 in the Department of Computer Science at ETH Zurich and Director of the Institute of Computational Science (2001-2005).

Petros Koumoutsakos has published 1 monograph, 3 edited volumes, 8 book chapters and over 170 peer reviewed articles. He is an elected Fellow of the American Physical Society and Fellow of the American Society of Mechanical Engineers. He is also recipient of the Advanced Investigator Award by the European Research Council (2013) and of the ACM Gordon Bell award in 2013.

COMPUTATIONAL CHALLENGES OF FAST DYNAMICS OF FLOWS WITH PHASE INTERFACES FOR BIOMEDICAL APPLICATIONS

NIKOLAUS ADAMS
Lehrstuhl für Aerodynamik und Strömungsmechanik - TU München

ABSTRACT

The simulation of two-phase flows with compressibility effects and turbulence is one of the current challenges for modern numerical models in predictive simulations. Different approaches promise the most efficient way to solution for different application scenarios. The interaction of phase interfaces with shock waves and the generation of shock waves by rapid phase change are essential flow phenomena for biomedical applications. In this talk we present recent developments in modeling and simulation of compressible flows with interfaces, address efficient computational approaches for interface tracking, multi-resolution approaches, and new physically motivated approaches for dynamic load balancing.

NIKOLAUS ADAMS

Nikolaus Adams recieved a Doctorate in Mechanical Engineering, from the Technische Universität München, Germany. Since 2004, Chair of Aerodynamics and Fluid Mechanics at the Technische Universität München. He has nearly 300 publications and was recipient of the Gordon Bell prize 2013.

His contributions are in flow physics, modelling and simulation of multi-scale flows and complex fluids and the dissemination of fundamental research into applications. Flow physics: Shock-turbulence interaction, shock-interface interaction, Richtmyer-Meshkov instabilities, cavitating flows, phase transition, real-gas mixing and combustion, fluid-structure interaction, contact and interface phenomena Modelling and Simulation: High resolution methods, large-eddy simulation models, physically consistent scale-separation models, smoothed-particle hydrodynamics, interface tracking and capturing methods, weakly-compressible approaches, large-scale simulations Application: Cavitation and erosion prediction, nanoparticle production, microfluidic generation of micro-droplets, chemical propulsion, buffeting in propulsion systems, biofluid mechanics, morphing structures for small aircraft and wind energy, automotive aerodynamics.

HIGH ORDER, SCALE RESOLVING MODELLING FOR HIGH REYNOLDS NUMBER RACING CAR AERODYNAMICS

SPENCER SHERWIN
Faculty of Engineering, Department of Aeronautics at Imperial College London

ABSTRACT

The use of computational tools in industrial flow simulations is well established. As engineering design continues to evolve and become ever more complex there is an increasing demand for more accurate transient flow simulations. It can, using existing methods, be extremely costly in computational terms to achieve sufficient accuracy in these simulations. Accordingly, advanced engineering industries, such as the Formula 1 (F1) industry, is looking to academia to develop the next generation of techniques which may provide a mechanism for more accurate simulations without excessive increases in cost.

Currently, the most established methods for industrial flow simulations, including F1, are based upon the Reynolds Averaged Navier-Stokes (RANS) equations which are at the heart of most commercial codes. There is naturally an implicit assumption in this approach of a steady state solution. In practice, however, many industrial problems involve unsteady or transient flows which the RANS techniques are not well equipped to deal with. In order to therefore address increasing demand for more physical models in engineering design, commercial codes do include unsteady extensions such as URANS (Unsteady RANS), and Direct Eddy Simulation (DES). Unfortunately even on high performance computing facilities these types of computational models require significantly more execution time which, to date, has not been matched with a corresponding increase in accuracy of a level sufficient to justify this costs. Particularly when considering the computing restrictions the F1 rules impose on the race car design.

Alternative high order transient simulation techniques using spectral/hp element discretisations have been developed within research and academic communities over the past few decades. These methods have generally been applied to more academic transient flow simulations with a significantly reduced level of turbulence modelling. As the industrial demand for transient simulations becomes greater and the computer "power per $" improves, alternative computational techniques such as high order spectral/hp element discretisations, not yet widely adopted by industry, are likely to provide a more cost effective tool from the perspective of computational time for a high level of accuracy. In this presentation we will outline the demands imposed on computational aerodynamics within the highly competitive F1 race car design and discuss the next generation of transient flow modelling that the industry is looking to impact on this design cycle.

SPENCER SHERWIN

Spencer Sherwin is the McLaren Racing/Royal Academy of Engineering Research Chair in the Department of Aeronautics at Imperial College London. He received his MSE and PhD from the Department of Mechanical and Aerospace Engineering Department at Princeton University. During his time at Imperial he has maintained a successful research program into the development and application of the high order spectral/hp element techniques with particular application to separated unsteady aerodynamics, biomedical flow and understanding flow physics through instability analysis.

Sherwin's research group also develops and distributes the openware spectral/hp element package Nektar++ which has been applied to direct numerical simulation and stability analysis to a range of applications including vortex flows of relevance to offshore engineering and vehicle aerodynamics and biomedical flows associated with arterial atherosclerosis. He has published over 120 peer-reviewed papers in international journals covering topics from numerical analysis to applied and fundamental fluid mechanics and co-authored a highly cited book on the spectral/hp element method. Currently he is an associate director of the EPSRC/Airbus funded Laminar Flow Control Centre and is the chair of the EPSRC Platform for Research in Simulation Methods (PRISM) at Imperial College London.

SALVINIA-INSPIRED SURFACES IN ACTION

CARLO MASSIMO CASCIOLA
University of Rome “La Sapienza”

ABSTRACT

Surfaces exhibiting extraordinary features exist in nature. A remarkable example is the Salvinia molesta. This water fern, due the presence of small hydrophilic patches on top of rough hydrophobic surfaces, is able to retain air pockets when submerged by stabilizing the resulting Cassie state against positive pressure fluctuations while, at the same time, preventing bubble detachment. A similar strategy is adopted by certain insects and spiders (e.g. Elmis Maugei and Dolomedes triton) to breath underwater, thanks to a stabilized air layer, the so-called plastron.

However, since CWT is a rare event beyond reach of brute force computations, the mechanism of wetting remains elusive and it is still difficult, if not impossible, to predict the transition from the Cassie to the fully wet Wenzel state. Using specialized techniques, it has been recently demonstrated that molecular dynamics is indeed capable to describe the Cassie-Wenzel transition on a simple model system. However, going beyond this proof-of-concept simulations, with the goal of reproducing real hydrophobic coatings and the complex morphology of natural surfaces, requires to combine a smart theoretical approach with a boost in computational resources.

We discuss here the results of massively parallel simulations on top-notch machines combined with advanced statistical mechanics techniques aimed at mimicking the Salvinia leaves and revealing its strategies for airtrapping. As will be shown, the results, obtained by exploiting the full potentialities of the Tier-0 computer architectures made available through the the WETMD project allocated by PRACE, have the potential to inspire next generation, biomimetic, superhydrophobic surfaces, as well as to provide benchmarks for continuum models of wetting and cavitation.

CARLO MASSIMO CASCIOLA

Carlo Massimo Casciola is presently full professor of Fluid Dynamics at the Mechanical and Aerospace Engineering Department of Sapienza University of Rome. He leads a research group working on the Fluid Dynamics of complex flows based at the Mechanical and Aerospace Department of Sapienza University of Rome.

The modus operandi of the group is chiefly theoretical and numerical, oriented to fundamental and numerical modeling. This approach brought the group members to collaborate with scientists belonging to several neighboring disciplines, such as mathematics, physics, material science, chemistry, and biology. The issuing multidisciplinary and multi scale expertise has already proved successful in dealing with such diverse problems as Aerodynamics, Turbulence, Combustion, Drag reduction, Particle Transport, Multiphase Flows, and Interfacial Phenomena like wetting, liquid slippage, and heterogeneous bubble nucleation. After the ERC-Advanced Grant 2013, BIC: Following Bubble form inception to collapse most activity focused on different fundamental aspects of cavitation.

HOT LATTICE QUANTUM CHROMODYNAMICS

Wednesday 13.30 - 15.30
Room 441

CHAIR: SANDOR KATZ
Institute for Theoretical Physics, Eötvös Loránd University, Budapest

SÁNDOR KATZ

Sándor Katz is a professor of physics, head of the Institute for Theoretical Physics at Eötvös Loránd University, Budapest. His research is focused on lattice calculations of Quantum Chromodynamics, the theory of strong interactions. Together with colleagues in the same group and in collaboration with other institutions they try to inderstand the properties of hot strongly interacting matter, such as the phase transition of hadrons to quark-gluon plasma and its equation of state

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SIMULATION OF STRONGLY INTERACTING MATTER FROM LOW TO HIGH TEMPERATURES

STEFAN KRIEG
Forschungszentrum Jülich

ABSTRACT

The rapid transition from the quark-gluon-plasma ‘phase’ to the hadronic phase in the early universe and the QCD phase diagram are subjects of intense study in present heavy-ion experiments (LHC@CERN, RHIC@BNL, and the upcoming FAIR@GSI). This transition can be studied in a systematic way in Lattice QCD. We report on a continuum extrapolated result for the equation of state (EoS) of QCD with and without dynamical charm degree of freedom. With these results, we will be able to close the gap between the low temperature region, which can be described by the hadron resonance gas model, and the high temperature region, which can be described by (hard thermal loop) perturbation theory. For all our final results, the systematics are controlled, quark masses are set to their physical values, and the continuum limit is taken using at least three lattice spacings.

STEFAN KRIEG

Stefan Krieg received his PhD in physics from Wuppertal University. He held Post-Doctoral positions at Forschungszentrum Jülich, Wuppertal University, and MIT. He is currently responsible for the Simulation Laboratory Nuclear and Particle Physics at Jülich Supercomputing Centre, Forschungszentrum Jülich. His research is focussed on Lattice Quantum Chromodynamics.

FROM QUARK NUMBER FLUCTUATIONS TO THE QCD PHASE DIAGRAM

CHRISTIAN SCHMIDT
University of Bielefeld

ABSTRACT

For the first few micro-seconds after the Big Bang, the universe was filled with a plasma of strongly interacting quarks and gluons, the QGP. Today, small droplets of QGP are created in heavy ion experiments. Recently, large experimental effort was undertaken to explore the phase diagram of QCD through a beam energy scan program of heavy ion collisions. We will review Lattice QCD computations of conserved charge fluctuations that are performed in order to make contact with these experiments. We then show that a comparison of fluctuations of conserved hadroinc charged from lattice QCD with experimental results allows to position the

so called freeze-out points on the QCD phase diagram.

Computational challenges, that boil down to a tremendous amount of inversion of large sparse matrices will be highlighted. Here, the method of choice is the iterative conjugate gradient solver, which in our case is bandwidth limited. On GPUs, e.g., we approach this problem by exposing more parallelism to the accelerator through inverting multiple right hand sides at the same time.

CHRISTIAN SCHMIDT

Schmidt received his PhD from Bielefeld University in 2003. After research appointments at the University of Wuppertal, the Brookhaven National Laboratory and the Frankfurt Institute for Advanced Studies, he is now back in Bielefeld, where his is currently holding a senior researcher position. He is an expert on the field of QCD simulations at nonzero temperature and density and has pioneered investigations of the QCD phase diagram through Taylor expansion. As a member of two large international collaborations, the HotQCD and the BNL-Bielefeld-CCNU.

LATTICE SIMULATIONS OF STRONG INTERACTIONS IN BACKGROUND FIELDS

MASSIMO D'ELIA
University of Pisa & INFN

ABSTRACT

The study of strong interactions in the presence of external sources, such as electromagnetic background fields or chemical potentials, offers the possibility to investigate the properties of strongly interacting matter in unusual conditions, which may be relevant to many contexts, going from heavy ion experiments to the physics of the Early Universe. Due to the non-perturbative nature of the problem, numerical lattice simulations are the ideal tool to obtain answers based on the first principles of Quantum Chromodynamics (QCD), which is the theory of strong interactions.

The last few years have seen a considerable and steady progress in the field. Because of the extremely high computational needs of the problem, this has been possible also due to a matching development in HPC infrastructures. In this talk I will review such progress, with a focus on results regarding the physics of QCD in strong magnetic fields.

MASSIMO D'ELIA

Massimo D'Elia received his degree in Physics from Scuola Normale Superiore and the University of Pisa, and his PhD in Physics from the University of Pisa in 1994 and 1998, respectively.

Associate Researcher at the University of Cyprus and at ETH Zurich in 1997 and 1998, Postdoc Fellow at the University of Pisa in 1999, Assistant Professor in Theoretical Physics at the University of Genoa (2000-2011). Since 2011 he is Associate Professor in Theoretical Physics at the Physics Department of the University of Pisa.

He is author of 170 publications in refereed journals and conference proceedings. His research is dedicated to the study of fundamental interactions, with a focus on the investigation of the properties of strongly interacting matter in extreme conditions by lattice QCD simulations.

COFFEE BREAK

Wednesday 15.30 - 16.00

MOLECULAR SIMULATIONS

Wednesday 16.00 - 18.00
Room 441

CHAIR: ILPO VATTULAINEN

Department of Physics at the Tampere University of Technology

ILPO VATTULAINEN

Ilpo Vattulainen is working as a professor at the Department of Physics, Tampere University of Technology (Finland). He is the director of the Biological Physics group (comprised of about 45 people), which focuses on molecular-scale simulations of biological systems, with a focus on lipids, proteins, and carbohydrates associated with cell membranes. He is the vice-chair in the Center of Excellence in Biomembrane Research chosen by the Academy of Finland for 2014-2019. He is also the principal investigator in an ERC Advanced Grant project, acts as the chair of the Customer Panel at the CSC – IT Center for Science (Espoo, Finland), and is a member of the Executive Committee of the European Biophysical Societies' Association. His group has been an active member of PRACE, CECAM, and other computational activities.

EFFICIENT LENNARD-JONES LATTICE SUMMATION TECHNIQUES FOR LIPID BILAYERS

ERIK LINDAHL
Department of Biochemistry and Biophysics at the University Stockholm

ABSTRACT

The introduction of particle-mesh Ewald (PME) lattice summation for electrostatics 20 years ago was a revolution for membrane simulations. It got rid of horrible cutoff effects, and removed the electrostatics cutoff's influence on important properties such as area and volume per lipid. However, over the last decade it has become increasingly obvious that the Lennard-Jones cutoff is also highly problematic. Dispersion corrections are not sufficient for membranes that are neither isotropic nor homogenous - altering the cutoff will still alter properties. Here I will present a new highly efficient and parallel technique for LJPME that is part of GROMACS version 5. We have solved the historical problem with Lorentz-Berthelot combination rules in lattice summation by introducing a series of approximations, first by using geometric combination properties in reciprocal space, and now also correcting for this difference in direct space terms. Not only does this improve molecular simulation accuracy by almost an order of magnitude, but it also achieves absolute LJPME simulation performance that is an order of magnitude faster than alternatives - in many cases it is within 10% of the previous cutoff performance in GROMACS.

ERIK LINDAHL

Erik Lindahl holds a PhD in Theoretical Biophysics, from KTH, Stockholm, Sweden. He is currently Professor of Biophysics, in the Dept. Biochemistry & Biophysics, Stockholm University and Professor of Theoretical Biophysics, at KTH Royal Institute of Technology. He was appointed Senior Research Fellow of the Swedish Research Council on Bioinformatics. He was and is principal investigator in numerous national end European research projects. He serves on the board of directors for the Swedish National Infrastructure for Computing leadership. He is the vice director, Swedish e-Science Research Center and a member of the PRACE Scientific Steering Committee. Erik Lindahl authored over 85 scientific publications.

ON THE ACTIVATION AND MODULATION OF VOLTAGE GATED ION CHANNELS

MOUNIR TAREK
CNRS & Université de Lorraine

ABSTRACT

Excitable cells produce electrochemical impulses mediated by the transport of ions across their membrane through proteins pores called ion channels. The most important family of channels propagating an electrical signal along the cell surface is the voltage-gated ion channel (VGCs) family. VGCs are essential physiological effectors: they control cellular excitability and epithelial transport. A myriad of genetic mutations found in the genes encoding their subunits cause channel malfunction. These so-called channelopathies have been incriminated in a variety of diseases, including, among others, epilepsy, pain syndromes, migraines, periodic paralyses, cardiac arrhythmias, hypertension and hypotension. Contemporary research will benefit from new insights into the minute molecular details in play which can contribute to a fine understanding of VGCs function, as well as its modulation by the environment or its disruption by specific mutations.

The working cycle of VGCs involves the complex conformational change of modular protein units called voltage sensor domains (VSDs). For over forty years, these rearrangements have been recorded as “gating” currents, intensities and kinetics of which are unique signatures of VGC function. In this Talk we show that the atomistic description of VSD activation obtained by molecular dynamics simulations and free energy calculations is consistent with the phenomenological models adopted so far to account for the macroscopic observables measured by electrophysiology. Most importantly, by providing a connection between microscopic and macroscopic dynamics, our results pave the way for a deeper understanding of the molecular level factors affecting VSD activation, such as lipid composition, amino acid mutations, and binding of drug molecules or endogenous ligands.

MOUNIR TAREK

Tarek is a Director of Research (DR2) CNRS, UMR 7565, CNRS-University of Lorraine, Vice-Chair of the department SRSMC (Structure and Reactivity of Complex Molecular Systems) with over 50 scientists. He is Member of the Steering committee of the Doctoral school “SESAMES”, Coordinator of the Physics Section of the ERASMUS exchange program for the University of Lorraine, and member of the Scientific Management Committee of the International Associated Laboratory EBAM that regroups eight major labs from France and Slovenia focussing on Electroporation based technologies and Treatments.

His research involves the use of computational methods to study membranes, proteins, ion channels and membrane transport proteins. The overall aim is to understand the relationship between (dynamic) structure and physiological function of membrane proteins. We are using molecular dynamics approaches to explore the conformational dynamics of proteins, and to relate their dynamical properties to biological function, and methods of structure prediction for proteins for which high-resolution structural data remain undetermined. We have expertise in rigorous atomistic MD simulations of potassium channels, and in particular of the voltage gated ones. Over the last 8 years, we studied many aspects of these channel properties, among which the effect of voltage sensor domain mutations and modulation by lipids, on the function of the channel. We have recently been allocated 140 million core hours by PRACE to study voltage gated channels kinetics.

EFFECT OF HYDROPHOBIC POLLUTANTS ON THE LATERAL ORGANIZATION OF BIOLOGICAL MODEL MEMBRANES

LUCA MONTICELLI
Institut de Biologie et Chimie des Protéines CNRS

ABSTRACT

Cell membranes have a complex lateral organization featuring domains with distinct composition, also known as rafts, which play an essential role in cellular processes such as signal transduction and protein trafficking. In vivo, perturbation of membrane domains (e.g., by drugs or lipophilic compounds) has major effects on the activity of raft-associated proteins and on signaling pathways. In live cells, membrane domains are difficult to characterize because of their small size and highly dynamic nature, so model membranes are often used to understand the driving forces of membrane lateral organization. Studies in model membranes have shown that some lipophilic compounds can alter membrane domains, but it is not clear which chemical and physical properties determine domain perturbation. The mechanisms of domain stabilization and destabilization are also unknown.

Here we describe the effect of six simple hydrophobic compounds on the lateral organization of phase - separated model membranes consisting of saturated and unsaturated phospholipids and cholesterol. Using molecular simulations, we identify two groups of molecules with distinct behavior: aliphatic compounds promote lipid mixing by distributing at the interface between liquid-ordered and liquid-disordered domains; aromatic compounds, instead, stabilize phase separation by partitioning into liquid-disordered domains and excluding cholesterol from the disordered domains. We predict that relatively small concentrations of hydrophobic species can have a broad impact on domain stability in model systems, which suggests possible mechanisms of action for hydrophobic compounds in vivo.

LUCA MONTICELLI

Luca Monticelli received a PhD in Chemistry from the University of Padova, Italy. He is at present Senior Researcher at the Institut de Biologie et Chimie des Protéines (CNRS, UMR 5086), Lyon, France.

His main interest is in membrane biophysics and in the interaction between biological membranes and nano-sized particles. In particular, he is interested in understanding how biological macromolecules (peptides, proteins) and man-made materials (carbon nanoparticles, industrial polymers, common pollutants) enter biological membranes and perturb their structure, dynamics, and function.

The main tools in his research are molecular simulations at different levels, from ab initio to atomistic and coarse-grained models. His research is coupled to the development of theoretical and computational methodologies for the study of complex biological systems, in the spirit of multi-scale modeling. Since 2005 he collaborates at the development of the MARTINI coarse-grained force field, which has emerged as one of the most powerful and most widely used model for studying large-scale behavior of biological macromolecules. Dr. Monticelli is the author of over 50 peer-reviewed papers.

HPC IN INDUSTRY

Wednesday 13.30 - 15.30
Room 442

HPC IN INDUSTRY IN IRELAND

CHAIR: LEO CLANCY
Division Manager ITC, IAD Ireland

LEO CLANCY

Leo heads IDA Ireland's Technology, Consumer and Business Services. IDA's role is to market Ireland to multi-nation investors and to support established investors in Ireland.

Prior to joining IDA Leo worked in the telecommunications industry, spending 13 years with Ericsson in engineering and management roles. This was followed by more than four years leading the technology function for an Irish fibre communications company. Leo holds a degree in Electronics Engineering from Dublin Institute of Technology.

SUBSURFACE IMAGING OF THE EARTH FOR EXPLORATION: METHODS AND HPC NEEDS

GARETH O'BRIEN
Tullow Oil

ABSTRACT

Imaging the subsurface of the Earth is a challenging task which is fundemental in determining resource location and management. Seismic wave propagation through the Earth is a key tool in geophysics and one of the best available methods for imaging the subsurface and studying physical processes in the Earth. Seismic imaging has moved from ray based imaging operators to numerical solutions to wave equations, usually termed full wavefield imaging. This methodology requires high performance computational (HPC) resources. The most recently implemented tools for imaging are Reverse Time Migration (RTM) and Full Wavefield Inversion (FWI). RTM imaging has been shown to be highly beneficial in imaging in complex geological regions whilst FWI has been used to develop high resolution velocity models, which leads to better subsurface images. The practical implementation needs expertise in imaging and in running HPC applications to reduce the overheads, not just in CPU costs but in turn-around times for quicker business decisions. As more expensive imaging tools are continually being developed, the size of the data being recorded in the field has approached the petabyte scale per survey. Thus, there is a continuing need for HPC, not just on cutting edge imaging algorithms but for updating traditional imaging codes. This presentation will discuss seismic imaging trends from a non-specialist point of view with focus on industry applications. The overall message being, the seismic exploration industry is still pushing the upper barrier of computational geophysics on HPC resources for processing and imaging methods. To extract the maximum benefit and throughput and minimise costs in CPU spend, a combination of cutting edge tools, advanced imaging specialists and geophysicists/physicists highly skilled in HPC are required.

GARETH O'BRIEN

Gareth O'Brien is currently a Lead Geophysicist in the Geophysical Technology and Operations Team at Tullow Oil plc working on all aspects of seismic imaging from building tools for wave propagation in challenging regions to running imaging projects. Along with the focus on imaging, a large aspect of the work involves technology evaluation and innovation within the geophysics group. He has been with Tullow Oil since September 2011, prior to that, he was been employed as a Senior Research Fellow in the School of Geological Sciences, University College Dublin, Ireland. His research focused on two main areas i) Computational Seismology and ii) Geophysical fluid dynamics: These topics have been applied to across a wide selection of problems including Earthquake gneiss, volcano seismology, passive and reactive containment transport, glacier dynamics and CO2 sequestration.

THE DNA DATA DELUGE - A PARALLEL COMPUTING APPROACH

BRENDAN LAWLOR
nSilico

ABSTRACT

A Formula 1 engine is powerful, highly engineered and capable of tremendous numbers of revolutions per second. To win races with such an engine, it's necessary to house it in a suitable chassis, and make sure that it gets fuel quickly. Similarly, a fast low-level algorithm, developed with a deep understanding of the target processor, needs to be correctly housed and fed in order to convert that sheer power into a useful solution.

NSilico is an Irish based SME that develops software to the life sciences sector, providing bioinformatics and medical informatics systems to a range of clients. Processing the exponentially growing amount of genomic sequence data is a major challenge to those clients. The Formula 1 engine in question is a SIMD C-language implementation of the Smith-Waterman algorithm, presented as a project of the PRACE SHAPE programme to this conference last year.

This talk outlines the technical challenges in harnessing this powerful implementation into a scalable, resilient service cluster at relatively low cost. The presented proof of concept solution uses the Scala language and the Akka framework to demonstrate how two primary abstractions - the Actor and the Stream - are suited to this task.

BRENDAN LAWLOR

Brendan Lawlor is NSilico's team leader in parallel computing and is a graduate of University College Cork and the Cork Institute of Technology. He is a practising software engineer with 25 years of experience in building enterprise systems in a variety of sectors and using a variety of platforms and technologies.

His current roles include providing Software Process and Architecture services to commercial software companies. In this capacity he designs and maintains software development infrastructure, he architects solutions for bespoke software systems, and executes those solutions using C++ and Java, and more recently Scala. He is also working towards a doctorate in Bioinformatics, with a view to putting the software engineering values he has acquired over his career to the service of this new and exciting field, and at the same time developing new skills in High Performance Computing and Big Data processing.

AN IRISH SME'S VIEW OF BIG DATA ANALYTICS

DAVE CLARKE
Asystec

ABSTRACT

The presentation will focus on giving a perspective on the relevance of Big Data Analytics to an Irish SME. With various assessments of where big data is on Gartner's Innovation Hypecycle, Dave's talk will review some of the key development tracks that big data has taken over the last 5 years. He will note some of the key challenges that he sees for Irish SME's notably the changing big data technology landscape and the need to collaborate with new people both internal and external to the organisation. These new stakeholders have diverse backgrounds and needs from DNA gene sequencing to supply chain administration to call centre service optimisation.

DAVE CLARKE

Dave Clarke joined Asystec in 2014 as Chief Data Scientist. Dave is leading the development of the new Asystec Big Data division, as well as the new multi-technology Executive Briefing Centre in Limerick.

Dave has worked in the IT industry for 20 years in software consulting, management consulting, project, program, and engineering team management, solutions

architecture, technology evangelist and data science roles. Dave has most recently been working with the EMEA start-up of Entercoms, a Dallas based supply chain analytics company. Previous to this, he spent 14 years with EMC. This included working with Pivotal/Greenplum, the cornerstone division of EMC's Big Data Analytics drive, where he spent his time consulting with senior business executives 1-to-1 and in large forums across the EMEA region. Previous to Greenplum, Dave worked in EMC's Solutions Group leading large multi-disciplinary teams developing EMC Proven Solutions in infrastructure management for Microsoft, Oracle and Greenplum Data Warehouse Appliance systems. Dave holds a Bachelor of Science degree in Applied Mathematics and Computing from the University of Limerick and a Masters of Science degree in Technology Management from University College Cork.

COFFEE BREAK

Wednesday 15.30 - 16.00

HPC IN INDUSTRY

Wednesday 16.00 - 18.00
President's Suite

CHAIR: LEE MARGETTS
Research Computing Services The University of Manchester

LEE MARGETTS

Lee Margetts is an expert in large-scale computational engineering. He has more than 15 years experience in HPC and started his career as a consultant in the UK National HPC Service, CSAR (1998-2008). Lee currently holds various posts at the University of Manchester, is a Visiting Research Fellow at the Oxford eResearch Centre, University of Oxford and an Affiliate Research Fellow at the Colorado School of Mines, USA. He leads the open source parallel finite element analysis project ParaFEM and is author of the accompanying text book, "Programming the Finite Element Method". He is an investigator on the EU FP7 European Exascale Software Initiative and his ambition is for ParaFEM to be one of the first engineering applications with Exascale capability. Lee has a particular interest in HPC technology transfer between academia and industry, holding an MBA with distinction in International Engineering Business Management. He contributes to international activities through his roles as Chairman of the NAFEMS HPC Technical Working Group; elected member of the PRACE Industrial Advisory Committee and academic lead on EPSRC's UK-USA HPC Network.

ON THE IMPACT OF AUTOMATIC PARALLELIZATION IN TECHNICAL COMPUTING FOR SCIENCE AND INDUSTRY

MANUEL ARENAZ
University of Coruña & CEO of Appentra Solutions

ABSTRACT

High Performance Computing is a key enabling technology to solve the big challenges of modern society and industry. The development of HPC programs is a complex, error-prone, tedious undertaking that requires a highly-skilled workforce well trained in HPC methods, techniques and tools. In the years to come, a large number of HPC experts are expected to retire. Thus, there is a growing urgency in mending the HPC talent gap, especially in market segments such as Oil&Gas and R+D/Government where HPC is competitive advantage.

Parallelism is the primary source of performance gain in modern computing systems, and compiler technology is at the heart of many developer tools available in the HPC marketplace. Thus, automatic parallelization is a key approach to address the HPC talent gap as it decouples the development of HPC programs from the features and complexity of the underlying parallel hardware. Overall, parallelizing compilers enable experts to focus on computational science and engineering methods, techniques and tools, getting them rid of learning HPC methods, techniques and tools.

Automatic parallelization is a long-lasting challenge for the HPC community. There have been many efforts world-wide in academia and industry to build parallelizing compilers that effectively convert sequential scientific programs into parallel-equivalents. Well-known examples are ICC, PGI, GCC, Polaris, SUIF, Pluto,... Recent advances in compiler technology to automatically extract parallelism from sequential scientific codes have solved the limitations of classical dependence analysis technology. A new hierarchical dependence analysis technology has been transferred from academia to industry by Appentra Solutions. The resulting product is Parallware, a new source-to-source parallelizing compiler for C programs that supports the OpenMP parallel programming standard. This talk will analyze the state-of-the-art in parallelizing compilers as well as their impact in modern science and industry from the point of view of performance, portability and productivity.

MANUEL ARENAZ

Manuel Arenaz is CEO at Appentra Solutions and professor at the University of A Coruña (Spain). He holds a PhD in Computer Science from the University of A Coruña (2003) on advanced compiler techniques for automatic parallelization of scientific codes. His specialty are compiler techniques for automatic extraction of parallelism and for automatic generation of parallel-equivalent code for a variety of multi/many-core computer systems. He has experience in the parallelization of a wide range of numerical methods using main parallel programming standards (e.g., MPI, OpenMP, OpenACC, vectorization/simdization). Recently, he co-founded Appentra Solutions to commercialize products and services that take advantage of the new Parallware technology. Parallware is a new source-to-source parallelizing compiler that automates the tedious, error-prone and time-consuming process of parallelization of full-scale scientific codes.

A SELF-MANAGED HPC CLOUD ECOSYSTEM FOR SIMULATION AND COLLABORATION

NICOLAS TONELLO
Director, Constelcom

ABSTRACT

Simulations, whether for virtual engineering, life sciences, or data processing and analysis in general are becoming essential to the creation of innovative products and scientific discoveries. Simulating ever larger and more complex problems to replace experiments or prototyping requires the kind of High Performance Computing (HPC) power traditionally only available in national research centres. However, whilst HPC capability is growing very fast, true supercomputing remains a specialist area often delegated to computing specialists as opposed to engineering and science discoverers, which restricts its uptake.

In this talk, we will present some of the ideas and concepts which we have evolved over the last five years to address the challenges and common requirements for all end-users and simulation applications, in order to foster Highly Collaborative Computing (HCC) supported by HPC and encourage utilisation by a much wider community of non-specialists through ease of access, ease of use and self-management, and which have led to the deployment of the first instance of ConstellationTM on the Hartree Centre's systems in the UK. The key elements and the need for close collaboration and interaction with supercomputing centres in order to develop this HPC Cloud ecosystem will be discussed, as well as plans for future developments and possibilities as wells as challenges to expand and create a pan-European connected community of users and resources.

NICOLAS TONELLO

Nicolas Tonello obtained a PhD in Aerospace Engineering, from the University of Michigan. Then he became multiphase flow and combustion projects leader for R&D and commercial editors in the USA and the UK, developing physical models and software for Computational Fluid Dynamics (CFD). In 2007 he became founder and Director of Renuda UK in London to provide consulting and software development CFD services in Europe.

In 2013 he founded Constelcom Ltd, to realise a larger, global vision for all simulation applications and activities requirements, different software delivery models, remote collaboration, and High Performance Computing (HPC).

Monday 25 May 2015

12.30		
12.30	**Women in HPC** Ballsbridge Hotel	**Scientific Steering Committee** (SSC) Meeting (invitation only) Ballsbridge Hotel
14.30	Coffee break	
15.00	**Women in HPC** Ballsbridge Hotel	**Scientific Steering Committee** (SSC) Meeting (invitation only) Ballsbridge Hotel
18.00		

Tuesday 26 May 2015

09.00	**Women in HPC** Ballsbridge Hotel	**Exascale** Aviva Stadium	**Scientific Steering Committee** (SSC) Meeting (invitation only) Ballsbridge Hotel
10.30	Coffee		
11.00	**Women in HPC** Ballsbridge Hotel	**Exascale** Aviva Stadium	**Scientific Steering Committee** (SSC) Meeting (invitation only) Ballsbridge Hotel
12.30	Lunch		
13.30	**Women in HPC** Ballsbridge Hotel	**Exascale** Aviva Stadium	**Registration** PRACEdays15
15.30	Coffee		
16.00	*President's Suite* **Welcome** Sergi Girona William Sellers **Fossils, physics and fast computers: unlocking a virtual past** Sascha Husa **Listening to black holes with supercomputers** Ange Caruso **HPC Simulation at EDF enabling energy challenges**		
18.00	**Cocktail Reception** and **Poster Sessions** *at Aviva Stadium President's Terrace*		

Wednesday 27 May 2015

09.00	*President's Suite* **Opening and Welcome** Sanzio Bassini, JC Desplat Masahiro Seki **Present Status of RIST in Promotion of High Performance Computing Infrastructure in Japan**		
10.30	Coffee		
11.00	Lee Margetts **Towards Exascale: The growing pains of industry strength CAE software** Augusto Burgueño Arjona **Implementing the European Strategy on High Performance Computing**		
12.30	Group Photo and Lunch		
13.30	*President's Suite* **European Research Council Projects** Session chair: Kenneth Ruud Liesbet Geris **Computational challenges in skeletal tissue engineering** Gabriel Staffelbach **HPC for combustion instabilities in gas turbines: the ERC INTECOCIS project in Toulouse** Matteo Valero **Runtime Aware Architectures**	*Room 441* **Hot Lattice Quantum Chromodynamics** Session chair: Sandor Katz Stefan Krieg **Simulation of strongly interacting matter from low to high temperatures** Christian Schmidt **From quark number fluctuations to the QCD phase diagram** Massimo D'Elia **Lattice simulations of strong interactions in background fields**	*Room 442* **HPC in Industry in Ireland** Session chair: Leo Clancy Gareth O'Brien **Subsurface Imaging of the Earth for exploration: Methods and HPC needs** Brendan Lawlor **The DNA Data deluge - a parallel computing approach** Dave Clarke **An Irish SME's view of Big Data Analytics**
15.30	Coffee		
16.00	*Room 442* **Computational Dynamics** Session chair: Petros Koumoutsakos Nikolaus Adams **Computational challenges of fast dynamics of flows with phase interfaces for biomedical applications** Spencer Sherwin **Spectral/hp element modelling of high Reynolds number complex geometry flows** Carlo Massimo Casciola **Salvinia-inspired surfaces in action**	*Room 441* **Molecular Simulations** Session chair: Ilpo Vattulainen Erik Lindahl **Large-scale ensemble simulation for efficient sampling of biomolecular systems** Mounir Tarek **On the activation and modulation of voltage gated ion channels** Luca Monticelli **Effect of hydrophobic pollutants on the lateral organization of biological model membranes**	*President's Suite* **HPC in Industry** Session chair: Lee Margetts Manuel Arenaz **On the impact of automatic parallelization in technical computing for science and industry** Nicolas Tonello **A self-managed HPC Cloud ecosystem for simulation and collaboration** Stefano Cozzini **Establishing HPC computational environments in industry: a view from inside**
18.00	**PRACE User Forum -**	**Free for All Session**	
19.00	**Networking Cocktail at**	**Ballsbridge Hotel**	
19.30	Dinner at Ballsbridge Hotel		

Thursday 28 May 2015

09.00	*President's Suite* Leo Clancy **International Technology Investment & HPC** Detlef Lohse **Towards ultimate Rayleigh-Benard and Taylor-Couette turbulence**		
10.30	Coffee		
11.00	**Panel Discussion** moderated by Tom Wilkie, Scientific Computing World **Science and Industry: Partners for Innovation** Sylvie Joussaume, INSU/CNRS Mateo Valero, Barcelona Supercomputing Center Anders Rhod Gregersen, Vestas Augusto Burgueño Arjona, European Commission **Award Presentation and Closing**		
12.30	Lunch		
13.30	**Industrial Advisory Committee** (IAC) (invitation only)	**User Forum (UF) Programme Committee** (invitation only)	**EESI2** Final Conference
15.30	Coffee		
16.00	**Industrial Advisory Committee (IAC)** (invitation only)		**EESI2** Final Conference

Friday 29 May 2015

09.00	**EESI2** Final Conference
10.30	Coffee
11.00	**EESI2** Final Conference
12.30	Lunch

As director of Constelcom Ltd, he is leading the development and delivery of ConstellationTM, a user-centric, web enabled, highly scalable platform with exceptional access and user experience to open up supercomputing and collaboration to all engineering, science and data processing communities. Our vision is to provide an all-encompassing, application agnostic environment for members to carry out all virtual engineering tasks, collaboratively and with seamless access to simulation software and HPC resources.

ESTABLISHING HPC COMPUTATIONAL ENVIRONMENTS IN INDUSTRY: A VIEW FROM THE INSIDE

STEFANO COZZINI
CEO eXact Lab

ABSTRACT

Stefano Cozzini will present the experience of an innovative startup to provide HPC computational environment in industry and beyond. eXact lab srl, founded just three years ago with the aim to provide High performance Computing services is still in its start-up phase but it is gaining experience and learning how to promote and establish what we define as an HPC computational environment f outside a purely research and academic world. Our idea of a computational environment will be discussed and some successful case studies illustrated. He will then close discussing the challenges ahead of us.

STEFANO COZZINI

Stefano Cozzini has over 15 years experience in the area of scientific computing and HPC computational e-infrastructures.

He is presently development scientist at CNR/IOM c/o Sissa in Trieste and CEO of exact lab srl, a company which he has cofounded in 2011 as a spin-off company of hist CNR/IOM institute. The company provides advanced computation services in the HPC arena and it is operating on wide range of services for several customers.

He has considerable experience in leading HPC infrastructure projects at national and international level. He served as Scientific Consultant for the International Organization Unesco, from 2003 to 2012, and UNDP/UNOPS during 2011 and 2012.

From 2014 he is also coordinator of the International Master in High Performance Computing promoted by Sissa and ICTP.

PRACE USER FORUM

Wednesday 18.00 - 19.00

PRACE User Forum Free For All Session

CHAIR: KOEN HILLEWAERT
CENAERO

ABSTRACT

The role of the PRACE User Forum (UF) is to provide a communication channel between the user community and the resource providers, as well as to sustain an open exchange forum between users. To both ends, open discussions are held during the general assembly organised at the occasion of the PRACEdays15, complemented with dedicated sessions at domain specific conferences.

All researchers that have participated in a PRACE computational project during the last 5 years can contribute to the User Forum. The activities of the UF are streamlined by the programme committee, who is responsible for the organisation of the sessions, as well as for summarizing and presenting the results of these discussions to PRACE aisbl and the concerned resource providers.

Previously identified discussion points concern project review, the need for enabling complex workflows, data retention policy and resource usage problems. These points will also be discussed during this general assembly, together with any new issues brought up by the participants. Also the renewal of the Programme Committee will be a part of the discussion.

PRESENT MEMBERS OF THE PROGRAMME COMMITTEE ARE:

Koen Hillewaert (chair), Cenaero, koen.hillewaert@cenaero.be
Turlough Downes, Dublin City University, turlough.downes@dcu.ie
Derek Groen, University College London, d.groen@ucl.ac.uk
Troels Haugbolle, University of Copenhagen, haugboel@nbi.dk
Gabriel Staffelbach, Cerfacs, gabriel.staffelbach@cerfacs.fr
Gustavo Yepes, Universidad Autonoma de Madrid, gustavo.yepes@uam.es

KOEN HILLEWAERT

Koen Hillewaert is the current chair of the PRACE User Forum. He is active in the development of CFD algorithms for nearly 20 years at VKI, Numeca and currently at Cenaero. He presently leads the Argo group, whose main activity concerns the numerical and industrial development of an adaptive high order and strongly scalable CFD code based on the discontinuous Galerkin method. This code aims at enablinga reliable and time-economic use of highly resolved LES of turbomachinery flows during design.

Within PRACE, the Argo group was awarded the industrial pilot “noFUDGE” and the two year project “PAdDLES”. The Argo group also occupies a prominent position in the high-order community, through its participation to the European research projects Adigma and IDIHOM, and the organisation of the international workshops on high-order CFD methods.

KEYNOTES AND PANEL

Thursday 09:00 - 12.30
President's Suite

INTERNATIONAL TECHNOLOGY INVESTMENT & HPC

LEO CLANCY
Division Manager ITC, IAD Ireland

ABSTRACT

Leo Clancy will focus in his presentation on global trends in international technology investment. His work at IDA (Industrial Development Authority) Ireland means that he has significant experience of this area. He will outline some of the areas where he sees HPC becoming more and more important in terms of these trends.

LEO CLANCY

Leo heads IDA Ireland's Technology, Consumer and Business Services. IDA's role is to market Ireland to multi-nation investors and to support established investors in Ireland. Prior to joining IDA Leo worked in the telecommunications industry, spending 13 years with Ericsson in engineering and management roles. This was followed by more than four years leading the technology function for an Irish fibre communications company. Leo holds a degree in Electronics Engineering from Dublin Institute of Technology.

ULTIMATE RAYLEIGH - BENARD AND TAYLOR - COUETTE TURBULENCE

DETLEF LOHSE
Faculty of Science and Technology University of Twente

ABSTRACT

Rayleigh-Benard flow - the flow in a box heated from below and cooled from above - and Taylor-Couette flow - the flow between two coaxial co- or counter-rotating cylinders - are the two paradigmatic systems in physics of fluids and many new concepts have been tested with them. They are mathematically well described, namely by the Navier-Stokes equations and the respective boundary conditions.

While the low Reynolds number regime (i.e., weakly driven systems) has been very well explored in the '80s and '90s of the last century, in the fully turbulent regime major research activity only developed in the last decade. This was also possible thanks to the advancement of computational power and improved algorithms and nowadays numerical simulations of such systems can even be done in the so-called ultimate regime of turbulence, in which even the boundary layers become turbulent. In this talk we review this recent progress in our understanding of fully developed Rayleigh-Benard and Taylor-Couette turbulence, from the experimental, theoretical, and numerical point of view, focusing on the latter. We will explain the parameter dependences of the global transport properties of the flow and the local flow organisation, including velocity profiles and boundary layers, which are closely connected to the global properties. Next, we will discuss transitions between different (turbulent) flow states.

This is joint work with many colleagues over the years, and I in particular would like to name Siegfried Grossmann, Roberto Verzicco, Richard Stevens, Erwin van der Poel, and Rodolfo Ostilla-Monico.

DETLEF LOHSE

Detlef Lohse got his PhD on the theory of turbulence in Marburg/Germany in 1992. As a postdoc in Chicago and later in Marburg and München he worked on single bubble sonoluminescence. In 1998 he was appointed as Chair of Physics of Fluids at the University of Twente, The Netherlands, where he still is.

Lohse's present research subjects are turbulence and multiphase flow, granular matter, and micro- and nanofluidics. Both experimental, theoretical, and numerical methods are used in his group.

Lohse is Associate Editor of Journal of Fluid Mechanics and several other journals. He is Fellow of the American Physical Society, Division of Fluid Dynamics, and of IoP. He is also elected Member of the German Academy of Science (Leopoldina) and the Royal Dutch Academy of Science (KNAW). He received various prizes such as the Spinoza Prize (2005), the Simon Stevin Prize (2009), the Physica Prize (2011), the George K. Batchelor Prize for Fluid Dynamics (2012), and the AkzoNobel Prize (2012).

COFFEE BREAK

Thursday 10.30 - 11.00

SCIENCE AND INDUSTRY: PARTNERS FOR INNOVATION

Moderator: **TOM WILKIE, Scientific Computing World**
Panelists: **SYLVIE JOUSSAUME**, INSU/CNRS
MATEO VALERO, Director Barcelona Supercomputing Center
ANDERS RHOD GREGERSEN, Vestas
AUGUSTO BURGUEÑO ARJONA, European Commission

ABSTRACT

During the last three days speakers from industry and academia presented results that would have not been achievable without HPC. Will continuing on the proven and successful track be sufficient to meet the goals that Europe sets itself to be a leader in innovation and scientific excellence. The panelists will discuss the respective expectations of industry, science, infrastructure providers, and funding agencies on future HPC technologies and services. They will explore opportunities for synergies and mutual transfer of know-how between the stakeholders. Questions from the audience are welcome and should be submitted to the panel chair prior to the session or via the open microphone during the discussion.

TOM WILKIE

Tom Wilkie is Editor-In-Chief of Scientific Computing World. He is Chairman, and one of the founder shareholders, of its publishing company, Europa Science Ltd, responsible for commercial and strategic oversight of the six publications the company produces.

With a background in mathematical physics and a PhD in the theory of elementary particle physics, he is a senior science writer and editor as well as company director. In the course of his career, he has been Features Editor of New Scientist and was Science Editor of The Independent newspaper for ten years, following the newspaper's launch in 1986.

Non-journalistic work has included a spell as an international civil servant for one of the specialised agencies of the UN system, and also time as Head of Bio-Medical Ethics at the Wellcome Trust. He is the author of three books on science and society.

SYLVIE JOUSSAUME

Sylvie Joussaume is a researcher within CNRS. She is an expert in climate modelling. She has been involved in IPCC assessment reports since the third report. Previously she was appointed as director of the Institut National des Sciences de l'Univers (INSU) from CNRS. She is chairing the scientific board of the European Network for Earth System modelling (ENES, http://enes.org) and coordinates the FP7 infrastructure project, IS-ENES, which integrates the European climate models in a common research infrastructure dealing with models, model data and high-performance computing for climate (http://is.enes.org) (2009-2017) and has published its infrastructure strategy for 2012-2022. She is chair of the PRACE Scientific Steering Committee (SSC) in 2015 and chairs the scientific committee of ORAP that promotes high-performance computing in France since 2010.

ANDERS RHOD GREGERSEN

Anders Rhod Gregersen is responsible for the High Performance Computing & Big Data efforts at Vestas Wind Systems A/S. He designed and operates the Firestorm supercomputer, the third largest commercially used supercomputer in the world at the time of installation. Before Vestas, Anders successfully enabled the University supercomputers in the Nordic countries to analyse the vast data streams from the largest machine in the world, the large hadron collider at CERN, Geneva. Besides Vestas, Anders is the Vice chairman of the Industrial Advisory Committee at PRACE.

MATEO VALERO

Mateo Valero, is a professor in the Computer Architecture Department at UPC, in Barcelona. His research interests focuses on high performance architectures. He has published approximately 600 papers, has served in the organization of more than 300 International Conferences and he has given more than 400 invited talks. He is the director of the Barcelona Supercomputing Centre, the National Centre of Supercomputing in Spain.

Dr. Valero has been honoured with several awards. Among them, the Eckert-Mauchly Award, Harry Goode Award, The ACM Distinguished Service award, the “King Jaime I” in research and two Spanish National Awards on Informatics and on Engineering. He has been named Honorary Doctor by the Universities of Chalmers, Belgrade and Veracruz in Mexico and by the Spanish Universities of Las Palmas de Gran Canaria, Zaragoza and Complutense in Madrid. “Hall of the Fame” member of the IST European Program (selected as one of the 25 most influential European researchers in IT during the period 1983-2008, in Lyon, November 2008)

Professor Valero is Academic member of the Royal Spanish Academy of Engineering, of the Royal Spanish Academy of Doctors, of the Academia Europaea, and of the Academy of Sciences in Mexico, and Correspondant Academic of the Spanish Royal Academy of Science, He is a Fellow of the IEEE, Fellow of the ACM and an Intel Distinguished Research Fellow.

AUGUSTO BURGUEÑO ARJONA

Augusto Burgueño Arjona is currently Head of Unit “eInfrastructure” at European Commission Directorate General for Communications Networks, Content and Technology. His unit coordinates the implementation of the European HPC strategy as well as the deployment of European research eInfrastructures such as Géant, PRACE, EUDAT, OpenAIRE and the European Grid Initiatiave (EGI). Previously he served as Head of Unit “Finance” Directorate General for Communications Networks, Content and Technology at European Commission and Head of inter-Directorate General Task Force IT Planning Office at European Commission.

Closing Session

ABSTRACT

PRACEdays15 will end with the presentation of the Best Poster Award and a preview about the venue for PRACEdays16 that will take place from 10-12 May 2016 in Prague, Czech Republic.

POSTERS

The following posters will be on display throughout the conference. On Tuesday from 18.00 to 19.30 the presenters will be available to discuss the posters. Members for the PRACE Scientific and Steering Committee will also select the best poster during this time. The award will be presented to the winner during the closing session on Thursday

NUMERICAL STUDY OF MIXING IN SWIRLING COAXIAL JETS. AN APPLICATION OF LARGE EDDY SIMULATION.

TERESA PARRA
University of Valladolid

ABSTRACT

Assessment of Large Eddy Simulation (LES) models of confined coaxial swirling jets is the aim of this work. The mid-term application is to improve the stabilization of flames of poor mixtures by means of a swirling flow. This provides saving of fuel as well as a reduction of contaminant emissions. Swirling burners have some advantages when compared with bluff bodies and cross flows. These are lower head losses and soot, less maintenance tasks. A possible application of the smallest burners is the food industry since baking with low emissions improves the taste of the product.

Despite the simple geometrical set-up of the benchmark, the flow pattern shows complex aerodynamic behavior. The simple burner considers the use of two coaxial nozzles: one axial with fuel and another annular with air. The expansion of the flow, when entering the chamber will produce the Outer Recirculation Zone. If the swirl number is large enough to let the flow turn back into the centre, the vortex breakdown phenomenon appears to form an Inner Recirculation Zone limited by two stagnation points located in the axis of the chamber. The region between both recirculation zones with high shear is where mixture of fuel-air occurs.

This work is devoted to isothermal flow to gain an insight of flow pattern associated to different swirl numbers and diffusers. Axial swirl injector is composed of 8 fixed vanes in the annular nozzle. It is responsible for the azimuthal momentum of annular jet. The swirl number is associated with the angle of the trailing edge of the vanes. Besides, the influence of conical diffusers in the mixture is analyzed.

Swirl numbers of 0.2 (low) 0.6 (intermediate) and 1.2 (strong) were tested. To sum up, the strong swirl number had the lead stagnation point near the discharge of the nozzles and provided a mixing length lower than half diameter of the chamber. Intermediate swirl number have bigger Outer Recirculation Zones and the mixing length is more than one diameter. Finally the low swirl number does not have any vortex breakdown and the mixing length is several diameters. Bearing in mind the influence of conical diffusers, it is more important in the case of intermediate swirl numbers since the diffuser reduces the mixing length. A 140º diffuser is able to avoid the Outer Recirculation Zone for Strong Swirls. The same diffuser setup operating with intermediate swirl number is able to prevent the formation of Taylor-Couette instabilities (counterrotating vortex rings) with the associated reduction of head losses.

These models were tested using the LES algorithm Scale Selective Discretization scheme. Temporal resolution is 10-5 s/timestep with spatial resolution 5 times larger than Kolmogorov scale. It was found that for mesh of 7-9 million cells without multigrid, the optimum is 64 processors. If the multigrid set up is modified to consider more cells in the coarsest level, the optimum number of processors can be increased to 128. Also, the increase of tolerance has an impact for efficient use of larger number of processors.

TERESA PARRA

Teresa Parra received her PhD in Mechanical Engineering in 1999. She is a researcher in the framework of Fluid Mechanics and Turbo-machinery at the University of Valladolid. Her research interests are in numerical simulation of turbulent and reactive flows using Reynolds Averaged Navier Stokes and Large Eddy Simulation approaches. Her basic research is applied to renewable energies (hydraulic and wind power) as well as ultra-low emissions of stabilized lean swirling flames. Since 2012, she is user of high performance computing infrastructures.

She has published among others in Combustion Explosions and Shock Waves, Journal of Engineering Computations, Combustion Science and Technology, Energy, Building and Environment, Applied Thermal Engineering.

NUMERICAL SIMULATION OF NON-PREMIXED SWIRLING FLAMES

RUBEN PEREZ
University of Valladolid

ABSTRACT

The present work focuses on the numerical simulation of diffusive flames in a confined swirl burner. The background motivation for the project arises from the greenhouse gas emissions. In methane operated burners, the methane slip due to incomplete combustion is a problem since methane is a harmful greenhouse gas. Lean flames produce less contaminant emissions and reduce fuel consumption, however they are unstable. The swirling flow is a stabilizer of the flame so that poor mixtures can be burned.

The governing equations for 3D, transient, reactive flow are solved with a second order scheme. The 3D mesh has 4 million hexahedral cells. No multi-grid was used for reactive cases because the averaging on temperature field is a precursor of the lack of accuracy on the reaction rate. As for the turbulence model, the k-□ was selected.

Numerical model for no swirl and high swirl burners have been carried out using heat and mass transfer for non reactive cases and a simplified mechanism of reaction for the reactive case. Regarding the reactive case: three stoichiometries were mixed and burned, stoichiometric (lambda = 1), lean (lambda = 1.2) and rich (lambda = 0.8) mixtures. The temporal resolution must be around 10-7 s/timestep, because of the stiffness of the reactive case.

Contrasting non reactive and reactive cases, the last one produces higher axial velocities to keep the mass balance. Hence, it is a precursor of smaller Inner Recirculation Zones (IRZ) in the case of strong swirls. The lead stagnation point of the IRZ plays an important role fixing the location of the flame front in swirling burners. Besides, the hot products of reaction of the IRZ help to warm the fresh mixture. Contrasting flames with swirl number null, 0.6 and 1 it is possible to conclude the decrease of the flame front thickness while increasing the swirl number.

Contrasting different stoichiometries, lean mixtures have lower equilibrium temperature and therefore, the thermal emission of nitrogen oxides is lower. However, strong swirls are needed for very poor mixtures in order to be burned in a stable way.

RUBEN PEREZ

Ruben Perez is a Ph.D. candidate in Mechanical Engineering at University of Valladolid, Spain, where he received his degree in Mechanical Engineering in 2011 and in Management Engineering in 2013. His research interests are in CFD for turbulent flows. He worked on design optimization of air radial impulse turbines for Oscillating Water Column Marine Power Plant and on HVAC and indoor air quality in operating rooms. Presently, he works on thermal analysis in the Spanish Interim Nuclear Waste Storage Facility and in power plant simulations as transient hydraulic calculations.

AMOEBA AND HPC – PARALLELISING POLARISABLE FORCE FIELDS

WERONIKA FILINGER
EPCC

ABSTRACT

For decades now classical and quantum mechanical based computational chemistry codes have been used to evaluate molecular properties and interactions in gas and condensed phases. However, there are a number of systems that cannot be simulated correctly using the currently available software as they are limited by the use of non-polarisable classical models. These models approximate electrostatic interactions by only using fixed charges, which means that the charges in atoms are not allowed to adapt to changes in their local environment. Hence these models are not capable of providing sufficiently accurate results for systems where the polarization and self-induced charges play a significant role in the interaction. Polarisation changes the geometry and energy of the system by distorting the bonds between atoms and it is a necessary intermolecular interaction when modelling chemical reactions in biological molecules and water-based systems. Therefore,

to tackle a wider range of problems in chemistry, biochemistry and material science where charges and polarization are important it is necessary to implement more realistic modelling of molecular forces that take into account these effects.

Thus efforts have been put into developing mutually polarisable models that enhance the fixed charge models by including the polarisation of atoms and molecules in the dynamics of these systems. These polarisable models are more accurate and more complex hence more computationally demanding. Typically the size and number of time steps in these simulations are selected so that the calculation can finish within a reasonable time period but they also need to be long enough to be relevant to the timescales of the process being simulated. For example, most proteins and DNA simulations need to span at least nanoseconds of simulated system time, which can take days to years of wall clock time on a single CPU. Moreover, the use of polarisable fields, which are necessary for most biological systems, will increase this time by ten-folds or more. Hence, there is a strong need to develop the software packages implementing polarisable force fields that are capable of exploiting current and emerging HPC architectures to make modelling ever more complex systems viable.

One of the more prominent polarisable models in this field is AMOEBA (Atomic Multipole Optimised Energies for Bimolecular Applications). This has been implemented and is widely used in codes such as TINKER and AMBER. AMOEBA replaces fixed partial charge with atomic multipoles and includes an explicit dipole polarisation, which allows atoms to respond to the polarisation changes in their molecular environment. AMOEBA has been shown to give more accurate structural and thermodynamic properties of various simulated systems. However, the time needed to calculate the effect of the induced dipoles alone is 15-20 times larger than the cost of one time step for a fixed charge model. If the computational time could be reduced then the AMOEBA force field could, for example, model a much broader range of protein-ligand systems than is currently possible or provide a means of refining in X-ray crystallography for large and challenging data sets such as ribosome crystals.

The larger computational costs associated with the calculation of polarisations needs to be mitigated by improved the parallelisation of codes such as TINKER. In this poster we give more details on the AMOEBA model as implemented in the TINKER molecular modelling package and present our efforts at improving its parallelisation through the use of hybrid MPI and OpenMP techniques.

WERONIKA FILLINGER

Weronika Fillinger joined EPCC in 2013 as an Application developer right after finishing EPCC's MSc in High Performance Computing. Weronika became interested in HPC when she was working on my MPhys master project, which was simulating Bootstrap Percolation on Complex Networks. The code Weronika wrote at that time required days to run and she realised that writing the code is only the first step in doing science via computer simulations. After that she completed the EPCC MSc in HPC and this time the subject of her dissertation was Optimising PLINK (a whole genome analysis toolset), which involved both parallelisation and serial optimisations of the code.

Working at EPCC, she have been involved in a variety of different collaboration projects centred on high performance computing including the European collaborative projects CRESTA and APES. Weronika is also involved in HPC training developing EPCC's online distance learning courses.

NOVEL MULTIPHASE SIMULATIONS INVESTIGATING CAVITATION BY USE OF IN-SITU VISUALISATION AND EULER/LAGRANGE COUPLING

MATHIS BODE
RWTH Aachen University

ABSTRACT

Flow configurations involving both liquid and gaseous fluids often occur in industrial applications. Engine injection systems, which are used to atomize liquid fuels, are one example. The performance of such atomizers depends on a cascade of physical processes, originating from the nozzle internal flow, cavitation, turbulence, and the mixing of a coherent liquid stream with a gaseous ambient environment. The transfer occurring between liquid and gas is governed by an interface topology. An accurate prediction of this mixing stage is crucial for reliable predictions of the overall system as it is typically the first physical process to be modeled in simulations and uncertainties here will influence, for example, the design and performance of engines all the way down to emission and pollutant formation.

IN recent years, engine experiments have shown that the impact of cavitation on the overall engine processes is much larger than current knowledge would predict. Due to the small size of injection systems, which have outlet diameters on the order of 100 micrometers, and the resulting bubbles, droplets and turbulence structures, which are even much smaller, a detailed investigation using experiments is very difficult and simulations can be quite helpful.

Accurate simulations of the whole atomization process have to include a broad spectrum of different length scales and resolve the interface topology in an exact and robust way, which is hard to achieve even with massively parallel code frameworks on Tier-0 HPC systems. However, recent developments with respect to interface tracking methods and a new simulation approach combining Eulerian and Lagrangian spray simulation techniques in order to decrease the computational cost in physically less important flow regions, enables us to study the impact of cavitation on the mixing process. Additionally, new in-situ visualization techniques enable a smart data management, which stores fully resolved data only in important flow regions leading to a higher information/data size ratio, which is crucial for model development.

This work presents the new simulation techniques as well as its application to realistic atomizers. The CIAO code framework was used on MareNostrum III and JUQUEEN for data generation and the data are studied focusing on the effect of cavitation on commonly used spray models in industrial context.

MATHIS BODE

Mathis Bode is a research assistant and Ph.D. student in Prof. Pitsch's group at the Institute for Combustion Technology at RWTH Aachen University. He received his Master of Science in Mechanical Engineering from RWTH Aachen University in 2012. His research interests include high fidelity simulations of multiphase flows on massively parallel computers.

MASSIVELY PARALLEL CODE TO SEARCH FOR GRAVITATIONAL WAVES FROM ROTATING NEUTRON STARS IN ADVANCED DETECTOR DATA

GEVORG POGHOSYAN
Steinbuch Centre for Computing at Karlsruhe Institute of Technology

ABSTRACT

Gravitational waves are the last prediction of general relativity still awaiting a direct experimental verification. Observations of gravitational waves will open a new field - gravitational wave astronomy. First science data from the global network of advanced gravitational wave detectors - LIGO, GE0600 and Virgo long arm interferometers, are expected in July 2015. The advanced detector network will be sensitive to signals all over the sky, although source positions can be determined by triangulation. For these reasons, searching for sources in noisy data is algorithmically challenging, since one has to simultaneously look for different types of signals, and computationally formidable, due to the large parameter space over which the searches must be carried out. To perform a rapid analysis of all data from the advanced LIGO and Virgo gravitational wave detectors' network, hundreds of millions of CPU hours will be required — the code utilizing the potential of massively parallel supercomputers is therefore mandatory.

Polgraw-Virgo group in cooperation with the Simulation Laboratory for Elementary- and Astro-Particles have developed a highly scalable computation code parallel PollGrawAllSky, which enables the data analysis of all-sky searches for gravitational wave signals at large scales on acceptable time scales. Benchmarking of the code in framework of PRACE Preparatory access on a Cray XE6 system was performed to show efficiency of our parallelization concept and to demonstrate scaling up to 50 thousand cores in parallel. To estimate the computational requirements when current version of code is used for analysis, we have performed representative tests with the Gaussian noise data at different band frequencies. For example, a serial search for GWs in one particular detection day at only 4 frequencies 600, 1000, 1700 and 2000 will require a total of 20 thousand CPU hours of computation, which is more than two years on a single CPU and correspondingly the output generated by this simulation would be ca. 4 GB.

To face the big challenge of the analysis of all the data that will be collected from the advanced detectors expected to be available by the year 2018, we are developing a hybrid parallelized PollGrawAllSky code able to scaling much above current 50000+ cores. To enhance the scalability of execution of many computations in parallel, we combine many instances consisting of different PolGrawAllSky executions that use different numbers of parallel sub-tasks. This feature is implemented using the dynamic process creation and grouping

framework of MPI, with different MPI sub-worlds also known as virtual groups that enables collective and dynamic communication operations across a subset of related tasks. The main PolGrawAllSky code with parallel sky loop is encapsulated into another code, named skyfarmer, equipped with internal scheduling and bookkeeping mechanism.

With further implementation of usage of coprocessors (hardware accelerators) like Graphical Processing Units in parallel code presently optimised to use only standard Central Processing Units we hope to reach scalability level allowing to analyse at least four times more resources, i.e., 1000 million CPU hours, to perform analysis of final data in 2018. These means performance of 1petaFLOPS computer working continuously for one year.

GEVORG POGHOSYAN

Gevorg Poghosyan is head of simulation laboratory for Elementary- and Astro-Particle Physics at Karlsruhe Institute of Technology. He is holding Ph.D. in Physics from Yerevan State University. As an expert for HPC in Astro- and Particle Physics he is working at Steinbuch Centre for Computing on joint research and development projects with scientific and industry groups to ease porting existing codes to supercomputing and enable optimal usage of present and future HPC systems for computational simulations. Gevorg have worked in University Rostock as DAAD Fellow and Institute of Physics of Basel University developing simulation codes for theoretical astrophysics, hydrodynamic and particle physics and studied correlation of superdense hybrid matter to evolution of stars, mergers and supernovae.

TOWARDS A QUANTITATIVE UNDERSTANDING OF THE QUARK-GLUON PLASMA

JON-IVAR SKULLERUD
Maynooth University

ABSTRACT

At extremely high temperatures (100,000 times those in the core of the Sun), the strong interaction, which holds quarks and gluons together to form protons, neutrons and other hadrons, undergoes a dramatic change of character. The quarks and gluons are no longer bound together, but instead form a new phase of matter called the quark-gluon plasma. At the same time, the quarks that make up ordinary matter become effectively massless as the chiral symmetry of the quarks, which is broken in ordinary matter, is restored. This state of matter existed in the first second after the Big Bang and is currently being produced in collisions between heavy ions (gold or lead) at CERN and Brookhaven.

The FASTSUM collaboration has been carrying out large-scale Monte Carlo simulations of strongly interacting matter at temperatures both above and below the transition to the quark-gluon plasma. These simulations have employed anisotropic lattices, where the lattice spacing in the temporal direction is much smaller than in the spatial directions. This allows a good resolution for temporal correlators, which is crucial to obtaining results for transport properties and survival of bound states in the plasma.

We will show results obtained for the electrical conductivity and charge diffusion as well as for states consisting of heavy (charm and beauty) quarks: the melting temperatures of the latter may be used as a “thermometer” of the quark-gluon plasma. We also show results for nucleons demonstrating the effects of chiral symmetry restoration. These results have been obtained from our “second generation” data ensembles generated with the use of PRACE resources. We are currently in the process of generating “third generation” ensembles which will double our temporal resolution and provide the first step towards a continuum extrapolation of our results.

JON-IVAR SKULLERUD

Jon-Ivar Skullerud is a lecturer in Mathematical Physics at Maynooth University, Ireland. He received his first degree in physics and philosophy at the University of Trondheim, Norway, and a PhD in theoretical physics from the University of Edinburgh. His main research interest is in non-perturbative studies of the strong interaction, in particular lattice QCD simulations at high temperature and density. He is also a national representative on the International Particle Physics Outreach Group.

EDGE-ELEMENTS FOR GEOPHYSICAL ELECTROMAGNETIC PROBLEMS: A NEW IMPLEMENTATION CHALLENGE

OCTAVIO CASTILLO REYES
Barcelona Supercomputing Center (BSC)

ABSTRACT

Electromagnetic Methods (EM) are an established tool in geophysics, finding application in many areas such as hydrocarbon and mineral exploration, reservoir monitoring, CO2 storage characterization, geothermal reservoir imaging and many others. The last decade has been a period of rapid growth of marine electromagnetics, mostly because of its industrial adoption.

The marine controlled-source electromagnetic (CSEM) method has become an important technique for reducing ambiguities in data interpretation in the offshore environment and a commonplace in the industry.

In the traditional configuration, the sub-seafloor structure is explored by emitting low-frequency signals from a high-powered electric dipole source towed close to the seafloor. By studying the received signal, the subsurface structures could be detected at scales of a few tens of meters to depths of several kilometers.

On the other hand, in the Finite Element Method for solving electromagnetic field problems, the use of Edge-based elements (Nédélec elements) has become very popular. In fact, Nédélec elements are often said to be a cure to many difficulties that are encountered (particularly eliminating spurious solutions) and are claimed to yield accurate results. However, the state of the art is marked by a relative scarcity in practice of robust codes to simulate geophysical electromagnetic problems. It’s may be attributed to their theoretical and implementational threshold. Indeed, more care and effort are required to implement them: basis functions, Piola mapping, edge directions and numbering strategy. Latter issues poses additional challenges.

Furthermore, the resultant data volumes of large-scale 3D modeling and simulations can easily overwhelm single core and modest multi core architectures. As a result, this kind of problems requires massively parallel computational resources in order to achieve a time frame acceptable to exploration process.

Based on previous ideas and considering the societal value of exploration geophysics, since this process is essential to among others, we present a novelty parallel implementation of Nédélec Elements for geophysical electromagnetic problems on unstructured meshes in 2D and 3D. The usage of unstructured meshes and mesh refinement make it possible to represent complex geological structures precisely and to improve the solution’s accuracy.

In particular, we present a simple, flexible and parallel implementation for Edge Elements in anisotropic mediums. The described software stack relies on a flexible solution which allows a general point of view. The efficiency and accuracy of the code is evaluated through a convergence test, scalability test, assembly time, and solver time, with a strong emphasis on the performance when the number of elements and degrees of freedom grows.

Since our target application is exploration geophysics, the results of this research stage shapes the future line of work to solve more complex problems such as forward modeling simulations and domain and functional decomposition.

OCTAVIO CASTILLO REYES

Octavio Castillo Reyes has his barchelor’s in Computer Systems engineering from Xalapa Institute of Technology, Mexico and M.Sc. In Networks and Telecommunications from Atenas Veracruzana University, Mexico. He has previously worked as lecturer at the University of Veracruz, particularly in the Master in Telematic Engineering and Bachelor in Administrative Computer Systems.

His scientific interests range in the broad fields of computational methods, finite element method, multiprocessor architectures, memory systems, performance and workload characterization.

Octavio Castillo Reyes is currently associate PhD student at Barcelona Supercomputing Center under the supervision of PhD. José María Cela Espín. He is working closely with REPSOL-BSC Research Center and his research focus is the Edge-based Finite Element Method and it’s coupling with geophysical electromagnetic problems in oil industry. Octavio Castillo is supported by a bursary from the Mexican National Council for Science and Technology (CONACYT).

GPU ACCELERATED FINITE ELEMENT METHOD FOR RADIO FREQUENCY ABLATED CANCER TREATMENT

PANCHATCHARAM MARIAPPAN
NUMA Engineering Services Ltd

ABSTRACT

Graphics Processing Units (GPUs) are nowadays used for numerical computation, beyond their original purpose of graphics accelerators. Mature hardware and GPU software tools and libraries support double precision and memory correction. GPU accelerated computational fluid dynamics has gained attention in both academia and industry. In this article, we investigate the importance of GPUs as accelerators in the field of biomedical engineering. We developed a software tool to predict the lesion development in cancer patients after the radio frequency ablation cancer treatment. We use Penne's bioheat model with appropriate boundary conditions and the finite element method for numerical discretization. From the finite element discretization of the bioheat equation, we observe that no explicit element integration is required. Since the problem domain is fixed, we find the neighbours of each node at the first time step and generate a compressed sparse row structured (CSR) matrix which can be used for the entire domain. After the CSR matrix is generated, we send the domain information such as nodes, elements and matrix information (e.g. the CSR matrix rows and columns) to the GPU. The Central Processing Unit (CPU) loads the initial data, finds the neighbours list, generates the CSR matrix and stores the results on the disk, whereas the GPU constructs the shape functions, assembles the local stiffness matrix into the global matrix in the CSR form and solves the sparse linear system with the help of the existing CUDA libraries such as CUBLAS and CUSPARSE.

In order to solve the linear system, we employed the ILU preconditioned BiCGStab algorithm, one of the fastest solvers among Krylov subspace solvers. At each time step, the GPU generates the heat source term and solves the cell death model, while the CPU saves the results in vtu/vtp files. The heat source term generation is based on our in-house point source model for approximating the Joule heating effect, and the cell death model is an adapted evolution equation, predicting whether cells near the tumour are alive or dead. The tasks assigned to the GPU are the most time consuming parts of the finite element method and the GPU accelerates them with the desired speed-up and accuracy. The major steps involved in this work are receiving the segmented CT scans of the patient from the doctors, generating the mesh, obtaining the needle position from the CT scans (approximately the centre of the tumour) and simulating them using our software tool. Existing software tools working on multi-core CPUs (Intel i5's) take 6 hours to predict a lesion for 26 minutes of real treatment time, for around 1 million elements. Our current work with the assistance of the GPU acceleration yields the result in approximately 3 minutes for the same number of elements, where the comparison is done with Intel Xeon CPU E5 – 2680 @ 2.8 GHz, and NVIDIA GeForce Titan Black GPU @ 3.5 GHz (2880 CUDA Cores).

PANCHATCHARAM MARIAPPAN

Panchatcharam Mariappan obtained a PhD in Mathematics from IIT Madras, Chennai, India in collaboration with TU Kaiserslautern, Germany. The title of the PhD Thesis was 'GPU accelerated finite point set method for fluid flow problems' He was lecturer at Vysya College, Salem, Tamilnadu, India and Online Tutor, with TWWI, Chennai, India.
He is now Software Development Engineer at NUMA Engineering Services Ltd, Dundlk, Co. Louth, Ireland

PARALLEL AGENT-BASED SIMULATION OF SOUTH KOREAN POPULATION DYNAMICS

CRISTINA MONTAÑOLA SALES
Universitat Politècnica de Catalunya

ABSTRACT

Changes in our society have created a challenge for policymakers, who confront a need of tools to evaluate the possible effects of their policies. Agent-based simulation is a promising methodology that can be used in the study of population dynamics. However, it has been little used in demographic research to help explaining dynamics. Simulation methodologies provide the opportunity to develop a virtual laboratory for exploring and validating current and new approaches. The purpose is to avoid conducting real social experiments, which may be expensive, unethical or even infeasible.

Agent-based simulation is commonly used for small scenarios because the number of agents and interactions between them can be extremely large in some of case studies, thus forcing the scientist to limit its number in order to execute the simulation in a standard computer. However, in the case of policy models, both the amount of compute power required and detailed micro-level data are significant. To deal with complex social models we can take advantage of parallel computation. Traditionally, parallel simulation has been applied in numerous scientific simulations such as networks or military. Nevertheless, the number of applications in the social sciences is scarce. One of the obstacles hindering the use of agent-based simulation is its scalability, especially if the analysis requires large-scale models. Currently there is no consensus on how to compute agent-based simulations in High Performance systems. Scalability issues cannot be solved just by distributing the computer workload on High Performance architecture. It depends on many factors, notably the execution platform and the complexity of the agent-based model, which in turn depends on the number of agents, their intelligent behavior and the complexity of their communication. It is not only important to address size problems but also to see whether more realistic agent-based models with complex behavior and communication network can be scaled-up to provide empirically and practically useful results.

A possible solution for scalability issues is to run the agent-based models on top of a scalable parallel discrete-event simulation engine. In our work, we use this solution in the design and development of a simulation framework that gives support for modeling and simulating agent-based demographic systems. It provides the placeholders for different demographic processes such as fertility, mortality, change in economic status, change in marital status, and migration. The main advantage of this approach is the ability to run large agent-based scenarios in High Performance Computing environments, when other current tools present limitations.

Moreover, we present a case study on forecasting demographics of South Korea during 100 years. South Korea is a country that shows the most unprecedented speed of aging in history. According to the latest projections, by 2050 South Korea may be the oldest country on earth. This situation could bring difficult challenges to face for the Korean government. Unless the country takes adequate measures to prepare for the demographic aging trend, it is expected that Korea will face a slower economic growth and living standards stagnation. With the application of agent-based simulation to this case we show how the life course of individuals is evolving, allowing expand on the movements, interactions, and behaviours of South Korean population. Our model is able to capture individual characteristics and to overcome some data-related limitations with assumptions on behavioural rules. With this real case scenario, we show the potential of parallel agent-based simulation methodology for demographics.

CRISTINA MONTAÑOLA SALES

Cristina Montañola Sales is a research assistant and Ph.D. student at inLab FIB (Barcelona informatics school laboratory), in the Universitat Politècnica de Catalunya (UPC) – BarcelonaTech. She is currently doing her research in collaboration with Barcelona Supercomputing Center (BSC). She holds an MSc in Computer Science from UPC. Her research interests include agent-based modeling, computer simulation, High-Performance Computing and computational social science.

MASSIVELY-PARALLEL MOLECULAR SIMULATION STUDIES OF ICE AND CLATHRATE-HYDRATE NANO-CRYSTAL AND PRECURSOR FORMATION

NIALL ENGLISH
Unversity College Dublin

ABSTRACT

Ice growth and decomposition was studied upon approximately spherical ice nano-particles of varying size surrounded by liquid water and at a variety of temperatures and pressures. The system box size was also varied for systems containing of the order of one million water molecules to almost ten million molecules, in order to establish system-size effects upon the growth and dissociation kinetics. It was found that there was a dependence upon system size on growth and dissociation, which points out the limitations of previous earlier simulation attempts in smaller simulation boxes.

Further, supercooled liquid water simulations were performed at various system sizes of the order to one to ten million water molecules, and the subtle re-arrangement of the structure and local density was explored as the system began to transition towards local ice-like conditions. Crucially, a system-size dependence was found upon these structural and dynamical rearrangements, which has been neglected in previous simulations.

The heterogeneous nucleation of ice nano-scale particles and the homogeneous nucleation of methane clathrate hydrates at water-methane interfaces were studied, again addressing the key question of the effect of system-size upon the results. It was found that both phenomena did depend on system-size, and that the subtle interplay between the frequency of box fluctuations and dilations with the underlying molecular rearrangements towards free-energy basins was quite important on influencing the outcome.

In the future, he would hope to continue these studies of clathrate and ice nucleation, growth and dissociation, especially with a view towards engineering applications, like the use of inhibitor compounds and temperature-/pressure-pulse strategies to regulate kinetics. Large-scale supercomputing is required to study these complex non-equilibrium processes without being plagued by the tyranny of small systems and periodic boundary conditions affecting results adversely. He expects that benefits to society will emerge from the greater understanding of these phenomena on a microscopic level, and the greater possibilities of devising kinetics-regulation strategies, e.g., to avoid pipeline blockage by hydrate plugs by inexpensive initial screening on supercomputing platforms, using molecular dynamics as an initial 'predictive' design tool.

NIALL ENGLISH

Niall English obtained a First Class Honours degree in Chemical Engineering from UCD in 2000. In 2003, Dr English completed a Ph.D. at UCD (Dept. of Chemical Engineering) on molecular simulation of electromagnetic (e/m)-field effects on methane-hydrate crystallisation. During 2004-2005, Niall carried out further simulation and theoretical studies on hydrate dissolution and on the effect of e/m fields on water and metal oxides at the National Energy Technology Laboratory, a U.S. DOE research facility in Pittsburgh, in conjunction with Dept of Chemical Engineering at the University of Pittsburgh. During 2005 to 2007, he worked for the Chemical Computing Group in Cambridge, GB. Here, Niall developed codes, protocols and methods for biomolecular simulation, chiefly for structure-based drug design applications in the pharmaceutical industry. Niall commenced his position as a lecturer in Chemical Engineering at UCD in 2007, being promoted to senior lecturer in 2014. His research interests encompass clathrate hydrates, solar and renewable energies, and simulation of e/m field effects.

USE OF GRAPHICS CARDS (GPU) TO SIMULATE ATOMS, MOLECULES AND NUCLEUS

JOSÉ MANUEL ALCARAZ-PELEGRINA
University of Córdoba

ABSTRACT

The realistic description of the physical properties of the microscopic systems with a finite number of particles, such as nuclei or atoms and molecules, isolated or confined inside of molecular complexes, is a basic goal in Physics. These studies, even in the most basic aspects, lead to the use of complex methods that require powerful techniques of calculation being the Quantum Monte Carlo (QMC), one of the most developed in the last years. However, it is well known that QMC methods are computationally expensive.

Recently, a programming approach for performing scientific calculations on a graphics processing units (GPUs) has been developed. GPUs have evolved into a highly efficient data-parallel computing device and first market companies have released programming tools to make use of these technologies.

The implementation of QMC codes in GPUs will result in a better knowlegde of the microscopic systems such as nuclei or atoms and molecules. A comparison between a GPU implementation of some QMC methods, a serial and a parallel code on CPU is presented for some systems.

JOSÉ MANUEL ALCARAZ-PELEGRINA

José Manuel Alcaraz-Pelegrina obtained a PhD in Physics from the University of Seville (Spain). He is presently Associate Professor at the Physics Department of the University of Córdoba (Spain). His current research interests include the use of GPU in modelling and simulation of non-linear systems and Monte Carlo methods in Atomic, Molecular and Nuclear Physics.

DEVELOPING A SCALABLE AND FLEXIBLE HIGH-RESOLUTION CODE FOR DIRECT NUMERICAL SIMULATION OF TWO-PHASE FLOWS

LENNON Ó NÁRAIGH
University College Dublin

ABSTRACT

TPLS (Two-Phase Level Set) is an open-source program for simulation of two- phase flows in 3D channel geometries using high resolution DNS. TPLS solves the incompressible Navier—Stokes equations for a two-phase flow. A regular grid finite-volume discretization is employed based on an idealized channel geometry with a range of different inlet conditions that can be prescribed by the user. The interface between phases is tracked with a Level-Set method. The code evolves the physical variables (pressure, fluid velocities, and interface configuration) through discrete time steps. At each timestep, the key computational tasks performed amount to the solution of large systems of sparse linear equations with tens of millions of unknowns, for the key physical variables. In addition, regular I/O is required to save the system state for later analysis and visualizsation, or to restart in the case of hardware failure.

The code is implemented in Fortran90, initially with MPI parallelization using a 2D domain decomposition and bespoke Jacobi/SOR iterative solvers. Over the last two years, we have improved the TPLS code in several respects to give better performance, scalability and usability, moving from an in-house code specialized for use by the original developers, to an open-source flexible program which can easily be used by others, including academic and industrial users. The culmination of this work is TPLS version 2.0 (presented herein), where we have re-implemented the two most computationally-expensive solvers – the pressure and momentum steps – with calls to the PETSc library. Initial tests using the GMRES with Block-Jacobi preconditioner showed a speedup of 80% in the pressure solver on 2048 cores, along with improved strong scaling behavior. The original gather-to-master I/O strategy which wrote text files has been replaced with the use of NetCDF. As a result, we have obtained an order-of-magnitude reduction in I/O time, a compression factor of 6.7 and removed the memory bottleneck of requiring rank 0 to gather the entire domain. In addition to the Level Set method, we have added a PETSc implementation of the Diffuse Interface method (DIM), which is available as an option to users. Finally, with the support of the Software Sustainability Institute, we have added the ability to configure the code through input files or command-line arguments, obviating the need for users to modify and recompile for every application.

Novelty and Originality of Project: TPLS is unique in several aspects. Unlike other solvers (e.g. those mentioned below), TPLS solver has been purpose-built for supercomputing architectures like ARCHER. Most open-source solvers like OpenFOAM, Gerris, Fluidity and commercial solvers like ANSYS-Fluent/CFX offer only one interface-capturing method (the volume-of-fluid method) thereby limiting the applicability of these solvers to either free-surface, stratified, or wavy-stratified flows. The TPLS solver offers the users a choice of two types of interface capturing mechanisms between Diffuse-Interface Method and the Level-Set method. This enables the solver to accurately simulate a wide variety of physical scenarios. A further key feature of the work is the interdisciplinary composition of the development team, including researchers in HPC applications development, applied mathematics, algorithms design, and the physics of fluid flows.

The need for HPC in the work: Due to the high computational cost of a typical three-dimensional simulation, parallelization is essential, and scaling of the methodology described above has been demonstrated to several thousand CPU cores.

Looking forward: TPLS has already been used to gain key fundamental insight into interfacial waves in two-phase flows, as well as in the hydrodynamics of evaporating droplets. Imminent future work will see TPLS applied to simulations of a much wider range of physical phenomena, with a view to gaining fundamental understanding of stratified-slug flow transitions, interfacial turbulence, contact-line motion, phase change, and heat transfer. We hope to enlarge the code's user base, not only among academics, but also with industrial partners, including but not limited to the oil-and-gas industries.

LENNON Ó NÁRAIGH

Lennon Ó Náraigh is a lecturer in Applied and Computational Mathematics in the School of Mathematical Sciences in UCD. He received his PhD in Applied Mathematics from Imperial College London, where he also worked as a research associated in the Department of Chemical Engineering, studying multiphase flow for the oil-and-gas industries. His current research interests are in hydrodynamic stability and high-end computing for multiphase incompressible flows.

INTELLIGENT WATER DROPS ALGORITHM WITH PERTURBATION OPERATORS FOR ATOMIC CLUSTER OPTIMIZATION

RITCHIE MAE GAMOT
University of Warwick

ABSTRACT

We present a modified version of the Intelligent Water Drops algorithm (MIWD) that has been adapted to allow it to be applied, for the first time, to global optimization of atomic clusters. Cluster perturbation operators were applied to further generate lower energies. The algorithm, dubbed as MIWD+PerturbOp, is an unbiased type of algorithm where no a priori cluster geometry information and construction were used during initialization which is not the case with other common search methods.

Four modifications were implemented: (a) The probability used to determine components for each agent in the population has factored in the pairwise potential energy; (b) The heuristic undesirability factor was based on an objective function used in a multi-start strategy study of LJ clusters by Locatelli, et al; (c) The total worst agent in each iteration has also been identified, aside from total best agent, and paths belonging to it updated. (d) L-BFGS was utilized to further relax clusters to its nearby local minimum.

Due to the iterative nature of the algorithm and the numerous combinations of parameters involved, HPC architecture was valuable in gathering results efficiently. Test runs reveal that a spherical bounding volume for the initial atom positions and grow-etch perturbation operator is a good combination for implementing final runs. Results achieved high success rates for sizes up to N = 104. This study outperformed the seeded runs of Basin Hopping with Occasional Jumping in terms of success rates for more problematic clusters namely, LJ38, LJ75 – 77, LJ98, LJ101, and LJ103-104.

A detailed property analysis of the clusters of up to 104 atoms against the results in Cambridge Cluster Database (CCD) will be discussed. Preliminary experiments also show the method's promise to binary LJ mixtures and Morse clusters which could be treated as a good indication of the method's applicability to ionic, nanoalloy clusters or nanoparticles in general. Initial experiments on small Janus clusters using a potential model with a modified orientation term suited for two-patch Janus particles show promising configurations.

RITCHIE MAE GAMOT

Ritchie Mae Gamot is a PhD student at the Centre for Scientific Computing, University of Warwick. She received her Bachelor's degree in Applied Mathematics at the University of the Philippines Mindanao and Master's degree in Computer Science at the University of the Philippines Diliman. Currently, her research focuses on utilizing a nature-inspired algorithm, called Intelligent Water Drops algorithm coupled with appropriate local search algorithms, to solve configurational optimization problems with specific focus on atomic clusters.

PORTABLE TASK-BASED PROGRAMMING FOR SEISMIC IMAGING

LIONEL BOILLOT
INRIA

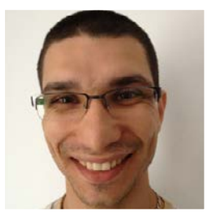
ABSTRACT

Seismic imaging is of high interest for oil or gas detection. The most accurate techniques used by oil companies are the RTM (Reverse Time Migration) and the FWI (Full Wave Inversion). These methods are based on seismic wave simulations, ideally in anisotropic elastic media, a generally accepted realistic modeling of the subsurface. The parallelization of these methods is a laborious task. The main difficulty comes from the heterogeneity, at several levels. First, the mesh is generally unstructured and the mesh cells are non-homogeneous in terms of number of degrees of freedom. Second, the anisotropy and the boundary conditions leads to unbalance computational zones. These two points lead to heterogeneous zones with different number of computations in each zone. Finally, the hardware heterogeneity prevents to obtain balanced subdomains in a domain decomposition context because even knowing the exact number of computations does not imply to know the exact time they require to execute, due to the vectorization capabilities, the different memory caches,... In addition, the dependencies between the different computational subdomains create complex data movement patterns.

Current algorithms in shared memory use OpenMP to exploit many-cores architectures, with positive outcomes. Integration with CUDA (or OpenCL) allows for access to the computational power of accelerators. Going outside the node boundary, existing algorithms are using a message passing library to exchange data between nodes, enabling distributed memory versions. At this point, mixing these different approaches in order to achieve high performance across heterogeneous platforms remains a complex, error-prone and time-consuming task. The upcoming heterogeneous manycore revolution motivated by the race toward Exascale will only emphasize this problem. Other programming paradigms, especially task-based approaches, seem to be a suitable approach for such levels of hardware complexity. Task-based programming has been successfully applied for to many computational domains leading to robust and efficient solvers: in dense linear algebra (e.g. the DPLASMA library); in sparse direct and iterative methods and fast algorithms (e.g. FMM or H-Matrix problems). However, this programming paradigm has yet to be applied to large industrial parallel codes and demonstrated that these codes may be turned into portable and efficient task-based programs.

Our study focuses on the integration of the 3D elastodynamics Total code DIVA (Depth Imaging Velocity Analysis) with the PaRSEC runtime system, a specialized runtime for task scheduling, developed at University of Tennessee. The code was initially based on the MPI library for the parallelism. The principle of task programming relies on rewriting the code flow as task executions, each task being a computational function. The description of the tasks with the data they need in input and output forms a DAG (Direct Acyclic Graph) of tasks. The arrows of the DAG contain the data movement information that the runtime uses to determine the data flow exhibiting the parallelism.

We first addressed shared memory architectures with a ccNUMA (cache coherent Non Uniform Memory Access) node and an Intel Xeon Phi accelerator, based on the Intel MIC (Many Integrated Cores) architecture. The preliminary results are very promising since we obtain a positive speed up in comparison with the MPI-based code. The most interesting results concerns the parallel efficiency which decreased with the MPI-based code and which is stable and very close to one with the task-based code. In addition, the performance is portable on these two architectures. These results encouraged us to continue our work and move across the node boundaries into the distributed memory architectures and especially clusters of hybrid multicore nodes.



LIONEL BOILLOT

Lionel Boillot is now an expert engineer in HPC at the INRIA Magique3D team project. He received a PhD in Applied Mathematics and Computer Science from "Université de Pau et des Pays de l'Adour" in 2014. The PhD thesis took place in the framework of a collaboration between the Inria research institute and the Total oil company. He has a previous experience of 2 years as HPC engineer and he is graduated from the SupGalilée engineering school and the University Paris 6 master class, both in the fields of applied mathematics and computer science. His main research interest falls in with HPC for CSE.

DYNAMICS OF BASIC HYDROLYSIS OF METHYL FORMATE – EFFECT OF MICROHYDRATION

IVAN CERNUSAK
Comenius University in Bratislava

ABSTRACT

Base catalyzed hydrolysis of methyl formate including one, two and three water molecules has been investigated using the ab initio molecular dynamics (MD) with the CP2K code. In MD calculations, we applied exchange functional by Perdew, Burke and Ernzerhof (PBE) with additional empirical dispersion correction (D3 method) by Grimme et al. For all atoms, basis sets of double-zeta quality with polarization in combination with the pseudopotentials proposed by Goedecker, Teter and Hutter (GTH) were used. The MD simulations were conducted at constant volume and temperature 298 and 350 K (NVT ensemble) maintained by CSVR thermostat with a time constant of 0.05 ps in the box of size 24 Å (open boundary conditions).

The study revealed that the important part of this micro-hydration assisted mechanism - the OH- attack on carbon in COH-group - strongly depends on the hydrogen-bonded network in the initial cluster. Several trajectories with different initial geometries of the hydrated CH3 O COH…OH- cluster and total length between 20-30 ps were analyzed. Only a fraction of these trajectories lead to traditional mechanism via BAC2 intermediate, while many end-up in stable but non-reactive hydrated ion coordinated to methyl formate.

Reaction profiles, geometry analysis and detailed participation of the solvent molecules (including animation of important trajectories) in selected cases are discussed.

IVAN CERNUSAK

Ivan Cernusak is professor in Theoretical Chemistry at Comenius University in Bratislava, Slovakia. Currently he is working on atmospheric chemistry problems associated with iodo-carbons and their reactivity in troposphere including the aspects of micro-hydration. He is involved also in theoretical calculations of thermo-kinetic parameters not easily amenable to experiment, e.g. in the primary circuit of a nuclear reactor, spectroscopic and electric properties of exotic diatomics and clusters.

GENDER INEQUALITY IN HPC

ATHINA FRANTZANA
EPCC

ABSTRACT

Gender inequality is a key problem across all scientific disciplines, both in academia and industry. HPC is a discipline that spans multiple traditional science subjects and relies on leading-edge scientific research. It would be plausible that the gender inequality issue, which has been identified and quantified across many fields of science and scientific research, is similarly present in HPC. To motivate action, we must measure and publicise the magnitude of the problem we face. To be effective, we must understand why women do not pursue careers in HPC so that our efforts can be appropriately targeted.

In 2014 the Software Sustainability Institute produced a study on software development in Russell Group Universities. This poster presents evidence of gender inequity in software development from further analysis of this study providing an initial insight into the group of people who use and develop HPC software. Our analysis shows that male researchers are more likely to develop software than female researchers (70% to 30%) and that men are more likely to receive training than women (63% to 39%). This has a profound effect on the people that developed their own software: 56% of the male respondents to the study had received training and developed their own software, whereas only 23% of the female respondents were trained and were developing software. Particularly important, as software developers in academia and HPC users are more likely to work with Linux or Mac. 66.2% of female respondents use Windows, with 33.8% using Mac, Linux or other operating system (Mac 25.7% , Linux 6.6 %). For the male respondents 42.2% use Windows, with the proportion of the male respondents using Mac (27.4%) or Linux (29.6%) doubling compared to men at 57.9%. The higher prevalence of Linux use in men and of Windows in women may be either the cause of the result of the lack of uptake in training by women. In this study we have also identified that women who responded to the survey are more likely to have less mature careers than men. Our analysis shows that there is not a considerable difference between the respondents that have less than 10 years of experience (66.9% of female and 57% of male). However, it is of great interest that 21.7% of the male respondents and only 9.7% of female have more than 20 years of experience.

This poster will present further details of this work and the potential impact of the findings on the HPC community.

ATHINA FRANTZANA

Athina Frantzana is currently in her second year of PhD research studies in the School of Physics and Astronomy. Her research involves the underrepresentation of women in the High Performance Computing (HPC) field and the identification of the reasons and possible solutions. Her scientific background and my previous involvement to the Women in Science (WISE) and the Women in HPC (WHPC) communities provide a better understanding of the female scientists' matters and support my research.

She is a member and fascilitator of Women in HPC Network by providing administrative support. She also was a member of the organising committee for the University of Edinburgh Women in Science and Engineering Workshop and member of the organising committee for the Women in High Performance Computing Network launch (April 2014).

PRACE: A FUNDAMENTAL RESOURCE IN PLASMA ASTROPHYSICS

EMANUELE CAZZOLA
KU Leuven

ABSTRACT

Coupling microphysics and macrophysics is the grandest of the grand challenges in almost all areas of science and engineering. Large scale system-wide effects can be triggered by the smallest scales in the system. An especially convenient field where the micro-macro coupling can be explored is the Earth space environment and its interaction with the incoming solar wind and cosmic rays. In this case we can access directly and measure both the system-wide scales as well as the smallest scales of interest. There are several space missions covering large regions of space surrounding the Earth (about 100 Earth radii, RE, in radius) capable of measuring the evolution of this environment. But from 12 March 2015 (the launch of the four spacecraft will be in about 12 hours at the moment of writing) we will have the Magnetospheric MultiScale (MMS) mission to probe the smallest scale of interest: the electron response scale that is about 100m in size. Needless to say simulating a sphere of 100 RE (or about 600,000 km) with a resolution of 100 meters is a grand challenge. A grand challenge that we at KU Leuven are attempting to solve using the best computing resources available via PRACE Tier-0 allocations.

In our recent work, we have consumed approximately 30 million CPU hours to achieve substantial advances that cover all major steps in the series of key processes developing in the Earth space environment. Like a bullet in the air, the Earth's space cocoon (called magnetosphere) cuts through the solar wind flow, creating a shock wave that compresses and heats up the solar plasma. We are performing simulations of this interaction, never done before, successfully capturing the physics of the entire planetary environment in a domain of 160 x 120 x 120 planet radii, and capturing the detailed physics of individual electrons. Each global simulation requires 750 000 cpu hours, and is used to detect the variations of the particle velocity distributions and pressure anisotropies across the shock, and the effects of the local small scale particle physics on the large scale dynamics.

Within this domain we zoom in on the most important regions of energy release where magnetic reconnection develops. This process allows magnetic field to dissipate enormous energies that are suddenly released in bursts, a phenomenon that has defied explanation for decades. We have performed highly resolved simulations of the most important regions of interest in 3D using up to 48,000 cores and showing several new processes not identified before: the presence of switch-off shocks and rotational discontinuities, multiple interconnected sites each forming interacting islands of magnetic field and magnetic flux ropes embedding points of zero magnetic field (called magnetic nulls). Results that are published in the most prestigious journals in the field.

Every new Tier-0 simulation allows us to get closer to the real dynamics and scales of the plasma environment of our planet, which help us to better understand the impact of the Sun on our life and our technology. Our

goal is to perform in the near future real scale, fully self-consistent, simulations of the full 3D environment of the Earth: the numerical magnetosphere.

EMANUELE CAZZOLA

Emanuele Cazzola obtained a Masters degree in energy and nuclear engineering at Politecnico di Torino (Torino – Italy) with the thesis “Dose and Radiation Effects During Future Missions on the Moon and Mars”.

He is currently a PhD candidate in the Plasma-Astrophysics section of the Department of Mathematics at KULeuven, Leuven, Belgium. His Phd thesis title will be “Models and Simulations of Magnetic Reconnection Processes in Plasmas for physics, laboratory and industrial purposes”, supervised by Giovanni Lepenta. His main research focus is currently “Particle In Cell simulations of asymmetric magnetic reconnection in the magnetopause”. His simulations routinely use as many as tens of thousands of cores and he has hands-on expertise with huge datasets (i.e. hundreds of GBs).

METAL OXIDE NANOCLUSTER MODIFED TiO_2 PHOTOCATALYSTS MODIFIED

MARCO FRONZI
Tyndall institute

ABSTRACT

TiO_2 photocatalysts, which use sunlight to generate chemically active electrons and holes that transform water or CO^2 into hydrogen or hydrocarbon fuels, have two key challenges: (1) to shift the TiO_2 band gap to the visible region, allowing solar energy to be used and (2) enhancing charge separation after photoexcitation. We discuss our modelling work, using density functional theory, on a new mechanism for band gap modification in TiO_2: surface modification of TiO_2 with metal oxide nanoclusters. Modifying TiO_2 with transition metal oxide nanoclusters induces visible light activity, which is achieved by introducing nanocluster derived electronic states above the original TiO_2 valence band edge, to shift the VB edge to higher energy. A model of the photoexcited state confirms the band gap reduction which is controlled by the coverage of transition metal oxide nanoclusters. A range of metal oxide nanoclusters including TiO_2, tin oxides, lead oxides, ZnO and CuO have been investigated and the mechanisms of band gap modification elucidated. Simple rules for modifying TiO_2 to induce visible light absorption are presented. We show that our models can predict the date of photoexcited holes and electrons and that the presence of low coordinated atoms is crucial. Experimental work from world-wide collaborators has confirmed the results of the simulations.

In performing these studies high performance computing using local resources, the ICHEC Stokes and Fionn infrastructure and the PRACE infrastructure (through DECI projects) was absolutely crucial. The simulations involve large atomistic models of TiO_2 based systems, the screening of many potential structures and compositions and associated analysis and post processing. In allowing us to carry out these calculations in the first place (capability) and provide the necessary throughput (capacity), the combined HPC ecosystem of our local, national and European HPC resources was entirely necessary.

Two of the most significant societal grand challenges we face are in Energy Supply (due to the decline in fossil fuel resources and increased fuel usage) and in CO^2 emissions (due to increased fuel usage and with extreme consequences). The photocatalyst materials we have developed mark a significant advance in this field providing a new pathway to photocatalyst development using widely available and safe materials. The ability to operate under visible light and to be sufficiently reactive to oxidise water and convert waste CO^2 to useful molecules has been demonstrated so that these photocatalysts are cutting edge materials in addressing the energy supply and emissions challenges we face into the near future.

MARCO FRONZI

Marco Fronzi is a Scientist Researcher at Tyndall National Institute, University College Cork (Ireland). Marco received my Laurea in Physics and my PhD in Computational Material Science at Tor Vergata University in Rome (Italy).

During the course of his career he has held research positions with a range of institutions across the world, including Osaka University and National Institute for Material Science in Japan, University of Sydney in Australia, University of Tor Vergata and Neuroscience Institute of the National Research Council in Italy, and University College of Cork in Ireland.

The main focus of his research concerns the application of theoretical-computational methodologies (e.g. Density Functional Theory calculations, as ,ab-initio and classical Molecular Dynamics simulations etc.), to understand and predict properties of surfaces, interfaces and bulk of materials of technological interest and to analyse their catalytic surface properties.

The results of his work have been published as scholarly articles in prestigious international journal (among which: Phys. Chem. Chem. Phys., J. Chem. Phys., Phys. Rev. B), and presented in international conferences (e.g. American Physical Society Meeting, American Vacuum Society Meeting, Australian Institute of Physics Congress, The Physical Society of Japan Meeting).

SATELLITE EVENTS

WOMEN IN HPC

Monday 13.30 - 18.00 The Ballsbridge Hotel
Tuesday 09.00 - 15.30 The Ballsbridge Hotel

WOMEN IN HPC :A HANDS-ON INTRODUCTION TO HPC

TONI COLLIS, EPCC
WERONIKA FILINGER, EPCC

In collaboration with the PRACE Advanced Training Centres (PATC), the UK National Supercomputing Facility, ARCHER, and the PRACE Scientific and Industrial Conference 2015 (PRACEDays15) we will be running a 1.5 day 'Hands on Introduction to HPC' training session. This course provides a general introduction to High Performance Computing (HPC) using the UK national HPC service, ARCHER, as the platform for exercises. Familiarity with desktop computers is presumed but no programming or HPC experience is required. Programmers can however gain extra benefit from the course as source code for all the practicals will be provided. This event is open to everyone interested in using HPC, but all our training staff will be women and we hope that this provides an opportunity for women to network and build collaborations as well as learning new skills for a challenging and rewarding career in HPC.

The lectures will be given by Toni Collis, EPCC, Weronika Filinger, EPCC

PROGRAMME

MONDAY 25 MAY 2015 - WOMEN IN HPC: HANDS-ON INTRODUCTION TO HPC PART 1
The Ballsbridge Hotel, Dublin

- 12.30 Welcome and introduction to course
- 12.45 LECTURE: Why learn about HPC
- 13:00 LECTURE: Using HPC: Image sharpening
- 13:15 PRACTICAL: Using HPC: Sharpen example
- 14:30 BREAK: Coffee
- 15:00 LECTURE: Parallel Programming
- 15:30 LECTURE: Building Blocks (CPU/Memory/Accelerators)
- 15:50 LECTURE: Building Blocks (OS/Process/Threads)
- 16:10 LECTURE: Fractals
- 16:15 PRACTICAL: Sharpen (cont.) and Fractal example
- 18.00 Close

TUESDAY 26 MAY 2015 - WOMEN IN HPC HANDS ON INTRODUCTION TO HPC PART 2
The Ballsbridge Hotel, Dublin

- 09.00 LECTURE: HPC Architectures
- 09:45 LECTURE: Parallel programming models
- 10:15 LECTURE: Batch systems
- 10:30 PRACTICAL: Computational Fluid Dynamics (CFD)
- 10:45 BREAK: Coffee
- 11:15 PRACTICAL: CFD (cont.)
- 12:00 LECTURE: Compilers
- 12:30 BREAK: Lunch
- 13:30 LECTURE: Parallel Libraries
- 14:00 LECTURE: Future of HPC
- 14:15 PRACTICAL: Compilers (CFD cont.) Finish exercises
- 15.00 Training finishes

TONI COLLIS

Toni Collis joined EPCC in 2011 as an Applications Developer and later as an Applications Consultant after completing a PhD in Molecular Simulation at the University of Edinburgh. Toni fell in love with HPC during my PhD as she studied EPCC's MSc in High Performance Computing(link is external) part time. She realised the best thing about her PhD was coding and helping her fellow scientists write better software, so a job in EPCC where she spend her time writing HPC code for scientists was perfect!

Her work includes teaching Parallel Numerical Algorithms to postgraduate students, as well as being involved in the ARCHER HPC training programme. Her project work has focused on a variety of topics form optimising Molecular Dynamics software, using solvers to improve current HPC codes, as well as introducing new techniques to port software to new architectures such as GPUs and helping scientists simulate anything from future Nuclear Fusion reactors to understanding the antimicrobial nature of designer molecules in cell membranes. In addition Toni is the Equality and Diversity Coordinator for the School of Physics and Astronomy at the University of Edinburgh and in 2013 she set up the Women in HPC initiative which aims to address the underrepresentation of women in HPC community.

WERONIKA FILLINGER

Weronika Fillinger joined EPCC in 2013 as an Application developer right after finishing EPCC's MSc in High Performance Computing. Weronika became interested in HPC when she was working on my MPhys master project, which was simulating Bootstrap Percolation on Complex Networks. The code Weronika wrote at that time required days to run and she realised that writing the code is only the first step in doing science via computer simulations. After that she completed the EPCC MSc in HPC and this time the subject of her dissertation was Optimising PLINK (a whole genome analysis toolset), which involved both parallelisation and serial optimisations of the code.

Working at EPCC, she have been involved in a variety of different collaboration projects centred on high performance computing including the European collaborative projects CRESTA and APES. Weronika is also involved in HPC training developing EPCC's online distance learning courses.

EUROPEAN EXASCALE PROJECTS

Tuesday 09.00 - 15.30

Enable Exascale in Europe for Industry

Dates: 26 - 28 May 2015
Location: Aviva Stadium, Dublin

Exascale research in Europe is one of the grand challenges tackled by the Seventh Framework Programme for Research and Technological Development (FP7) and becomes even more important in Horizon 2020, the next European framework programme. Started in 2007 and with a total budget of over €50 Billion, the idea is to respond to Europe's needs in terms of jobs and competitiveness, and to maintain leadership in the global knowledge economy. The "European Exascale Projects" represent the collective efforts of multiple collaborative projects funded by the European Commission to investigate and develop hardware and software for Exascale supercomputers.

One of the strategic objectives is to strengthen the scientific and technological base of European industry. Following this aim, the European Exascale projects will organize a European Exascale workshop with a particular focus on industry, in conjunction with PRACEdays15. More information about the European Exascale projects can be found at www.exascale-projects.eu.

Agenda

09:00 Welcome address by EC, Dr. Panagiotis Tsarchopoulos
09:15 Welcome & Introduction by Prof. Dr. Thomas Lippert, Head of Jülich Supercomputing Centre
09:30 Keynote: Exascale Needs & Challenges for Aeronautics Industry, Eric Chaput, Airbus
10:30 – 11:00 Coffee break
11:00 DEEP & DEEP-ER: Innovative Exascale Architectures in the light of user requirements, Gabriel Staffelbach, Estela Suarez & Marc Tchiboukdjian
11:45 Mont-Blanc: High Performance Computing from Commodity Embedded Technology, Filippo Mantovani, Yoon K Ho
12:15 – 13:15 Lunch break
13:15 CRESTA: Developing Software and Applications for Exascale Systems, Mark Parsons
13:45 EPiGRAM: Software in Support of Current and Future Space Missions, Stefano Markidis
14:15 EXA2CT: Mining Chemical Space Annotation to tackle the Phenotypic Challenge of Pharma Industry, Hugo Ceulemans
14:45 NUMEXAS: Embedded Methods for Industrial CFD Applications, Riccardo Rossi
15:15 Panel Discussion moderated by Gilad Shainer
15:15 Conclusion & Farewell

Abstracts

Keynote: Exascale Needs & Challenges for Aeronautics Industry

Eric Chaput, Airbus - Flight-Physics Capability Strategy
Exascale computing is seen as a key enabling technology for future aircraft design to be developed and optimised in a fully multi-disciplinary way, making a wide use of design systems that provide integrated analysis and optimisation capabilities which allow for a real-time/interactive way of working. The move from RANS to unsteady Navier-Stokes simulation, (ranging from current RANS-LES to full LES) and/or Lattice Boltzmann method will significantly improve predictions of complex flow phenomena around full aircraft configurations with advanced physical modelling. For instance moving LES capability from Petascale to Exascale computing will accelerate the understanding of noise generation mechanisms and will enable the elaboration of flow control strategy for noise reduction. Multi-disciplinary analysis and design, and real time simulation of aircraft manoeuver, supported by affordable CFD-based aerodynamic and aero elastic data prediction will be a significant change of paradigm in aeronautics industry. The challenges faced by our industry at the horizon of 2025 will be presented together with the expectations on Exascale computing likely to bring operational benefits at that time.

DEEP & DEEP-ER: Innovative Exascale Architectures in the Light of User Requirements

Estela Suarez, Jülich Supercomputing Centre; Marc Tchiboukdjian, CGG; Gabriel Staffelbach, CERFACS
When developing new architectures for the Exascale era, the chicken-or-egg question arises of what to work on first: new hardware or new codes actually able to fully exploit Exascale systems. In the DEEP and DEEP-ER projects we tackle this challenge by adopting a comprehensive, holistic approach. We have come up with an innovative hardware concept, called the Cluster-Booster architecture. At the same time we develop the software stack and work very closely with our application partners to thoroughly integrate all three aspects. For our pilot applications, on the one hand we optimise their codes for our system, and on the other hand we are developing the system design based on the Exascale requirements that our users have. In this session we will explain our basic concept and share two of our use cases: Our industry partner CGG will talk about seismic imaging in the oil and gas industry, and our partner CERFACS on computational fluid dynamics. These two use cases will clearly demonstrate the potential the DEEP architecture offers at Exascale, not least for industrial users.

Mont-Blanc: High Performance Computing from Commodity Embedded Technology

Filippo Mantovani, Barcelona Supercomputing Center
In this session, the coordinator of the Mont-Blanc project will present an overview and status of this European project together with RR HPC Tech Lead Specialist-Aerothermal Methods at Rolls-Royce, a member of the Industrial End-User Group. He will present their observations from the process of testing the low-energy HPC prototypes produced by the project.

CRESTA: Developing Software and Applications for Exascale Systems

Mark Parsons, EPCC, the University of Edinburgh
The CRESTA project was one of three complementary Exascale software projects funded by the European Commission. The recently completed project employed a novel approach to Exascale system co-design, which focused on the use of a small set of representative applications to inform and guide software and systemware developments. The methodology was designed to identify where problem areas exist in applications and to use that knowledge to consider different solutions to those problems, which inform software and hardware, advances. Using this approach, CRESTA has delivered on all of its outputs, producing a set of Exascale focused systemware and applications.

EPiGRAM: Software in Support of Current and Future Space Missions

Stefano Markidis, KTH Royal Institute of Technology
During the preparation of NASA and ESA space missions, several simulations of different scenarios in space are carried out on HPC systems. These large scale simulations allow scientists to plan the space missions and to investigate possible phenomena of interest. In this talk, we present the new software developed by the EPiGRAM project to increase the scalability of these codes, the performance of the I/O activities and the amount of useful data for analysis. The impact of the EPiGRAM software on the current NASA Magnetospheric Multiscale Mission (MMS) and on the proposed ESA THOR mission (http://thor.irfu.se/) is discussed.

NUMEXAS: Embedded Methods for Industrial CFD Applications

Riccardo Rossi, CIMNE - International Centre for Numerical Methods in Engineering
A problem of paramount importance in the simulations of real engineering problems is the construction of a suitable discretization. It is widely acknowledged that the meshing step required to obtain a suitable geometry may take 90% of the time needed to obtain an engineering result. The objective of our work is to develop a technology to embed "dirty" geometries within a background mesh, which is then adapted to fit the requirements of the simulation. The technique employed results in a methodology, which is both robust and scalable on modern HPC hardware.

EXA2CT: Mining Chemical Space Annotation to tackle the Phenotypic Challenge of Pharma Industry

Hugo Ceulemans, Janssen
The trajectory from a biological concept to a drug available to patients is expensive and typically spans over a decade. Drug discovery starts by mapping a disease mapped to a scalable experiment in a test tube. This enables the screening libraries of chemicals for hits or active compounds, from which chemical starting points or leads are selected. These leads are then taken through a cascade of follow-up assays and animal models to optimize their potency on the intended protein targets implicated in disease, while controlling their activity on undesired targets associated with side effects. Finally, the compound is transferred to drug development, where the candidate drugs are tested in human subjects in three subsequent clinical phases. Still, the vast majority of candidates that enter drug development do not make it through to approval. One current trend to mitigate the high attrition rate is to do the initial screening in more complex, so-called phenotypic assays, which are believed to emulate the disease much better than biochemical assays, and that do not rely on the limiting knowledge of which targets are critical for effect. The phenotypic approach, however, presents challenges of their own: their throughput is lower, implying a need for more compact libraries. Secondly, many of the existing compound optimization processes require knowledge of the target. Both of these challenges can be addressed by improving the industries capabilities to predict the activities of chemical on not just the intended protein target, but on as many proteins and processes as possible. To this end, we propose scaled-up machine learning approaches that can mine extensive but heterogeneous information on biological activities of chemicals that is accessible to the industry, to learn to predict it comprehensively. Moreover, we believe computational approaches enable us to extract much more relevant primary information for these exercises from industry standard screens; for instance, by more extensive image analysis, feature selection and machine learning microscopy based screens. Finally, progress is being made in not only formulating predictions, but also quantifying the reliability of predictions, not just for each model for a certain target, but even for individual prediction of a given chemical at a given concentration on a given target.

SPEAKERS

Eric Chaput, Airbus - Flight-Physics Capability Strategy

Eric Chaput joined Airbus in 1992 after a Ph.D. in Energetics and Optimisation, Post-doctoral positions in Experimental and Numerical Simulation at University of Poitiers, and six years' experience at Airbus Defence & Space working for ARIANE and HERMES programmes. He became subsequently CFD Research Manager, before managing Aerodynamics Methods and in 2004, Senior Manager of Flight-Physics Methods. He is currently the leader of Airbus Flight-Physics capability strategy and a Senior Expert in Aerodynamics Flow Simulation Methods. He has long experience and interest in HPC, driving within the HPC Steering Board the needs and investment for Airbus Engineering, and for more than 15 years member of the Management Board of CERFACS, a research organization and Center of Competence in HPC serving a wide range of industrial sectors.

Estela Suarez, Jülich Supercomputing Centre

Estela Suarez is the project manager for DEEP & DEEP-ER, two European funded Exascale research endeavors. She works at Juelich Supercomputing Center in Germany and holds a PhD in Physics from the university of Geneva. Already early on Estela has engaged intensively in scientific simulations and computing. Her passion for this research area made Estela follow a career in an HPC environment and enter the Exascale world.

Marc Tchiboukdjian, CGG

Marc Tchiboukdjian currently works as IT Architect for CGG, a fully integrated geoscience company providing leading geological, geophysical and reservoir capabilities to the oil and gas industry. He holds a PhD from the University of Grenoble and has been active in the field of Exascale research for the last four years. Within the DEEP project, Marc is working on mapping seismic imaging algorithms on the DEEP architecture and evaluating their performance.

Gabriel Staffelbach, CERFACS

Gabriel Staffelbach is a senior researcher at Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique (CERFACS). He has been working on numerical simulation of combustion and high performance computing since 2002 and is an active user of most HPC systems available to the scientific community via both the PRACE and INCITE programs.

Stefano Markidis, KTH Royal Institute of Technology

Stefano Markidis is Assistant Professor in High Performance Computing at the KTH Royal Institute of Technology. He is a recipient of the 2005 R&D100 award and author of more than 50 articles in peer-reviewed articles. His research interests include large scale simulations for space physics applications.

Mark Parsons, EPCC, the University of Edinburgh

Mark Parsons joined EPCC, the supercomputing centre at The University of Edinburgh, in 1994 as a software developer working on several industrial contracts following a PhD in Particle Physics undertaken on the LEP accelerator at CERN in Geneva. In 1997 he became the Centre's Commercial Manager and subsequently its Commercial Director. Today he is EPCC's Executive Director (Research and Commercialisation) and also the Associate Dean for e-Research at Edinburgh. He has many interests in distributed computing ranging from its industrial use to the provision of pan-European HPC services through the PRACE Research Infrastructure. His research interests include highly distributed data intensive computing and novel hardware design.

Riccardo Rossi, CIMNE - International Centre for Numerical Methods in Engineering

Riccardo Rossi, holds a PhD in Civil Engineering from the Technical University of Catalonia (UPC) and is Senior Researcher at CIMNE and tenure-track lecturer at UPC BarcelonaTech. He has extensive experience in the field of Computational Solid and Fluid Dynamics and in the solution of Fluid-Structure Interaction problems, using both body fitted and embedded approaches. He is one of the authors of the multiphysics code KRATOS and author of 36 JCR papers and some 50 conference presentations in the field, including a plenary lecture. Dr. Rossi is also a member of the executive committee of SEMNI and has contributed to the organization of ECCOMAS conferences.

Filippo Mantovani, Barcelona Supercomputing Center

Filippo Mantovani is a postdoctoral research associate of the Heterogeneous Architectures group at the Barcelona Supercomputing Center (BSC). He graduated in Mathematics and holds a PhD in Computer Science from University of Ferrara in Italy. He has been a scientific associate at the DESY laboratory in Zeuthen, Germany, and at the University of Regensburg, Germany. He spent most of his scientific career in computational physics, computer architecture and high performance computing, contributing to the Janus, QPACE and QPACE2 projects. He joined BSC's Mont-Blanc project in 2013, becoming recently technical coordinator of the project.

Hugo Ceulemans, Janssen

Hugo holds an M.D., an M.Sc. in Bioinformatics and a Ph.D. in Molecular Biology from the University of Leuven, and did postdoctoral fellowships in molecular and computational phosphatase biology at the University of Leuven and in structural bioinformatics at the EMBL in Heidelberg. He joined Janssen in 2008 as a computational biologist supporting the Infectious Diseases and Vaccines franchise with models that predict the clinical efficacy of multi-drug regimens in HIV patients given viral sequences. Over the years, his responsibilities extended to cover additional computational approaches and all disease franchises in Janssen. Three years ago, these activities were consolidated in a new Computational Systems Biology unit, which now offers the analysis and integration of sets of chemical, biochemical, omics, phenotypic and clinical data and the formalization of drug discovery knowledge in predictive quantitative models. Mining the extensive, but heterogeneous annotation of the various biological effects of millions of chemicals is one of the major activities of the unit.

Gilad Shainer, HPC Advisory Council Chairman

Gilad Shainer is an HPC evangelist who focuses on high-performance computing, high-speed interconnects, leading-edge technologies and performance characterizations. Mr. Shainer holds an M.Sc. degree (2001, Cum Laude) and a B.Sc. degree (1998, Cum Laude) in Electrical Engineering from the Technion Institute of Technology in Israel. He also holds patents in the field of high-speed networking.

EESI2 FINAL CONFERENCE

Thursday 13:30 - 18.00
Friday 09:00 - 12.30

The second European Exascale Software Initiative, EESI2, organises its final international conference from noon to noon on 28 and 29 May, 2015 in Dublin back-to-back with the PRACEdays15 (26 – 28 May). More information about the program can be found on the EESI website.

EESI2 is an EC-funded FP7 project. The main goals of EESI2 are to elaborate an evolutive European vision and roadmap and to propose recommendations to address the challenges of Extreme Data and Extreme Computing for the new generation of Exascale computers expected in 2020 and beyond.

More than 120 experts have been involved in the project during the last two years and documents including recommendations have already been published.

The EESI2 project will present its works, vision and recommendations to a large public in a final two days conference, on 28 – 29 May 2015 in Dublin. This major event is organized by SURFsara and funded by the European Commission. The public includes worldwide experts, scientists, engineers, policy makers from different European member states and representatives of the European Commission.

The first day of the event will focus on the technical challenges and recommendations in the areas of “Tools and Programming Models”, “Ultra Scalable Algorithms” and “Data Centric Approaches”, each of them being underlined by the needs of specific user applications. Discussion on the technical aspects of the recommendations will be facilitated through a panel at the end of the day.

The second day will look forward into the future of the European ecosystem for High Performance Computing, in particular into the dawning era of Exascale computing and Big Data challenges. Insights from industry, co-design, education and the perspective of the EC will be discussed, finally resulting in a panel session with focus on the position of Europe in the Exascale roadmap and opportunities. The conference is targeted to worldwide specialists, scientists, engineers, policy makers from different European member states and representatives of the European Commission.

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PRACE days 15