

# EuroHPC Summit Week 2019



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## Report of Contributions

Contribution ID: 1

Type: **not specified**

# Challenges of First Principle Modelling and Role of HPC in Magnetic Fusion

*Tuesday, 14 May 2019 11:00 (45 minutes)*

Scientific Keynote

**Presenter:** BECOULET, Marina (CEA)

**Session Classification:** Plenary

Contribution ID: 2

Type: **not specified**

## **Water Resource Modelling**

*Tuesday, 14 May 2019 11:45 (45 minutes)*

Industrial keynote

**Presenter:** Prof. HAROU, Julien

**Session Classification:** Plenary

Contribution ID: 3

Type: **not specified**

## **Convergence of Big Data and HPC**

*Wednesday, 15 May 2019 08:30 (30 minutes)*

**Presenter:** KEYES, David (KAUST)

**Session Classification:** Plenary

Contribution ID: 4

Type: **not specified**

## **Workflows for continuum computing platforms (from edge to HP computing)**

*Wednesday, 15 May 2019 09:00 (30 minutes)*

**Presenter:** BADIA, Rosa M. (BSC)

**Session Classification:** Plenary

Contribution ID: 5

Type: **not specified**

## **In Memoriam - Dimitri Komatitsch**

*Thursday, 16 May 2019 08:30 (45 minutes)*

Scientific Keynote

**Presenter:** MONTEILLER, Vadim

**Session Classification:** Plenary

Contribution ID: 6

Type: **not specified**

## **Modeling and simulation issues at EDF enabling energy challenges**

*Thursday, 16 May 2019 09:15 (45 minutes)*

Industrial Keynote

**Presenter:** CARUSO, Ange (EDF)

**Session Classification:** Plenary

Contribution ID: 7

Type: **not specified**

## **How the 4 major regions will implement this HPC-Data-Edge cyber-infrastructures**

*Wednesday, 15 May 2019 09:30 (1 hour)*

(15 minutes each) China, EU, Japan, US

China (Dr. Jingheng Xu, Tsinghua University)

Japan (Pr. Satoshi Matsuoka, RIKEN)

United States (Dr. Pete Beckman, ANL)

EU (Leonardo Flores Añover, European Commission)

**Session Classification:** Plenary



Contribution ID: 8

Type: **not specified**

## Opening & Welcome

*Tuesday, 14 May 2019 08:30 (5 minutes)*

**Presenter:** BOGAERTS, Serge (PRACE)

**Session Classification:** Opening & Welcome

Contribution ID: 9

Type: **not specified**

## Opening & Welcome

*Tuesday, 14 May 2019 08:45 (30 minutes)*

**Presenter:** LIPPERT, Thomas

**Session Classification:** Opening & Welcome

Contribution ID: **10**

Type: **not specified**

## Opening & Welcome

*Tuesday, 14 May 2019 08:35 (10 minutes)*

**Presenter:** MEYER, Norbert (PSNC)

**Session Classification:** Opening & Welcome

Contribution ID: 11

Type: **not specified**

## **Investigating supersymmetry with GAMBIT**

*Tuesday, 14 May 2019 14:30 (30 minutes)*

**Presenter:** KVELLESTAD, Anders (Imperial College London)

**Session Classification:** PRACEdays Scientific Track 1

Contribution ID: 12

Type: **not specified**

## **Status of non-supersymmetric dark matter theories with GAMBIT**

*Tuesday, 14 May 2019 15:00 (30 minutes)*

**Presenter:** SCOTT, Pat (Imperial College London)

**Session Classification:** PRACEdays Scientific Track 1

Contribution ID: 13

Type: **not specified**

## **Revealing the complex flows around young planets**

*Tuesday, 14 May 2019 15:30 (30 minutes)*

**Presenter:** MCNALLY, Colin (Queen Mary University of London)

**Session Classification:** PRACEdays Scientific Track 1

Contribution ID: 14

Type: **not specified**

## **Multi-scale Reionization**

*Tuesday, 14 May 2019 16:00 (30 minutes)*

**Presenter:** BIANCO, Michele (University of Sussex)

**Session Classification:** PRACEdays Scientific Track 1

Contribution ID: 15

Type: **not specified**

## **DNA Structure and Dynamics: Two Successful Stories using HPC**

*Tuesday, 14 May 2019 14:30 (30 minutes)*

**Presenter:** PUIGGRÒS, Pablo D. Dans (IRB Barcelona, Spain)

**Session Classification:** PRACEdays Scientific Track 2



Contribution ID: 16

Type: **not specified**

## **Conformational and transport properties of small circular DNA molecules in dilute solution: A detailed molecular dynamics simulation study**

*Tuesday, 14 May 2019 15:00 (30 minutes)*

**Presenter:** ALEXIOU, Terpsichori (University of Patras & FORTH/ICEHT)

**Session Classification:** PRACEdays Scientific Track 2

Contribution ID: 17

Type: **not specified**

## **Molecular dynamics simulation of complex systems**

*Tuesday, 14 May 2019 15:30 (30 minutes)*

**Presenter:** POGHOSYAN, Armen (The International Scientific-Educational Center of NAS RA)

**Session Classification:** PRACEdays Scientific Track 2

Contribution ID: **18**

Type: **not specified**

## **Chemical properties emerging from structural disorder**

*Tuesday, 14 May 2019 16:00 (30 minutes)*

**Presenter:** LA PENNA, Giovanni (National research council of Italy)

**Session Classification:** PRACEdays Scientific Track 2

Contribution ID: 19

Type: **not specified**

## **Making global coupled 15km climate simulations possible**

*Tuesday, 14 May 2019 17:00 (30 minutes)*

**Presenter:** CASTRILLO, Miguel (Barcelona Supercomputing Center)

**Session Classification:** PRACEdays Scientific Track 3

Contribution ID: 20

Type: **not specified**

## **Towards HPC-based shallow flow simulations for Various Problems**

*Tuesday, 14 May 2019 17:30 (30 minutes)*

**Presenter:** MINOLA GINTING, Bobby (Technical University of Munich)

**Session Classification:** PRACEdays Scientific Track 3

Contribution ID: 21

Type: **not specified**

## **Supporting the research lifecycle of GEO-Geohazard Supersites and Natural Laboratories initiative through HPC and research objects**

*Tuesday, 14 May 2019 18:00 (30 minutes)*

**Presenter:** PALMA, Raul (Poznań Supercomputing and Networking Center)

**Session Classification:** PRACEdays Scientific Track 3

Contribution ID: 22

Type: **not specified**

## Monitoring dust orientation

*Tuesday, 14 May 2019 18:30 (30 minutes)*

**Presenter:** TSEKERI, Alexandra (National Observatory of Athens)

**Session Classification:** PRACEdays Scientific Track 3

Contribution ID: 23

Type: **not specified**

## **Modelling mechanism of reactions and active sites in heterogeneous catalysis, looking for reactivity indicators in supported ziegler-natta nano-systems**

*Tuesday, 14 May 2019 17:00 (30 minutes)*

**Presenter:** D'AMORE, Maddalena (University of Turin)

**Session Classification:** PRACEdays Scientific Track 4



Contribution ID: 24

Type: **not specified**

## **Silica for drug-delivery: when simulation can complement experiment**

*Tuesday, 14 May 2019 17:30 (30 minutes)*

**Presenter:** DELLE PIANE, Massimo (University of Bremen, Germany)

**Session Classification:** PRACEdays Scientific Track 4

Contribution ID: 25

Type: **not specified**

## **Shear rheology of polymer melts and nanocomposites via nonequilibrium molecular dynamics simulations**

*Tuesday, 14 May 2019 18:00 (30 minutes)*

**Presenter:** TSALIKIS, Dimitrios (University of Patras)

**Session Classification:** PRACEdays Scientific Track 4

Contribution ID: 26

Type: **not specified**

## **The peptide bond condensation reaction at the air/water interface catalyzed by the “salt of the life”**

*Tuesday, 14 May 2019 18:30 (30 minutes)*

**Presenter:** SIRO BRIGIANO, Flavio (University of Evry Val D'Essonne, University of Paris Saclay)

**Session Classification:** PRACEdays Scientific Track 4

Contribution ID: 27

Type: **not specified**

## **Presentation of the Peer Review Process**

*Wednesday, 15 May 2019 11:30 (1h 30m)*

**Session Classification:** PRACEdays User Forum Open Session

Contribution ID: 28

Type: **not specified**

## **A Virtual Universe for the ESA Euclid Satellite: the Flagship v2.0 Simulation**

*Wednesday, 15 May 2019 14:30 (30 minutes)*

**Presenter:** STADEL, Joachim (University of Zurich)

**Session Classification:** PRACEdays Scientific Track 5

Contribution ID: 29

Type: **not specified**

## **Searching for new superfluid effects by means of numerical experiments**

*Wednesday, 15 May 2019 15:00 (30 minutes)*

**Presenter:** WLAZŁOWSKI, Gabriel (University of Technology, Poland)

**Session Classification:** PRACEdays Scientific Track 5

Contribution ID: **30**

Type: **not specified**

## **Radiation imprint of ultra-intense laser heating of solids**

*Wednesday, 15 May 2019 15:30 (30 minutes)*

**Presenter:** GARTEN, Marco (Helmholtz-Zentrum Dresden - Rossendorf, Germany)

**Session Classification:** PRACEdays Scientific Track 5

Contribution ID: **31**

Type: **not specified**

## **The Stellar Initial Mass Function from Isothermal MHD Turbulence**

*Wednesday, 15 May 2019 16:00 (30 minutes)*

**Presenter:** HAUGBØLLE, Troels (Niels Bohr Institute Københavns Universitet)

**Session Classification:** PRACEdays Scientific Track 5



Contribution ID: 32

Type: **not specified**

## **Advanced non-linear MHD simulations for fusion research**

*Wednesday, 15 May 2019 17:00 (30 minutes)*

**Presenter:** FUTATANI, Shimpei (Polytechnic University of Catalonia, Spain)

**Session Classification:** PRACEdays Scientific Track 7

Contribution ID: 33

Type: **not specified**

## **XCompact3d: a powerful framework to study turbulent flows with turbulence-resolving simulations**

*Wednesday, 15 May 2019 17:30 (30 minutes)*

**Presenter:** BARTHOLOMEW, Paul (Imperial College London, UK)

**Session Classification:** PRACEdays Scientific Track 7

Contribution ID: 34

Type: **not specified**

## **Energy cascade in rotating turbulent flows**

*Wednesday, 15 May 2019 18:00 (30 minutes)*

**Presenter:** BUZZICOTTI, Michele (University of Rome Tor Vergata, Italy)

**Session Classification:** PRACEdays Scientific Track 7

Contribution ID: 35

Type: **not specified**

## **Breaking new ground in magnetic fusion: stepping GYSELA towards exascale computing**

*Wednesday, 15 May 2019 18:30 (30 minutes)*

**Presenter:** DIF-PRADALIER, Guilhem (CEA, France)

**Session Classification:** PRACEdays Scientific Track 7

Contribution ID: 36

Type: **not specified**

## **Massively parallel sequence alignment using PCJ-BLAST**

*Wednesday, 15 May 2019 14:30 (30 minutes)*

**Presenter:** BAŁA, Piotr (University of Warsaw, Poland)

**Session Classification:** PRACEdays Scientific Track 6

Contribution ID: 37

Type: **not specified**

## **Molecular Dynamics investigation on the regulatory mechanism of the SHP-2 protein**

*Wednesday, 15 May 2019 15:00 (30 minutes)*

**Presenter:** BOCCHINFUSO, Gianfranco (Tor Vergata University of Rome, Italy)

**Session Classification:** PRACEdays Scientific Track 6

Contribution ID: 38

Type: **not specified**

## **Computer-aided drug design for oncogenic mutant proteins using HPC resources**

*Wednesday, 15 May 2019 15:30 (30 minutes)*

**Presenter:** COURNIA, Zoe (Biomedical Research Foundation, Academy of Athens, Greece )

**Session Classification:** PRACEdays Scientific Track 6

Contribution ID: 39

Type: **not specified**

## **Mechanistic effects of lipids and protein post-translation modifications on signaling over human cell membranes**

*Wednesday, 15 May 2019 16:00 (30 minutes)*

**Presenter:** PLUHACKOVA, Kristyna (ETH Zürich, Switzerland)

**Session Classification:** PRACEdays Scientific Track 6



Contribution ID: 40

Type: **not specified**

## **Verified Exascale Computing for Multiscale Applications (VECMA)**

*Wednesday, 15 May 2019 17:00 (30 minutes)*

**Presenter:** COVENEY, Peter (University College London , UK)

**Session Classification:** PRACEdays Scientific Track 8

Contribution ID: 41

Type: **not specified**

## **FEniCS-HPC mesh adaptivity on the heterogeneous architecture**

*Wednesday, 15 May 2019 17:30 (30 minutes)*

**Presenter:** KRISHNASAMY, Ezhilmathi (KTH, Germany)

**Session Classification:** PRACEdays Scientific Track 8

Contribution ID: 42

Type: **not specified**

## **Multi-scale Quantum Transport Simulations in thousands of cores**

*Wednesday, 15 May 2019 18:00 (30 minutes)*

**Presenter:** GARCIA AGUILAR, Jose Hugo (Catalan Institute Of Nanoscience and Nanotechnology, Spain)

**Session Classification:** PRACEdays Scientific Track 8

Contribution ID: 43

Type: **not specified**

# **Exascale Matrix Factorization: Using Supercomputers and Machine Learning for Drug Discovery**

*Wednesday, 15 May 2019 18:30 (30 minutes)*

**Presenter:** VANDER AA, Tom (imec, Belgium)

**Session Classification:** PRACEdays Scientific Track 8

Contribution ID: 44

Type: **not specified**

## **SHAPE – Helping SMEs onto the HPC ladder**

*Wednesday, 15 May 2019 14:30 (30 minutes)*

**Presenter:** JOHNSON, Chris (University of Edinburgh)

**Session Classification:** PRACEdays Industrial Track

Contribution ID: 45

Type: **not specified**

## Helping SMEs via SHAPE projects

*Wednesday, 15 May 2019 15:00 (30 minutes)*

**Presenter:** DE MIER, Monica (Barcelona Supercomputing Center, Spain)

**Session Classification:** PRACEdays Industrial Track

Contribution ID: 46

Type: **not specified**

## **Immersion Cooling, High Performance Cooling for HPC.**

*Wednesday, 15 May 2019 15:30 (30 minutes)*

**Presenter:** RISPOLI, Daniele (Submer, Spain)

**Session Classification:** PRACEdays Industrial Track

Contribution ID: 47

Type: **not specified**

## Recent Industrial Applications in HPC

*Wednesday, 15 May 2019 16:00 (30 minutes)*

**Presenter:** MCGINTY, Brendan (University of Illinois at Urbana-Champaign, USA)

**Session Classification:** PRACEdays Industrial Track



Contribution ID: 48

Type: **not specified**

## **Performance of low emissions swirling flames. Influence of diffusers.**

*Wednesday, 15 May 2019 17:00 (30 minutes)*

**Presenter:** PARRA, Teresa (University of Valladolid, Spain)

**Session Classification:** PRACEdays Industrial Track

Contribution ID: 49

Type: **not specified**

## **High fidelity simulation of vortex induced vibrations for flow control and energy harvesting**

*Wednesday, 15 May 2019 17:30 (30 minutes)*

**Presenter:** LEHMKUHL, Oriol (Barcelona Supercomputing Center, Spain)

**Session Classification:** PRACEdays Industrial Track

Contribution ID: 50

Type: **not specified**

## **Control of shock wave/boundary layer interaction by means of micro vortex generators**

*Wednesday, 15 May 2019 18:00 (30 minutes)*

**Presenter:** GRÉBERT, Arnaud (ISAE-SUPAERO, University of Toulouse, France)

**Session Classification:** PRACEdays Industrial Track

Contribution ID: 51

Type: **not specified**

## **Towards clean propulsion with synthetic fuels: Hierarchical, cluster-modularized simulations with node-level optimization and deep learning**

*Wednesday, 15 May 2019 18:30 (30 minutes)*

**Presenter:** BODE, Mathis (RWTH Aachen University, Germany)

**Session Classification:** PRACEdays Industrial Track

Contribution ID: 53

Type: **not specified**

## **Centres of Competence**

(private meeting, by invitation only)

Contribution ID: 54

Type: **not specified**

## **Centres of Competence**

(private meeting, by invitation only)

Contribution ID: 55

Type: **not specified**

## **GÉANT: Why NRENs are essential for a successful EuroHPC**

*Tuesday, 14 May 2019 09:45 (30 minutes)*

**Abstract:** The EC has defined three pillars for HPC: Next generation technologies, access for industry and academia and HPC application delivery and use. All three require a high end network, reliable security services and a trustworthy identity and access management infrastructure. The European National Research and Education Networks (NRENs) and GEANT have together built a network and set of services to meet the demands of HPC. And they will further develop this to meet the future demands of the EuroHPC programme delivering a quality and targeted set of services that distinguishes NRENs from commercial Internet providers.

**Presenter:** HUIZER, Erik

**Session Classification:** GÉANT

Contribution ID: 56

Type: **not specified**

## **HPC resources access and equality: some data**

*Tuesday, 14 May 2019 14:30 (15 minutes)*

**Presenter:** TESTI, Debora (CINECA)

**Session Classification:** Equality and Diversity in HPC



Contribution ID: 57

Type: **not specified**

## **Improving equality and diversity through policies, practices, action plans and culture**

*Tuesday, 14 May 2019 15:00 (15 minutes)*

**Presenter:** MARGETTS, Lee (University of Manchester, UK)

**Session Classification:** Equality and Diversity in HPC

Contribution ID: 58

Type: **not specified**

## **Women in STEM an academic perspective**

*Tuesday, 14 May 2019 14:45 (15 minutes)*

**Presenter:** LÓPEZ, Núria (ICIQ)

**Session Classification:** Equality and Diversity in HPC

Contribution ID: 59

Type: **not specified**

## **How BSC is facing the challenge of the gender issue**

*Tuesday, 14 May 2019 15:15 (15 minutes)*

**Presenter:** BADIA, Rosa M. (BSC)

**Session Classification:** Equality and Diversity in HPC

Contribution ID: **60**

Type: **not specified**

## **HPC: Challenge Accepted.**

*Tuesday, 14 May 2019 15:30 (15 minutes)*

Sharing my failures, mistakes and efforts in my HPC master.

**Presenter:** INCA, Julita (EPCC)

**Session Classification:** Equality and Diversity in HPC

Contribution ID: **61**

Type: **not specified**

## **Inputs from audience and open discussion with the panel**

*Tuesday, 14 May 2019 17:00 (2 hours)*

**Session Classification:** Equality and Diversity in HPC