

# PRACE Scientific & Industrial Conference 2018



HPC for  
Innovation:  
When Science  
Meets Industry

29–31 May 2018

University of Ljubljana  
Ljubljana, Slovenia





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# Welcome

Dear Participant, It gives us great pleasure to welcome you to the **PRACE Scientific and Industrial Conference 2018** - the fifth edition of PRACEdays, hosted by PRACE and the University of Ljubljana under the motto: **HPC for Innovation: When Science Meets Industry** This year, the conference takes place in Ljubljana, Slovenia's capital city and largest city. It is known for its university population and green spaces, including expansive Tivoli Park. The curving Ljubljanica River, lined in outdoor cafes, divides the city's old town from its commercial hub. Ljubljana has many museums, including the National Museum of Slovenia, displaying historic exhibitions, and the Museum of Modern Art, home to 20th-century Slovene paintings and sculptures.

The University of Ljubljana (UL) is proud to welcome this high-level scientific and industrial conference to the capital of Slovenia. UL is Slovenian representative in PRACE and Slovenian member in PRACE IP projects. As the largest higher education institution, it is striving to increase the uptake of HPC technology among professors, researchers and students all around Slovenia on one hand and to transfer this knowledge to business sector on the other hand.

In 2018 the third edition of the European HPC Summit Week is organised by European Extreme Data & Computing Initiative (EXDCI) project and PRACEdays18 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.

PRACEdays18 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 Thomas Skordas, Director *"Digital Excellence and Science Infrastructure"* Directorate General for Communications Networks, Content and Technology (DG CONNECT), European Commission to give a talk on *"The European HPC Strategy and the EuroHPC Joint Undertaking"* on Wednesday. On Tuesday the conference programme offers

parallel sessions with selected speakers from different research domains including CFD & Engineering, Materials & Chemistry, Plasma & Energy, Life Sciences & Chemistry, and Industry. We recommend you join one of those to get a "flavour" of HPC in industry and academia on Tuesday afternoon.

On Thursday the panel session will be moderated by Jacki Davis, an experienced journalist, speaker and moderator of high-level events both in Brussels and in EU national capitals. The panel gathers renowned panellists to discuss the topic: *"CoEs and HLSTs, what problems can they solve for me?"* For the third 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.

PRACEdays18 will also offer to you – dear participant – a social programme including a conference dinner at and tour of the Postojna Cave, a 24,340 m long karst cave system created by the Pivka River. It is the second-longest cave system in the country.

We would like to take this opportunity to thank all those who have made this event possible: the local host University of Ljubljana (UL), the Organisation and Programme Committee, the PRACE Communications Team, the PRACE Scientific Steering Committee, the PRACE Industrial Advisory Committee, the PRACE User Forum, the EXDCI Project partners, PRACE-5IP Project partners, the PRACE Board of Directors, the European Commission, and the PRACE Council. 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!**



**Anwar Osseyran**  
Chair of the PRACE Council



**Serge Bogaerts**  
Managing Director, PRACE

# Committees

## ORGANISATION & PROGRAMME COMMITTEE (OPC)

<b>Serge Bogaerts</b>	PRACE aisbl, Chair of the OPC
<b>François Bodin</b>	EXDCI Scientific Director, Vice-Chair of the OPC
<b>Maike Gilliot</b>	ETP4HPC
<b>Renata Giménez</b>	BSC (Spain), EXDCI Dissemination Team
<b>Troels Haugbølle</b>	NBI (Denmark), Chair of the PRACE User Forum
<b>Dimitri Komatitsch</b>	LMA CNRS-MRS, Member of the PRACE SSC
<b>Leon Kos</b>	University of Ljubljana, Local host 2018
<b>Silke Lang</b>	PRACE aisbl, PRACE Communications Officer
<b>Núria López</b>	Institute of Chemical Research of Catalonia, Vice-Chair of the PRACE SSC
<b>Lee Margetts</b>	University of Manchester (UK), Chair of the PRACE IAC
<b>Jean-Philippe Nominé</b>	ETP4HPC
<b>Marjolein Oorsprong</b>	PRACE aisbl, PRACE Communications Officer
<b>Janez Povh</b>	University of Ljubljana, Local host 2018
<b>Matej Praprotnik</b>	University of Ljubljana, Member of the PRACE SSC
<b>Sinéad Ryan</b>	Trinity College Dublin, Chair of the PRACE SSC
<b>Veronica Teodor</b>	FZ Jülich, PRACE PMO

## SCIENTIFIC STEERING COMMITTEE (SSC)

<b>Marina Becoulet</b>	CEA
<b>Carlo Massimo Casciola</b>	University of Rome
<b>Luke Drury</b>	Dublin Institute for Advanced Studies
<b>Claudia Filippi</b>	University of Twente, Faculty of Science and Technology
<b>Frauke Gräter</b>	Heidelberg Institute for Theoretical Studies (HITS)
<b>Laura Grigori</b>	INRIA/University Pierre and Marie Curie
<b>Dimitri Komatitsch</b>	LMA CNRS-MRS
<b>Petros Koumoutsakos</b>	ETH Zürich
<b>Erik Lindahl</b>	KTH Royal Institute of Technology
<b>Núria López (Vice Chair)</b>	Institute of Chemical Research of Catalonia
<b>Ignacio Pagonabarraga Mora</b>	University of Barcelona
<b>Antonio Navarra</b>	CMCC
<b>Mike Payne</b>	University of Cambridge, EPSRC Centre
<b>Matej Praprotnik</b>	Faculty of Mathematics and Physics, University of Ljubljana
<b>Sinéad Ryan (Chair)</b>	University Dublin, Trinity College Dublin, School of Mathematics
<b>Per Stenström</b>	University of Technology, Göteborg
<b>Julia Yeomans</b>	University of Oxford, Rudolf Peierls Centre for Theoretical Physics
<b>Claudio Zannoni</b>	University of Bologna

## INDUSTRIAL ADVISORY COMMITTEE (IAC)

<b>Henk Coenen</b>	NXP
<b>Enric Gibert</b>	PHARMACELERA
<b>Tomi Iljaš</b>	Arctur
<b>Dieter Jahn (Vice-Chair)</b>	BASF
<b>Lee Margetts (Chair)</b>	NAFEMS
<b>Alain Martin</b>	EDF
<b>Marc Morere</b>	Airbus
<b>Martin Winter</b>	CEFIC

## Committees

### PRACE BOARD OF DIRECTORS (BoD)

<b>Serge Bogaerts (Chair)</b>	PRACE aisbl
<b>Florian Berberich</b>	FZ Jülich
<b>Maria Grazia Giuffreda</b>	ETH Zurich/CSCS
<b>Sinéad Ryan</b>	UCD, Dublin, Chair of SSC
<b>Oriol Pineda</b>	BSC
<b>Stephane Requena</b>	GENCI
<b>Debora Testi</b>	CINECA

### EVENT ORGANISER

<b>Jean-Baptiste De Bock</b>	Of <sup>2</sup> Cores
<b>Harold Carniyan</b>	Of <sup>2</sup> Cores
<b>Freek Wambeke</b>	Of <sup>2</sup> Cores
<b>Leila Aleksandra Jelić</b>	3DTA

### USER FORUM (UF)

<b>Koen Hillewaert</b>	Centre de recherche en Aéronautique (Cenaero)
<b>Troels Haugbøelle (Chair)</b>	University of Copenhagen
<b>Marc Baaden</b>	CNRS
<b>Carmen Domene</b>	King's College London
<b>Turlough Downes</b>	Dublin City University
<b>Derek Groen (Vice Chair)</b>	Brunel University London
<b>Stefano Fabris</b>	CNR-IOM DEMOCRITOS
<b>Maria-Teresa Parra</b>	University of Valladolid
<b>William Sellers</b>	University of Manchester
<b>Gabriel Staffelbach</b>	Cerfacs
<b>Jorge Vieira</b>	Instituto Superior Técnico
<b>Gustavo Yepes</b>	Universidad Autonoma de Madrid (UAM)

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 PRACEdays18.

<b>Stelios Erotokritou</b>	CaSToRC
<b>Anni Jakobsson</b>	CSC
<b>Silke Lang</b>	PRACE aisbl
<b>Tiina Leiponen</b>	CSC
<b>Janina Liebmann</b>	FZ Jülich
<b>Leon Kos</b>	University Ljubljana
<b>Mateja Maffi</b>	University Ljubljana
<b>Marjolein Oorsprong</b>	PRACE aisbl
<b>Karina Pesatova</b>	IT4Innovations
<b>Cornelia Staub</b>	JKU/RISC
<b>Veronica Teodor</b>	FZ Jülich
<b>Nikos Nikoloutsakos</b>	GRNET
<b>Timotej Hrga</b>	University of Ljubljana
<b>Dejan Penko</b>	University of Ljubljana
<b>Gregor Simič</b>	University of Ljubljana
<b>Matic Brank</b>	University of Ljubljana
<b>Ivona Vasileska</b>	University of Ljubljana
<b>Alenka Maffi</b>	University of Ljubljana

### PROJECT MANAGEMENT ORGANISATION (PMO)

<b>Thomas Lippert</b>	FZ Jülich, Project Coordinator
<b>Florian Berberich</b>	FZ Jülich, Project Manager
<b>Veronica Teodor</b>	FZ Jülich, Deputy Proj. Manager
<b>Janina Liebmann</b>	FZ Jülich, Assistant

### MEDIA CREW

<b>Ramon Vila</b>	Vision film, producer
<b>Antonio Iglesias</b>	Vision film, video/photo crew
<b>Chiara Colalelli</b>	Vision film, producer



You will easily recognise them as they all wear a blue PRACEdays18 T-shirt.

# European HPC Summit Week 2018

28 May-  
1 June 2018  
Ljubljana  
Slovenia

The European HPC Summit Week 2018 (EHPCSW18) offers a wide variety of workshops covering a number of application areas where supercomputers are key, as well as HPC technologies and infrastructures. This third edition will include even more HPC workshops than the 2017 edition, covering a range of application areas including life sciences, chemistry, astronomy, energy or material sciences, as well as HPC future technologies. This year's edition will take place 28 May – 1 June 2018 in Ljubljana, Slovenia, and will be hosted by PRACE's Slovenian Member ULFME – University of Ljubljana, Faculty of Mechanical Engineering. It will be a great opportunity to network with all relevant European HPC stakeholders, from technology suppliers and HPC infrastructures to HPC scientific and industrial users in Europe.

The programme of the week contains workshops from various HPC initiatives in Europe in order to find synergies among all parties of the HPC ecosystem:



**EXDCI Workshop**  
Monday 28 May (afternoon)



**PRACEdays18**  
Tuesday 29 May  
to Thursday 31 May



**ALLScale, ANTAREX, READEX and ExCAPE projects: High-Performance Computing Approaches for Monitoring, Exploring, Optimizing and Autotuning**  
Tuesday 29 May (afternoon)



**NextGenIO, SAGE Working Towards Exascale IO**  
Tuesday 29 May (afternoon)



**EOSC Pilot Meeting; Recommendations on Governance and Rules of Participation**  
Tuesday 29 May (afternoon)



**Workshop on Energy Efficiency in HPC**  
Wednesday 30 May (afternoon)



**HPE: Memory-Centric Architectures for Exascale Systems: Scientific and Industrial Requirements**  
Wednesday 30 May (afternoon)



**EUDAT Workshop**  
Wednesday 30 May (afternoon)



**EAP Connect: Deep Learning & Medical Data Mining**  
Wednesday 30 May (afternoon)  
**EAP Connect: Containers in HPC**  
Thursday 31 May (afternoon)



**EuroEXA, ExaNeST, ExaNoDe, EcoScale: Towards Exascale HPC Systems: Co-design and technology development within the EuroEXA, ExaNeST, ExaNoDE and ExaScale Projects**  
Thursday 31 May (afternoon)



**EuroLab-4-HPC**  
Thursday 31 May (afternoon)



**ComPat: Computing Patterns for High Performance Multiscale Computing**  
Thursday 31 May (afternoon)

## General Information



### PRACEdays18

From Tuesday 29 May to Thursday 31 May 2018

### VENUE

University of Ljubljana, Faculty of Law  
Poljanski nasip 2, 1000 Ljubljana, Slovenia  
Tel: +386 1 42 03 100 / +386 1 42 03 115

### REGISTRATION DESK

The main registration and information desk is situated at the entrance of the Atrium of the Faculty of Law building from Monday to Friday.

<b>Monday 28 May</b>	08:00 to 18:00
<b>Tuesday 29 May</b>	08:00 to 18:00
<b>Wednesday 30 May</b>	08:00 to 18:00
<b>Thursday 31 May</b>	08:00 to 18:00
<b>Friday 1 June</b>	08:00 to 13:00

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

Image copyright: Ljubljana Convention Bureau  
[www.visitljubljana.com/en](http://www.visitljubljana.com/en)

### COFFEE BREAKS AND LUNCHES

Morning and afternoon coffee breaks will be served at the first floor. The lunches will be served at the Atrium, ground floor.

### WELCOME RECEPTION

**Tuesday 29 May 2018**

**Hall of Faculty of Law 19:30 - 21:00**

Included in the registration fee.

This reception will be held at the Hall and terrace of the Faculty of Law. 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 30 May 2017**

Visit to Postojna Cave and Conference Dinner.

After the group picture, buses will leave from the venue to the Postojna Cave at 17:30.

The visit of the Cave is from 18:30 - 20:30.

The Dinner is from 20:30 - 22:00.



# Useful Information

## CURRENCY AND PAYMENTS

The official currency of Slovenia is the euro (€). Most shops across the country accept international credit and debit cards.

## CITY BUSES

If you want to use the city buses you need to have an Urbana card on which you put credit for bus rides. Every bus ride costs 1,20€ and you can use as many buses as you want in 90 minutes for this price. You can buy Urbana cards at Ljubljana Bus Station, selected offices of the post office, at Tourist Information Centres or with the help of Mobile App Urbana.

## BICIKELJ - BICYCLE-SHARING SYSTEM

Open 7 days a week, 24 hours a day, the Bicikelj system enables you to travel freely by day or night. Whether you use the system regularly or just occasionally, you can make an unlimited number of trips over the period of your subscription. In addition to an e-mail address, you need to have a credit card, but you do not need an Urbana city card. Upon registration, you will receive to your e-mail address your user number and a 4-digit PIN code, which are required for every bike rental. The registration fee for weekly use of the Bicike(LJ) system is 1 Euro.

## TIME

Slovenia is in the Central European Time zone (CET)

## IMPORTANT NUMBERS

Slovenia: +386

113 – Police

112 - Emergency Reporting Centre  
(fire and rescue station)

## ELECTRICITY

230V/16A

## WIFI

All delegates will have free wifi at the venue.

Free wifi is also available around the city:

- Connect to the WiFreeLjubljana network.
- Go to [www.wifreeLjubljana.si](http://www.wifreeLjubljana.si)
- Enter your mobile phone number.
- You receive an SMS with your WiFree code.
- Enter your WiFree code.
- You can use WiFreeLjubljana free for up to 60 minutes
- further details to access the free wifi will be published on the registration badge

## SIGHTSEEING IN LJUBLJANA

Ljubljana is small enough that you can experience it on foot but there are also very good city bus connections. Taking a walk through the picturesque streets of Ljubljana is a perfect way to see most of the city's major architectural sights, get to know some of the distinctive local features, and meet people. Climb the castle hill, spend some wonderful moments in the castle courtyard and along the ramparts, and let stunning city views make you fall in love with Ljubljana. Find your favourite spot on the relaxing Ljubljanica river embankments, treat yourself to a picnic in the scenic Tivoli Park, marvel at the diversity of plants at the Ljubljana Botanic Garden, and explore the city's unique alternative quarter, Metelkova. Should your feet be tired while you still want more, take a free ride on board a Kavalir electric vehicle, part of the green transport system in the pedestrianized city centre. Due to Ljubljana and Central Slovenia's rich and unique artistic and historical heritage, visiting the region's museums is quite an experience.

[www.visitljubljana.com/en/visitors/things-to-do/art-and-culture/article/museums-in-ljubljana-and-its-surrounding-areas](http://www.visitljubljana.com/en/visitors/things-to-do/art-and-culture/article/museums-in-ljubljana-and-its-surrounding-areas)

Univerza v Ljubljani

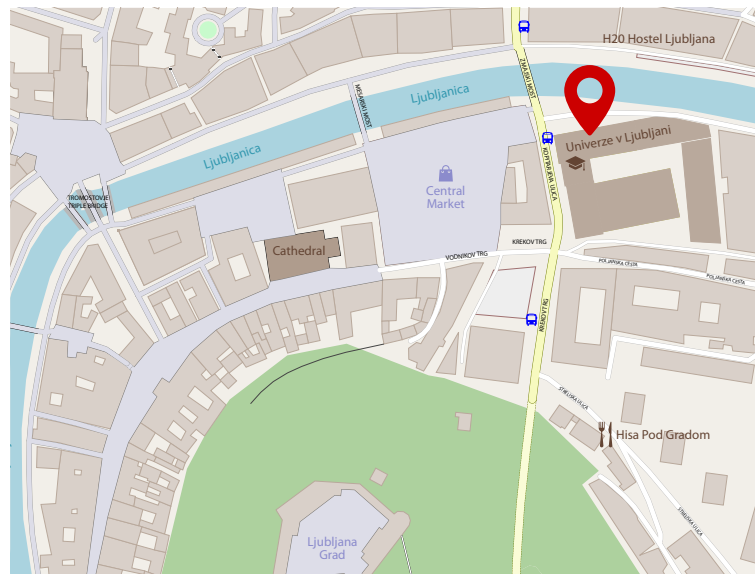


University of Ljubljana, Faculty of Law  
Poljanski nasip 2, SI-1000 Ljubljana

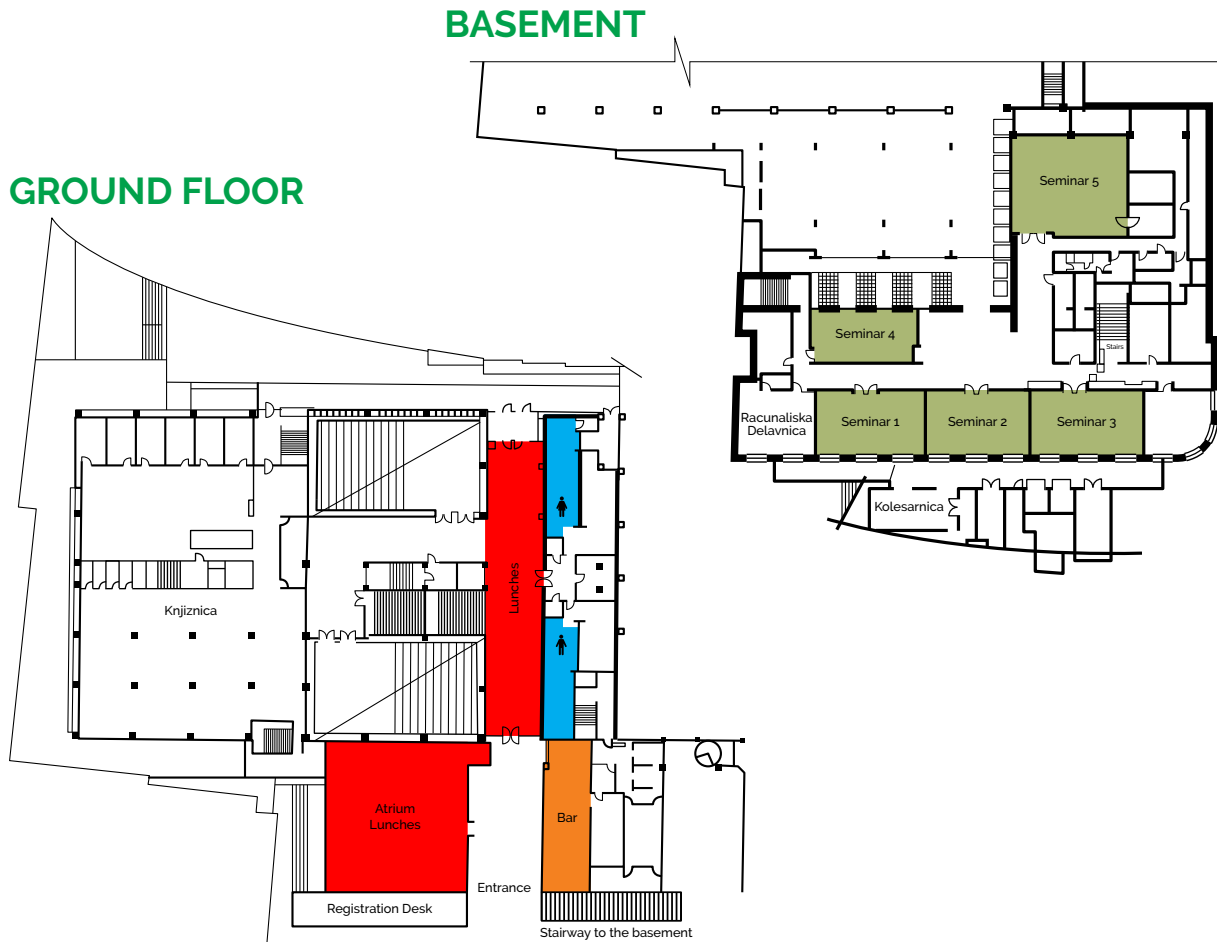
**Tel:** +386 1 42 03 100

**Fax:** +386 1 42 03 115

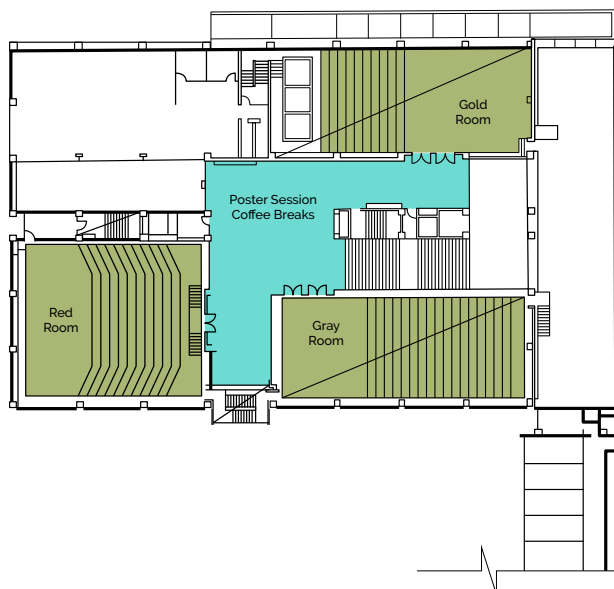
**Web:** [www.pf.uni-lj.si](http://www.pf.uni-lj.si)



# Floorplan of Faculty of Law



## FIRST FLOOR



- Poster Sessions / Coffee Breaks
- Plenary Sessions, Parellel Sessions & Meetings
- Lunches
- Bar
- Rest Rooms

# Keynotes

## PLENARY SESSION

TIME: 09:00 - 10:30  
ROOM: RED **TUE**

### Chair

#### **SERGI GIRONA, Vice-Chair of the PRACE Council**

Sergi Girona holds a PhD in Computer Science from the Technical University of Catalunya. Currently he is Director of the Operations Department of the Barcelona Supercomputing Center (BSC) and the manager of the Spanish Supercomputing Network (RES). He has been closely linked to PRACE since its creation: between 2013 and 2015 he was both Chair of its Board of Directors and Managing Director. In June 2016 he was appointed Council Vice-Chair, a role that he currently performs. He joined BSC in 2004 for the installation of MareNostrum in Barcelona, which was at that time the largest supercomputer in Europe, a position that maintained for 3 years. Sergi was responsible for the site preparation and the coordination with IBM for the system installation. His responsibilities nowadays include managing the Operations group with the responsibilities of User Support and System Administration of the different HPC systems at BSC. He is Spanish delegate at e-IRG, and member of the ESFRI Health and Food Strategic working group. The list of projects he has participated in include: DEISA, PRACE, EUDAT, EESI, Human Brain Project, RDA, EXDCI, ELITRANS, iCordi, HPC Europa, Red de eCiencia and RES. Before joining BSC, he was Director of the Spanish branch of EASi Engineering since its creation, and its R&D Director for its German headquarters.



### Opening of EHPCSW & PRACEdays18

#### **SERGE BOGAERTS, Managing Director of PRACE, Chair of the EHPCSW & PRACEdays OPC**

Serge Bogaerts graduated in 1992 as Mechanical and Electrical Engineer at the Free University of Brussels (ULB). Researcher in numerical fluid mechanics at the von Karman Institute, then design engineer in nuclear safety at Tractebel Engineering, and, in 2003, researcher in CFD-Multiphysics at Cenaero, Serge knows the challenges of numerical simulation. He managed the operations of Cenaero supercomputers from 2006 which allowed him to build up an in-depth experience in leading projects for the procurement and operation of HPC infrastructures. In October 2012, he was appointed Belgian Delegate to the PRACE Council on which he also served as Council Secretary from October 2015 onwards. He left Cenaero to take up the position of PRACE Chair of the Board of Directors and Managing Director on 1 February 2017.

# Keynotes

## PLENARY SESSION

TIME: 09:00 - 10:30  
ROOM: RED **TUE**

### Welcome

#### **ANWAR OSSEYRAN, Chair of the PRACE Council**

Prof. dr. Anwar Osseyran is since 2001 the CEO of SURFsara (formerly SARA), The Dutch national HPC Center and since January 2015 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 Master in Electrical Engineering and a PhD in Applied Physics. He was 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 for Supercomputing, member of the Executive Board of Nederland 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). Prof. Osseyran has three patents to his name.



### Slovenian Government

#### **MAJA MAKOVEC BRENČIČ, Ministry of Education, Science and Sport**

PhD in management and organisation and Full Professor of International Business at the Faculty of Economics of the University of Ljubljana In 2013, Maja Makovec Brenčič was appointed Vice-Rector of the University of Ljubljana responsible for knowledge transfer, cooperation between the academia and the industry and the wider social environment, and internationalisation. Between 2010 and 2013 she headed the Council of the newly established Quality Assurance Agency for Higher Education of Slovenia. At the Faculty of Economics, she was Vice Dean for strategy development, internationalisation and quality. She is very familiar with ensuring quality of education, development trends in education and science, international education and scientific environment and connecting the academia with the industry and wider social environment. She is also involved in some activities connected with the organisation of sport in Slovenia.

# Keynotes

## PLENARY SESSION

TIME: 09:00 - 10:30  
ROOM: RED **TUE**

### University of Ljubljana

#### IGOR PAPIČ, Rector of the University of Ljubljana

Prof. Dr. Igor Papič is a professor at the Faculty of Electrical Engineering at the University of Ljubljana. He is the Head of the Laboratory of Electricity Networks and Devices, and he was the Vice-Dean for Education from 2011 to 2013 and the Dean of the Faculty from 2013 to 2017. He received his bachelor's degree in 1992, his master's degree in 1995 and his doctorate in 1998 from the Faculty of Electrical Engineering at the University of Ljubljana. From 1994 to 1996, he trained at Siemens' Power Transmission and Distribution department in Erlangen, Germany. In 2001, he taught as a guest professor at the University of Manitoba in Winnipeg, Canada. His research includes active compensators, FACTS (Flexible AC Transmission System) devices, power quality and smart grid concepts.

Prof. Dr. Igor Papič has also led numerous domestic and international research and development projects. In 2009, he and his partners established Reinhausen 2e, d. o. o., a spin-off company of the University of Ljubljana. The company's two main activities include engineering and the development of passive, hybrid and active compensators. He was elected and is serving as Rector of the University of Ljubljana for the mandate from 1 October 2017 to 30 September 2021.



### CEF Call 2018 and Results of the CEF Call 2017

#### LEONARDO FLORES AÑOVER, European Commission

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 has 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 establishment of the EuroHPC Joint Undertaking and for the support to the European HPC ecosystem. He is Project Officer for the PRACE Implementation Projects and other research and innovation actions.

**10:30 - 11:00 Coffee Break**

# Keynotes

## PLENARY SESSION

TIME: 11:00 - 13:10  
ROOM: RED **TUE**

### Chair

#### **SAI NARASIMHAMURTHY, Seagate and Vice-President for Industry ETP4HPC**

Dr. Sai Narasimhamurthy is currently Principal Engineer at Seagate, working on Research and Development for next generation storage systems. He has actively led and contributed to many Extreme Scale Computing and Cloud research initiatives, currently leading the SAGE H2020 project. Sai also holds the position of Vice-Chair of Industry for the ETP4HPC organisation and leads the storage and I/O working group for developing ETP4HPC's Strategic Research Agenda (SRA). Previously, Sai was CTO and Co-founder at 4Blox, inc, a venture capital backed storage infrastructure software company in California in the area of Storage Area Networks(SANs). Sai obtained his PhD from Arizona State University (2005) in the area of Internet Protocol(IP) Storage and has been involved with storage systems starting from the early days of IP SANs (iSCSI). Sai also worked with Intel R&D and was a contributing participant in the first stages of the RDMA consortium for IP Storage and 10GbE.



### **Binary Neutron Stars: Einstein's Richest Laboratory**

**LUCIANO REZZOLLA, Goethe University, Frankfurt, Germany**

#### **ABSTRACT**

I will argue that if black holes represent one the most fascinating implications of Einstein's theory of gravity, neutron stars in binary systems are arguably its richest laboratory, where gravity blends with astrophysics and particle physics. I will discuss the rapid recent progress made in modelling these systems and show how the inspiral and merger of a binary system of neutron stars is more than a strong source of gravitational waves. Indeed, while the gravitational signal can provide tight constraints on the equation of state for matter at nuclear densities, the formation of a black-hole-torus system can explain much of the phenomenology of short gamma-ray bursts, while the ejection of matter during the merger can shed light on the chemical enrichment of the universe.

#### **LUCIANO REZZOLLA**

Luciano Rezzolla received his PhD in Astrophysics in 1997 at the International School for Advanced Studies (SISSA) in Trieste. After being a Research Associate at the University of Illinois at Urbana-Champaign, he returned to SISSA in 1999 as Associate Professor and Director of the Computing Centre. From 2006 to 2013 he joined the Albert Einstein Institute in Potsdam (Max-Planck Institute for gravitational physics) as the Head of the Numerical-Relativity Research. Since 2013 he is Chair of Theoretical Relativistic Astrophysics and Director of the Institute of Theoretical Physics in Frankfurt. In 2013 he was awarded an ERC Synergy Grant and is the recipient of the 2017 Karl Schwarzschild Prize. He has worked in several areas of relativistic hydrodynamics and relativistic astrophysics, ranging from the investigation of fundamental issues to the construction of advanced numerical codes for the simulation of sources of gravitational waves and accretion flows onto astrophysical compact objects

# Keynotes

## PLENARY SESSION

TIME: 11:00 - 13:10  
ROOM: RED **TUE**

### Cloud HPC and Containers Supporting Science and Engineering

**WOLFGANG GENTZSCH, President & Co-Founder UberCloud Online Marketplace**

#### ABSTRACT

In the first part we will provide a general view and actual status of cloud computing for scientists and engineers, the challenges and benefits, and the major HPC cloud providers. We will look at some of the most severe hurdles for cloud adoption: often still the very limited license models of the many different commercial software providers, and the different proprietary cloud platforms of several larger software providers. In the second part we will zoom in on novel software novel containers for HPC, based on Docker and on Singularity, which come with a number of great benefits for the HPC users, such as ease of software packaging and porting to any Linux environment, user-friendly access and use of software, workflows and data, while still maintaining application scalability.

#### WOLFGANG GENTZSCH

Wolfgang Gentsch is President and co-founder of the UberCloud Online Marketplace for engineers and scientists to discover, try, and buy computing on demand, in the cloud. Wolfgang was Chairman of the International ISC Cloud Conferences from 2010 to 2015. Previously, he was an Advisor to EUDAT & DEISA, directed the German D-Grid and the North Carolina Statewide Grid, and was a member of the Board of Directors of the Open Grid Forum and of the US President's Council of Advisors for Science and Technology, PCAST. Before, Wolfgang was a professor of computer science at several universities in the US and Germany previously and held leading positions at the North Carolina Grid and Data Center in Durham, Sun Microsystems in California, the DLR Aerospace Center in Germany, and MPI Plasmaphysics in Munich. In the 1990s, he founded HPC company Gridware (Sun Grid Engine) which was acquired by Sun in 2000.



# Keynotes

## PLENARY SESSION

TIME: 11:00 - 13:10  
ROOM: RED **TUE**

### Building a World-Class Supercomputer Infrastructure

JEAN-PIERRE PANZIERA, Chair of ETP4HPC

#### ABSTRACT

ETP4HPC is committed to developing a European world-class HPC technology value chain. An important vehicle for this development are the Research and Innovation projects funded by the European Commission. With the HPC contractual Public-Private Partnership (cPPP) signed with the European Commission, ETP4HPC has been contributing to the definition of the Horizon 2020 HPC Work Programme. The new EuroHPC initiative launched in Rome in March 2017 is providing a new impetus to the European HPC ecosystem. ETP4HPC fully supports the proposition to organise EuroHPC as a Joint Undertaking. EuroHPC will be operational in 2019; it will manage the acquisition and operation of world-class supercomputing machines. This legal structure will make it possible to merge multiple sources of funding in order to provide the European research and science community with the supercomputing capacity they need. ETP4HPC will play a pivotal role in the EuroHPC Joint Undertaking which will also organise and coordinate the Research and Innovation HPC programme. This should replace the current cPPP framework. ETP4HPC will be one of the private members together with the Big Data Value Association (BDVA) and will be part of the Research and Innovation Advisory Group.

#### JEAN-PIERRE PANZIERA

Jean-Pierre Panziera is the Chair of the ETP4HPC since December 2016 and has been actively involved in the life of the association since its inception, contributing to technical papers. Concurrently, Jean-Pierre is the Chief Technical Director for HPC at Bull (now part of Atos) since 2009. His role consists in defining the company's HPC strategy. Prior to that, he was Chief Engineer at SGI where he had worked for 20 years. Jean-Pierre holds an engineering degree from Ecole Nationale Supérieure des Mines de Paris.

# Keynotes

## PLENARY SESSION

TIME: 11:00 - 13:10  
ROOM: RED **TUE**

### Presentation of the PRACE Scientific Case

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

#### ERIK LINDAHL

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.

**13:10 - 14:30 Lunch**

# Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED **TUE**

## Chair

### **LEE MARGETTS, Senior Lecturer in Structural Integrity, University of Manchester, UK**

Dr Lee Margetts is Chair of the PRACE Industrial Advisory Committee, representing the international trade association NAFEMS. He is also Chair of the NAFEMS HPC Working Group. Dr 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). Dr 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", Wiley, 2014. Dr Margetts was a Senior HPC Consultant in the UK National HPC Service CSAR (2001-2006) and continued in a similar role at Manchester until 2015. He is currently a Senior Lecturer (Associate Professor) in the School of Mechanical, Aerospace and Civil Engineering at the University of Manchester. His main research activity is the development of HPC software for the multi-scale modelling of complex materials; with applications ranging from nuclear graphite to ultra high performance concrete to dinosaur bone. He was one of the investigators in the EU's *European Exascale Software Initiative* and strongly supported the project's recommendation that the EC provide funding for the HPC Centres of Excellence. Dr Margetts is currently an investigator in two Horizon 2020 projects, ECO-COMPASS, which is investigating the development of biodegradable plant-based composites for aerospace applications and EXDCI-2, the European Extreme Data and Computing Initiative. He is also the co-investigator on a 5 Year EPSRC Fellowship titled *GEMS: Geometric Modelling of Solids*: which aims to deliver one of the greatest mathematical advances in the modelling of solids since the invention of the finite element method.

# Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED **TUE**

## DNS of Interfacial Heat and Mass Transfer in Bubble Swarms

NÉSTOR BALCÁZAR, Technical University of Catalonia, Spain

### ABSTRACT

Bubbly flow with interfacial heat or mass transfer is a complex phenomenon, that is difficult to understand, predict or model. Experimental measurements of bubbly flows can be hard due to limitations in optical access, whereas analytical methods can be applied only for the most simple cases. On the other hand, the development of computers has promoted Direct Numerical Simulations (DNS) of the Navier-Stokes equations as another means to design controlled numerical experiments of bubbly flows. This work is focused on combining High Performance Computing (HPC) and DNS to explore the complexities of bubbly flows, including interfacial heat or mass transfer, from first principles. With this purpose, the Navier-Stokes equations, energy equation, and chemical species concentration equations are solved using a finite-volume approach on a collocated unstructured grid. A novel methodology is presented in the framework of a multiple-marker interface capturing approach, which can reproduce the physics of bubble collisions in long time simulations of bubbly flows. These methods are used to perform high-fidelity simulations of thermocapillary-driven bubble swarms in micro-gravity environments, for Reynolds number  $Re \sim O(10)$  and Marangoni number  $Ma \sim O(10)$  as well as heat and mass transfer processes in gravity-driven bubbly flows with  $Re \sim O(100)$  and low Schmidt number.

### NÉSTOR BALCÁZAR

Dr. Néstor Vinicio Balcázar Arciniega holds a Ph.D. in Thermal Engineering from the Technical University of Catalonia-BarcelonaTech (UPC), awarded in September-2014. From December 2014 up to March 2016, he was a post-doctoral researcher at the Heat and Mass Transfer Technological Center-UPC. Since April 2016, he is a researcher at Termo Fluids S.L., Spain. He has participated as a researcher in more than 10 HPC projects, including 2 Tier-0 PRACE projects: "DNS of gravity-driven bubbly flows" (PRACE Call 10, 22M hours), and "DNS of bubbly flows with interfacial heat and mass transfer" (PRACE Call 14, 18M hours). His research is focused on the development of numerical methods for DNS of gas-liquid multiphase flows on unstructured grids, including variable surface tension, phase change, interfacial heat and mass transfer. He is the author of 8 papers in JCR journals (5 as the first author), 15 papers in peer-reviewed international conference proceedings, and has supervised 1 Ph.D. thesis at UPC.

## Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED **TUE**

### Oil Reservoir Simulations in HPC

**IOANNIS PAPAEFSTATHIOU, Synelxis Solutions SA and School of Electrical and Computer Engineering at the Technical University of Crete, Greece**

#### ABSTRACT

Reservoir simulations (RS) are state-of-the-art technology used to predict field performance under several possible production schemes. They combine the physical laws applying to the oil production process and involve differential equation numerical solution techniques, in order to come up with a prediction of the future oil and gas production. The complexity of the differential equations involved together with the dense time and 3D space discretisation using unstructured grids renders a simulation run as a computationally intensive task that can only be executed on dedicated HPC clusters. In our work we are employing, at different grid points, the Rachford-Rice equation. The algorithm that solves the Rachford-Rice equation is the Newton-Raphson method. The respective OpenCL kernels used in this work are Hyperbolic and Michelsen and provide a fast convergence in solving the Rachford-Rice equation for oil reservoir simulations. We have executed our code in an HPC system under development within the ECOSCALE project. In that respect we are using an HPC platform which employs reconfigurable devices (i.e. FPGAs) in the nodes. Based on our results our implementations in reconfigurable cores are 20%-30% faster than the corresponding ones on a state-of-the-art multi-core CPU while consuming an order of magnitude less power.

#### IOANNIS PAPAEFSTATHIOU

Ioannis is a Manager at Synelxis Solutions SA and a Professor at the School of Electrical and Computer Engineering at the Technical University of Crete. He is working in the design and implementation of methodologies for systems with tightly coupled design parameters and highly constrained resources. He was granted a PhD in computer science at the University of Cambridge in 2001, an M.Sc. (Ranked 1st) from Harvard University in 1996 and a B.Sc. (Ranked 2nd) from the University of Crete in 1996. He has published more than 100 papers in IEEE and ACM-sponsored journals and conferences. He has participated in many European R&D Programmes (e.g. OSMOSIS, FASTCUDA, HEAP, FASTER, COSSIM ECOSCALE, EXTRA); in total he has been Principal Investigator in 12 competitively funded research projects in Europe (in 7 of them he was the technical manager), in the last 7 years, where his cumulative budget share exceeds €5 million.

# Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED

TUE



## Supercomputing for Everyone: Meeting the Growing Needs of Businesses

**ROMAIN KLEIN, Co-founder & CTO at Aeromines, Mines Paristech - Transvalor**

### ABSTRACT

Aeromines is a scientific computing cloud platform for computational fluid dynamics developed for Mines Paristech and marketed by Transvalor to industrial clients in several domains: Aerospace, Defense, Automotive, Construction, Energy, etc. We will present several industrial test cases that rely on this unique project. Based upon cluster virtualization technology from IBM: it also brings students, researchers and industries together in a secure, flexible and collaborative high-performance computing environment – reducing the costs of complex computational modeling, providing unlimited storage and total security and shortening the time taken to test new ideas by 91%. Additionally, this session will cover the advantages of this innovative solution and highlights the benefits of this collaboration including: A flexible hybrid-cloud infrastructure tailored for HPC providing on-premise performance and the ability to easily burst to the cloud as required; A complete PaaS solution to easily host the Aeromines software stack with enterprise grade scheduling; Security, with isolated resources to either a shared cluster or dedicated clusters for clients with highly confidential data; Flexibility with the ability to grow or shrink resources depending on client demands. A live demo will be also be shown as a conclusion.

### ROMAIN KLEIN

Romain is Co-founder of Aeromines, a High Performance Cloud Computing Platform for MINES ParisTech, powered by IBM Spectrum Computing. Today, as CTO of the platform at Transvalor, he is responsible to ensure that the projects are delivered according to requirements and make use of the best architectural components in a practical manner -balancing architectural correctness, leading edge and the ability of the implementation team to deliver. He is a graduate engineer from Ecole Centrale d'Electronique in Paris and also obtained a Master of Science in Engineering at Aalborg Universitet, Denmark.

## Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED **TUE**

### SHAPE: Removing barriers to HPC for SMEs

PAUL JOHN GRAHAM, SHAPE Co-ordinator, and EPCC, University of Edinburgh

#### ABSTRACT

SHAPE (SME HPC Adoption Programme in Europe) is a pan-European initiative supported by the PRACE (Partnership for Advanced Computing in Europe) project. It can be challenging for SMEs to adopt HPC. They may have no in-house expertise, no access to hardware, or be unable to commit resources to a potentially risky endeavour. This is where SHAPE comes in, by making it easier for SMEs to make use of high-performance computing in their business - be it to improve product quality, reduce time to delivery or provide innovative new services to their customers. Successful applicants to the SHAPE programme get effort from a PRACE HPC expert and access to machine time at a PRACE centre. In collaboration with the SME, the PRACE partner helps them try out their ideas for utilising HPC to enhance their business. This talk will describe the mechanism of SHAPE and present some of the success stories from the SMEs that have worked with PRACE.

#### 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.

## Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED

TUE



### SHAPE: Virtual Prototyping in Development Cycle of 3D Printed Cranial Orthoses

**AUTHOR:** MGA. ALEŠ GRYGAR (left), Co-Founder, Chief designer, Invent Medical**PRESENTER:** TOMÁŠ KARÁSEK, Head of parallel algorithms research lab

IT4Innovations, VŠB – Technical University of Ostrava, Ostrava, Czech Republic

#### ABSTRACT

Orthoses are custom-designed external devices used to control the effect of an actual or developing deformity. The cranial orthoses are devices used to correct the plagiocephaly, brachycephaly, and scaphocephaly condition in children aged 4 to 18 months old. The orthosis is designed for the individual head shape of the child based on non-invasive scanning. The supporting system of the 3D printed orthosis consists of plastic shells coupled with a locking mechanism. The stiffness of inner shell must be determined based on medical advice. Currently stiffness of new design of the inner shell is established by physical experiment. The aim of this work supported by PRACE SHAPE program was to create a virtual prototyping tool to determine the stiffness of supporting structure during a designing process to guarantee its required properties i.e. flexibility. The work in this project was divided into two stages. The first stage was devoted to laboratory testing of one selected structure. The experiment results were used to verify a strongly nonlinear computer model that correctly describes the real structure during physical testing. The obtained knowledge was used in the second stage for idealization of the model and automatization of the whole process. During second stage, numerical simulation on three variants of structures were performed to test developed workflow. In this presentation, the whole toolchain together with the simulation results and their validation by physical experiment will be presented.



## Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED

TUE



### SHAPE: Optimising 2D Simulations For Faster, Better Steam Turbine Design

NICOLAS TONELLO, Renuda, United Kingdom

#### ABSTRACT

As part of a SHAPE project, Renuda UK Ltd and EPCC, the HPC centre at the University of Edinburgh, collaborated to improve the performance of Renuda's industrial and power generation steam turbine modelling code, referenced as CodeX for this project. The code was first investigated to identify areas for improvement and to identify the most suitable optimisation approach to take. CodeX was then refactored and restructured to allow for the parallelisation of the code, but also to make improvements in the serial performance. Lastly, the code was parallelised using OpenMP directives, ensuring portability across platforms. Benchmarks performed during the project indicate that for runs of typical operational models, the optimised serial code is over twice as fast as the original. For parallel runs this enhancement is reflected further, with a headline figure of over 27x faster than the original code on 16 cores. The end result of this process is an optimised, parallelised version of CodeX, which can be used to perform simulations in a significantly shorter timescale, thus enabling Renuda to offer enhanced services to their customers. The presentation will outline the work performed during the project, including the technical approach, code analysis and final results.

#### NICOLAS TONELLO

Following a PhD Aerospace Engineering at The University of Michigan, Ann Arbor, MI, USA, specialising in detonations and supersonic reactive flow, Dr Tonello worked in the USA for several years developing multiphase, reactive flow CFD software for aerospace applications. After moving to the UK to take up a position leading the implementation of two-phase flow Eulerian modelling and radiation for a leading CFD software provider, Dr Tonello founded Renuda in the UK and is now director of Renuda in the UK and France, which specialises in developing software applications and conducting fluid flow and thermal studies. Dr Tonello has 20+ years' experience in CFD and fluid mechanics applied to a large variety of industrial problems and flow regimes, from nuclear to the process industry, with a keen interest and expertise in High Performance Computing (HPC).

# Industrial Track

TIME: 14:30 - 16:30  
ROOM: RED

TUE



## On Flexibility of HPC

**DANIEL VLADUŠIČ**, Chief Research Officer, XLAB Research, XLAB

### ABSTRACT

High Performance Computing today is still rather inflexible. Batch oriented job management, the absence of APIs for self-service and strict requirements from the HPC provider regarding the software environment on the physical nodes, present a big hurdle for the average IT user or even developer. On the other hand, with the advent of distributed computing (cloud, fog concepts) and its dependence on artificial intelligence (or at least analytics), HPC could be utilised better. After all, HPC providers offer GDPR-compliant and highly secure EU-based compute facilities. Looking at the overall EU picture, where more than 99% of enterprises are SMEs, HPC providers could indeed collect a significant number of businesses, which are dependent on flexible and safe data and number crunching. Some of the models for this already exist (e.g. UberCloud, Fortissimo Marketplace and NERSC Shifter), however they are not enough - they still follow the traditional models heavily. On the other hand, big public infrastructure providers are enabling HPC (e.g. Azure with Cray offering) - the window of opportunity for the independent HPC providers is thus closing. HPC, if it counts on diversification of clientele, must simplify and automate access to its resources.

### DANIEL VLADUŠIČ

Dr. Daniel Vladušič received his PhD in computer science from the University of Ljubljana in 2005, in the field of artificial intelligence. His professional path includes a combination of research and business, as from academia, he moved to a research intensive SME - XLAB. He applied his research and know-how in the field of artificial intelligence to distributed systems and worked also as a technical advisor, developer and evaluator in several FP6, FP7 and H2020 projects (MOSAICA, Odyssey, XtremOS, Giraff+, FORTISSIMO, FORTISSIMO2) as well as on the level of national projects (DEDI, DEDI II). He was the coordinator of H2020 ICT-07-2014: Advanced Cloud Infrastructures and Services project - MIKELANGELO. His current position is Chief Research Officer at XLAB.

16:30 - 17:00 Coffee Break

## Industrial Track

TIME: 17:00 - 18:00  
ROOM: RED **TUE**

### CFD Software Verification on an Electric Airplane Utilizing HPC

**MATEJ ANDREJAŠIČ**, Head of Aerodynamics Department  
Pipistrel Vertical Solutions d.o.o., Slovenia

#### ABSTRACT

Software verification is one of the most important aspects of the engineering work. Before using any kind of software for the design purposes, it needs to be verified against established numerical benchmarks or even better, against experimental measurements. The same goes for the computational fluid dynamics (CFD) simulations, where calculations with different software (on the high level) and different parameter set-ups, numerical schemes, turbulence models, etc. (on the low level) can converge to different solutions. In this presentation a verification of different software against experimental measurements of Pipistrel's Alpha Electro airplane will be shown. Since the aerodynamic characteristics of the complete airplane were under comparison, HPC had to be utilized in order to run CFD simulations. A flight test campaign was carried out in order to obtain the polar curve of a clean airplane without the influence of a propeller.

#### MATEJ ANDREJAŠIČ

Matej Andrejašič finished his undergraduate studies at the Faculty of Mathematics and Physics, University of Ljubljana, Slovenia, in 2009. After the graduation he was employed at Pipistrel d.o.o. Ajdovščina as a researcher in the Research and Development department. He received his PhD degree in physics at the University of Nova Gorica, Slovenia, in 2014 with the thesis entitled "Optimization of Aerodynamic Surfaces using Pressure Based Functionals". For the past three years he has been the Head of the Aerodynamics Department, where he is responsible for aerodynamic studies and CFD simulations done for internal and external projects, as well as for European research projects.

## Industrial Track

TIME: 17:00 - 18:00  
ROOM: RED **TUE**

### Enabling HPC-Cloud Services from the Research Environment to the Industrial Context

STEFANO COZZINI, eXactLab, Seville, Spain

#### ABSTRACT

In this short presentation I will discuss the many challenges and some success stories in our restless effort, as an SME, to promote HPC/Cloud services toward the industrial market. Our company, founded as a research spin-off is now evolving and is competing in the growing HPC industrial market with a blend of technical/scientific competences associated with appropriate customer care. I will report on this evolution discussing the lessons learned so far and open issues in front of us.

#### STEFANO COZZINI

Dr Stefano Cozzini is a development scientist at CNR-IOM Trieste with over 20 years experience in the area of scientific computing and HPC computational e-infrastructures. At the end of 2011, he cofounded a spin-off company of the CNR/IOM institute eXact lab srl which has been steadily growing since then. The company provides advanced computation services by means of its own HPC/CLOUD infrastructure, ranging from raw computational times to complex highly customised solutions. Among its clients are primary industries of the Northern Eastern part of Italy. Stefano is passionate about HPC education; he has organised more than 20 HPC training events all around the world and he is presently actively involved in the Master in High Performance Computing promoted by SISSA and ICTP ([www.mhpc.it](http://www.mhpc.it)) and in the recently launched master degree on *Data Science and Scientific Computing* at University of Trieste.



### Helping SMEs With HPC

TOMISLAV ŠUBIĆ, CEO, Yotta Advanced Computing, Croatia

#### ABSTRACT

Large worldwide and European enterprises from different sectors are successfully embracing high performance computing. They have gained competitive advantages, created innovative products and solutions using HPC technology. There are a variety of areas, where HPC can bring many benefits: ranging from foundries, manufacturers of plastic products, design studios to financial services companies. But large companies have the means to invest in infrastructure and research and development in HPC. Small and medium enterprises often do not have the necessary resources to step into high performance computing and to make use of it. Not only do they lack infrastructure and knowledge, but many of them are also not aware of the opportunities it offers. Even if they are familiar with it, they are not comfortable with "sharing" their data and intellectual property with big cloud providers. We will talk about how we recognised a business opportunity in offering HPC services and cloud or bare-metal infrastructure to SMEs, what their concerns and problems are, and how they want to use HPC in their business.

# Industrial Track

TIME: 17:00 - 18:00  
ROOM: RED **TUE**

## **TOMISLAV ŠUBIĆ**

Tomislav Šubić is the CEO of Yotta Advanced Computing, a young Croatian start-up that helps businesses improve their products and services using HPC. He worked on several EU projects like NextGenIO, Fortissimo and SESAMENet. He holds a Master's degree in Informatics from the Department of Informatics at the University of Rijeka. During his studies he worked as a teaching assistant at the BioSFLab University of Rijeka where he did his own research, but also provided technical support for other researchers. His interests include distributed systems, GPGPU, cloud and high performance computing.



## **Performance Optimization on High Performance Computers**

**GUANGMING TAN, Professor, Institute of Computing Technology, Chinese Academy of Sciences**

### **ABSTRACT**

This talk will introduce some recent work on both developing HPC systems and performance optimization at the Institute of Computing Technology, Chinese Academy of Sciences. Three important performance tuning issues are summarized and the corresponding solutions are presented. The key idea is an architecture-driven optimization methodology for HPC applications.

### **GUANGMING TAN**

Guangming Tan is the Professor at the Institute of Computing Technology, Chinese Academy of Sciences. His research interests includes parallel programming and algorithms, domain-specific architecture and bioinformatics. He has published more than 50 papers in top conference/journals like SC, PLDI and TPDS. He is serving as Associate Editor of IEEE Transactions on Parallel Distributed Systems.

# CFD & Engineering

TIME: 14:30 - 16:30  
ROOM: GOLD **TUE**



## Chair

**LAURA GRIGORI, Senior Researcher, Inria, Paris**

In INRIA in France, Laura leads the Alpines group, a joint group between INRIA and J.L. Lions Laboratory, Sorbonne University, Paris. Her field of expertise is in numerical linear algebra and high performance scientific computing. She co-authored 2008 papers introducing communication avoiding algorithms that minimize communication, for which she was awarded with her co-authors the SIAM Siag on Supercomputing Best Paper Prize 2016 for the most outstanding paper published in 2012-2015 in a journal in the field of high performance computing. She leads several projects on preconditioning, communication avoiding algorithms and associated numerical libraries for large scale parallel/multicore machines. She was the co-chair of the Algorithms Area, Supercomputing 2013 conference and the Program Director of the SIAM special interest group on supercomputing, 2014-2015, then the Chair of this interest group, 2016-2017. She has been a member of PRACE Scientific Steering Committee since 2016 and a member of SIAM Council since January 2018.



## A Hybrid Monte Carlo Algorithm for Sampling Extreme Events in Turbulence and Stochastic Models

**GEORGIOS MARGAZOGLU, University of Rome, Tor Vergata,  
Department of Physics, Italy & Cyprus Institute, Cyprus**

### ABSTRACT

Extreme and rare events are a defining feature of turbulence but present a severe challenge to standard computational approaches that struggle to systematically sample these events. Here, we present a Monte Carlo importance sampling method that is capable of selectively exploring those remote areas of phase space associated with extreme and rare events. We propose a novel computational approach, based on the path integral formulation of stochastic dynamics, and employ an accelerated Hybrid Monte Carlo (HMC) algorithm for this purpose. As a proof of concept, we investigate the one-dimensional Burgers' equation subject to random noise that is white-in-time and power-law correlated in Fourier space and benchmark our results with standard CFD methods. Furthermore, we present first examples of constrained sampling around saddle-point instanton field configurations (optimal fluctuations) that describe the tails of the probability distribution functions of velocity differences and gradients.

### GEORGIOS MARGAZOGLU

Georgios completed his BSc Degree in Physics at the National and Kapodistrian University of Athens in 2014. In 2015 he completed a MSc Degree in Physics at the University of Rome, "Tor Vergata". He then progressed to complete a PhD in Physics, with the project: HPC-LEAP European Joint Doctorate University of Rome, "Tor Vergata" & Cyprus Institute. The topic of the thesis was "Hybrid Monte Carlo (HMC) approach for stochastic hydrodynamical systems". His thesis supervisors were Luca Biferale and Constantia Alexandrou.

# CFD & Engineering

TIME: 14:30 - 16:30  
ROOM: GOLD **TUE**

## Numerical Simulations of Multiphase Flows in Injection Systems and Generic Nozzles

**THERESA TRUMMLER**, Technical University of Munich, Department of Mechanical Engineering, Chair of Aerodynamics and Fluid Mechanics, Germany

### ABSTRACT

In pressure atomizers a liquid is highly accelerated before it is discharged. The acceleration results in a local decrease of the static pressure even below vapor pressure which leads to partial evaporation (cavitation) of the fluid. Liquid-embedded vapor structures are subsequently advected into regions of higher pressure where they collapse and emit intense shock waves with post-shock pressures of more than 10,000 bar. These collapse events can cause severe damage of the injector which is called 'cavitation induced erosion'. On the other hand, the collapse-induced turbulence can enhance the spray break up, which is a desired effect. In order to numerically investigate the effects of cavitation we employ a density based finite volume method that takes into account full compressibility of all phases to capture the shock wave after the collapse. For the numerical model an implicit large eddy approach is utilized, where the truncation error of the discretization scheme serves as a physically consistent subgrid-scale model for turbulence. Compressible Large Eddy Simulations of realistic geometries are challenging because of the required high spatial and temporal resolutions and without HPC our research projects would not be feasible.

### THERESA TRUMMLER

Theresa is a Research assistant and PhD candidate at the Institute of Aerodynamics and Fluid Mechanics, Technical University Munich since August 2015. Her Research fields are Numerical modelling of cavitating multiphase flows, gas modelling and gas effects in cavitating flows and Numerical Prediction of cavitation erosion. She is also part of the code-developing team of CATUM (CAvitation Technical University Munich). CATUM is a density based, compressible flow solver utilizing the volume of fluid method. For the large-scale simulations, the in-house code is MPI-parallelized and performance optimized. Theresa has obtained some High Performance Computing (HPC) experience on the Supercomputer SuperMUC from the Leibniz Rechen Zentrum under various projects. Theresa completed her Masters at TU Munich in Mechanical Engineering with major subjects in numerical methods and thermo-fluid-dynamics. Her Master's Thesis title was "Gasmodelling in Cavitating Flows".

# CFD & Engineering

TIME: 14:30 - 16:30  
ROOM: GOLD **TUE**

## Using high Order DGM for Generating DNS and LES Databases in Complex Geometry

KOEN HILLEWAERT, Centre de Recherche en Aeronautique (Cenaero), Belgium

### ABSTRACT

In industry, it is commonly accepted that if statistically averaged turbulence modeling (RANS) can predict turbomachinery performance reliably near the design optimum, it usually fails at off-design. Moreover, current design trends lead to complex blade designs and increased loading, further reducing the reliability of RANS. Industry therefore invests continuously in the improvement of these models, as well as in the development of more advanced methods capable of directly resolving turbulent flow features in full scale machines, using Large Eddy Simulation. A stumbling block for turbulence model development is the limited availability of high quality reference data on industrially relevant flows. Whereas numerical databases are regularly generated on simple configurations, for complex configurations often only experimental data are available. Such data sets are not very detailed and often difficult to reproduce numerically. The continuous increase in computational resources enables the generation of data bases on industrially relevant geometries with growing complexity. Such benchmarks should remain as close as possible to the actual configuration, but may deviate in order allow a reproducible numerical specification. The talk discusses practical aspects of two dedicated PRACE projects, namely R2Wall (airfoil NACA4412 near stall,  $Re=1.6$  million) and FullStuP (full span LP turbine cascade MTU T161,  $Re=90.000$ ). Joint work with Ariane Frère and Michel Rasquin, Cenaero.

### KOEN HILLEWAERT

Graduated as a mechanical engineer from Ghent University. Koen became researcher at the von Karman Institute and developer at Numeca before joining Cenaero in 2002 to work on high order CFD methods (HOM). This lead to his PhD at the Université Catholique de Louvain and the high order multiphysics platform Argo, developed for high resolution LES of turbomachinery in collaboration with the SAFRAN group. Since 2016 he is responsible for coordinating research in numerical fluid dynamics. He is involved in many initiatives surrounding high resolution CFD, including European projects Adigma, IDIHOM and Tilda, the International Workshop on High Order CFD Methods, the CGNS standard and the ERCOFTAC community. He is PI of several PRACE projects applying HOM for DNS and LES on industrially relevant geometries, with current allocations generating reference data for improving industrial RANS methods, whereas a recent INCITE project targets LES of a multistage compressor together with Safran.



# CFD & Engineering

TIME: 14:30 - 16:30  
ROOM: GOLD **TUE**

## HPC for the Simulation of Turbulent Combustion in Aeronautical Engines

VINCENT MOUREAU, CORIA CNRS-UMR6614,  
Normandie Université, INSA et Université de Rouen, France

### ABSTRACT

Despite the strong increase in computational power, modern super-computers are more and more difficult to exploit. First, massively parallel computers now feature hundreds of thousand cores, which require CFD codes with excellent, strong and weak scaling. Second, the largest super-computers rely on very different architectures and processors: Many Integrated Cores (MIC) and Graphics Processing Units (GPU) are both well represented along with more traditional processing units. The porting and optimization of CFD codes on these new platforms has become challenging and depends on choosing the most suitable numerical methods for exascale. The talk will describe some recent work, where modern supercomputing architectures have been used to address complex and unsteady CFD problems in the aeronautical industry. The talk will also highlight how these modern computing platforms and their massive parallelism can be exploited. Lessons learned from the development of high-performance CFD solvers will be outlined and the envisioned roadblocks for the next generation of CFD solvers will be discussed.

### VINCENT MOUREAU

Vincent Moureau is a CNRS researcher at CORIA in the combustion modeling group. He received his Master of Science from Ecole Centrale Paris in 2001 and obtained his PhD from Institut Français du Pétrole and Ecole Centrale Paris in 2004. After a two-year postdoctoral fellowship at Stanford University in the Center for Turbulence Research, he joined Turbomeca, SAFRAN group, as a combustion engineer from 2006 to 2008. Since 2009, his research focuses on turbulent combustion and spray modeling. He also works on the development of the YALES2 solver for Large-Eddy Simulation and Direct Numerical Simulation of turbulent flows in complex geometries using massively parallel computers. He received the Yves Chauvin award for his PhD thesis in 2005, the 3rd prize of the Bull Joseph Fourier award for the promotion of numerical simulation in 2010 and an IBM faculty award in 2011. He is the coordinator of the Scientific Group SUCCESS which is devoted to the promotion of super-computing for the CFD of complex flows in realistic geometries.

# Materials & Chemistry

TIME: 14:30 - 15:30  
ROOM: VIOLET **TUE**



## Chair

**CLAUDIA FILIPPI, MESA+ Institute for Nanotechnology,  
University of Twente, The Netherlands**

Claudia Filippi is professor in Computational Chemical Physics at the University of Twente in the Netherlands. She completed her undergraduate studies in Physics at the University of Trento, Italy, in 1991, and obtained her PhD at Cornell University, USA, in 1996. After a postdoc at the University of Illinois at Urbana-Champaign, USA, she was a lecturer in Physics at University College Cork, Ireland, from 1998 to 2001. She then moved to the Netherlands as assistant professor at the University of Leiden and, since 2008, is professor at the University of Twente. Her research is in the field of electronic structure and multiscale simulations and, currently, focuses on the methodological development of novel and more effective approaches for investigating light-induced phenomena in complex (bio)molecular systems.



## Construction and Relaxation of Metallic Heterointerfaces Including Point Defects For DFT Simulations

**ROBERTO IGLESIAS, University of Oviedo, Department of Physics, Spain**

### ABSTRACT

Metallic multilayers with nano-sized interlayer spacings have been proposed to be part of the first wall in future nuclear fusion reactors and technological applications where highly resistant materials are needed. A high concentration of interfaces promises high resistance to radiation damage accumulation. Non-coherent interfaces are intrinsically difficult to examine via DFT because of the large unit cells required. The construction of non-coherent interfaces built from fcc/bcc metals combinations, i.e., Cu/Nb, Cu/W and W/W in different orientations, starting from bulk systems will be shown. The interfaces have been relaxed to optimize the interlayer separation distances. Subsequently, monovacancies and He impurities have been introduced. A detailed energetic and mobility analysis has been performed. Both types of defects tend to move close to the interface and form a helium-vacancy complex. A site immediately adjacent to the interface seems to be preferred. Our results show a strong dependence of defect behaviour with the relative orientation of the metallic surfaces forming the interface.

# Materials & Chemistry

TIME: 14:30 - 15:30  
ROOM: VIOLET **TUE**

## ROBERTO IGLESIAS

Roberto Iglesias is an associate professor at the Department of Physics of the University of Oviedo, Spain. He is specialized in structural, diffusive and magnetic properties simulation of critical raw materials (CRM) and alloys subject to extreme conditions, through electronic structure calculations using ab initio and atomistic codes. He is co-author of more than 30 peer-reviewed articles, 55 conference communications and presentations. He is PI of a FP7 project, has participated in about 15 other projects and 8 supercomputational projects at national and international research facilities. He is the organiser of an international workshop and reviewer of 4 international journals. Awarded a PhD dissertation extraordinary prize in Physics at the University of Oviedo, he was also a member of several scientific societies: SSDN, SETN, AUSE, CEMAG, and the Nuclear Fusion Institute (IFN-UPM). Three positive research activity evaluations, granted by the Spanish National Research Activity Evaluation Commission. He is the PhD thesis supervisor of a student and of five Dipl. Eng. and one B. Sc. Theses.



## Molecular Design of Bio-Based Polyurethanes

**BELA FISER, Institute of Chemistry, University of Miskolc, Hungary**

### ABSTRACT

Polyurethanes (PUs), as the sixth most widespread group of polymers, has reached ~18Mt in global market. PUs are made by reacting di- or oligo-isocyanates with polyols to form various versatile materials (e.g. heat insulators). The complicated and expensive recycling of PUs initiated the design of natural-polyol based materials that can be sustainable for production. The potential application of different bio-polyols (glucose etc.) in polyurethane synthesis was explored using computational tools. The reactivity of the studied sugars was compared by computing all the possible reaction pathways. All in all, more than 500 quantum chemical calculations were performed using a local HPC cluster (University of Miskolc) and additional resources from the NIIF HPC (Hungary). Based on our results, the most promising molecules were selected, and novel fully carbohydrate-based polyurethanes were synthesized. The designed bio-based PUs have the potential for future industrial use as eco-friendly polymers and thus replace the conventional polyurethanes in some applications. The research was conducted in collaboration with our industrial partner, BorsodChem Zrt. It was supported by the European Union and the Hungarian State, co-financed by the European Regional Development Fund in the framework of the GINOP-2.3.4-15-2016-00004 project, aimed to promote the cooperation between the higher education and industry.

## Materials & Chemistry

TIME: 14:30 - 15:30  
ROOM: VIOLET **TUE**

### **BELA FISER**

Is a research fellow at the University of Miskolc (Hungary) and lecturer at the Ferenc Rákóczi II. Transcarpathian Hungarian Institute (Ukraine). He works on various projects including molecular design of new materials, computational study of antioxidants and modeling of homogeneous catalytic processes. He was a Marie Curie Early Stage Researcher at the University of the Basque Country, Spain (2013-2016) where he received his first PhD in Synthetic and Industrial Chemistry under the supervision of Prof. Enrique Gómez Bengoa. He received his second PhD in Materials Science and Technology under the supervision of Prof. Béla Viskolcz at the University of Miskolc in 2017. He is a member of the Marie Curie Alumni Association and secretary of the Hungarian Chapter. His scientific activity includes: 2 dissertations, 3 book chapters, >33 articles, presenting author of 25 oral presentations & 18 posters, co-author of 11 oral presentations & 61 posters. Domain: Chemistry, Computational Chemistry.

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# Life Sciences & Chemistry

TIME: 15:30 - 16:30  
ROOM: VIOLET **TUE**

## Chair

**CLAUDIA FILIPPI**, MESA+ Institute for Nanotechnology,  
University of Twente, The Netherlands

Please read CV on page 34.



## A Massively Parallelized, Systematic Method for Efficient Prediction of Multiple Drug Binding

**CSABA HETENYI**, University of Pécs, Department of Pharmacology  
and Pharmacotherapy, Hungary

### ABSTRACT

Multiple (allosteric or prerequisite) binding of drugs is often involved in their mechanism of action affecting e.g. signal transduction in various forms of cancer. While experimental structure determination methods cannot identify multiple drug binding in many cases, cheminformatics offers an alternative solution for this problem. Here, we feature recent developments of our method Wrap 'n' Shake ([www.wnsdock.xyz](http://www.wnsdock.xyz)) for the detection of multiple drug binding sites and modes. The method combines the advantages of a systematic, fast, computational blind docking search and molecular dynamics calculations with explicit water model. Beyond internal parallelization of molecular dynamics, the updated version of the method involves additional parallelisation for the sets of drug-target complexes producing fast and systematic solutions. While molecular dynamics is often considered as a time consuming step of structural calculations, the massive parallelization of Wrap 'n' Shake allows the use of its benefits rather than its limitations. For example, with explicit water model and full flexibility, targets of large conformational changes can be handled and precise binding modes of even bulky, and highly hydrated peptide ligands can be calculated. We expect that Wrap 'n' Shake will become a routine tool for drug developers and molecular biologists in academia and industry, as well.

### CSABA HETENYI

Csaba Hetényi is a Qualified Chemist, a PhD, and a Doctor Habilitatus in Pharmacy. He has co-authored research articles in prestigious journals J Am Chem Soc, PNAS, EMBO Reports, Bioinformatics, and is also a co-inventor of US patents. Dr. Hetényi has received more than 1600 independent citations for his research results, has a Hirsch-index of 19 and his works were favorably evaluated by several review articles and research papers. In 2011, Dr Hetényi won a Talentum Academy Award for his research achievements. His present research interest is focused on the development and application of pharmacoinformatics tools and investigation of molecular pathomechanisms of diseases. Dr Hetényi presently works with a group of three PhD students and four undergraduate researchers. He has successful collaborations with researchers in Sweden, Estonia, Spain, and the USA. Recent results of his research group can be found at [www.mobywat.com](http://www.mobywat.com) and [www.wnsdock.xyz](http://www.wnsdock.xyz)

# Life Sciences & Chemistry

TIME: 15:30 - 16:30  
ROOM: VIOLET **TUE**

## Modelling the Mechano-Chemical Interactions of Fluid Membranes

**DANIEL SANTOS-OLIVÁN**, Polytechnic University of Catalonia  
Universitat Politècnica de Catalunya, LaCàN, Spain

### ABSTRACT

Fluid surfaces are ubiquitous in cell and tissue biology. For instance, lipid bilayers constitute the main separation structure of cells, such as the plasma membrane and of organelles. At tissue level, epithelial monolayers can also be seen as fluid surfaces. Apart from their biological interest, these are fascinating systems from a mechanical point of view: they behave as fluid in-plane, while they exhibit a solid behavior out-of-plane. This mechanical duality provides structural stability and adaptability, allowing fluid surfaces to build relatively stable structures that can nevertheless undergo dynamic shape transformations, such as those required in vesicular trafficking, cell motility and migration, mechano-adaptation to stretch and protein diffusion. We model these different fluid surfaces following Onsager's variational principle, which brings together all the mechano-chemical interactions in these biological systems in a non-linear and thermodynamically consistent way. We solve numerically the resulting equations by means of finite element simulations. For that, we have developed HiPerLiFE, a High Performance Library for Finite Elements that can be applied to general fluid surfaces. This code is designed to manage complex unstructured grids, which deal with the complex geometries required to model fluid surfaces, in systems with distributed memory with MPI being able to handle the multiphysics nature of the fluid surfaces described above.

### DANIEL SANTOS-OLIVÁN

Daniel Santos-Oliván works as a post-doc researcher at LaCàN in the Polytechnic University of Catalonia. After completing his undergraduate studies at the University of Zaragoza, he moved to Barcelona where he completed a Master in Astrophysics and Particle Physics. In 2017, he received his PhD in Physics from the University of Barcelona (UB) and the Institute of Space Sciences (IEEC-CSIC). During this period, he studied the numerical evolution of scalar fields in curved spacetimes focusing on the critical collapse in Anti-de Sitter and in the AdS/CFT correspondence using Pseudo-Spectral Methods for achieving the resolution needed for collapsing geometries. Currently, he studies the modeling of fluid surfaces at biological systems using incorporating HPC methods to their numerical computations.

# Plasma & Energy

TIME: 14:30 - 15:30  
ROOM: SEMINAR 1 **TUE**

## Chair

**MARINA BECOULET, Senior Research Physicist in French Atomic Energy Commission, Institute of Magnetic Fusion Research**

Marina is presently employed as a Senior Research Physicist in the French Atomic Energy Commission, Direction of Fundamental Science, Institute of Magnetic Fusion Research, Activity: Theory, experiment, modeling in tokamak plasmas, non-linear MHD

Titles: Research Director of CEA, International expert of CEA

Diploma: "Habilitation à diriger des recherches" (HDR) in Science of Maters University Aix-Marseille1-2009; PhD in Physics and Mathematics of the Institute of Applied Mathematics, Russian Academy of Science in Moscow (1985). Graduate from Moscow State University, Physics Department, Plasma Physics Division (1981)

Work: 1981-1993. Institute of Applied Mathematics, Russian Academy of Science, Moscow, Russia. 1991-1992. JET, Joint European Torus, UK. CEA/DRFC, St Paul-lez-Durance, France-1993. 1998- present time. Senior Research Physicist, CEA/DRF/IRFM/SPPF, France.

Publications: H-factor: 40 (<http://apps.webofknowledge.com>).



## High Performance Computing of Non-linear MHD Simulations for Fusion Plasmas

**SHIMPEI FUTATANI, Senior Research Fellow, Physics Department, Universitat Politècnica de Catalunya (UPC), Barcelona, Spain**

### ABSTRACT

This work is dedicated to the nuclear fusion physics research in close collaboration with existing experimental fusion devices and the ITER organisation which is a huge international nuclear fusion R&D project. The goal of the ITER project is to demonstrate a clean and safe energy production by nuclear fusion which is the reaction that powers the sun. Fusion energy production requires magnetically confined plasmas keeping the high pressure. 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 damage the fusion device. 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. This 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.

# Plasma & Energy

TIME: 14:30 - 15:30  
ROOM: SEMINAR 1 **TUE**

## SHIMPEI FUTATANI

Shimpei Futatani completed his PhD at Kyoto University, Japan in 2008. He received 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. 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 2014, he was appointed as a senior researcher at Barcelona Supercomputing Center. Since 2018, he works at Physics Department of Technical University of Catalonia (UPC: Universitat Politècnica de Catalunya). He was awarded a Ramon y Cajal grant (2015-2020) which is a highly competitive research funding programme from the Spanish Ministry of Economy and Competitiveness. For the HPC research, he was awarded computing time on Marconi, RES (Spanish Supercomputing Network) and PRACE project resources as the Principal Investigator.



## Optimization of Plasma Confinement Through Supercomputation: Towards Clean and Efficient Energy Sources

**JERONIMO GARCIA, Alternative Energies and Atomic Energy Commission (CEA), Department of Physics, France**

### ABSTRACT

The search of alternative energy sources able to alleviate the dependence on fossil fuels is a priority of modern societies. The generation of energy by means of fusion reactions could be one of these alternatives. The international megaproject ITER, presently under construction in south of France, aims to demonstrate the scientific and technological feasibility of fusion energy. One of the main uncertainties in ITER is the impact of different isotopes of hydrogen on the thermal energy confinement time. For more than thirty years, these phenomena have not been explained, leading to the so-called isotope effect. In the framework of the PRACE supported project ZONALGENE the role of large fluctuation scales has been analysed. We have used the GENE code to solve the gyrokinetic equation, i.e. the Vlasov equation, for plasmas reduced from 6-D to 5-D by means of a gyro-averaging method. Our massive parallel simulations performed on MareNostrum show that the isotope effect can be understood as a complex nonlinear multiscale interaction involving a variety of physical mechanisms. Our results have strong consequences for future devices as ITER which will work with a Deuterium and Tritium isotope fuel mixture and will therefore likely benefit from improved thermal energy confinement.



# Plasma & Energy

TIME: 14:30 - 15:30 **TUE**  
ROOM: SEMINAR 1

## **JERONIMO GARCIA**

Jeronimo Garcia is a senior researcher with strong physics, computational physics and management skills with experience in a wide range of areas, including innovative plasma ideas, experimental plasma physics, and gyrokinetic theory. Currently working at the "French Alternative Energies and Atomic Energy Commission" he obtained his Ph.D. in plasma physics by the Technical University of Catalonia (UPC), Barcelona, Spain in 2006. Since then, he has published more than 70 papers with a broad variety of topics, including equilibrium and far from equilibrium thermodynamics, computational plasma physics and kinetic theory applied to plasmas. Recently, HPC has become one of his main interests leading to being awarded computational resources for the PRACE supported ZONALGENE.

# Astro & Particle

TIME: 15:30 - 16:30  
ROOM: SEMINAR 1 **TUE**

## Chair

**IGNACIO PAGONABARRAGA, CECAM Director, CECAM, EPFL**

Director of CECAM, since 2011 he is Full Professor in Condensed Matter Physics at the University of Barcelona. He has developed and exploited mesoscopic computational methods to model the dynamics of soft matter and complex fluids. Recently, he has also extended his interests to study the behaviour of biological systems at molecular and cellular scale. He has attracted funding from the Catalan and Spanish Governments, and from the European Union, as well as from industrial companies and private foundations. He has been involved in 54 scientific projects competitively funded, as Principal Investigator. He is member of the External Council Board of the School of Mathematics and Physics of the University of Lincoln (UK). He has published 160 papers in peer reviewed international journal.



## Multi-scale Reionization: The Physics of the First Billion Years of the Universe

**ILIAN ILIEV, Reader in Astronomy, Dept. of Physics and Astronomy, University of Sussex**

### ABSTRACT

Over the first billion years of cosmic evolution, radiation from the first galaxies initiated the process of cosmic reionization, which eventually ionized and heated the universe. This inherently multi-scale process, mostly driven by stellar radiation from low-mass galaxies, had profound effects on the cosmic structures. The star formation inside such galaxies is strongly affected by complex radiative and hydrodynamic feedback effects. I will present the latest results from our several PRACE supported Tier-0 and Tier-1 projects in recent years. These include massively-parallel N-body, radiative transfer and radiative-hydrodynamics simulations covering the full, vast range of relevant scales (dynamic range of more than a million), using a variety of advanced numerical techniques, including Adaptive Mesh Refinement (AMR), artificial neural networks and GPU acceleration. Some of the key questions we are aiming to address are: 1) How does the radiative feedback from the First Stars affect the formation of early structures and later star formation? 2) What are the observational signatures of the first galaxies? 3) How important is the effect of local modulation of the star formation in minihaloes due to differential supersonic drift velocities between baryons and dark matter? 4) How are these feedback effects imprinted on large-scale observational features?

# Astro & Particle

TIME: 15:30 - 16:30  
ROOM: SEMINAR 1 **TUE**

## ILIAN ILIEV

Dr. 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. Dr. Iliev is the Project Leader of four Tier-0 and three Tier-1 PRACE supported 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, Co-Coordinator of the Full Numerical Simulations Focus Group within the Square Kilometre Array Epoch of Reionization project. To date he has published 97 refereed papers.



## Gravitational Waves from Early Universe Phase Transitions

DAVID WEIR, Department of Physics, University of Helsinki, Finland

### ABSTRACT

Gravitational waves have been receiving a great deal of attention as a new tool in astrophysics. In the future they may be able to tell us a lot about the early universe, too. In 2034, the European Space Agency will launch the LISA detector. LISA may be able to see gravitational waves produced when the Higgs boson 'turned on'. This might have been a violent process, emitting lots of gravitational waves from collisions of bubbles of the new Higgs phase. To make accurate predictions of what LISA might see, large simulations are required. Several length scales must be resolved, including thickness of the bubble walls, the bubble radius, and the size of the universe. Simulations must also run for a long time to see everything from the bubbles nucleating and colliding through to the turbulent aftermath. I will present the results of my PRACE project, the aim of which was to make precision predictions for the LISA mission, and discuss the role HPC in general and PRACE resources in particular have made to advancing the state of the art in this field. I will also discuss related research making use of HPC, including Monte Carlo simulations of the underlying theories.

### DAVID WEIR

David Weir is a postdoctoral researcher at the University of Helsinki. He performs large-scale simulations of the physics of the early universe, and explores the production of gravitational waves from cosmological sources. Prior to returning to the University of Helsinki he was a Marie Curie intra-European Fellow at the University of Stavanger, where he was also awarded resources in the PRACE 10th Project Access call. He is a member of the Cosmology Working Group of the space-based LISA gravitational wave mission.

16:30 - 17:00 Coffee Break

# Keynotes

## PLENARY SESSION

TIME: 18:00 - 19:30  
ROOM: RED **TUE**



### Chair

**LEON KOS, University of Ljubljana**

Dr. Leon Kos is an HPC promoter that builds digital relationships for research, teaching, and getting the job done by using many programming languages and Unix flavours. He likes embedded systems the same as big machines. Advocates open science and data provenance. His research areas at University of Ljubljana include plasma physics, fusion, CAD kernel and 3D scientific visualisation, where he frequently encounters software development requests by HPC related projects. Leon advises national HPC centre initiative, administers university cluster, organises HPC training courses in Slovenia and coordinates PRACE MOOC, Summer of HPC and serves as a EHPCSW&PRACEdays18 local organiser.

# Keynotes

## PLENARY SESSION

TIME: 18:00 - 19:30  
ROOM: RED **TUE**

### HPC as a Key Enabler for Digital R&D

**HORST WEISS, Vice-President Digitalization Advanced Materials  
& Systems Research, Data Sciences BASF SE, Germany**

#### ABSTRACT

HPC as a key enabler for digital R&D. HPC continues to advance at a remarkable rate. Sheer computing power combined with rapid advances in scientific algorithms offer the promise to reduce and target experimentation following the results of modelling and simulation. Predictive power and cost efficiency are the most crucial issues related to modeling in industrial applications. Modeling is supposed to deliver insight and provide experimentalists the information that would not be as easily available otherwise. Thus, the experimental results could be interpreted and later predicted. Expected main benefits are: Helps to find and better understand the correlation between chemical and physical properties (i.e. to bridge chemistry to application performance); Helps to save cost and time by avoiding "trial and error" type of experimentation; Builds up formalized knowledge in terms of usable models, thus avoiding to repeat mistakes; Supports screening of properties of new materials to narrow down solution space; Avoids unnecessary handling of expensive or dangerous materials; Helps with production scale up; All in all, reduces time to market. It is in fact our experience and will be highlighted, that modeling can be used to predict the properties of materials and chemicals that have not yet been developed/produced.

#### HORST WEISS

Horst Weiss received his PhD in Theoretical Chemistry (group of R. Ahlrichs, Karlsruhe) and joined BASF in May 1994. He worked as a quantum chemist with applications in catalysis, and polymer chemistry. In 2001, he started the first Molecular Modeling Group in BASF's Materials Research. The modeling portfolio comprises methods from quantum chemistry, atomistic simulations, mesoscopic models, continuum FEM methods and data driven modeling. Application areas cover a broad spectrum of BASF chemistry, from small molecules chemistry to mechanics and processing of materials. Main interest is to connect chemical details to macroscopic performance and properties to support product and process development. Since 2015, he is Vice President Materials Modeling. In October 2016, he co-founded the new "Digitalization in R&D" central department which reports directly to BASF's CTO & CEO (since May 2018) Martin Brudermüller. In this function, he is responsible for Digitalization in Materials Research and coordinator Data Sciences including HPC.

# Keynotes

## PLENARY SESSION

TIME: 18:00 - 19:30  
ROOM: RED **TUE**

### Large Scale Multiphysics and Multiscale Simulations Based on Meshless Methods

BOŽIDAR ŠARLER, Faculty of Mechanical Engineering, University of Ljubljana, Slovenia.

#### ABSTRACT

Structure of a novel meshless solution procedure for calculation of solid and fluid mechanics problems, coupled with the electromagnetic fields, is presented. The discretisation of the governing coupled set of partial differential equations is defined on a set of nodes which can be non-uniformly distributed. The domain and boundary of interest are divided into overlapping influence areas. On each of them, the fields are represented with radial basis functions collocation on a sub-set of nodes, present in the influence area. The micro-scale problems are tackled through transition rules between the nodes. All governing equations are solved in their strong form. The polygonisation is not present. The large deformation and growth problems are handled by node redistribution and activation of additional nodes. The solution procedure can be adapted in node redistribution and/or refinement sense, which is of utmost importance when coping with the fields exhibiting sharp gradients. The method is extremely simple to code and accurate, allowing straightforward parallelisation. Besides this, the inclusion of complicated physics is transparent, reducing the development time. The coding in 2D or 3D is almost identical. Applications to several large-scale industrial problems are shown, particularly in the field of thermomechanical processing of steel and aluminium alloys.

#### BOŽIDAR ŠARLER

Professor Šarler's research interest is focused on multiphysics and multiscale computational modelling and simulation of materials and processes. He received several domestic and international recognitions for development of meshless methods with radial basis functions. He has published 150 archival journal papers, numerous book chapters, and edited dozen of books with selected papers from international conferences. He has managed several international projects within COST, COPERNIKUS, EU frameworks, NATO, National Academies USA, Research Grants Council of Hong Kong, Chinese Academy of Sciences, Helmholtz Association, Germany, etc. He has organised numerous special sections on international conferences and edited special numbers of distinguished journals. He presented keynotes at conferences of the prestigious type like EUROMAT, EUROSIM (EU), THERMACOMP (UK), ICCES (USA), TMS (USA) and Asian Congress on Computational Mechanics (Singapore). His research efforts are connected with large international research centres and global industry.

19:30 - 21:00 Welcome Reception & PRACEdays18 Poster Session

# Keynotes

## PLENARY SESSION

TIME: 09:00 - 10:30  
ROOM: RED **WED**

### Chair

**SERGE BOGAERTS, Managing Director of PRACE, Chair of the EHPCSW & PRACEdays OPC**

Please read CV on page 12



## Building a World-Class National High Performance e-Infrastructure for Australian Research and Innovation

**ALLAN WILLIAMS, Associate Director (Services and Technologies),  
National Computational Infrastructure**

### ABSTRACT

This presentation will cover a little history of HPC in Australia and some of the drivers that have shaped the development of HPC nationally. In particular the impact of the National Collaborative Research Infrastructure Strategy (NCRIS) and how that has helped shape the current integrated research environments that we have built integrating cloud, data and HPC. The presentation will also highlight some of the research that has been undertaken across the country delivering national benefits as well as some collaborative projects that our centres are involved in internationally. Finally, the presentation will present the some of the future directions that we will be taking and highlight opportunities to collaborate with Europe.

### ALLAN WILLIAMS

Allan Williams has been the Associate Director responsible for Services and Technology at the National Computational Infrastructure since 2013. In this current role, he is responsible for the delivery of both high-quality and innovative integrated research infrastructure services supporting Australia's leading researchers. Prior to his start at NCI, he was Director of IT Services for the ANU responsible for University Wide Corporate and Student IT services including networking, cybersecurity and telephony. He has held a number of different roles within Universities and Industry including campus IT Security Manager, contract IT trainer, Unix administrator and Web developer. He developed one of the earliest web sites in Australia (number 800 in the world) and was involved in running a national conference on Artificial Intelligence while studying. He holds an honours science degree in Physics and Pure Mathematics and a postgraduate diploma in Computer Science.

# Keynotes

## PLENARY SESSION

TIME: 09:00 - 10:30  
ROOM: RED **WED**

### The European HPC Strategy and the EuroHPC Joint Undertaking

**THOMAS SKORDAS, Director "Digital Excellence and Science Infrastructure"  
DG Communications Networks, Content and Technology, European Commission**

#### ABSTRACT

High Performance Computing (HPC) is at the core of major advances and innovations in the global digital economy, and it is a key technology for science, industry, and society at large. Access to HPC capabilities and technologies is a vital and strategic resource for the future of EU's scientific leadership, industrial competitiveness and sovereignty. However, our efforts in HPC are not at the level of our economic and human potential. The EU does not have the most performant supercomputers and those existing depend on non-European technology. Europe needs a strong joint action in HPC to implement a true European HPC strategy and close the investment gap with our world competitors by bringing together national and European funding with complementary private support. This need has been recognised by several European countries in the EuroHPC declaration where they commit to work together and with the European Commission for jointly acquiring, deploying and operating across the EU an integrated world-class HPC and data infrastructure. The European HPC strategy will be implemented through a specific instrument: the EuroHPC Joint Undertaking (JU). The EuroHPC JU will allow the EU to co-invest with Member States to support a thriving full European HPC ecosystem capable of deploying a world-class HPC and data infrastructure with exascale capabilities by 2022/2023, securing our own independent and competitive HPC technology supply, and achieving excellence in HPC applications.

#### THOMAS SKORDAS

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. On 1st March 2017 he was appointed Director "Digital Excellence and Science Infrastructure".

10:30 - 11:00 Coffee Break



# Keynotes

## PLENARY SESSION

TIME: 11:00 - 11:45  
ROOM: RED **WED**

### Chair

**LEE MARGETTS, Senior Lecturer in Structural Integrity, University of Manchester, UK**

Please read CV on page 19



### Memory Driven Computing

**FRANZ-JOSEF PFREUNDT, Division Director at Fraunhofer****Head of the Competence Center for HPC at the Fraunhofer ITWM**

#### ABSTRACT

Simplifying distributed computing on large data volumes is a major challenge in industry and academia. Large shared memory systems are very costly and are one solution. High speed networks and byte addressable storage devices pave the way to distributed solutions with a very large memory footprint. Asynchronous RDMA programming API's allow the creation of large partitioned global address spaces and hide latency. Based on this technology, changes to modern databases and big data frameworks can create environments that simplify data access and make the life of a programmer easier. But we are not there yet. At Fraunhofer we have been working for a few years on a new purely software based solution that puts a large virtual memory space in the center of a future programming and execution environment. It manages all data transfers and completely decouples programming from coordination. The main challenge in this software system named ADIOS was the development of a generic parallel programming approach that generates all data transfers and makes efficient use of a very large virtual memory space in tuning both data movement and code movement. The talk will cover the general ideas, planned future work and use cases in ML, Big Data and parallel computing domains.

#### FRANZ-JOSEF PFREUNDT

Dr Franz-Josef Pfreundt studied Mathematics, Physics and Computer Science resulting in a Diploma in Mathematics and a PhD degree in Mathematical Physics (1986). He was cofounder of the Fraunhofer ITWM and is Division Director and Head of the "Competence Center for HPC. He has been awarded the Fraunhofer Research and the IBM Faculty award. He is PI for a variety of parallel computing research projects including the development of new parallel programming frameworks. His main research focus are parallel filesystems (BeeGFS) new parallel programming approaches (GPI) and the use of these technologies for various industrial environments. Recent activities include the development of distributed storage technologies for the renewable energy market.

# PRACE User Forum

## OPEN SESSION

TIME: 11:45 - 13:00  
ROOM: RED **WED**

### Chair

**TROELS HAUGBØLLE, Chair of the PRACE User Forum**

#### ABSTRACT

The PRACE User Forum provides a communication channel between PRACE and the researchers and users 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, and where we will present a survey of current and past users opinions. This year, the general assembly will also include a discussion of the Peer Review process with Maria-Grazia Giuffreda, Member of the PRACE Board of Directors, and a presentation from Luciano Rezzolla and Luca Marsella about the role of the PRACE access committee in the final ranking of proposals, and what they look for to identify excellent proposals.

#### TROELS HAUGBØLLE

Troels Haugbølle is a computational astrophysicist who is currently specialising in star and planet formation. After graduating at the University of Copenhagen he was a postdoctoral fellow at the University of Aarhus in Denmark and the Autonomous University in Madrid, Spain, before returning to Copenhagen, where he joined the Centre of Star and Planet formation in 2011. He is now associate professor and part of the faculty at the Niels Bohr Institute at University of Copenhagen. He has developed several large-scale codes used for understanding kinetic plasmas, the evolution of the interstellar medium, and the formation of stars and planets. He is involved in an international initiative for developing next generation exa-scale ready multi-physics, multi-scale astrophysics codes. He has been the PI of three PRACE projects, and in addition Co-I on three other projects.

# PRACE User Forum

## OPEN SESSION

TIME: 11:45 - 13:00  
ROOM: RED **WED**

### PRACE Tier-0 Review Process: Overview

**MARIA GRAZIA GIUFFREDA, Chair of the PRACE User Forum and ETH Zurich/CSCS**

#### ABSTRACT

The overarching goal of PRACE is to provide a federated European supercomputing infrastructure that is science driven and globally competitive. It builds on the strengths of European science providing high-end computing and data analysis resources. To provision a federated world-class Tier-0 supercomputing infrastructure, PRACE has put in place a strong transparent Peer Review Process exclusively based on scientific excellence, which will be presented together with Project Access.

#### MARIA GRAZIA GIUFFREDA

PhD in Computational Chemistry in Belgium followed by a post-doc at ETH Zurich in the Physical Chemistry Department. Since 2006 working at ETH Zurich – Swiss National Supercomputing Centre (CSCS) first as Application Analyst, then as Group Leader of the User Support Group. From 2013 Associate Director and head of the User Engagement and Support Unit. I am also responsible for the User Lab Program and the CSCS National and Tier-0 Calls for Proposals.

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### Historical Context of The Work of The AC and The RAS Meeting

**ERIK LINDAHL, Member of the PRACE Scientific Steering Committee**

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# PRACE User Forum

## OPEN SESSION

TIME: 11:45 - 13:00  
ROOM: RED **WED**

### PRACE Peer Review Process: How to Prepare a Good Proposal

**LUCA MARSELLA, Computational Scientist, Swiss National Supercomputing Centre, Eidgenössische Technische Hochschule Zürich (Switzerland)**

#### ABSTRACT

The PRACE Peer Review Process includes two types of assessment: technical and scientific. The two assessments are carried out separately by different groups of experts. The technical review seeks to assure that the proposal is technically feasible for the system(s) requested. The presentation will focus on the technical aspects of the proposals submitted for a PRACE Project Access on a Tier-0 system: applicants will need to access the target system(s) beforehand through a PRACE Preparatory Access, in order to collect the required scalability and performance data for their large-scale computational projects. Best practices and guidelines on how to present the required technical information in the application will be presented from the technical reviewer's point of view.

#### LUCA MARSELLA

Luca Marsella graduated in Physics at the University of Cagliari (Italy) and holds a PhD in statistical and biological physics from the International School for Advanced Studies in Trieste (Italy). He has been working in the field of computational materials science and biophysics at the University of Padua (Italy), at the Ecole Normale Supérieure in Lyon (France) and at the University of Split (Croatia). He currently works as HPC technical advisor at the Swiss National Supercomputing Centre (CSCS) in Lugano (Switzerland) within the User Engagement & Support Unit, where he is responsible for maintaining the scientific software applications portfolio and providing support to CSCS users.

**Co-presenter: LUCIANO REZZOLLA, Goethe University, Frankfurt, Germany**

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**12:45 – 13:00 Open Discussion & Questions from the Audience**

**13:00 - 14:30 Lunch Break**

# Keynotes

## PLENARY SESSION

TIME: 09:00 - 10:30  
ROOM: RED **THU**

### Chair

**SINÉAD RYAN, Trinity College Dublin, Chair of the PRACE SSC**

Sinead Ryan is Chair of Theoretical High Energy Physics at Trinity College, Dublin, Ireland. Her research focus is the numerical simulation of quantum chromodynamics, the theory of the strong nuclear force, in an approach known as lattice QCD. A particular interest of hers is understanding strong exotic matter and the physics of the early universe. Precision lattice QCD calculations require state-of-the-art HPC resources and the field has been at the forefront of hardware and software development for more than 30 years. Sinead's research has been enabled at leadership HPC resources through the US INCITE and European PRACE programmes.



### HPC as an Opportunity for Innovative SMEs

**TOMI ILIJAŠ, CEO & President, Arctur, Slovenia**

#### ABSTRACT

Arctur is Research & Development oriented SME, active in the field of ICT. Established in 1992, Arctur has progressed to become the main Slovenian commercial supplier of HPC (High Performance Computing) services and solutions. Arctur has its own HPC and Cloud Computing infrastructure to be used as the technological foundation for advanced HPC and Cloud computing solutions and innovative web services in a distributed, high-redundancy environment. The company has extensive experience in server virtualization and deployment, integration of disparate IT-systems, IT support of project-management and server farm leverage for the deployment of Software as a Service (SaaS), specialized for small and media enterprises (SME). In recent years, Arctur is active in the field of mobile solutions, interlacing them with web and Cloud platforms. The company has also entered the fast developing field of 3D printing, both in data acquisition and 3D modelling, supported with remote rendering and parallel computations in a dedicated Cloud-based ecosystem. Endeavours related to 3D technologies are often pertinent to the field of cultural heritage.

#### TOMI ILIJAŠ

Tomi Ilijaš is founder and president of Arctur and he holds a MSc degree from Ljubljana University. Mr. Ilijaš is an entrepreneur with focus on Hi-Tech innovation and has shared his knowledge and experience to many start-ups and spin-offs in the region. Recently, he is researching new business models in HPCaaS and successfully breaking the barriers in bringing HPC to manufacturing SMEs.

# Keynotes

## PLENARY SESSION

TIME: 09:00 - 10:30  
ROOM: RED

THU



### Phoretic Active Matter and Micromachines

MARISOL RIPOLL, Theoretical Soft Matter and Biophysics,  
Institute of Complex Physics, Forschungszentrum Jülich, Germany

#### ABSTRACT

Thermophoresis refers to the directed motion of colloidal particles in the presence of a temperature gradient, which can occur towards cold (thermophobicity) or warm areas (thermophilicity). Together with the colloid motion, the temperature gradient also induces a thermoosmotic flow of the surrounding solvent. This flow can eventually translate into the formation of thermophoretic crystals, or be used to generate diverse flow patterns in microfluidic environments. The thermophoretic effect can also be exploited to build micromachines, which we investigate by means of a mesoscopic simulation technique known as multiparticle collision dynamics simulations (MPC). Asymmetric microgears locally heated in a cooled surrounding solvent can be shown to rotate spontaneously and unidirectionally. Microscale turbines rotating in the presence of external fields can be constructed by assembling anisotropic blades in a chiral manner based on the so-called anisotropic thermophoretic effect, characteristic of elongated objects. These devices have potentially a huge economic impact, since they are able to transform waste heat energy into kinetic motion. Self-propelled motion due to thermophoresis can be induced for particles with asymmetric properties such as Janus or dimer colloids, which display very interesting single and collective hydrodynamic behavior such as clustering or swarming. Interestingly, most of these concepts are also valid in the case of diffusiophoresis which relies on the existence of concentration gradients, as those produced in the presence of catalytic surfaces.

#### MARISOL RIPOLL

Marisol Ripoll studied Theoretical Physics in Universidad Complutense de Madrid (Spain), and did her PhD in between UNED (Spain) and Utrecht University (The Netherlands). She went to Forschungszentrum Jülich (Germany) for a postdoctoral stay, where she was later awarded with the lead of Young Investigators Group, becoming in 2014 a senior scientific researcher. In her research, she typically uses mesoscopic simulations to understand the properties and behaviour of soft matter and biological systems such as colloids, polymers, or liquid crystals. Of special interest are hydrodynamic interactions, shear induced effects, microfluidics, phoresis, active systems, or synthetic micromachinesol.

10:30 - 11:00 Coffee Break

## Panel Session

TIME: 11:00 - 13:00  
ROOM: RED **THU**

### Chair

**SERGE BOGAERTS**, Managing Director of PRACE, Chair of EHPCSW & PRACEdays OPC

Please read CV on page 12

## CoEs and HLSTs, What Problems Can They Solve for Me?

Moderator: **JACKI DAVIS**, EDITOR/Journalist and AnalystPanellists: **LEE MARGETTS**, University of Manchester, UK and IAC Chair**SINEAD RYAN**, Trinity College Dublin, Chair of the PRACE SSC**XIAOXIANG ZHU**, Winner of the PRACE Ada Lovelace Award for HPC**PAUL GIBBON**, Forschungszentrum Juelich GmbH, Germany**ERWIN LAURE**, KTH, Sweden**LUCA MARSELLA**, CSCS, Switzerland

### Moderator

**JACKI DAVIS**, EDITOR/Journalist and Analyst

Jacki Davis is a leading commentator and analyst on European Union affairs. She is a very experienced journalist, speaker and moderator of high-level events both in Brussels and in EU national capitals. She is the editor of many publications, a regular broadcaster on television and radio news programmes and documentaries commenting on EU issues, and both a Senior Adviser and member of the Governing Board at the Brussels-based think tank, the European Policy Centre. She has been based in Brussels for 25 years, and was previously Communications Director of the European Policy Centre; launch editor and editor-in-chief of E!Sharp, a monthly magazine on EU affairs launched in 2001; the launch editor of European Voice, a Brussels-based weekly newspaper on EU affairs owned by The Economist Group, from 1995-2000 (which has now become Politico); and the Brussels correspondent of a British national newspaper.



### Panellist

**ERWIN LAURE****Director PDC, Center for High Performance Computing KTH****Royal Institute of Technology Stockholm, Sweden**

Erwin Laure is Professor for High Performance Computing and Director of the PDC - Center for High Performance Computing Center at KTH, Stockholm. He has more than 20 years experiences in High Performance Computing and is the coordinator of several leading European Exascale projects (e.g. "EpiGRAM", "ExaFLOW", and "BioExcel") and actively involved in major e-infrastructure projects (particularly PRACE and EUDAT). His research interests include programming environments, languages, compilers and runtime systems for parallel and distributed computing, with a focus on exascale computing.

## Panel Session

TIME: 11:00 - 13:00  
ROOM: RED **THU**



### Panellist

**PAUL GIBBON**, Head of Computational Science Division, Juelich Supercomputing Centre, Forschungszentrum Juelich GmbH, Germany

Paul Gibbon received the B.Sc. degree in physics from the University of Bristol, Bristol, U.K., in 1985 and a Ph.D. in plasma physics from Imperial College London, London, U.K. in 1988 under the supervision of A. R. Bell. He then held postdoctoral positions at several European institutes including Darmstadt University of Technology, Germany, CEA Saclay, and the University of Jena, Germany. Since 2001, he has been with Forschungszentrum Jülich GmbH in Germany, where he now heads the Computational Science Division of the Jülich Supercomputing Centre, and also holds a part-time appointment as Associate Professor at the Katholieke Universiteit Leuven teaching computational physics. His current research interests are centred on topical challenges in plasma physics, where he has authored over 100 peer-reviewed publications. On the European HPC stage, Dr Gibbon currently co-manages the Energy-Oriented Centre of Excellence (EoCoE) and coordinates the JSC part of the PRACE High-Level Support Team.



### Panellist

**LEE MARGETTS**  
Structural Integrity,  
University of Manchester, UK  
Chair of the PRACE IAC  
Please Read CV on page 19



### Panellist

**XIAOXIANG ZHU**,  
Winner of the PRACE  
Ada Lovelace Award for HPC  
Please Read CV on page 58



### Panellist

**SINEAD RYAN**, SSC Chair  
Trinity College, Dublin, Ireland  
Chair of the PRACE SSC  
Please Read CV on page 53



### Panellist

**LUCA MARSELLA**  
ETH Zurich/CSCS, Switzerland  
Please Read CV on page 52



# Keynotes

## PLENARY SESSION

TIME: 11:00 - 13:00  
ROOM: RED **THU**

### EUDAT: The pan European Collaborative Data Infrastructure

GIUSEPPE FIAMENI, Cineca, Italy

#### ABSTRACT

There is a growing awareness that the "rising tide of data" requires new approaches to data management and that data preservation, access and sharing should be supported in a seamless way. EUDAT's vision is data shared and preserved across borders and disciplines and its mission is to enable data stewardship within and between European research communities through the EUDAT Collaborative Data Infrastructure. EUDAT offers a common model and service infrastructure for managing data spanning all European research data centres and community data repositories. EUDAT is the largest pan-European data infrastructure and is conceived as a network of collaborating, cooperating centres, combining the richness of numerous community-specific data repositories with the permanence and persistence of some of Europe's largest scientific data and computing centres. Covering both access and deposit, from informal data sharing to long-term archiving, and addressing identification, discoverability and computability of both long-tail and big data, EUDAT services aim to address the full lifecycle of research data. The purpose of this presentation is to present the complete EUDAT services suite and the results of the collaboration activity carried on with PRACE in implementing cross-infrastructure use cases.

#### GIUSEPPE FIAMENI

Giuseppe Fiameni, leader of the HPC Services group at Cineca and member of the EUDAT CDI Executive Board. Responsible of the "Data federation and data intensive computing technology" work package of the Human Brain SGA2 project.

# PRACE Ada Lovelace Award for HPC

TIME: 12:00 - 13:00  
ROOM: RED **THU**



## Winner

**XIAOXIANG ZHU, Professor/Department Head Signal Processing in Earth Observation, Technical University of Munich/Department of EO Data Science, Remote Sensing Technology Institute at German Aerospace Center**

Xiaoxiang Zhu is the professor for Signal Processing in Earth Observation (SiPEO, [www.sipeo.bgu.tum.de](http://www.sipeo.bgu.tum.de)) at Technical University of Munich (TUM) and the German Aerospace Center (DLR), Germany. She is also the founding head of the department of EO Data Science in DLR's Earth Observation Center. Zhu received the Master (M.Sc.) degree, her doctor of engineering (Dr.-Ing.) degree and her "Habilitation" in the field of signal processing from TUM in 2008, 2011 and 2013, respectively. She was a guest scientist or visiting professor at the Italian National Research Council (CNR-IREA), Naples, Italy, Fudan University, Shanghai, China, the University of Tokyo, Tokyo, Japan and University of California, Los Angeles, United States in 2009, 2014, 2015 and 2016, respectively. Her main research interests are remote sensing and Earth observation, signal processing, machine learning and data science, with a special application focus on global urban mapping. Xiaoxiang has been a master user of LRZ and GSC since 2012, and used grants of 46 million core hours on SuperMUC of Leibniz Supercomputing Centre.

## 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)



**The following PRACE Awards will also be presented:  
Best Scientific Presentation**

## Closing of the Conference

**SERGE BOGAERTS, Chair of EHPCSW 2018 & PRACEdays18 OPC**

## Posters

NAME	POSTER TITLE	AFILIATION
<b>Oscar Antepara</b>	DNS of rising bubble with path instability	Heat and Mass Transfer Technological Center (CTTC) - Technical University of Catalonia (UPC)
<b>Jon May</b>	Numerical Solution of Elastodynamics equations using Finite Differences & Dynamic calls on GPUs'	University of L'Aquila
<b>Ruben Perez</b>	Numerical Simulation of Non-premixed swirling flames	ICAI
<b>EUDAT</b>	Coupling HPC and data services together	EUDAT
<b>Andrej Kastrin</b>	Elixir HPC Course	University Ljubljana
<b>Janez Povh</b>	High-Performance Computing in Combinatorial Optimization	University of Ljubljana, Faculty of Mechanical Engineering, Ljubljana
<b>Božidar Šarler</b>	Meshless Modelling of Materials and Processes	University of Ljubljana, Faculty of Mechanical Engineering, Ljubljana
<b>Jernej Stare</b>	Can multiscale simulation explain neuropsychiatric disorders?	National Institute of Chemistry, Ljubljana
<b>Leon Kos</b>	Parallel Power Deposition on Plasma Facing Components	Faculty of Mechanical Engineering, University of Ljubljana
<b>Vesna Ribic</b>	First-Principles Calculation of Gd-doped BiFeO <sub>3</sub>	Institute for Multidisciplinary Research, University of Belgrade







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Marjolein Oorsprong, PRACE aisbl

Stelios Erotokritou, CaSToRC

#### MEDIA PARTNERS

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#### EVENT ORGANISERS

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#### HOST

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The Implementation Phase of PRACE receives funding from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 730913. For more information, see [www.prace-ri.eu](http://www.prace-ri.eu)



**PRACE aisbl is funded by the PRACE Members**  
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