PRACE
Scientific & Industrial Conference 2017

HPC for Innovation: When Science Meets Industry

Conference Programme & Abstracts

Vertex Building Campus Nord UPC
Barcelona, Spain, 16-18 May 2017
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A tabled overview of all sessions during PRACEdays17 can be found on pages 30 to 31.
Welcome

It gives us great pleasure to welcome you to the PRACE Scientific and Industrial Conference 2017 - the fourth edition of PRACEdays, hosted by PRACE and the Barcelona Supercomputing Center under the motto: HPC for Innovation: When Science Meets Industry For the second time the conference takes place in Barcelona in Spain, the PRACEdays series started here in 2014. The cosmopolitan capital of Catalonia offers a wide variety of historical, architectural and culinary highlights.

The Barcelona Supercomputing Center (BSC) is proud to welcome this high-level scientific and industrial conference to Barcelona. BSC, the national supercomputing centre in Spain is at the service of the international scientific community and of industry requiring HPC resources. MareNostrum, managed by BSC, is one of the 7 supercomputers of the PRACE Research Infrastructure. Hosting PRACEdays17 is another opportunity for BSC to significantly contribute to supporting the European HPC ecosystem.

In 2017 the second edition of the European HPC Summit Week is organised by European Extreme Data & Computing Initiative (EXDCI) project and PRACEdays17 forms the central part of this week, alongside various HPC-related workshops representing a wide range of HPC topics, from services to technology, including application development.

PRACEdays17 features keynote speakers from international academia and industry who will present their work on different HPC-related topics. It is a pleasure for PRACE to welcome Khalil Rouhana, Deputy Director-General, DG CONNECT, European Commission to give a talk on “The European HPC strategy - the European Data Infrastructure (EDI)” on Tuesday.

On Tuesday and on Wednesday the conference programme offers parallel sessions with selected speakers from different research domains including Astrophysics, Climate & Environment, Fluid Dynamics, Life Science, Material Science, and Industry. Three industrial parallel sessions presented by experts one of the sessions is from our host country Spain. We recommend you join one of those to get a “flavour” of HPC in industry on Tuesday afternoon.

On Thursday the panel session will be moderated by Inma Martinez, considered by FORTUNE and TIME as one of the world’s leading digital media strategists. The panel gather renowned panellists to discuss the topic: “Support to HPC code: The gap between scientific code development and exascale technology. The software challenges for extreme scale computing faced by the Community”. For the second time PRACE will present the PRACE Ada Lovelace Award for HPC to a woman who is making an outstanding contribution to and impact on HPC in Europe at a global level.

PRACEdays 17 will also offer to you – dear participant – a social programme including a conference dinner at Fàbrica Moritz Restaurant, serving traditional Catalans cuisine as well as international delicacies.

We would like to take this opportunity to thank all those who have made this event possible: the Organisation and Programme Committee, the PRACE Council, the PRACE Board of Directors, the PRACE Scientific Steering Committee, the PRACE Industrial Advisory Committee, the User Forum, the European Commission, the local host BSC 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!
Committees

ORGANISATION & PROGRAMME COMMITTEE (OPC)

Serge Bogaerts  
Chair of the OPC, Managing Director of PRACE aisbl (Belgium)

Veronica Teodor  
Vice-Chair of the OPC, FZ Jülich (Germany)

Erik Lindahl  
Chair of the PRACE SSC, KTH Royal Institute of Technology (Sweden)

Anders Rhod Gregersen  
Chair of the PRACE IAC, Vestas (Denmark)

Lee Margetts  
Vice-Chair of the PRACE IAC, The University of Manchester (United Kingdom)

Koen Hillevaart  
Chair of the PRACE User Forum, CENAERO (Belgium)

Renata Gimenez  
Local host, BSC (Spain)

Sara Ibañez  
Local host, BSC (Spain)

Marjolein Oorsprong  
PRACE Communications Officer, PRACE aisbl (Belgium)

Silke Lang  
PRACE Communications Assistant, PRACE aisbl (Belgium)

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Chair of the SSC; KTH Royal Institute of Technology (Sweden)

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Vice-Chair of the SSC, Free University of Berlin (Germany)

Marina Bécoulet  
CEA (France)

Carlo Massimo  
Casciola University of Rome (Italy)

Luke Drury  
Dublin Institute for Advanced Studies (Ireland)

Claudia Filippi  
University of Twente, Faculty of Science and Technology (The Netherlands)

Laura Grigori  
INRIA/University Pierre and Marie Curie (France)

Dimitri Komatitsch  
LMA CNRS-MRS (France)

Núria López  
Institute Catalan of Chemistry Research (Spain)

Ignacio Pagonabarraga  
Mora University of Barcelona (Spain)

Antonio Navarra  
CMCC (Italy)

Mike Payne  
University of Cambridge EPSRC Centre (United Kingdom)

Matej Praprotnik  
National Institute of Chemistry/University of Ljubljana, Faculty of Mathematics and Physics (Slovenia)

Sinead Ryan  
University Dublin, Trinity College Dublin, School of Mathematics (Ireland)

Per Stenström  
University of Technology, Göteborg (Sweden)

Julia Yeomans  
University of Oxford, Rudolf Peierls Centre for Theoretical Physics (United Kingdom)

Claudio Zannoni  
University of Bologna (Italy)

INDUSTRIAL ADVISORY COMMITTEE (IAC)

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Chair of the IAC; Vestas (Denmark)

Lee Margetts  
Vice-Chair of the IAC; NAFEMS (United Kingdom)

Henk Coenen  
NXP (The Netherlands)

Gibert Enric  
Pharmacelera (Spain)

Christoph Gümbel  
Porsche AG (Germany)

Dieter Jahn  
BASF (Germany)

Jean-François Lavignon  
ETP4HPC (France)

Marc Morere  
Airbus (France)

Jean-Denis Muys  
Audionamix (France)

Stéphane Tanguy  
EDF (France)

Paul Walsh  
Nsilico (Ireland)

Martin Winter  
CEFIC - European Chemical Industry Council (Germany)
Committees

**PRACE BOARD OF DIRECTORS (BoD)**

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<td>Serge Bogaerts</td>
<td>Managing Director PRACE aisbl (Belgium)</td>
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<td>Florian Berberich</td>
<td>FZ Jülîch, Germany</td>
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<td>Sergio Bernardi</td>
<td>CINECA (Italy)</td>
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<td>Maria Grazia Giuffreda</td>
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<td>Erik Lindahl</td>
<td>KTH, Chair of the SSC (Sweden)</td>
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<td>Oriol Pineda</td>
<td>BSC (Spain)</td>
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<td>Stephane Requena</td>
<td>GENCI (France)</td>
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**PROJECT MANAGEMENT ORGANISATION (PMO)**

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<tr>
<td>Thomas Lippert</td>
<td>FZ Jülîch, Project Coordinator (Germany)</td>
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<tr>
<td>Florian Berberich</td>
<td>FZ Jülîch, Project Manager (Germany)</td>
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<tr>
<td>Veronica Teodor</td>
<td>FZ Jülîch, Deputy Project Manager (Germany)</td>
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**USER FORUM (UF)**

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<tr>
<td>Koen Hillewaert</td>
<td>Chair of the User Forum; Centre de recherche en Aéronautique (Cenaero) (Belgium)</td>
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<tr>
<td>Troels Haugboelle</td>
<td>University of Copenhagen, Vice Chair of the User Forum (Denmark)</td>
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<td>Marc Baaden</td>
<td>CNRS (France)</td>
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<td>Carmen Domene</td>
<td>King’s College London (United Kingdom)</td>
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<td>Turlough Downes</td>
<td>Dublin City University (Ireland)</td>
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<td>Derek Groen</td>
<td>Brunell University London (United Kingdom)</td>
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<td>Stefano Fabris</td>
<td>CNR-IOM Democritos (Italy)</td>
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<tr>
<td>Maria-Teresa Parra</td>
<td>University of Valladolid (Spain)</td>
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<tr>
<td>William Sellers</td>
<td>University of Manchester (United Kingdom)</td>
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<tr>
<td>Gabriel Staffelbach</td>
<td>Cerfacs (France)</td>
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<tr>
<td>Jorge Vieira</td>
<td>Instituto Superior Técnico (Portugal)</td>
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<tr>
<td>Gustavo Yepes</td>
<td>Universidad Autonoma de Madrid (UAM), (Spain)</td>
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**MEDIA CREW**

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<tr>
<td>Ramon Viã</td>
<td>Vision film, producer</td>
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<tr>
<td>Antonio Iglesias</td>
<td>Vision film, video/photography crew</td>
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<tr>
<td>Marta Lacima</td>
<td>Vision film, producer</td>
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The PRACEdays staff will welcome you at the on-site registration desk but likewise they will be happy to help you if you have any questions during PRACEdays17.

You will easily recognise them as they all wear a blue PRACEdays17 T-shirt.
European HPC Summit Week

MONDAY 15 MAY
- EXDCI Workshop

TUESDAY 16 - THURSDAY 18 MAY
- PRACEdays17

TUESDAY 16 MAY
- HPC for renewable energies: New programming models and strategies for the emerging exascale architectures (EoCoE).
- ENES / ESIWACE HPC Workshop.

WEDNESDAY 17 MAY
- Mathematics for Exascale and Digital Science.
- EuroLab-4-HPC: The Future of High-Performance Computing.

THURSDAY 18 MAY
- Round-Table: Exploiting the Potential of European HPC Stakeholders in Extreme-Scale Demonstrators.
- EUDAT workshop: Coupling HPC and Data Resources and services together.

FRIDAY 19 MAY
- POP User Forum: Help us, help you! Help us improve the POP Service so that we can help you improve your HPC Applications.
- Closed ETP4HPC SRA Workshop (registration only for ETP4HPC SRA working group leaders and selected partners only).
- Closed ETP4HPC Steering Board Meeting (registration open to the ETP4HPC Steering Board Members and invited guests only).
- NextGenIO / SAGE workshop: Working towards Exascale IO.
General Information

**PRACEdays17**
*From Tuesday 16 May to Thursday 18 May 2017*

**VENUE**
Vertex Building,
Campus Nord UPC,
Plaza Eusebi Güell,
Barcelona Supercomputing Centre.
Tel. (+34) 93 413 77 16
Website: [www.bsc.es](http://www.bsc.es)

**REGISTRATION DESK**
The main registration and information desk is situated at the entrance of the Auditori hall of the Vèrtex building from Monday to Friday.

- **Tuesday 16 May**: 08:00 – 18:00
- **Wednesday 17 May**: 08:00 – 18:00
- **Thursday 18 May**: 08:00 – 13:00

The registration staff will be happy to help you with any local information, social events and internet access.

**COFFEE BREAKS AND LUNCHES**
Morning and afternoon coffee breaks and lunches will be served at the hall of the Auditori or outdoors at the gardens.

**WELCOME RECEPTION**
*Tuesday 16 May 2017*
Auditori Hall, 18:30 – 20:30
Included in the registration fee.
The reception will be held at the Auditori hall.
The reception is held in conjunction with a poster session which gives the delegates an opportunity to browse the posters as well as connect with colleagues and friends.

**CONFERENCE DINNER**
*Wednesday 18 May 2017*
Sala 39 - Fàbrica Moritz
20:00 – 22:00
Included in the registration fee.
Shuttle buses will be available in front of the Vertex building at 19:30.
Useful Information

**WHAT TO SEE IN BARCELONA**

**Discover the City on Foot**
Barcelona is a big city, but it’s the perfect size to discover on foot. Spend a day away from the metro and the tourist bus, and take your time strolling around and stopping to taste the city’s great gastronomic options. If you are in the mood for visiting some of the most impressive buildings and parks, you will want to see all the Parc de la Ciutadella has to offer as well as the Parc de Joan Miró, and the Montjuïc castle, but there’s also a Barcelona you won’t find in guidebooks. Get off the beaten path and head up to Horta, get to know the charm of the Sant Andreu district, see a lesser-known side of the Eixample and take in breathtaking panoramic views.

**Explore Gaudí and Modernisme**
Without a doubt, one of Barcelona’s top attractions for tourists (as well as for those who live here) is admiring the city’s modernist architecture and the works of Antoni Gaudí in particular. Just walking around you’ll come across various examples of Gaudí’s work throughout the city, be they civil or religious buildings. The most famous are the Sagrada Familia, impressive both outside and in; Park Güell, a space that’s out of a fairy tale and emulates an English garden city; and La Pedrera. But don’t miss the opportunity to visit other Gaudí buildings that sometimes occupy smaller space in guidebooks, such as Palau Güell, Casa Batlló, Torre Bellesguard, Casa Vicens and (if you have time to venture a bit outside Barcelona) the crypt of the Colònía Güell, in Santa Coloma de Cervelló. But Gaudí wasn’t the only modernista architect who left his mark on Barcelona. Also worth a visit are Casa Amatller and the Palau de la Música, works by Puig i Cadafalch, Casa Lleó Morera, designed by Domènech i Muntaner; and Casa de les Terrades. Another example is the Hospital de la Santa Creu i Sant Pau, a World Heritage Site and whose gardens are an oasis in the bustle of the city.

**CURRENCY**
The currency in Spain is €.

**CREDIT CARDS**
Major credit cards are widely accepted.

**ELECTRICITY**: 220V/16A
Please bring a suitable adaptor for an E type sockets.

**TIME**
Spain is in the Central European Time zone (CEST).

**IMPORTANT NUMBERS**
Emergency number: 112; Taxi: +34 93 225 00 00

**WIFI**
All delegates will have free WiFi at the Vertex building and Eduroam will also be available.

1. Select the network “XSF-UPC”
2. Open the browser. You will be automatically redirected to the login site.
3. Then you have two options:
   3.1 For http and https access only, use the “Guest” button
   3.2 For full access, use either of the following:
      Username: EXDCI Password: Barcelona2017
      Username: xsf.convidat Password: 2017Mecanica
Vertex Building, 
Campus Nord UPC, 
Plaza Eusebi Güell, 
Barcelona Supercomputing Centre. 
Tel. (+34) 93 413 77 16 
Website: www.bsc.es
Floorplan of Vertex Building

MINUS 2 FLOOR

- Plenary Sessions
- Parallel Tracks
- Poster Session, Coffee, Lunch & Cocktail Reception
- Garden: Coffee, Lunch & Cocktail Reception
- PRACE Staff Room
Keynotes
PLENARY SESSION

Chair
SERGE BOGAERTS, Managing Director of PRACE aisbl
Serge Bogaerts graduated in 1992 as a Mechanical and Electrical Engineer from the Free University of Brussels (ULB), then as a researcher in numerical fluid mechanics at the von Karman Institute. He studied engineering in nuclear safety at Tractebel Engineering, and in 2003 worked as a researcher in CFD-Multiphysics of supercomputers at Cenaero. Serge knows the challenges of numerical simulation. He managed the operations of Cenaero supercomputers from 2006 which allowed him to gain experience in leading projects of procurement and operation of HPC infrastructures. In October 2012 he was appointed as Belgian Delegate to the PRACE Council and since October 2015 has also served as Council Secretary. He left Cenaero to take on the role as Chair of the Board of Directors and Managing Director of PRACE aisbl in February 2017.

Opening of PRACEdays17
ERIK LINDAHL, Chair of the PRACE Scientific Steering Committee; Stockholm University
Erik Lindahl received a PhD from the KTH Royal Institute of Technology in 2001, and performed postdoctoral research at Groningen University, Stanford University and the Pasteur Institute. He is currently professor of Biophysics at Stockholm University, with a second appointment as professor of Theoretical Biophysics at the Royal Institute of Technology. Lindahl’s research is focused on understanding the molecular mechanisms of membrane proteins, in particular ion channels, through a combination of molecular simulations and experimental work involving cryo-EM and electrophysiology. He has authored some 130 scientific publications and is the recipient of an ERC starting grant. Lindahl heads the international GROMACS molecular simulation project, which is one of the leading scientific codes to exploit parallelism on all levels from accelerators and assembly code to supercomputers and distributed computing. He is co-director of the Swedish e-Science Research Center as well as the Swedish National Bioinformatics Infrastructure, and lead scientist of the BioExcel Center-of-Excellence for Computational Biomolecular Research. His research work has been awarded with the Prix Jeune Chercheur Blaise Pascal, the Sven and Ebba-Christian Högberg prize, and the Wallenberg Consortium North prize. Lindahl is currently the chair of the PRACE Scientific Steering Committee.
Keynotes

PLENARY SESSION

Opening of EHPCSW

SERGI GIRONA, EXDCI Co-ordinator

Sergi Girona is Director of the Operations Department of the Barcelona Supercomputing Center (BSC). He has belonged for many years to the BoD of PRACE since its creation in 2010, and was both its Chair and Managing Director until September 2015. He was lately appointed as Council Vice-Chair, in June 2016, a role that he performs currently. He holds a PhD in Computer Science from the Technical University of Catalunya. In 2001, EASI Engineering SL 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. In July 2017, MareNostrum 4 is scheduled to enter in production. Currently, he is managing the Operations group with the responsibilities for User Support and System Administration of the different HPC systems at BSC. He is also project coordinator of EXDCI, the EHPCSW organizer.

Welcome

ANWAR OSSEYRAN, Chair of the PRACE Council

Anwar Osseyran is since 2001 the CEO of SURFsara (formerly SARA), the Dutch national HPC Center and since January 2015 is a member of the Executive Board of SURF, the Dutch Cooperative of Research and Education. He is part-time Professor of Business Analytics and Computer Science at the University of Amsterdam and has worked before with various companies including Philips, Digital Equipment, HISCOM and Omron. He has a Masters in Electrical Engineering and a PhD in Applied Physics. He has been elected in June 2016 as Chair of the PRACE Council. He is also the chair of the Advisory board of the Swiss National Supercomputing Centre, member of the of the Scientific Advisory Council of The Cyprus Institute (CaSToRC), member of the Executive Board of Netherlands ICT (the Dutch ICT association), member of the Amsterdam Climate Council and Chair of Green IT Consortium Amsterdam. Anwar Osseyran is (co-)author of the books “Broadband in a world of Glass” (ISBN 903952449), Sustainable ICT (ISBN 9789012582285), Green ICT & Energy (ISBN 9780415620963), The Big Data Revolution (ISBN 9789082199314) and Industrial Applications of High Performance Computing (ISBN 9781466596801). Anwar Osseyran has three patents to his name.
Keynotes
WELCOME BY LOCAL HOST

LOCAL HOST
JOSEP MARIA MARTORELL, Associate Director of the Barcelona Supercomputing Center
Josep Maria Martorell is the Associate Director of the Barcelona Supercomputing Center. Dr Martorell has a PhD in Computer Science from Ramon Llull University and a degree in Physics from the University of Barcelona. He has ample knowledge of the research environment, with a twelve years of experience in this sector, five of which as Director General of Research of the Government of Catalonia. Since April 2016 he is Associate Director of the BSC.

LOCAL HOST
FRANCESC SUBIRADA I CURCÓ, Director General for Research
Frances Subirada I Curcó has a bachelor’s degree in Chemical Engineering from the Institut Quimic de Sarrià (IQS) and a master’s degree in Business Administration from the Open University Business School (UOBS, United Kingdom). Between 1989 and 1999, he was responsible for a number of strategic, technical and business areas at IBM. From 2000 to 2004, he was associate director of the IBM-UPC joint research institute. He was also director of the IBM Centre for Advanced Studies in Barcelona. In 2005 he helped found the Barcelona Supercomputing Center (BSC) and was associate director of the public consortium from its creation until his appointment as Director General for Research. Subirada has been a member of a number of European councils and boards on research and development in information and communication technology, focusing especially on the European supercomputing strategy. He has continuously been involved with international and national universities and public and private research and development centres throughout his career.
The European HPC strategy  
– The European Data Infrastructure (EDI)

KHALIL ROUHANA, Deputy Director-General, DG Connect, European Commission,

ABSTRACT
Digitisation is in the heart of the Digital Single Market and it is impacting all areas of our life and economy. High Performance Computing (HPC), Big Data and Cloud are critical technologies that are driving major scientific, industrial and social innovations in the global digital economy. The European Cloud Initiative is one of the key elements of the Commission’s strategy for the Digitisation of Industry. This initiative aims to put Europe in the driving seat of the global data-driven economy, based on the capacity to manage, store and analyse the huge volumes of information generated by the data revolution. The European Cloud Initiative will establish an ambitious European Data Infrastructure of world-class HPC, high-speed networks, and data capabilities. The goal is to provide the scientific community, the public sector and industry with leading-edge technologies and solutions benefiting all areas in science, business and society. The European Cloud Initiative also foresees actions to establish a complete European HPC ecosystem to acquire leadership-class supercomputers, secure its own independent HPC technology and system supply, and deploy HPC services to industry and SMEs. No single Member State will have the human or financial resources to acquire exascale capabilities and develop the necessary HPC ecosystem on its own in the same time frame as the US, Japan or China. The European Cloud Initiative will require the coordination of national and European investments in an EU-wide strategy to reach the ambitious goals and provide the HPC capabilities required for Europe to realise its potential and compete globally.

KHALIL ROUHANA

Khalil Rouhana is the Deputy Director-General in DG Connect (Communications Networks, Content & Technology) since 1/12/2016. His responsibilities include the policies for digital economy and society and notably for research, innovation and industrial strategies, digital solution for societal challenges and governments as well as cybersecurity. Before that he was Director for “Digital Industry” in DG Connect supporting the competitiveness of core digital sectors in Europe and the digitisation of all industrial sectors of the economy. In his previous experiences in the Commission, he was the Director for “Digital content & Cognitive systems”, the Head of Unit in charge of ICT research and Innovation strategy, and started as a project officer in the ESPRIT programme in the areas of High Performance Computing and Future and Emerging technologies. Before joining the Commission in 1992, he was director of an institute and a school of engineering (Grande Ecole) in France for 5 years. He started his career as research and development engineer for the aeronautics industry, worked for the French University in Beirut and also created his own engineering company. He has a master degree in electrical and electronic engineering from “Ecole Supérieure d’Electricité” (Supelec, France).
Vlasiator: Understanding Near-Earth Space in Six Dimensions
MINNA PALMROTH, Professor in Computational Space Physics
Department of Physics, University of Helsinki, Finland

ABSTRACT
The constant flow of solar wind from our star, the Sun, builds the richest reachable plasma laboratory with spatial and temporal scales not attainable in terrestrial laboratories. Plasma phenomena within the near-Earth space create space weather, referring to harmful effects that can endanger technological systems or human life in space. Space weather predictions are mostly at an empirical stage, while future forecasts will be based on numerical simulations. Up to now, large-scale space weather simulations are based on a very simple theory assuming that plasma is a fluid. Vlasiator is a newly developed large-scale space physics model. Vlasiator modelling targets are immense: To model the entire near-Earth space with a breakthrough resolution, using a description going far beyond the existing large-scale plasma simulations. Therefore, Vlasiator includes advanced high-performance computing techniques available from load-balancing to highly scalable grids to allow massively parallel computations. Due to the unprecedented accuracy at global scales, Vlasiator has been used to discover phenomena that no one thought would exist. The presentation introduces Vlasiator, and some of the recent science results. Future application areas may include space weather, 6D fusion modelling, and spacecraft instrument specification definitions, along with acting as benchmark code to test new facilities and architectures. Based on the work of Minna Palmroth (please have look on Vlasiator http://vlasiator.fmi.fi) a new game Mars Mania has developed.

MINNA PALMROTH
Minna Palmroth is a professor in computational space physics at the University of Helsinki. She received a PhD degree in 2003. In 2011, she became the Head of Department at the Finnish Meteorological Institute to lead more than 60 researchers in fields ranging from radar and space technology to earth observation and space weather. At age 41, she has managed research grants worth over €4.5M, including two European Research Council grants, and two PRACE Tier-0 grants. She is an internationally distinguished researcher and holds important national and international positions of trust both in science and in the private sector: she is, e.g., the Chair of the Space Advisory Group for the European Commission, and a member of Advisory group for Vapa Media, the leading digital media company in Finland. She is highly active both in outreach and societal impact, and interested in coupling science with public and private sectors.
Keynotes

PLENARY SESSION

Quantitative Supply Chain Optimization Using Big-Data Methodologies in The Chemical Industry

TELLI VAN DER LEI, Senior Scientist, DSM Chem Tech R&D BV, The Netherlands

ABSTRACT
Supply chain is an important function within the chemical industry business as it is responsible for the timely transformation of raw materials, into intermediates, and eventually end-products that need to be delivered to customers. Inventory assets, for example, are part of OWC and help reflect the status of a company’s liquidity and solvency. Within DSM, supply chain optimization helps to improve operational efficiency. Model based simulation and optimization can generate insights about the behavior of the supply network in relation to planned production and (future) customer demand. Over the years different generations of supply chain models have improved DSM operations and through PPP projects new forms of modelling are actively being explored. Two trends drive this need for continuous model improvement: increasing amounts of data that are available need to be harnessed, and growing awareness that the supply chain is a complex and dynamic global network that requires the right models to help understand policy effects. Within DSM, the Business and Operations works streams of the DSM Big Data Program aim at finding solutions for the challenges these trends provide. Solutions are being developed for e.g. Data Driven Growth, Sales Forecasting, Statistical Forecasting, Finance OWC & Risk, and Supply Chain Optimization.

TELLI VAN DER LEI
Telli van der Lei is Senior Scientist in Supply Chain & Process Modeling at DSM. She is responsible for the Business and Operations research projects done within the DSM Big Data Program which she helped to set up as lead scientist. Next to this, she focuses on business projects for data driven growth. Telli has a MSc in Science & Policy from the University of Utrecht and a PhD from Delft University of Technology in quantitative problem structuring methods used for operations research. She worked as a post doc and assistant professor at the department of Engineering Systems and Services (ESS) which focused on the design of system architectures and market mechanisms that enable the transition to renewable energy, sustainable mobility and ubiquitous computing. Her research focused on asset management and model based decision support for energy and industry. For example, introducing agent based modelling to Shell Global Solutions by developing a network simulation model for stranded gas fields.
Keynotes
PLENARY SESSION

Presentation of the Upcoming Call for Proposals of the Connecting Europe Facility (CEF) Telecom 2017
LEONARDO FLORES AÑOVER,
Senior Expert in the HPC and Quantum Technologies Unit of DG Connect
Leonardo Flores Añover is a Computer Scientist from the Polytechnic University of Madrid and worked in industrial R&D in the fields of Telecommunication & Space before joining the European Commission in 1995. In the EC, he had several positions as Project Officer in the areas of distributed systems, Computer Science, Embedded Systems and High Performance Computing (HPC). He is currently a Senior Expert in the HPC and Quantum Technologies Unit of Directorate General CONNECT dealing with the European HPC strategy, in particular for the coordination and integration of the HPC, communication and data infrastructures into a European Data Infrastructure and for the support to the European HPC ecosystem. He is Project Officer for the PRACE Implementation Projects, several Centres of Excellence on HPC and other research and innovation actions.

Developing European Technology to Serve the HPC Ecosystem
JEAN-PIERRE PANZIERA, ETP4HPC Chair
Chief Technology Director for Extreme Computing at Atos
The European HPC ecosystem is one of the best in the world with a large HPC user base, an outstanding HPC applications development community and a set of Tier-0 HPC datacentres. The purpose of the ETP4HPC (European Technology Platform for High Performance Computing) is to develop the last component: a complete European HPC technology ecosystem. This talk will present the current efforts undertaken under the Horizon 2020 programme to foster the development of European technologies for HPC and Big Data.

JEAN-PIERRE PANZIERA
Jean-Pierre Panziera is the Chief Technology Director for Extreme Computing at Atos. He started his career in 1982 developing new algorithms for seismic processing in the research department of the Elf-Aquitaine oil company. Then he moved to the Silicon Valley as an application engineer and took part in a couple of start-up projects, including a parallel supercomputer for Evans & Sutherland in 1989. During the following 20 years, he worked for SGI successively as application engineer, leader of the HPC application group and Chief Engineer. In 2009, he joined Bull, now an Atos company, where he is responsible for the HPC developments. Jean-Pierre holds an engineer degree from Ecole Nationale Supérieure des Mines de Paris.

13:00 - 14:30 Lunch
Materials Science
SCIENTIFIC PARALLEL TRACK 1

Chair
MATEJ PRAPOTNIK, University of Ljubljana, Slovenia

Matej Praprotnik is head of Molecular Modeling at the National Institute of Chemistry, Ljubljana, Slovenia. He studied physics at the University of Ljubljana. From 1998 to 2003 he worked as a young researcher at the National Institute of Chemistry, Ljubljana, where he also obtained his PhD in 2003. He has been employed at the National Institute of Chemistry since then. He joined the Theory group at the Max Planck Institute for Polymer Research, Mainz, Germany as a postdoc in 2004 and stayed until the end of 2008. In 2008, he received his habilitation in physics at the University of Ljubljana and he has been an associate professor of physics at the Faculty of Mathematics and Physics, University of Ljubljana since 2013. In 2008, he was a visiting scientist at the Institute for Mathematics and Its Applications (IMA), University of Minnesota, USA, for a month. In 2009 and 2010, he was a visiting scientist at the ETH Zurich, Switzerland for 6 months and a member of KITP, UCSB, Santa Barbara, CA for 2 months in 2012. In 2013, he was also a visiting scientist at the Kavli Institute for Theoretical Physics China (KITPC) at the Chinese Academy of Sciences, Beijing, China. Since 2015 he has been the President of the Slovenian Biophysical Society. Since 2016, he has been a member of PRACE Scientific Steering Committee (SSC). His research interest is focused on multiscale modeling & simulation of soft and biological matter.

Bioinspired Surfaces For Robust Submerged Superhydrophobicity: Insights from Molecular Dynamics
ALBERTO GIACOMELLO, University of Rome Sapienza, Italy

ABSTRACT
Superhydrophobicity is a class of surface properties of enormous technological interest, including self-cleaning, anti-fouling, drag-reduction, which stems from the presence of a gas layer (plastron) entrapped within surface roughness. This state is fragile, as changes in the environmental conditions, such as pressure, may break down these microscopic bubbles. The main challenge of the PRACE Project “SLIP - Salvinia-inspired surfaces in action: slip, cavitation, drag reduction” to develop new design criteria for robust submerged superhydrophobicity: underwater, pressure variations can be significant and the plastron must survive for the whole duration of the application. The key findings were inspired by the remarkable properties of an infesting water fern, the Salvinia molesta whose leaves evolved topographically and chemically complex hairs that allow the plant to preserve a gas layer under extreme environmental conditions. We thus employed massively parallel molecular dynamics simulations to investigate how the surface chemistry and the geometry of roughness can be combined to resist both positive pressures and negative ones (suction) and to optimize the durability of superhydrophobicity: bioinspiration revealed that a re-entrant geometry and a heterogeneous surface chemistry guarantee robust superhydrophobicity over the broadest range of pressures.
ALBERTO GIACOMELLO
Alberto Giacomello graduated in 2010 in Mechanical Engineering from Sapienza University of Rome and in 2011 from the Polytechnic Institute of New York University. In 2014 he obtained a PhD in “Theoretical and Applied Mechanichs” from Sapienza; his thesis was selected among the top 5 in Europe in the field of flow, turbulence, and combustion (ERCOTAC da Vinci competition). Subsequently, he joined the Max Planck Institute for Intelligent Systems in Stuttgart as a post-doc. Presently, he is researcher (assistant professor) in the Department of Mechanical and Aerospace Engineering at Sapienza where he works in the group of Prof. Casciola within an ERC-ADG on cavitation. His research area is in fluid and interfacial problems at the micro- and nanoscale, focusing on nucleation, superhydrophobicity, and contact angle hysteresis. During the tenth call, he obtained access to PRACE infrastructure through the two-year project “SLIP” investigating the properties of nanostructured surfaces for underwater applications.

Optimized Monte Carlo and Molecular Dynamics Algorithms for modelling the self-organization of two classes of materials: semifluorinated alkanes and semiconducting polymers based on thiophenes
FLORA TSOURTOU, PhD student, University of Patras, Greece

ABSTRACT
Monte Carlo is a very promising method for overcoming the problem of long relaxation times plaguing molecular dynamics methods in atomistic simulations of complex soft matter systems. In Monte Carlo, system equilibration is effected by using efficient moves which do not follow the natural trajectory of the system; instead, they can be totally unphysical thus dramatically accelerating the rate with which the system samples new states in phase space. We are developing efficient Monte Carlo algorithms to simulate three classes of materials: semifluorinated alkanes (SFAs), polymer semiconductors based on thiophene (substituted and unsubstituted), and polypeptides (e.g., poly-L-alanine and glycine), all of which present morphology at the nanoscale. To predict chain self-organization and long range molecular ordering in these systems, it is absolutely necessary to work with large simulation cells containing hundreds of thousands of atomistic units. To cope with the corresponding large requirements in CPU time, we then identify the subroutines with the largest demand in computational resources and run in parallel by utilizing multithreading on NVIDIA graphics processing units (GPUs) or by implementing MPI. This improves code performance by almost one order of magnitude with some spectacular results concerning the predicted morphologies.
FLORA TSOURTOU
Flora Tsourtou obtained her Diploma (in 2010) and then her Master’s (in 2013) in Chemical Engineering, both from the University of Patras, Greece. Since then, she has been a PhD student in the same Department, in the Laboratory of Statistical Thermodynamics and Macromolecules directed by Prof. Vlasis G. Mavrantzas. She implements highly complicated, state-of-the-art Monte Carlo moves for the atomistic Monte Carlo simulation of polymeric systems with emphasis on chain self-organization at the nanoscale. In the past, these moves had been developed for simpler systems. She currently redesigns them for two more complex families of polymeric systems, thiophene-based polymer semiconductors and polypeptides. The Monte Carlo codes she develops is optimized to run on Graphics Processing Units (GPUs) or in parallel by implementing MPI. She developed an expertise in parallel programming and her codes run on several supercomputing environments via the PRACE and LinkSCEEM projects.
Spanish Industry
INDUSTRIAL PARALLEL TRACK 1

Chair
José María Cela, CASE Department Director at BSC, Spain

José M. Cela gained a PhD in Telecommunication Engineering from Universitat Politècnica de Catalunya (UPC) and is Professor of Computer Architecture at the same university since 1996. He is Director of the Department of Computer Applications in Science and Engineering (CASE) at the Barcelona Supercomputing Center (BSC) since 2007. He has directed more than 25 R&D projects (and participated in more than 40), has published over 80 articles and has participated in more than 100 international conferences. His research is related to numerical simulation in engineering and high performance computing (HPC). In recent years, his research has focused on the energy sector. He directs the joint research center Repsol-BSC. In addition, he is responsible for the macro-research project with Iberdrola renewables and several other projects in the field of fusion energy.

In Silico Drug Discovery and Computation
Robert Soliva, Nostrum Biodiscovery, Barcelona, Spain

ABSTRACT
Knowledge-driven drug discovery and personalized medicine have completely shifted the way pharmaceutical and biotech companies operate. 25 years ago, computers were just an auxiliary tool that played a secondary role. Currently, it is impossible to conceive the development of new therapies without a heavy use of computation. From target-based approaches in early discovery to the analysis of tons of genomic and clinical data, computers are now at the center stage. Nostrum Biodiscovery (NBD) is a newly created company specializing in the development and exploitation of simulation techniques for the discovery of new therapies. During the presentation, some examples of the proprietary technologies of NBD will be given, all of them demanding heavy computational power.

Robert Soliva took his BSc in Molecular Biology and Biochemistry at the University of Barcelona (UB). Later, he took his PhD in protein and nucleic acid molecular recognition thanks to a CIRIT grant in the group of Dr. Modesto Orozco (also at the UB). He worked in the Drug Discovery unit of Laboratorios Uriach and Palau Pharma for more than 12 years during which he actively contributed to the development of several clinical candidates that were licensed to top-tier pharma companies. During the last 5 years, he worked for the firm ZBM Patents & Trademarks as patent agent and has now taken the role of Chief Scientific Officer at Nostrum Biodiscovery, a spin-off company participated by the Barcelona Supercomputing Center, the Institute of Research in Biomedicine, ICREA, the University of Barcelona and Fundación Marcelino Botín.
Vortex Bladeless: A New Way to Harvest Wind Energy

JOSE F. VIYEIRA, R&D Project Engineer, Vortex Bladeless

ABSTRACT

The aim of Vortex Bladeless’ device is to harvest energy from the wind taking advantage of a phenomenon called Vortex Induced Vibrations (VIV). The geometry of the device is designed in such a way that vortices generated all along the structure are synchronized. To manufacture a prototype and test it within controlled environments is very useful for the technical development of the device. However, it really is far from being the most efficient strategy, because big efforts are spent on experimental assays that might not answer the questions nor within the time frame acceptable for a project like this. Hence, HPC allows a very close approximation to the reality giving accurate, fast and truthful answers to what is asked for, permitting a faster development of the device. At the same time, it gives the opportunity to make a very extensive understanding of what is actually happening within the fluid and its interaction with the structure. This approach is helping us to improve the geometry and the scalability of the device.

JOSE F. VIYEIRA

Jose Viyeira is an Aerospace Engineer (Universidad Politécnica de Madrid). His passion for space, planes and cars made him highly interested in Fluid Dynamics. He worked in many different projects such as the Formula Student Kart Competition at the University of Hertfordshire (IAESTE scholarship). He also worked for the Airbus A350 program (ATOS), in Design and Systems Departments. Afterwards, he made his Final Degree Thesis at the Politecnico di Torino. His main role in Vortex Bladeless as CFD Engineer, is to generate models to compute and analyze the complex interactions between the air and the structure. Nevertheless, as a part of the R&D team, Jose manages other tasks such as logistics, prototyping, external collaborations and every other aspect that helps to develop the technology. Lots of failure and success has brought to him here, so he feels proud of them both.
Chair
CHRISTOFF SCHÜTTE, President, Zuse Institute Berlin (ZIB), Germany

Christof Schütte is the President of the Zuse Institute Berlin (ZIB), Berlin’s Competence Center for Computing and Data Science. Simultaneously, he is a full-professor of mathematics at the Freie Universität Berlin, and co-chair of the Research Center MATHEON and of the Einstein Center for Mathematics. He received his diploma in Physics and his PhD in Mathematics and is author and of over 150 Peer Reviewed publications in multiscale modeling and simulation of complex system, numerical mathematics, computational biology, chemistry as well as data science. Presently, he acts as the Vice-Chair of the Scientific Steering Committee of PRACE.

A Multiscale Model of Chromatin at the bp-level
JÜRGEN WALTHER, PhD student, IRB Barcelona, Spain

ABSTRACT
The three dimensional organization of chromatin inside the cell nucleus is expected to strongly depend on sequence specific properties of nucleosomal and linker DNA. However, recent experiments cannot yet capture the characteristics of chromatin arrangement on the resolution level of a single base-pair. To model the chromatin fiber with bp-level accuracy we first developed a coarse-grained DNA model (CG) to investigate sequence dependent DNA properties (with the simulation times ~10⁵ times faster than conventional all atom molecular dynamics (MD) simulations). In our model, DNA is represented intrinsically at base pair level with an elastic potential representing the interactions between adjacent base pairs. Coupling terms between base pairs are extracted from atomistic MD simulations of DNA with the new parmbsc1 force field. A comparison of DNA structures generated by CG and by all atom MD reveals striking similarity of important features such as the distribution of helical parameters and bending properties. To extend the DNA model towards chromatin, a linker DNA is described as above in the CG model, secondly the nucleosome is introduced as a rigid object in between two linkers and thirdly electrostatic and steric potentials account for long-range intra-fiber interactions. This representation of chromatin makes it possible to study the characteristics of few kb-long chromatin fibers of arbitrary linker sequence and length at base pair level accuracy. Among other things we find out that a long linker separating a set of nucleosome strings of equal linker lengths can play an important role in the formation of self-associating domains in the genome.
Rapid, Accurate, Precise and Reliable Relative Free Energy Prediction Using Ensemble Based Thermodynamic Integration

AGASTYA P. BHATI, PhD student, University College London, UK

ABSTRACT
The use of in silico methods to predict binding affinities of ligands to proteins has been largely confined to academic research until recently, primarily due to the lack of their reproducibility, as well as lack of accuracy and time to solution. In the last few years, an ensemble based molecular dynamics approach has been proposed that provides a route to reliable predictions of free energies. Here, we describe our approach to thermodynamic integration, known as TIES, which substantially improves the speed, accuracy, precision and reliability of calculated relative binding free energies. We report the performance of TIES when applied to a diverse set of protein targets and ligands. The results are in very good agreement with experimental data (90% of the predictions agree to within 1 kcal/mol) while the method is reproducible by construction. Statistical uncertainties of the order of 0.5 kcal/mol or less are achieved. This methodology, which is being pursued in the CompBioMed Centre of Excellence (www.compbiomed.eu), has the potential to positively impact the drug design process in the pharmaceutical domain as well as in personalised medicine, with concomitant major industrial and societal impact. TIES is an automated workflow that can be completely run in 8 hours or less, depending on the architecture and hardware available.

AGASTYA P. BHATI
Agastya P. Bhati is a PhD student at the Centre for Computational Science, Department of Chemistry, University College London. He is interested in developing methods based on statistical thermodynamics to make accurate, precise and reproducible ligand-protein binding affinity predictions in a short time using classical molecular dynamics simulations. He is currently focussing on the development and automation of a workflow which yields accurate, precise and reproducible relative binding affinities for alchemical tranformations between two ligands bound to a traget protein as well as protein mutations in ligand-protein complexes. The workflow is highly scalable substantially improving its applicability in the pharmaceutical domain and personalised medicine.
PCJ-BLAST – Massively Parallel Sequence Alignment Using NCBI Blast and PCJ Java library

PIOTR BAŁA, ICM, University of Warsaw

ABSTRACT (Marek Nowicki, Davit Bzhalava, Piotr Bała)

With the development of Next Generation Sequencing there is a high demand in the area of computational biology to extract useful information from the databases. The most widely used is the BLAST algorithm and its implementation is developed by NCBI. In this contribution, we present novel massively parallel execution of the blast algorithm on thousands of processors, available on supercomputers and HPC clusters. Our work is based on the optimal splitting up the set of queries running with the non-modified NCBI-BLAST package for sequence alignment which makes our solution flexible and extensible. The work distribution and search management are implemented in Java with the PCJ (Parallel Computing in Java) library. The PCJ-BLAST package is responsible for reading input sequence, splitting it up and starting multiple NCBI-blast executables. Since processing of individual pieces can take different CPU time, our implementation has mechanisms to achieve good load balancing which significantly improves scalability and reduces search time. The load balancing is dynamic and does not require previous knowledge of the time for processing individual chunks. We have tested our solution on Cray XC40 with Aries interconnect and x86 cluster with Infiniband. Our results show very good performance and efficiency up to thousands of cores.

PIOTR BAŁA

Piotr Bała graduated in physics in 1988 and received a PhD in physics in 1993 at N. Copernicus University (Toruń, Poland). He has been studying quantum effects in molecular system using high performance computing (HPC). Since 2000 he is a leader of the team at ICM University of Warsaw which developed grid tools for molecular biology. He was strongly involved in national and European grid projects, and is member of the UNICORE Forum. The main focus of his current research is on the development of new methods for parallel and distributed computing. In particular he is leader of the team developing a PCJ library for parallel computing in Java and coordinator of the HPDCJ project (CHIST-ERA). The PCJ library received an HPCC award at SC’14. Piotr Bała is an author and co-author of more than 130 scientific papers.
Industry & Engineering
INDUSTRIAL PARALLEL TRACK 2

Chair

DIETER JAHN, BASF, Germany

Dieter Jahn studied chemistry and joined BASF SE in 1979 as a scientist in central research. He continued in various positions there until December 2012, when he retired from the position of Senior Vice President Science Relations and Innovation Management. He was a member of the Research & Innovation Programme council of the European Chemical Industry Council (CEFIC) and Chairman of the Innovation Committee of the German Chemical Industry Association (VCI). In 2006 and 2007 he was President of the German Chemical Society (GDCh) and between 2010 and 2015 he was a permanent member of the Senat Commissions of the Helmholtz Association of German Research Centers. Now he serves as a member of the IAC of PRACE, as Transfer Ambassador to the Government of the State of Rheinland-Pfalz and as a member of the Supervisory Board of the High-Tech Gründerfonds.

FTL Systems' Commercial ExaScale Systems Designed & Manufactured in Europe

JOHN WILLIS, CEO, FTL Systems B.V. Groningen, The Netherlands

ABSTRACT

Scaling TeraScale and PetaScale to realize commercially practical ExaScale runs into practical problems. Conventional CPU and GPU architectures require compilers and programmers to decompose and synchronize many millions of independent, concurrent operation sequences. For most commercial applications this is impractical. The energy cost of so many conventional processors is a practical obstacle to taking machines from a “hero” project into the marketplace. FTL Systems B.V. is realizing a commercially viable ExaScale answer to the above challenges. We are consolidating our corporation’s more than 22 years of experience in advanced computing technology around a new development and manufacturing facility in Groningen (NL). We have previously realized our own processor cores in the 1 to 10 TeraFLOP range. New technology pushing each core beyond 1/10th PetaFLOP results in an ExaScale system with less than 110 racks. Meeting the above challenges requires many innovations, for most of which FTL Systems has proven capability. Electro-optical techniques allow precisely controlled timing in the 50 GHz to 1 TeraHertz range. Asynchronous logic techniques manage jitter and skew at these high frequencies. Low temperature logic requires breakthrough innovations. Novel architecture and compiler techniques facilitate the formally correct use of multi-threaded, CSP, functional and generalized artificial intelligence (self-learning) application paradigms.
Industry & Engineering
INDUSTRIAL PARALLEL TRACK 2

JOHN WILLIS
John Willis completed a MS/PhD degree from Carnegie Mellon University following a BS in electrical engineering from Cornell. He has authored more than 50 academic papers and more than 40 patents related to computer architecture, RF/MW systems, design automation and solar energy. Previously he worked as a computer system architect for Carnegie's Robotics Institute (robotics machine vision and military signal processing), Philips Research (Strand) and then IBM (AS/400) before joining FTL Systems in 1995 as CEO. He worked on several European Union Frame projects. Centralisation of FTL Systems' headquarters, research, development and manufacturing in Groningen, the Netherlands has absorbed much of his time over the last two years. Home is in the Netherlands, England and the US. In his spare time he is serving as the editor for his latest revision of VHDL, and enjoys yoga and cycling.

16:30 - 17:00 Coffee
Fluid Dynamics
SCIENTIFIC PARALLEL TRACK 3

Chair
CARLO CASCIOLA, University of Rome Sapienza, Italy
Carlo Massimo Casciola is full professor of Fluid Dynamics at the University of Rome La Sapienza, Department of Mechanical and Aerospace Engineering, where he leads a research group working on complex flows. Most of his research topics involve the coupling of macroscopic flows with a micro-structure. After being awarded the ERC Advanced Grant 2013, BIC: Following Bubbles from Inception to Collapse, most of this research has been focused on different aspects of cavitation, e.g. heterogeneous nucleation, bubble collapse modeling, bubble-wall interactions, bio-medical applications of cavitation. The tools employed span from Direct and Large Eddy Simulation, to Phase Field Models, Free Energy Methods, and Molecular Dynamics techniques specialized for Rare Events.

Climate Change Mitigation: Prediction of CO₂ Dissolution in Geological Reservoirs
MARCO DE PAOLI, Vienna University of Technology, Austria

ABSTRACT
A major proportion of global energy consumption comes from fossil fuels combustion, which has led to a corresponding increase of carbon dioxide (CO₂) concentration in the atmosphere, which is likely responsible for the greenhouse effect. The remedy to this global problem is still a topic of debate and large-scale injection and storage of CO₂ into deep geological reservoirs is proposed to mitigate climate change. In this work, high-resolved Direct Numerical Simulations are used to analyse the dynamics of injected CO₂. An efficient pseudo-spectral scheme (Fourier-Chebyshev) is adopted to discretize the governing equations. Due to the wide range of scales explored in time (from seconds to centuries) and in space (from millimeters to tens of meters), huge computational costs have to be sustained. The results have been achieved with parallel algorithms on HPC infrastructures. We developed and ran our parallel code on several facilities - i.e. Fermi and Marconi (Italy), VSC3 (Austria), Mira (USA) - using more than 20 million core-hours. The results obtained in this study give an accurate description of the dissolution phenomena and may lead to an increase of the CO₂ stored, i.e. a reduction of the anthropogenic emissions, within the next 20-30 years.

MARCO DE PAOLI:
Marco De Paoli earned his PhD (2017) in Environmental and Energy Engineering Science from the University of Udine. He received his Bachelor's (2011) and Master’s (2013) degrees in Mechanical Engineering from the University of Udine, where he collaborated with Professors A. Soldati, C. Marchioli and F. Zonta. He was visiting student at the Institute de Mecanique des Fluides de Toulouse (IMFT, 2013) and at the Vienna University of Technology (2016), where he is actually researcher. Since 2014, his interests have focused on HPC systems. He is currently working on flows in porous media and multiphase flows, using pseudo-spectral methods and massively parallelized tools.
# TUESDAY 16 MAY 2017

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<td>08:00</td>
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<td><strong>AUDITORI</strong> Chaired by: Serge Bogaerts. Chair of the PRACEdays17 Organisation and Programme Committee</td>
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<td>09:00</td>
<td>Opening of EHPCSW: Sergi Girona. EXDCI Co-ordinator &amp; Opening of PRACEdays17: Erik Lindahl. Chair of the SSC Welcome: Anwar Osseyran. PRACE Council Chair and CEO of SURFsara, Netherlands Josep Maria Martorell. BSC Associate Director &amp; Francesc Subirada. Director General for Research of the Government of Catalonia</td>
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<td>09:45</td>
<td>Keynote: Khalil Rouhana. Deputy Director-General, DG Connect, European Commission, The European HPC Strategy – The European Data Infrastructure (EDI)</td>
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<td>11:45</td>
<td>Keynote: Telli van der Lei. DSM Chem Tech R&amp;D BV. Quantitative Supply Chain Optimization Using Big-Data Methodologies in The Chemical Industry</td>
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<td>Presentation of the Call for proposals of Connecting Europe Facility (CEF) Telecom 2017: Leonardo Flores Añover. Project Officer, European Commission</td>
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<td>12:00</td>
<td>Presentation: Jean-Pierre Panzier. ETP4HPC, Developing European Technology to serve the HPC Ecosystem</td>
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<td>14:30</td>
<td>VS208 MATERIALS SCIENCE - Scientific Parallel Track 1</td>
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<td>Chair: Matej Prapatnik. University of Ljubljana, Slovenia</td>
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<td>Alberto Giacomello. University of Rome Sapienza, Italy Bioinspired Surfaces For Robust Submerged Superhydrophobicity: Insights from Molecular Dynamics</td>
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<td>Flora Tsourtou. PhD student, University of Patras, Greece Optimized Monte Carlo and Molecular Dynamics Algorithms for modelling the self-organization of two classes of materials: semifuorinated alkanes and semiconducting polymers based on thiophenes</td>
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<td>15:30</td>
<td>VS208 LIFE SCIENCE – Scientific Parallel Track 2</td>
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<td>Chair: Christoff Schütte. Free University of Berlin, Germany</td>
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<td>Jürgen Walther. PhD student, IRB Barcelona, Spain A Multiscale Model of Chromatin at bp-level.</td>
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<td>Agastya P. Bhati. PhD student, University College London, UK Rapid, Accurate, Precise and Reliable Relative Free Energy Prediction Using Ensemble Based Thermodynamic Integration</td>
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<td>Piotr Bala. University of Warsaw PCJ-BLAST - massively parallel sequence alignment using NCBI Blast and PCJ Java library</td>
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<td>VS208 FLUID DYNAMICS – Scientific Parallel Track 3</td>
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<td>Chair: Carlo Casciola. University of Rome, Italy</td>
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<td>Marco De Paoli. Vienna University of Technology, Austria Climate Change Mitigation: Prediction of CO2 Dissolution in Geological Reservoirs</td>
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<td>Ursula Rasthofer. ETH Zurich, Switzerland Large Scale Simulation of Cloud Cavitation Collapse</td>
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<td>Alessio Roccon. TU Wien, Vienna, Austria Viscosity-Modulated Breakup &amp; Coalescence of Large Drops in Bounded Turbulence</td>
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<tr>
<td>18:30</td>
<td><strong>AUDITORI</strong> Chaired by Serge Bogaerts. Chair of the PRACEdays17 OPC</td>
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<tr>
<td>19:00</td>
<td>6 Poster Presentations Shortlisted for PRACE Best Poster Award</td>
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<tr>
<td>19:30</td>
<td>Welcome Reception &amp; Poster Session</td>
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**Calendar of Events**
### WEDNESDAY 17 MAY 2017

<table>
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<th>Time</th>
<th>Session</th>
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<tr>
<td>11:00</td>
<td><strong>AUDITORI</strong> Chaired by: Serge Bogaerts. Chair of the PRACEdays17 Organisation and Programme Committee</td>
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<tr>
<td></td>
<td>Opening &amp; Welcome</td>
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<td>MoU PRACE-RIST-XSEDE</td>
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<td></td>
<td>Keynote: Xue-Feng Yuan, School of Engineering Science for Intelligent Manufacturing, Guangzhou University, People’s Republic of China</td>
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<td>Innovation of Intelligent Manufacturing Driven by Cloud HPC</td>
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<td>Keynote: Nuria Lopez, Institute of Chemical research of Catalonia, ICIQ, Tarragona, Spain. Modeling of Catalysts With Industrial Applications</td>
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<tr>
<td>12:45</td>
<td>EHPCSW Group Photo</td>
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<tr>
<td>13:00</td>
<td>LUNCH</td>
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<tr>
<td>14:00</td>
<td><strong>VS208 ENERGY &amp; PARTICLE PHYSICS – Scientific Parallel Track 4, Chair: Marina Bécoulet, CEA, France</strong></td>
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<tr>
<td></td>
<td>Shimpei Futatani, Senior Researcher, Barcelona Supercomputing Center</td>
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<td></td>
<td>High Performance Computing for Non-linear MHD Simulations of Pellet Triggered ELMs in Fusion Devices</td>
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<td>Enrico Calore, University of Ferrara, Italy. Design &amp; Optimization of a Portable Lattice QCD Monte Carlo Code for Heterogeneous HPC Architectures, using OpenACC</td>
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<tr>
<td>15:30</td>
<td><strong>VS208 ASTROPHYSICS – Scientific Parallel Track 5, Chair: Luke Drury, Dublin Institute for Advanced Studies, Ireland</strong></td>
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<td></td>
<td>Ilian T. Iliev, School of Mathematical and Physical Sciences, University of Sussex, UK. Multi-scale Reionization</td>
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<td>Luca Franci, Department of Physics and Astronomy, University of Florence, Italy</td>
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<td>Hybrid 3D Simulations of Turbulence and Kinetic Instabilities at Ion Scales in the Expanding Solar Wind</td>
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<td>16:30</td>
<td>COFFEE</td>
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<tr>
<td>17:00</td>
<td><strong>VS208 CLIMATE &amp; ENVIRONMENT – Scientific Parallel Track 6, Chair: Dimitri Komatitsch, LMA CNRS-MRS, France</strong></td>
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<tr>
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<td>Jose Manuel Redondo, UPC Barcelona Tech. (University of Cambridge ), Spain (UK). Turbulence Cascades. Fractal intermittency and Ocean Pollution</td>
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<td></td>
<td>Kim Serradell Maronda, Earth Sciences Department, Barcelona Supercomputing Center, Spain. Software Stash Deployment for Earth System Modelling using SPACK</td>
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<td>Ilias Sibgatullin, Moscow State University &amp; Institute of System Programming and Oceanology Institute of Russian Academy of Sciences</td>
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<td>Mixing Due to Large Amplitude Internal Waves and Convection</td>
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<td>18:30</td>
<td><strong>AUDITORI</strong> Chaired by Koen Hillewaert, Chair of the PRACE User Forum</td>
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<td>PRACE USER FORUM OPEN SESSION</td>
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<td>Roxana Dascalu &amp; John Clifford, PRACE aisbl, PRACE Access</td>
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<td>Toni Collis, EPCC. How to recruit and retain women in the PRACE HPC community</td>
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<td>Open Discussion - Free for All</td>
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<tr>
<td>20:00</td>
<td>Networking Cocktail &amp; Dinner, Fabrica Moritz Restaurant (19:30 Buses will begin to depart to the Restaurant. Buses depart for hotels at 22.30)</td>
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### THURSDAY 18 MAY 2017

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
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<tr>
<td>09:00</td>
<td><strong>AUDITORI</strong> Chaired by Serge Bogaerts. Chair of the PRACEdays17 OPC</td>
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<td>Opening &amp; Welcome, Serge Bogaerts. Chair of the PRACEdays17 OPC. Keynote Industrial: Henri Calandra, TOTAL (TBC)</td>
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<tr>
<td>10:00</td>
<td>COFFEE</td>
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<tr>
<td>10:30</td>
<td><strong>PANEL DISCUSSION – Support to HPC code: The Gap Between Scientific Code Development and Exascale Technology.</strong></td>
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<td>The Software Challenges For Extreme Scale Computing Faced by The Community</td>
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<td>Henri Calandra, TOTAL; Lee Margetts, IAC Vice-Chair; Frauke Gräter, Heidelberg Institute for Theoretical Studies (HITS); Thomas Skordas, European Commission; Erik Lindahl, SSC Chair, Moderated by Inma Martinez, Considered by FORTUNE and TIME as One of The World’s Leading Digital Media Strategists</td>
</tr>
<tr>
<td>12:00</td>
<td><strong>PRACEdays17 Award Session</strong></td>
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<td></td>
<td>Closing &amp; Announcement of PRACEdays18: Serge Bogaerts, Chair of the PRACEdays17 OPC</td>
</tr>
<tr>
<td>13:00</td>
<td>LUNCH</td>
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Large Scale Simulation of Cloud Cavitation Collapse

URSULA RASTHOFER, ETH Zurich, Switzerland

ABSTRACT

Cloud cavitation collapse is encountered in engineering and medical applications such as marine propulsion and shock-wave lithotripsy. The underlying physics of cloud cavitation collapse remain largely unexplored. Experiments and simulations must address a wide range of spatio-temporal scales involved in the bubble collapses and their interactions with the flow field. Here, we present simulations of this process with clouds of up to fifteen thousand resolved bubbles. Therefore, we use a highly efficient compressible, multi-component flow solver based on a finite-volume formulation with diffuse interface description. We investigate the collapse process by considering spherical clouds of gas bubbles in quiescent liquids subject to different ambient pressures. Three stages of the collapse process are identified: (I) the initiation of the process by collapses of individual bubbles at the outer layer, which come along with emanating micro-jets and cap-like bubble deformations, (II) the formation of an inward-propagating spherical velocity front and pressure wave and (III) the final focusing of these waves at the center of the cloud, which induces pressures orders of magnitude higher than the ambient pressure. These results challenge existing low order models of cloud cavitation collapse and provide the necessary information for their improvements.

URSULA RASTHOFER

Ursula Rasthofer obtained her diploma in aeronautics and aerospace from Technische Universität München (TUM) in 2009, and her PhD in mechanical engineering from TUM in 2015. She is a postdoctoral researcher at ETH Zürich since 2015. Dr Rasthofer’s research interest focuses on modelling and simulation of turbulent flow, numerical methods for multiphase flow and high performance computing.
Viscosity-Modulated Breakup and Coalescence of Large Drops in Bounded Turbulence

ALESSIO ROCCON, TU Wien, Vienna, Austria

ABSTRACT
In this work, we examine the influence of viscosity on breakup and coalescence of a swarm of large drops in a wall-bounded turbulent flow. We consider several values of surface tension and a wide range of drops to fluid viscosity ratios, while we maintaining the same density for drops and carrier fluids. Drops can coalesce and break following a complex dynamics that are primarily controlled by the interplay between turbulence fluctuations, surface tension (measured by We). We use Direct Numerical Simulations (DNS) coupled with a Phase Field Method (PFM) to describe the drops dynamics. We observe a consistent action of increasing λ, which, especially for the larger Weber numbers decreases significantly the breakup rate of the drops. Qualitatively, an increase of drop viscosity decreases the breakup rate, very much like an increase of surface tension does. The mechanism by which drop viscosity acts is a modulation of turbulence fluctuations inside the drop, which reduces the work surface tension has to do to preserve drop integrity. We believe that this may give important indications in many industrial applications to control drop coalescence and fragmentation via the ratio of drop-to-fluid viscosity.

ALESSIO ROCCON
Alessio Roccon is a PhD Student, Institute of Fluid Mechanics and Heat Transfer, TU Wien (2014 to present). Previously he studied in the University of Udine, where he completed an M.S. in Mechanical Engineering (2012-2014) and a B.S. in Mechanical Engineering (2009-2012). Alessio’s area of interest is in Computational Fluid Mechanics, in particular direct numerical simulations (DNS) of multiphase system in turbulent regime.
European Industry
INDUSTRIAL PARALLEL TRACK 3

Chair
ANDERS RHOD GREGERSEN, Chief Specialist, Vestas Wind Systems A/S
Anders Rhod Gregersen is the chief specialist and responsible for high performance and data heavy computing at Vestas Wind Systems A/S. At Vestas he has 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 (LHC) at CERN, Geneva. He is the current chair for the Industrial Advisory Committee of PRACE.

The MaRS (Matrix of RNA-Seq) Project.
FABIEN PIERRAT, Acobiom, Montpellier, France

ABSTRACT
Recent years have seen a dramatic increase in the amount of genomic and transcriptomic data. Our research program focused on transcriptomic data and the RNA-Seq approach (which reflects the genes expression). RNA-Seq approach is used in identifying disease-related genes, analyzing the effects of drugs on tissues, and providing insight into disease pathways. The RNA-Seq is widely used to characterize gene expression patterns associated with tumor formation. RNA-Seq data can be digitalized and then easily and reliably compared in silico with the growing library of RNA-Seq databases generated for normal and pathological situations in other laboratories around the world (more than 27000 human libraries, more than 120To of data). We will highlight challenges that emerge from this flood of data, such as downloading data, parallelization of algorithms execution, (de-)compression of genomic sequences, and execution of complex scientific workflows. This project will aim at the development of the Generic platform called MaRS (Matrix of RNA-Seq) with one innovative method to analyze, integrate and contextualize largescale biological data in the fields of Human Health. MaRS is made timely by the exponential increase in the throughput of molecular (Omics) approaches to cover the unmet needs in the specific fields of Health.

FABIEN PIERRAT
In 2003 Fabien completed a Masters in Genetics at the University Henri Poincare, Nancy, France. Following that in 2004 he completed a Master’s Degree in BioInformatics in the University of Montpellier II, France. Fabien’s is a Bioinformatics Engineer with expertise in transcriptome, NGS data analysis and exploration and database development for biology.
FORTISSIMO and SHAPE: Helping SMEs Access HPC

PAUL JOHN GRAHAM, Software Architect, EPCC, University of Edinburgh

ABSTRACT

High Performance Computing (HPC) and High Performance Data Analytics (HPDA) can transform the products and services companies offer by enabling better design, performance and efficiency. The uptake of these technologies by SMEs has been slow because of high barriers to entry and this talk will look at two initiatives – FORTISSIMO and SHAPE – designed to improve this position. SHAPE is the PRACE Research Infrastructure’s initiative to stimulate the use of the PRACE HPC systems by SMEs and help them prepare their modelling and simulation applications. Through SHAPE, SMEs can get compute time and expert assistance to see how HPC can help their business. FORTISSIMO is a pair of projects focussed on helping manufacturing SMEs take their first steps in HPC and HPDA through engagement in set of “experiments”. With a combined total of over 90 experiments and 200 partners, FORTISSIMO is showing how business products, processes and services can be transformed, in experiments ranging from the aerodynamics of hypercars to the pouring of liquid steel in a foundry. All of these experiments are developing success stories which have been used to create the FORTISSIMO Marketplace – a commercially-focussed website where companies can access compute and modelling applications on demand.

PAUL JOHN GRAHAM

Paul Graham is a Software Architect at EPCC at the University of Edinburgh, and is the coordinator of SHAPE (SME HPC Adoption Programme in Europe), a pan-European programme that promotes High Performance Computing adoption by SMEs (small to medium sized enterprises), supported as part of the PRACE initiative. Paul graduated in 1995 with a BSc (Hons) in Computational Physics from Edinburgh University, and then went to work at the ICI Wilton Research & Technology Centre in Middlesbrough as a member of their Computer Modelling Team. Paul subsequently joined EPCC in 1998, and in the years since has worked on a broad range of projects, principally with industrial and commercial partners, as both project manager and technical lead. Technical highlights include data mining for a national bank, software performance optimisation for Rolls Royce, parallelisation of electro-magnetic modelling code for the oil industry, modelling virtual musical instruments using GPUs, and many projects with local SMEs, enabling the technology transfer of EPCC’s High Performance Computing expertise.
European Industry
INDUSTRIAL PARALLEL TRACK 3

Presentation of the SESAME Net Project:
“Roadmap for improving SME uptake of HPC”
and “HPC4SME Assessment Process”
TOMI ILIJAŠ, ARCTUR, Coordinator of SESAME Net Project

ABSTRACT
SESAME Net is a network of over 25 HPC Centres that was established within the project and it is contributing to the implementation of the European HPC strategy, in particular to foster the use of HPC by SMEs. The objectives of the SESAME Net project are to promote access to computational expertise anywhere in Europe and to enable the dissemination of best practice in HPC industrial use particularly for SMEs. One of its most important results is a “EU roadmap” for improving SME uptake of HPC. The roadmap is structured for both sides – SMEs and HPC Centres. Both parties can find useful information on “how to start”. We realized that there is quite a small number of SMEs in EU who are ready to use HPC in the Cloud and that the same ones appear in many EU funded projects as experiments. To raise the awareness and build the demand among more than 2MIO SMEs in EU, we developed a web application – the HPC4SME Assessment Tool. Now SMEs have the opportunity to assess their potential to use HPC in Cloud for free, with the help of Sesame Net partner. A Europe-wide campaign to encourage SMEs to do the assessment was started in March with more than 1000 SMEs expected to go through the process until May 2017. In the future, other assessment tools are planned to assess the readiness of HPC centres and independent Software vendors (ISVs) to offer services to SMEs and governments to assess their readiness to support SMEs on their way to become HPC success stories.

TOMI ILIJAŠ

Working as Arctur’s CEO since 1992, Tomi Ilijaš has hands-on experience both in SME management and in the specialized area of ICT. As business manager he established a firm and expanded it into one of most prominent programming companies in Slovenia, but also launched and took active part in some important intra-business initiatives, such as establishment of ICT Branch Association at Slovenian Chamber of Commerce. As a strong advocate of cooperation between industry and academia he initiated a number of national and international projects in which Arctur linked up with various research institutes and universities, both from Slovenia and abroad. During the last decade, an important part of Mr. Ilijaš’s ICT activities has been devoted to research and development of methodologies for various business processes – especially for project management – and related ICT solutions. During the last couple of years, a substantial part of his efforts were allocated to the field of high-performance computing business. He played a crucial role in establishing one of the most powerful supercomputers in the region, which is promptly becoming a strong infrastructural foundation for Arctur’s strategic orientation towards R&D in the field of HPC and cloud-computing. Tomi took part in evaluation of project proposals for EU e-Content programme.
Keynotes
PLENARY SESSION

Future GÉANT network plans in Europe
MARK JOHNSTON, Chief Operations officer, GÉANT

ABSTRACT
The mission of the GÉANT network is to provide unconstrained high performance infrastructure and trusted access to scientific instruments and resources of the global R&E community. GÉANT also provides access to a portfolio of services and testbeds that support research and development. This session will focus on how GÉANT ensures the network is built to support large data flows and the network services that GÉANT offers e-infrastructures. It will also cover GÉANT’s future evolution plans to meet the realities of ever increasing data flows and exponential network traffic increases.

MARK JOHNSTON
Mark joined GÉANT in 2013 and is responsible for the network infrastructure serving Europe’s research and education community to deliver real value and benefit to society by enabling research communities across Europe, and the world, to transform the way they collaborate on ground-breaking research. Mark holds a MBA, Business Administration and Management from the University of Edinburgh.

19:00 Presentations shortlisted for PRACE Best Poster Award

19:30 - 21:30 Welcome Reception & Poster Session
Innovation of Intelligent Manufacturing Driven by Cloud HPC

XUE-FENG YUAN, CPhys FinstP FRSC, School of Engineering Science for Intelligent Manufacturing, Guangzhou University, People’s Republic of China

ABSTRACT

Enormous advances in the subject area over last decades have rapidly transformed traditional industrial sectors in foods, personal care products, pharmaceuticals, paints, lubricants, ceramics, polymers, liquid crystals, high performance fibers, oil exploration and production into a digital era of formulation design and precision control over processing conditions from molecular viewpoint, and fertilizing a new industrial revolution. In this talk, I shall review current development of computational rheology in China, present an integrated multiple scale simulation platform including finite volume, lattice Boltzmann, immersed boundary numerical techniques etc. and simulation results of semi-dilute polymer solutions in a wide range of Wi-Re number regime relevant to ink-jet printing flows. I shall then discuss future challenge in cloud-HPC modelling of complex systems, including digital manufacturing, living system and social-economic system, which exhibits a hierarchical structure and is composed of self-regulated multi-functional and control centres, through strongly correlated chemical, physical and social processes at the length and time scales spanning over many order of magnitude.
Modeling of Catalysts With Industrial Applications
NURIA LOPEZ, Group Leader, Institute of Chemical research of Catalonia, ICIQ, Tarragona, Spain

ABSTRACT
Modeling of materials that present catalytic properties and can be employed by the industry represent a main challenge due to the different time and length scales involved. Even at the molecular level the increasing complexity of the systems investigated with large molecules, complex reaction networks and the role of solvent needs to be solved to implement new catalytic solutions that allow the change in paradigm from oil-derived to renewable sources. In the talk, I will show the challenges that have been partially solved, and some new strategies to apply methodologies that can benefit from the extensive use of HPC to address them.

NURIA LOPEZ
Since 2005 Professor Nuria Lopez had been Group Leader at the Institute of Chemical Research of Catalonia, ICIQ. Her research area is the Modeling of materials with catalytic properties. She has worked on PI (2010-2015) ERC Starting Grant Bio2Chem-d; (2016) Proof-of-Concept BigData4Cat and Partner in A-LEAF, POROUS4APP and ELCOREL European projects. She has completed Industrial projects with Bayer Materials Science, Haldor-Topsoe, and Repsol. She is a member of the Scientific Steering Committee in PRACE and the Editorial Advisory Board ACS Catalysis. Nuria has published 150 papers in Physics, Chemistry, and Materials Science, more than 6500 citations h=40.
High Performance Computing for Non-linear MHD Simulations of Pellet Triggered ELMs in Fusion Devices

SHIMPEI FUTATANI, Senior Researcher, Computer Applications in Science and Engineering (CASE) Department, Barcelona Supercomputing Center

ABSTRACT
Magnetically confined plasmas require a sufficiently high pressure in order to produce fusion energy. One of the difficulties of the steady operation of the fusion plasma is caused by MHD (MagnetoHydroDynamic) instabilities at the plasma boundary, called ELMs (Edge Localized Modes). ELMs lead to energy bursts onto the plasma facing components which could be damaged in future tokamak devices like ITER. The injection of pellets (small deuterium ice bodies) into the plasma to trigger small ELMs is a promising ELM mitigation method for the steady operation of ITER. The work aims to improve the understanding of the physics processes involved in ELM control by pellet injection, using the non-linear 3D MHD code JOREK which simulates pellet ablation physics self-consistently with the MHD activity in order to improve the physics basis for the application of this ELM control method in fusion plasmas of existing fusion reactors, and for implications of ITER plasmas. The dependence of the pellet sizes on the particle and the energy loss due to the pellet triggered ELM will be presented. The power deposition asymmetry on the divertor target will be presented.
SHIMPEI FUTATANI
Shimpei Futatani completed his PhD at Kyoto University, Japan in 2008. He has another independent PhD from Aix-Marseille University, France in 2009. In 2010, he was appointed as a postdoctoral researcher at the ITER Organization via Monaco Postdoctoral Fellowship (a highly competitive fellowship awarded to only 5 people from across the world once every two years). In ITER, he contributed to the development of an advanced non-linear MHD simulation code (JOREK) by incorporating the physics process involved in the pellet ablation which controls MHD instabilities. In 2013, he was appointed as a postdoctoral researcher at the Ecole Centrale de Lyon in France to study the self-organization through the MHD dynamo process. In 2014, he was appointed as a senior researcher at Barcelona Supercomputing Center. He leads the project of the computational analysis of MHD simulations of pellets injected in ITER plasma with close collaborations with existing experimental fusion devices.

Design and Optimization of a Portable Lattice QCD Monte Carlo Code for Heterogeneous HPC Architectures, using OpenACC
ENRICO CALORE, University of Ferrara, Italy

ABSTRACT
The present panorama of HPC architectures is extremely heterogeneous, ranging from traditional multi-core CPU processors, to many-core CPUs such as the Intel KNL, and various accelerators, such as GPUs. In this scenario, code portability become necessary for easy maintainability of applications, in particular for scientific computing, where code changes are very frequent, making it tedious and prone to error to keep different code versions aligned. Moreover, apart from code portability, also performance portability would be desiderable. In this work we present the design and optimization of a state-of-the-art production-level LQCD application, using the directive-based OpenACC programming model. OpenACC abstracts parallel programming to a descriptive level, relieving programmers from specifying how codes should be mapped onto the target architecture. We describe the implementation of a code fully written in OpenACC, and show that we are able to target several different architectures, including state-of-the-art traditional CPUs and GPUs, with the same code. We also measure performance, evaluating the computing efficiency of our OpenACC code on several architectures, comparing it with GPU-specific implementations and showing that a good level of performance-portability can be reached.
Energy & Particle Physics
SCIENTIFIC PARALLEL TRACK 4

ENRICO CALORE
Enrico Calore received the Bachelor’s and Master’s Degree in Computer Engineering at Università degli Studi di Padova (Italy) in 2006 and 2010 respectively. In the meanwhile he worked at INFN (The Italian National Institute of Nuclear Physics) thanks to some fellowship programs. He received his PhD in Computer Science from Università degli Studi di Milano in 2014 and is now a Postdoctoral Researcher at Università degli Studi di Ferrara and INFN Ferrara. His main interests are in the fields of HPC, scientific computing, parallel and distributed computing, code optimization and energy awareness in computing.
Astrophysics

SCIENTIFIC PARALLEL TRACK 5

Chair
LUKE DRURY, Dublin Institute for Advanced Studies, Ireland
Luke Drury is a theoretical astrophysicist working on high-energy astrophysics, plasma astrophysics and particle acceleration, in particular the problems associated with the origin of cosmic rays. A native of Dublin he studied pure mathematics and experimental physics at Trinity College Dublin before going on to do a PhD at the Institute of Astronomy in Cambridge, England. He then worked at the Max-Planck-Institut fuer Kernphysik in Heidelberg, Germany, before returning to Dublin as Senior Professor in the Dublin Institute for Advanced Studies where he is currently the Director of the School of Cosmic Physics. He was heavily involved in setting up the Irish Centre for High-End Computing and has a long-standing interest in e-Infrastructures. He currently chairs E-CAM, one of the eight e-infrastructure centres of excellence funded by the EU under H2020, and is also the chair of the European Space Agency’s Astronomy Working Group. Luke Dury is member of PRACE SSC.

Multi-scale Reionization
ILIAN T. ILIEV, Reader in Astronomy, Department of Physics & Astronomy, School of Mathematical and Physical Sciences, University of Sussex, UK

ABSTRACT:
The first billion years of cosmic evolution remain one of the last largely uncharted territories in astrophysics. During this key period, the cosmic web of structures we see today first took shape and the very first stars and galaxies formed. The radiation from these first galaxies started the process of cosmic reionization, which eventually ionized and heated the entire universe. This inherently multi-scale process, mostly driven by stellar radiation from low-mass galaxies, had profound effects on the cosmic structures, leaving a lasting impression. The star formation inside such galaxies is strongly affected by complex radiative and hydrodynamic feedback effects, including ionizing and non-ionizing UV radiation, shock waves, gas cooling and heating, stellar winds and enrichment by heavy elements. I will present results from our several PRACE projects, based on massively-parallel N-body, radiative transfer and radiative-hydrodynamics simulations covering the full, vast range of relevant scales using a variety of numerical techniques, including AMR and GPU acceleration. Sample questions we aim to address are: 1) how do the radiative feedback affect the formation of early structures and subsequent star formation?; 2) how different is high-redshift galaxy formation compared to the present? 3) How are the feedback effects imprinted on large-scale observational features?
Astrophysics  
SCIENTIFIC PARALLEL TRACK 5

ILIAN T. ILIEV  
Ilian Iliev is computational astrophysicist whose research is focused on the formation of cosmological structures throughout cosmic time, from the First Stars to the present day. Of particular interest are studies of the Epoch of Reionization, the formation of the first stars and galaxies and their radiative feedback on the intergalactic medium and observable signatures. This work is done through massively-parallel simulations using a variety of numerical techniques, including N-body, radiative transfer and hydrodynamics. Iliev is the Project Leader of three Tier-0 and two Tier-1 PRACE projects, and a co-investigator on two Innovative and Novel Computational Impact on Theory and Experiment (INCITE) awards by the USA Department of Energy. He is core member of the LOFAR Epoch of Reionization Key Science Project and Co-Coordinator of the Full Numerical Simulations Focus Group within the Square Kilometre Array Epoch.

Hybrid 3D Simulations of Turbulence and Kinetic Instabilities at Ion Scales in the Expanding Solar Wind  
LUCA FRANCI, Postdoctoral Research Fellow, Department of Physics and Astronomy, University of Florence, Italy  

ABSTRACT:  
The solar wind and planetary magnetospheres are exceptional laboratories for plasma astrophysics. A vast collection of data from past and present space missions is available and will further increase thanks to upcoming ones. Spacecraft in-situ observations indicate that kinetic interactions are active in the solar wind and small-scale processes are fundamental in determining the plasma evolution during the expansion from the solar corona outwards. Observations need to be directly compared with theoretical models, provided by more and more accurate numerical simulations. Thanks to the intensive use of HPC resources, we provide space missions with a very accurate and rapid computational support by performing state-of-the-art hybrid (kinetic ions, fluid electrons) numerical simulations. By performing a large collection of high resolution 2D and 3D hybrid simulations of plasma turbulence, we investigated the physics of the solar wind from large fluid scales to small kinetic scales, also taking into account the effects of the expansion. We focused on the development of turbulence and on its interplay with kinetic instabilities, on the nature of the ion-scale spectral break in solar wind spectra and on the properties of the small-scale fluctuations. We recovered a remarkable qualitative and quantitative agreement with many features of spacecraft observations.
LUCA FRANCI

Luca Franci is a Postdoctoral Research Fellow at the Department of Physics and Astronomy of the University of Florence. He investigates the physics of astrophysical plasmas by performing state-of-the-art hybrid (kinetic ions, fluid electrons) simulations of solar wind turbulence. Although he started his research activity in this field in 2014, he has already published many papers about solar wind turbulence in international Peer Reviewed journals and given oral presentations at the most prestigious international conferences in the field of geosciences and space sciences (e.g., EGU 2015 and 2016, AGU 2015 and 2016). He has years-long experience in optimizing and running codes for computational astrophysics on many different HPC systems. Since 2013, he has been the PI of six HPC projects and he was in the team of a PRACE awarded project. Currently, he is the PI of a DECI-13 awarded project. He was a poster presenter at the PRACEdays16 conference.

16:30 - 17:00 Coffee
I am a CNRS Research Director (Directeur de Recherche CNRS) in the Laboratory of Mechanics and Acoustics at CNRS/University of Aix-Marseille, France. My research interests include adjoint/inverse imaging problems based on acoustic waves in industrial, oceanic or geophysical structures, and the study of associated effects related to strong local heterogeneities and/or steep topography, as well as the numerical study of acoustic or seismic wave propagation in complex media. I also work on numerical modeling and imaging in the context of non destructive testing. I use a variational formulation of the equations of elastodynamics, and solve it in three dimensions (3-D) using the so-called spectral-element method, a high-order version of the finite-element method, which can be shown to be very accurate at low cost, and particularly well suited to an efficient implementation on parallel computers.

Turbulence Cascades, Fractal Intermittency and Ocean Pollution

JOSE MANUEL REDONDO, Professor, Dept. Fisica (Visiting DAMTP), UPC Barcelona Tech., Spain, (University of Cambridge) (UK)

ABSTRACT

When investigating and predicting the role of the ocean surface in the diffusion of pollutants (such as oil spills) it is fundamental to understand what are the causes of dispersion are at all the range of scales (and times) within the environmental turbulence processes. Coupling of satellite information, in situ data and numerical experiments help to predict real pollution events. The full potential of E.S.A. satellite information needs further understanding. Fractal (multi-fractal) analysis is also used in order to estimate the complex diffusion of pollutants in the ocean, where the relevance of the large scale structures and the cascades of energy and vorticity are fundamental as pollutants mix. The flows are influenced by rotation and buoyancy in self-similar but complex behavior that we may use to parametrise mixing at both limits of the Rossby Deformation Radius scale, $RL$ (where Rotation and Stratification balance). Operational satellite control and analysis of the appearance and spreading of oil slicks on the sea surface from satellites equipped with the Synthetic Aperture Radar (SAR) are modeled as likely sources of pollution drift and transformation with operational numerical methods that include Wind, Currents and Waves. We have shown how to identify SAR signatures and at the same time provide calibrations for the different local configurations of topological structures such as: vortices, spirals, langmuir, antropo-genic oil spills; Natural tensio-active slicks and weather fronts that eventually may be parametrized and quantified in statistical progresses, and the processes...
Climate & Environment
SCIENTIFIC PARALLEL TRACK 6

involved. Scale to scale processes and Intermittency are also examined. Measurements also confirm the picture of other Laboratory flow visualization studies. The fluid is stirred within the mixing region with relatively small amounts of molecular or reactive mixing, function of Damkohler and molecular effects, which are believed only to dominate on longer time scales.

JOSE MANUEL REDONDO
Jose M. Redondo graduated from Madrid Complutense University in 1979 as Licenciado en Fisicas, after a M. Sc. in Physics in USA Virginia Politecnich Institute (1981). He began a research period in Nuclear Thermohydraulics at the Spanish Air Force and Navy. After working as research student and post doctoral fellow at DAMTP in Cambridge University since 1984. He completed a Doctorate degree in Physics at the University of Barcelona and in Applied Mathematics in Cambridge at Trinity College (1990). He has been professor of applied physics at UPC since 1991, teaching at the Civil Engineering School of Barcelona, The Building Engineering School and the Aeronautical Engineering School of UPC. He is regularly Visiting Professor at DAMTP, Cambridge, ENS, Paris, MIO, Toulon, ITM, Prague, UAE, Tanger, IPD, Madrid, RAS, Moscow, etc. He coordinates the Pan European Laboratory of Non-Homogeneous Turbulence of ERCOFTAC, and is vice-chairman of the NP division of the EGU (European Geoscience Union). Presently he coordinates a EU Hit research group for “Fractal Turbulence” at the Max Plank Institute and is principal investigator of the European Space Agency (EGU).

Software Stack Deployment for Earth System Modelling using SPACK
KIM SERRADELL MARONDA, Computational Earth Sciences group leader
Earth Sciences Department, Barcelona Supercomputing Center, Spain

ABSTRACT
Nowadays, the complexity of the frameworks on which current weather and climate models need to be built, run and configured properly requires additional components apart from the original source code. Models are built following a long list of dependencies in the form of libraries, open source and/or commercial software packages or any other piece of software, like system commands. In the framework of the H2020 Center of Excellence in Simulation of Weather and Climate in Europe (ESiWACE), we will present the research done to build a methodology to select, configure and install a complete Earth System Model (ESM) software stack, making much easier the deployment of models and reducing the time to start simulations in an HPC facility, and, such, the time to solution from idea to published result. We will present Spack and its application to the ESM needs. Spack is a package management tool designed to support multiple versions and configurations of software on a wide variety of platforms and environments. It was
Mixing Due to Large Amplitude Internal Waves and Convection

ILIAS SIBGATULLIN, Professor in Fluid Mechanics at the Faculty of Mechanics and Mathematics of Moscow State University; Research Fellow at the Institute of System Programming and Oceanology Institute of Russian Academy of Sciences.

ABSTRACT

Mixing processes in stratified media are extremely important in oceanology and atmospheric sciences. Mixing is much more complicated in media with background stratification due to density, because conventional direct cascade does not explain actually observed transport of heat and sediments. Background stratification can be both stable and unstable. Due to tidal motions over orography and intensive transfer of energy from barotropic to baroclinic motions, stably stratified abyssal waters can suffer intensive mixing due to instabilities of large amplitude waves and overturnings. Convective motion is a natural mixer, and stably and unstably stratified layers may interact to produce penetrative convection which is common in planetary sciences. Numerical simulation already allowed to understand many features of instabilities and turbulence in stratified media. Here our essential goals are to continue numerical research for two experiments being made in Ecole Normal Superieur de Lyon and Universidad Politecnica de Catalunya. In stably stratified fluids we would describe energy cascade in internal wave’s attractors, three-dimensional interactions in internal wave’s attractors, Lagrangian mixing.
biharmonic external forcing and find semiempirical relations for parametrisation of the vertical mixing. For convection problems we would build the bifurcation diagrams for the experimental box developed in UPC both for conventional and penetrative convection and compare energy eddy spectrum for different lateral boundary conditions. To make such research possible we use high-resolution and high-order numerical approaches: Fourier-Chebyshev pseudospectral and nek50000 code based on spectral element approach with Largangian functions on Gauss-Lobatto-Legendre points in each element. To study interference with particles for moderate supercriticalities we use OpenFOAM solvers. The resolution needed for resolving nonlinear dynamics of 3D small-scale structures (due to high Schmidt-Prandtl number) may be up to 2048^3 and the codes we are using are highly scalable on parallel computers.

ILIAS SIBGATULLIN

PRACE User Forum
OPEN SESSION – FREE FOR ALL

Chair
KOEN HILLEWAERT, Argo team leader, Cenaero

ABSTRACT
The PRACE user forum provides a communication channel between PRACE and the researchers involved in PRACE computational projects. Its aim is to identify generic issues and needs that users encounter during all steps related to computational projects awarded by PRACE. The yearly general assembly is held during PRACEdays. As usual, the main feature is the open discussion in which users can voice their opinion and bring up new issues. This year, the general assembly will also include a discussion of the peer review process with the PRACE review officers Roxana Dascalu and John Clifford, and a presentation from Toni Collis about “Women in HPC”.

KOEN HILLEWAERT
Koen Hillewaert is a specialist in numerical fluid dynamics, finite elements and turbomachinery. After graduating as a mechanical engineer from the University of Ghent, he was a researcher at the von Karman Institute and developer at Numeca. In 2002 he joined Cenaero as CFD developer working on high order methods, leading to his PhD at the Université Catholique de Louvain. He is now the main developer of the high order multiphysics platform Argo, aimed at enabling highly detailed large eddy simulation of turbomachinery during design. He is also responsible for coordinating research in the domain of fluid dynamics and involved in many international initiatives surrounding high order CFD methods, including three high profile European research projects (Adigma, IDIHOM and Tilda) and the organisation of the International Workshop on High Order Methods. He was PI of two PRACE projects on DNS and LES of turbomachinery flows using new high order finite element methods.
How to Recruit and Retain Women in the PRACE HPC Community

TONI COLLIS, Co-Founder of Women in HPC and Applications Consultant in HPC Research & Industry, EPCC, University of Edinburgh.

ABSTRACT
This session will discuss ‘Women in HPC’, the work currently going-on worldwide to improve diversity, and open a discussion with the PRACE User Forum on recruiting women and retain a diversity. The under-representation of women is a challenge that the entire supercomputing industry faces. As a community we are only just beginning to measure and understand how ‘leaky’ our pipeline is, but attrition rates are likely as high as the general tech community: 41% of women working in tech eventually leave the field (compared to just 17% of men). This session will discuss how this issue impacts PRACE and will finish with a discussion on how PRACE can address the barriers facing women accessing PRACE resources, training and education.

TONI COLLIS
Toni Collis is co-founder of Women in HPC (WHPC), and an Applications Consultant in HPC Research and Industry at EPCC, the University of Edinburgh’s Supercomputing Centre. Within EPCC Toni provides technical expertise on a range of research projects using HPC in academic software, from engineering to biology and teaches on courses in the EPCC MSc in High Performance Computing. Toni is also part of the team that provides technical assistance to the UK national HPC service (ARCHER) community to help users port and optimise codes on ARCHER, and the provision of training for ARCHER users. As lead of WHPC, Toni is responsible for providing strategic guidance on its direction and the events that it runs and is also working on research into diversity in the HPC community. She has been on the organising committee for a variety of workshops and conferences including SC16, EuroMPI 2016, multiple WHPC events and is on the Executive Committee for SC17.
Overview of PRACE Access

JOHN CLIFFORD and ROXANA DASCALU, Peer Review Officers at PRACE.

ABSTRACT
Excellence in research highly depends on the quality of the process and procedures used to select the proposals for funding and/or supporting. Envisioned to create a world-class competitive and persistent pan-European Research Infrastructure (RI) HPC Service, the Partnership for Advanced Computing in Europe (PRACE) has developed a unified European open and fair Peer Review process of calls for proposals. The aim of the presentation is to show PRACE Peer Review principles and the different phases of the assessment process established by PRACE for Preparatory Access and Project Access calls, supported with hypothetical proposals assessment examples.

JOHN CLIFFORD
John is a Peer Review Officer at the Partnership for Advanced Computing in Europe (PRACE) in Brussels, Belgium. This role entails the management of the Peer Review process, which results in offering world class HPC resources and services to scientists and researchers from academia and industry in Europe, and contributes to promoting the PRACE Programme to the different research communities. After graduating with a BSc from University College Dublin, John undertook a PhD at Imperial College London. His research focused on the chemical and physical properties of new materials such as dyes and polymers and their utilisation in applications. After several years’ experience as a researcher and coordinator of European projects, he now uses his expertise to guide scientists and engineers from many different fields to successfully secure funding to carry out their research using some of the most cutting edge High Performance Computing systems available in the world today.

ROXANA DASCALU
Roxana Maria Dascălu, PhD is a Peer Review Officer at the Partnership for Advanced Computing in Europe (PRACE) in Brussels, Belgium. Prior to joining PRACE, Roxana worked as a Programme Officer for the Central Management Unit of the Ambient Assisted Living Association in Brussels, responsible for the central management and monitoring of a portfolio of AAL international research and innovation projects. She also worked for EACEA, the European Commission, monitoring projects focused on cooperation between European companies and universities. Roxana has a valuable experience in programme management, consultancy, managing public communication campaigns and managing EU funded projects in education and research. She has worked in Bucharest, Berlin and Brussels and has earned 2 bachelor’s degrees, in Political Sciences and in Public Administration, an MSc in Project Management and a PhD in Communication Sciences.

Networking Cocktail & Dinner
FÀBRICA MORITZ RESTAURANT (19:30 BUSES TO DINNER)
Keynote
PLENARY SESSION

Chair
SERGE BOGAERTS, Chair of the PRACEdays17 OPC
Please find his CV on Page 12

Challenges of Increased HPC Complexity and Value Delivery for the O&G Industry
HENRI CALANDRA, TOTAL ESA

ABSTRACT
Over the past several decades, growing world-wide demand for energy has driven a significant increase in the volume of hydrocarbons produced by the Oil & Gas industry. To meet this demand, exploration and production operations are driven to deeper and more remote fields with increased geological complexity, both in the subsurface and above-ground. However, these developments are increasingly economically challenging due to a renewed pressure to reduce costs. In this presentation, we will review Total’s experience in HPC and demonstrate the value that HPC has delivered to the O&G industry. We will see that, despite the above challenges, the industry can still leverage the rapid evolution in computing capability, which is highlighted by new “players” taking advantage of advances in HPC technologies. We will also discuss how the increasing complexity of HPC systems is driving the need for more advanced tools and integration of classical HPC and computational scientists on teams with domain application specialists.

HENRI CALANDRA
Henri Calandra obtained his MSc in mathematics in 1984 and a PhD in mathematics in 1987 from the Université des Pays de l'Adour in Pau, France. He joined Cray Research France in 1987 and worked on seismic applications for 2 years. In 1989 he joined the applied mathematics department of the French Atomic Agency and in 1990 he started working for Total ESA. After 12 years working in high performance computing and Pre-stack Depth Migration Research as project leader, in 2002 he started and led Total USA’s Geophysics Research Group for 3 years in Houston. Back to France in 2005 he coordinated the Depth Imaging Research activity for TOTAL, becoming an expert in numerical algorithms and High Performance Computing for Geo-sciences in 2008. In January 2014, as VP at TOTAL EP R&T USA in Houston, Henri started and led the Computational Science and Engineering Dept (CSE). Since January 2017 Henri is back in France as an expert in numerical algorithms and High Performance Computing for Geoscience for TOTAL E&P and scientific advisor for the TOTAL CSE corporate program.

10:00 - 10:30 Coffee
Support to HPC Code: The Gap Between Scientific Code Development and Exascale Technology. The Software Challenges For Extreme Scale Computing Faced by the Community

ABSTRACT
Thanks to the efforts of Tom Wilkie, the PRACE panel discussion has become one of the most anticipated items on the PRACEdays conference agenda. Those who attended last year will remember that Tom has retired as moderator and so it is our great pleasure to welcome Inma Martinez to the role. This year, we will examine the views of academia, industry and the European Commission regarding the role of open source in the development of software for HPC systems. Why is this topic our chosen theme? As the HPC community knows too well, computer hardware evolves quite quickly through generational shifts every few years, whilst scientific HPC codes develop much more slowly. This mismatch in time-scales is partly because using the latest hardware requires the development of extremely complex algorithms and software, and partly because it is becoming increasingly difficult to express sufficient parallelism to make existing algorithms use hundreds of thousands of processors. What is of particular concern to our community is that in the next few years, we are at risk of facing a serious impasse where it might not be possible to transform advances in supercomputer hardware into solving more advanced problems in academia and industry. With Inma’s help, the panel will discuss the challenges we are facing, strategies for bridging the gap and whether we can find new ways to align efforts in hardware and software design.

Moderator: INMA MARTINEZ
Panelists: HENRI CALANDRA, TOTAL
LEE MARGETTS, IAC Chair
FRAUKE GRÄTER, Heidelberg Institute for Theoretical Studies (HITS)
THOMAS SKORDAS, European Commission
ERIK LINDAHL, SSC Chair
Panel Discussion

Moderator
INMA MARTINEZ, Venture Partner responsible for Data Sciences and Product Innovation at Deep Science Ventures

Inma Martinez has been a pioneer in the mobile and digital industries since the 1990s, leading successful exits and growth in a number of high-profile tech start-ups in the UK and Finland, and an internationally recognized female tech entrepreneur that has paved the way for others. Fortune and Time have described her as one of Europe’s top talents in social engagement through technology. Silicon Valley’s Red Herring ranked her amongst the top 40 women in tech innovation, and Fast Company labelled her a “firestarter”. A data scientist who built one of the first AI systems for personalising mobile data services, she is currently a venture partner at Deep Science Ventures, a sci-tech accelerator and investment fund launched by Imperial College London. Inma is also involved in a number of data projects in the private sector, ranging from FinTech, cyberspace in education and smart cities to precision livestock farming and has been behind the product innovation strategies of big multinational corporates. Since 2001 she has served as an independent technology advisor to the EU Technology Commission, as a digitalization and Big Data expert, collaborating with various digital working groups across Europe. In 2010 she was appointed by the British government to serve as a spoke person on technology development and entrepreneurship at the UK Trade & Industry Catalyst Programme. Inma’s most requested keynotes focus on the digital acceleration affecting Life, Work and Play, and how businesses should reorganise their Human Capital and products and services to address the transformational forces of A.I. and Digitalisation, increasing their innovation by harnessing disruptive technologies. In addition, she often presents new approaches to emerging sectors such as FinTech, IoT, Smart Cities and Artificial Intelligence deployed to create products and services.

Panellist
THOMAS SKORDAS, Director “Digital Excellence and Science Infrastructure”
DG Communications Networks, Content and Technology, European Commission

Thomas Skordas received his diploma in Electrical Engineering in 1984 from University Aristotle of Thessaloniki, Greece, and the PhD in Computer Science in 1988, from the Institut National Polytechnique de Grenoble, France. From 1988 to 1995, Thomas worked in Grenoble, France as a Research Fellow and as project leader in EU-funded R&D projects in the areas of Information Technology and Robotics. In 1995, Thomas joined the European Commission as a Research Programme Officer in the Information Society Technologies Programme, part of the Directorate General Information Society & Media (DG INFSO). Ever since, Thomas worked in various units of DG INFSO (which, in 2012 became DG CONNECT) dealing with ICT research in the context of EU’s Research Framework Programmes. From 2006 to 2009, he was Deputy Head of Unit in ICT Security and Trust. In July 2009, Thomas was appointed Head of the Photonics Unit and since 1st February 2014, Head of the Flagships Unit. In March 2017 he was appointed Director “Digital Excellence and Science Infrastructure”.
Panel Discussion

**Panellist**

ERIK LINDAHL,
Chair of the PRACE Scientific Steering Committee;
Stockholm University

Please find his CV on Page 13

**Panellist**

HENDRI CALANDRA, TOTAL

Please find his CV on Page 53

**Panellist**

LEE MARGETTS, Vice-Chair of the PRACE Industrial Advisory Committee; NAFEMS (UK)

Lee Margetts is Vice-Chair of the PRACE Industrial Advisory Committee, representing the international trade association NAFEMS. He is also Chair of the NAFEMS HPC Working Group. Lee Margetts holds a PhD in "Parallel Finite Element Analysis" (University of Manchester, UK) and an MBA (with distinction) for the dissertation "Wealth Generation from Open Source Software" (Alliance Manchester Business School, UK). Lee Margetts is the founder of the open source software project ParaFEM (http://parafem.org.uk) and author of the accompanying textbook "Programming the Finite Element Method". Lee Margetts was Senior HPC Consultant in the UK National HPC Service CSAR (2001-2006) and continued in a similar role at Manchester before being appointed Lecturer in 2015. He was one of the investigators in the EU’s European Exascale Software Initiative.

**Panellist**

FRAUKE GRÄTER, Group leader Molecular Biomechanics (MBM)
Heidelberg Institute for Theoretical Studies (HITS)

Frauke Gräter is head of the research group “Molecular Biomechanics” at the Heidelberg Institute for Theoretical Studies (HITS) and Professor at Heidelberg University. She investigates how proteins have been designed to specifically respond to mechanical forces in the cellular environment or as a biomaterial, e.g. in the process of blood coagulation, in spider silk fibers or in composite materials like nacre. To this end, her group uses and further develops various simulation techniques from the molecular to the mesoscopic scale.

**Panellist : Winner of PRACE Ada Lovelace Award for HPC**

FRAUKE GRÄTER, Group leader Molecular Biomechanics (MBM)
Heidelberg Institute for Theoretical Studies (HITS)

Frauke Gräter is head of the research group “Molecular Biomechanics” at the Heidelberg Institute for Theoretical Studies (HITS) and Professor at Heidelberg University. She investigates how proteins have been designed to specifically respond to mechanical forces in the cellular environment or as a biomaterial, e.g. in the process of blood coagulation, in spider silk fibers or in composite materials like nacre. To this end, her group uses and further develops various simulation techniques from the molecular to the mesoscopic scale.
PRACE Ada Lovelace Award for HPC

At PRACEdays17 PRACE will present for the second time the PRACE Ada Lovelace Award for HPC to a female scientist who is making an outstanding contribution to and impact on HPC in Europe, at a global level. The winner of this award will be a young female scientist (PhD +10 years max, excluding parental leave) who is currently working in Europe or has been working in Europe during the past three years; who has made an outstanding impact on HPC research, computational science or service provision at a global level; who works in academia or industry; and who is a role model for women beginning careers in HPC.

The winner of the Award will be invited to participate in the concluding Panel Session at PRACEdays17, and will receive a cash prize of €1000 as well as a certificate and an engraved crystal trophy.

The Selection Committee is composed of:

- **Jürgen Kohler**: ex-Chair of the PRACE Industrial Advisory Committee, Daimler AG, Germany, and member of the Selection Committee since 2016
- **Mateo Valero**: SC15 award winner for outstanding contribution to HPC, Director of the Barcelona Supercomputing Center (BSC), Spain, and member of the Selection Committee since 2016
- **Richard Kenway**: ex-Chair of the PRACE Scientific Steering Committee, Tait Professor of Mathematical Physics, UK, and Member of the Selection Committee since 2016
- **Laura Grigori**: Member of the PRACE Scientific Steering Committee, and Director of Research at INRIA/University Pierre and Marie Curie, France
- **Christoph Schütte**: Vice-Chair of the PRACE Scientific Steering Committee, Professor of Mathematics and Computer Science at the Free University of Berlin, Germany
- **Suzanne Talon**: CEO of Calcul Québec, Canada

The following PRACE Awards will also be presented: Best Poster, Best Student Poster, Best Scientific Presentation and Best Industrial Presentation.

**AUGUSTA ADA KING, Countess of Lovelace**

Augusta Ada King, Countess of Lovelace (née Byron; 10 December 1815 – 27 November 1852) was an English mathematician and writer, chiefly known for her work on Charles Babbage’s early mechanical general-purpose computer, the Analytical Engine. Her notes on the engine include what is recognised as the first algorithm intended to be carried out by a machine. As a result, she is often regarded as the first computer programmer. (source: Wikipedia)

**Closing of the Conference**

SERGE BOGAERTS, Chair of the PRACEdays17 OPC
## Posters

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## Student Posters

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CO-ORDINATION
Silke Lang, PRACE aisbl

PROOF READING
John Clifford, PRACE aisbl
Marjolein Oorsprong, PRACE aisbl
Stelios Erotokritou, CaSTROC
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