

ICTP International Symposium on “The Future of Scientific Computing: A Global Perspective”

Date: Monday 27 May 2024

Place: Budinich Lecture Hall, ICTP, Trieste, Italy

Leading scientists, policymakers, and industry experts from around the world will gather at ICTP's International Symposium to discuss the opportunities offered by scientific computing in tackling key scientific challenges, with a global perspective. The symposium will explore how artificial intelligence, high-performance computing and recent advancements in quantum computing will impact the scientific discovery process across scientific fields, including climate science, molecular chemistry, and materials science. Reflecting ICTP's core mission, the symposium will emphasize a global and inclusive approach that can address the needs of scientific communities working in the world's less developed regions. The symposium is part of ICTP's 60th anniversary celebrations taking place throughout 2024, culminating in a high-level event in November 2024. Outcomes of the symposium will be presented and discussed during a panel session at this November event.

Programme:

9:00-9:30

Opening

Speakers:

Atish Dabholkar (ICTP), Alessandro Curioni (IBM & AI Alliance), Sandro Scandolo (ICTP)

9:30-10:20

Session 1 - Scientific Cases

Moderator: Stefano Baroni (SISSA)

Speakers:

Giulia Galli (University of Chicago), Andrea Cavalli (CECAM, Lausanne), Erika Coppola (ICTP)

Synopsis

Scientific computing has emerged as the third pillar of the scientific method, along with theory and experiment, and has provided insights where theory or experiment alone could not, for example in the projection of future climate changes, in the design of new materials for clean energy, and in the analysis of cosmological observations. This session will highlight the scientific challenges that lie ahead, and how computational approaches hold the promise to tackle and solve these challenges in the next decades.

10:20-10:50 Coffee break

10:50-11:40

Session 2 - Artificial Intelligence

Moderator: Roberto Trotta (SISSA)

Speakers

Marc Mezard (Bocconi, Milano), Eiman Kanjo (NTU/Turing Institute/ICL), Teodoro Laino (IBM), Guido Sanguinetti (SISSA), Nicola Marzari (EPFL, NCCR MARVEL)

Synopsis

This session will focus on the more recent advancements in the AI fields, giving particular attention to AI models for scientific discovery. Large language models and foundational models are revolutionizing AI, but will these models, trained on a very big set of unlabeled data, replace task-specific models traditionally implemented to solve scientific problems? Other themes on the agenda will be: societal challenges related to the rapid advancement of AI; AI's public perception; and the potential risks associated with the AI revolution, such as the divide between those having access to large computational resources and those who do not. The session will emphasize how the development of trustworthy AI and open foundational models may help bridge this gap and improve the public understanding and usage of this disruptive technology.

11:40-12:30

Session 3 - Quantum Computing

Moderator: Marcello Dalmonte (ICTP)

Speakers

Peter Zoller (University of Innsbruck and IQOQI), Mark Jackson (Quantinuum), Martin Mueller (GESDA), Francesco Petruccione (NITheCS, South Africa)

Synopsis

This session will discuss present opportunities and future perspectives of quantum computing. Questions on the agenda will include: what are the problems that quantum computing can contribute to solving, in science and for the larger benefit of society? What are the corresponding time scales? How do quantum technologies interface with other emerging ones (e.g., AI and HPC)? What is the role that companies, public infrastructures, and institutions can play?

12:30-14:00 Lunch break

14:00-14:50

Session 4 - New Technologies for Scientific Computing

Moderator: Stefano Cozzini (Area Science Park)

Speakers

Thomas Schulthess (CSCS, Switzerland), Gabriel Fonseca-Guerra (Intel/Neuromorphic Lab), Marc Bettencourt (NVIDIA), Nicola Venuti (Amazon Web Services)

Synopsis

Advanced computing and high-performance computers (HPC) have been used to model, simulate and analyse scientific problems in different fields, from astrophysics to climate science, since the dawn of the modern computing era. In the last half century, the models studied by HPC systems have increased exponentially both in scale and resolution. Next-

generation computers are expected to operate at the exascale (10^{18} flops per second), thanks to new types of accelerators, such as the latest generation of GPUs installed on exascale supercomputers (NVIDIA Grace Hopper). The downside of GPU computing is power consumption. Data computation and data transfer are responsible for a large part of this consumption, and the rapid development of Machine Learning and AI neural network models is adding even more demand. Since we have reached the end of Moore's law, the need for a shift in perspective on HPC technologies has become necessary. Big data analysis and exascale computing require a data-centric computing approach. This new paradigm is characterised by high-speed memory transfer, and a hardware system revolution, based on new technologies (e.g. Neuromorphic chips or Quantum Accelerators) and new infrastructures better suited for dynamic workflows (e.g. cloud). The performance of the computing system, in particular the energy efficiency, sets the fundamental limit of AI/ML capability. This panel session will investigate the capabilities of new technologies (e.g. Neuromorphic computing, quantum) and new HPC infrastructures (e.g. cloud), highlighting the pros and cons of each.

14:50-15:40

Session 5 - HPC Infrastructures: A Global Perspective

Ivan Girotto (ICTP)

Speakers

Happy Sithole (NICIS, South Africa), Robert Basmadjian (Toubkal Supercomputer, Morocco), Fabio Affinito (CINECA), Thomas Schulthess (CSCS, Switzerland)

Synopsis

Several challenges hinder the deployment and efficient exploitation of large-scale computational infrastructures in the global South, among them limited access to technological advances, brain drain, and lack of computing "ecosystems". The session aims at surveying the current status of large/middle-scale HPC infrastructures in the global South, and assessing their long-term sustainability vis-a-vis the above challenges. Remote access to high-end computer infrastructures through transboundary actions will also be discussed.

15:40-16:10 Coffee break

16:10-17:00

Session 6 - Global Initiatives

Sandro Scandolo (ICTP)

Invited speakers

Sara Bonella (CECAM), Alessandro Curioni (IBM & AI Alliance), Alessia D'Orazio (National HPC, Big Data e Quantum Computing Research Centre, ICSC), Elisa Molinari (Univ. Modena and MaX Center of Excellence), Jon Stumpf (Mass Open Cloud Alliance)

Synopsis

This session will present new international initiatives (EuroHPC, ICTP's Consortium, AI Alliance, MOC Alliance), focused on HPC, AI, and cloud development, aiming to provide global and inclusive access to HPC and cloud technologies for scientific computing,

together with the educational tools necessary to use these technologies effectively. This is a necessary action to address the computational needs of scientific communities working in less-developed regions of the world.