MaX Conference on the Materials Design Ecosystem at the Exascale: High-Performance and High-Throughput Computing

29 - 31 January, 2018 Trieste, Italy

Materials are crucial to scientific and technological advances and industrial competitiveness, and to tackle key societal challenges - from energy and environment to healthcare, information and communications, manufacturing, safety and transportation. Computational science, with the current accuracy and predictive power, can play a very relevant role in this respect by boosting materials design and discovery.

In this scenario, scientific objectives and computational technological perspectives are nowadays more intertwined than ever. The MaX Centre (Materials Design at the Exascale), one of the nine Centres of Excellence for computing applications funded by the EU since 2015, has been acting along two core lines, namely, high-performance computing (HPC), in view of the transition to exascale architecture, and high-throughput computing (HTC), with the final aim of building a materials modelling ecosystem. The MaX Centre takes the opportunity of its general conference to share with the scientific community its current efforts and future perspectives, as well as to underline the state of the art of both the scientific and the technological innovation which can disruptively impact on material discovery in the next decade.

This conference aims at gathering scientists active in the field of materials modelling, together with HPC and HTC experts to discuss the most recent advancements in the field, including, but not limited to:

- Advances in high performance computing for materials science
- New avenues from data analytics/artificial intelligence in materials science
- High throughput computing for materials discovery
- Trends in high performance computing and codesign towards

Further information: http://indico.ictp.it/event/8004/ smr3161@ictp.it management@max-centre.eu

ØRIMING

THE EXASCALE

TRANS/ITION

Organizers:

STEFANO BARONI (SISSA) ELISA MOLINARI (CNR-NANO) SANDRO SCANDOLO (ICTP)

ICTP Scientific Contacts:

IVAN GIROTTO RALPH GEBAUER

Invited Speakers include:

ANU BABY, UNIVERISTÀ DI MILANO BICOCCA (IT) STEFANO BARONI, SISSA (IT) LUCA BENINI, UNIVERSITÀ DI BOLOGNA (IT) & ETH (CH) STEPHAN BLÜGEL, FZ-JUELICH (DE) PIETRO BONFÀ, CINECA (IT) LUIGI BROCHARD, LENOVO HPC (FR) ROBERTO CAR, PRINCETON UNIVERSITY, NJ (USA) IVAN CARNIMEO, SISSA (IT) JUAN F. CARRASQUILLA, PERIMETER INSTITUTE (CA) CARLO CAVAZZONI, CINECA (IT) ALESSANDRO CURIONI, IBM (CH) THIERRY DEUTSCH, CEA-INAC (FR) MASSIMILIANO FATICA, NVIDIA (USA) MARIVI FERNANDEZ-SERRA, STONY BROOK UNIVERSITY (USA) LUCA GRISANTI, SISSA (IT) **GEOFFROY HAUTIER, UCL-NAPS (BE)** JUERG HUTTER, UNIVERSITY OF ZURICH (CH) KARSTEN W. JACOBSEN, TECHNICAL UNIVERSITY OF DENMARK (DK) ANTON KOHZENVNIKOV, CSCS (CH) BORIS KOZINSKY, HARVARD UNIVERSITY (USA) LIN LIN, UNIVERSITY OF CALIFORNIA, BERKELEY, CA (USA) **STEPHAN MOHR, BSC (ES)** NICOLAS MOUNET, EPFL (CH) PABLO ORDEJON, ICN2 (ES) DIRK PLEITER, JUELICH SUPERCOMPUTING CENTER (DE) DEBORAH PREZZI, CNR NANO (IT) MARIA CLELIA RIGHI, UNIMORE (IT) DAVIDE SANGALLI, CNR-ISM (IT) STEFANO SANVITO, TRINITY COLLEGE DUBLIN (IE) FILIPPO SPIGA, ARM (USA) THOMAS STERLING, INDIANA UNIVERSITY (USA) LEOPOLD TALIRZ, EPFL (CH) DAVID WILKINS, EPFL (CH) ZEILA ZANOLLI, RWTH (DE)

- exascale
- Novel algorithms for first principles simulations

Poster proposals can be submitted together with the online application.

How to apply:

Online application: http://indico.ictp.it/event/8004/

Female scientists are encouraged to apply.

There is no registration fee.

Deadline:

20 January 2018







