

PRACE Scientific
& Industrial
Conference 2016



HPC for Innovation: When Science Meets Industry

10–12 May 2016

Orea Hotel Pyramida, Prague, Czech Republic





Some numbers...

- 218 participants
- 6 parallel sessions
- 8 international keynotes
- Running under the European HPC Summit Week

HPC for Innovation: when Science meets Industry

PRACE Scientific and Industrial Conference

Prague, 10–12 May 2016

TUESDAY 10 MAY 2016

13:30 REGISTRATION PRACEdays16 (13:30–15:30)

15:30 WELCOME COFFEE

CINEMA HALL

Chaired by Petros Koumoutsakos, Chair of the PRACE SSC

16:00 **Welcome:** Sergi Girón, Chair of the PRACEdays16 OPC
Presentation: Leonardo Flores Añover, EC Project Officer, *High Performance Computing (HPC): a key element of the European Cloud Initiative*

16:15 **Keynote:** Hans-Thomas Janka, Max-Planck-Institute for Astrophysics, *Solving the Mysteries of Supernova Explosions by 3D-Simulations*

17:00 **Keynote:** Martin Winter, The European Chemical Industry Council, *Digital in the Chemical Industry*

17:45 **Keynote:** Sharon Brode Geva, Director of Advanced Research Computing (ARC), University of Michigan, United States
Beyond Hardware: Scaling Up the Approach to Advanced Research Computing

18:30 WELCOME RECEPTION & POSTER SESSION

WEDNESDAY 11 MAY 2016

CINEMA HALL

Chaired by Sergi Girón, Chair of the PRACEdays16 OPC

09:00 **Opening and Welcome:** Sarzio Bassini, Chair of the PRACE Council, and Vít Vondrák, IT4Innovations

09:45 **Keynote:** Max Lemke, Head of Unit for Complex Systems and Advanced Computing, European Commission
Digitising European Industry: a key role for Europe's digital competence centres

Presentation: Jean-François Lavignion, ETP4HPC, *Development of HPC technology to serve the European HPC ecosystem*

10:30 COFFEE

11:00 **Keynote:** Carme Rovira Virgili, University of Barcelona, *Computer simulation to understand how enzymes work*

11:45 **Keynote:** Christoph Gümbel, Director Virtual Vehicle, Porsche A.G., *HPC as a critical success factor for the competitiveness of the car industry*

12:30 GROUP PHOTO

12:45 LUNCH

13:30 CONGRESS HALL 1
ASTRO/PHYSICS
Scientific Parallel Session 1
Chair: Luke Drury,
Dublin Institute for Advanced Studies

Parallel Talk 1.1
Giovanni Lapenta, KU Leuven
Magnetic Nulls in Kinetic Simulations of Space Plasmas

Parallel Talk 1.2
Oriane Roos, CEA-Saclay
Cosmic Scene Investigation using HPC

Parallel Talk 1.3
Ilian Iliev, University of Sussex
Multi-scale reionization

CONGRESS HALL 2
CHEMISTRY/LIFE SCIENCES
Scientific Parallel Session 3
Chair: Erik Lindahl,
KTH Royal Institute of Technology

Parallel Talk 3.1
Åke Nordlund, Niels Bohr Institute,
University of Copenhagen
DISPATCH: A code framework for the exascale era

Parallel Talk 3.2
Adriana Pietropaolo, University of Catania
Controlling and predicting the switchable screw-sense in self-assembling polymers

Parallel Talk 3.3
Matthieu Chavent, University of Oxford
Membrane Protein Crowding: filling the gap between computations and experiments

CINEMA HALL
CZECH INDUSTRY
Industrial Parallel Session 1
Chair: Vít Vondrák, IT4Innovations

Industrial Talk 1.1
Johan Nicolai Hartnack, DHI Group
High Performance Computing in an Operational Setting

Industrial Talk 1.2
Jan Kometa, Borcad CZ s.r.o.
HPC Technologies in Product Design Cycle

Industrial Talk 1.3
Tomáš Blejchař, Orgrez a.s.
Numerical Simulation of Complex Physical Phenomena in the Power Industry

Keynotes

Keynotes

Parallel Sessions

15:30 COFFEE

Parallel Sessions

16:00 CONGRESS HALL 1
ENGINEERING
Scientific Parallel Session 2
 Chair: Petros Koumoutsakos, ETH Zürich

Parallel Talk 2.1
 Luca Biferale, University of Rome Tor Vergata
Turbulence under rotation: Eulerian and Lagrangian statistics

Parallel Talk 2.2
 Sergio Pirazzoli, University of Rome La Sapienza
Unravelling wall turbulence with supercomputers

Parallel Talk 2.3
 Marjorie Bertolus, CEA, DEN, DEC/SESC/LLOC
Investigation of nuclear fuel materials under irradiation at the atomic scale

CONGRESS HALL 2
ENVIRONMENT
Scientific Parallel Session 4
 Chair: Dimitri Komatitsch, LMA CNRS-MRS

Parallel Talk 4.1
 Thierry Penduff, CNRS / LGGE
The first ensemble of global ocean simulations: the OCCIPUT project

Parallel Talk 4.2
 Gianmaria Sannino, ENEA, SSPT-MET
How much do tides affect the simulated climate of the Mediterranean Sea?

Parallel Talk 4.3
 Jost von Hardenberg, ISAC-CNR
Climate SPHINX: High-resolution climate simulations with an improved representation of small-scale variability

CONGRESS HALL 3
EUROPEAN INDUSTRY
Industrial Parallel Session 2
 Chair: Anders Rhod Gregersen, Vestas Wind Systems A/S

Industrial Talk 2.1
 Niels Aage, Technical University of Denmark
Ultra large scale structural optimisation-topology optimized wing structure

Industrial Talk 2.2
 Mathis Bode, RWTH Aachen University
Novel simulations of fuel injection systems investigating spray characteristics by use of high-fidelity multiphase methods and supercomputers

Industrial Talk 2.3
 Denis Wouters, CybeleTech
Numerical simulations for plant breeding optimization

User Forum

18:00 CINEMA HALL
PRACE User Forum Open Session - Free for All
 Chair: Koen Hillewaert, Conaero

- Richard Tavares, PRACE aisbl: *Overview of the PRACE Peer Review Process*
- All: *User Forum General Assembly*
- Leonardo Flores Añover, Senior Expert in the E-Infrastructures Unit (DG Connect), European Commission: *HPC for e-Infrastructure Work Programme 2018-2020*
- John Chevers, Géant: *GÉANT's support for HPC*

20:00 Networking Cocktail & Dinner, U Flekú Restaurant, (19:45 buses will begin to depart to the city centre)

THURSDAY 12 MAY 2016

Keynotes

CINEMA HALL
 Chaired by Sergi Girona, Chair of the PRACEdays16 Organising and Programme Committee

Opening and Welcome: Alison Kennedy, Chair of the PRACE Board of Directors

09:00 Keynote: Omar Ghattas, University of Texas at Austin, *Extreme-scale Bayesian Inverse Problems for Non-Newtonian Geophysical Flows*

09:45 Keynote: Merle Giles, NCSA University of Illinois, *HPC from Solver to Economic Impact*

10:30 COFFEE

Panel Session

11:00 Panel Session
 Moderated by Tom Wilkie, Europa Science Ltd.
"How can we assess European competitiveness in the global HPC race?"

- Anders Rhod Gregersen, Chair of the PRACE IAC
- Petros Koumoutsakos, Chair of the PRACE SSC
- Augusto Burgueño Arjona, European Commission
- Merle Giles, NCSA University of Illinois
- PRACE Ada Lovelace Award for HPC Winner

12:00 PRACE Awards for Best Poster, Best Scientific Presentation, Best Industrial Presentation and PRACE Ada Lovelace Award for HPC

Closing of the Conference: Sergi Girona, Chair of PRACEdays16 OPC

12:30 LUNCH



- Austria
- Belgium
- China
- Croatia
- Cyprus
- Czech Republic
- Denmark
- Deutschland
- Finland
- France
- Germany
- Greece
- Hungary
- Ireland
- Italy
- Japan
- Mexico
- Netherlands
- Poland
- Portugal
- Slovakia
- Spain
- Sweden
- Switzerland
- Turkey
- United Kingdom
- United States



Housekeeping

- Registration desk at the entrance of the hotel
- WiFi connection details announced in all rooms
- Please keep your badge with you also for the Cocktail and the Dinner
- #PRACEdays16 and @PRACE_RI for social media (Twitter)

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Coffee Breaks & Lunches

- Coffee breaks between plenary sessions in the foyer of the Cinema Hall
- Coffee breaks between parallel sessions in the foyer of the Congress Halls
- Lunches in the Bohemia Restaurant, 1st floor

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Poster Session & Cocktail

- Tuesday 10 May
- Energy Restaurant and Lobby of the Orea Pyramida Hotel

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Dinner at Restaurant U Flekù

- Wednesday 11 May
- Busses will depart at 19:45, very sharp
- Busses will go back to the Orea Pyramida Hotel

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