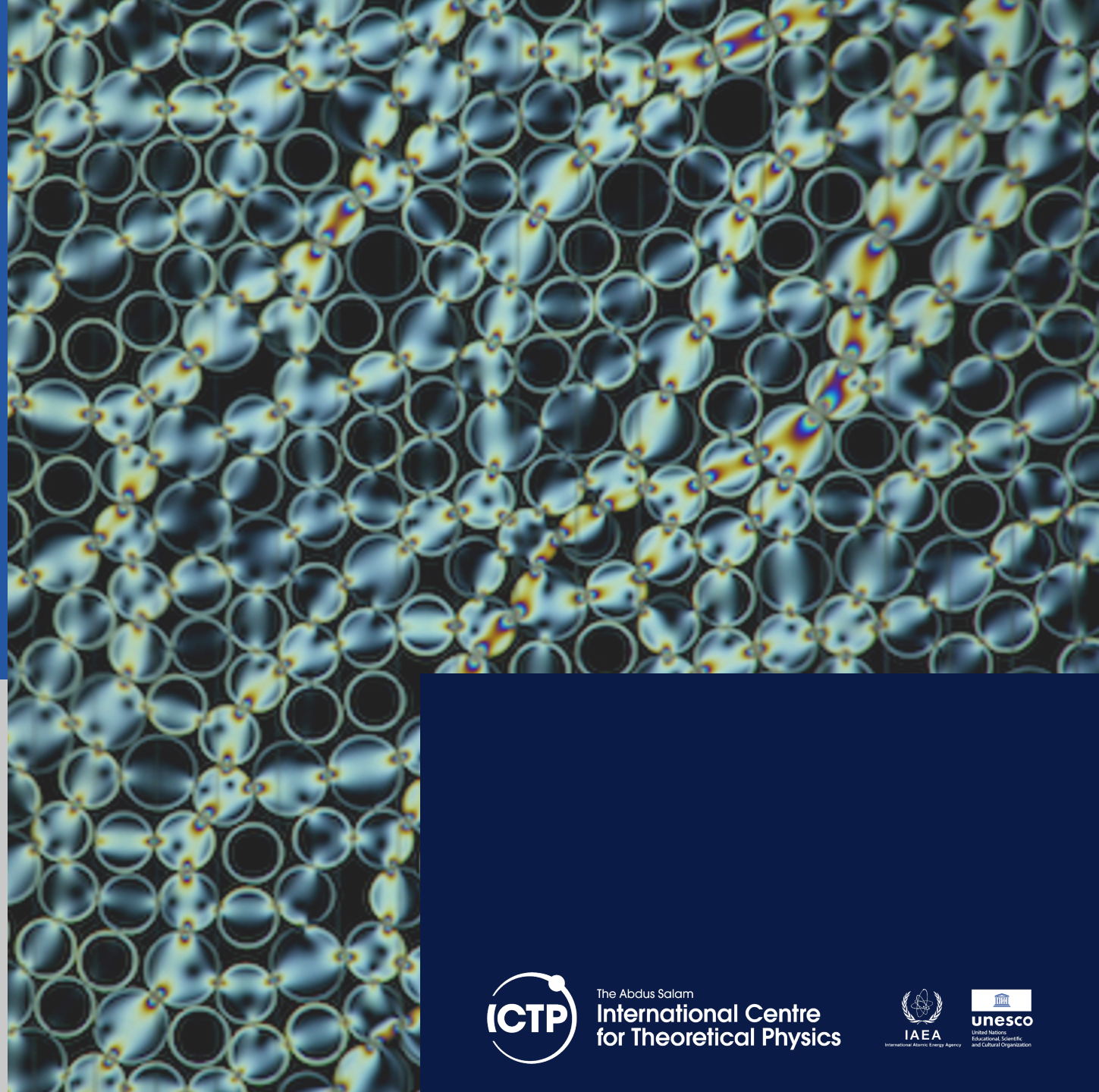
ICTP:

World-class Research and a Successful Model of International Collaboration

Public Information Unit

ICTP 1964–2024



The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency

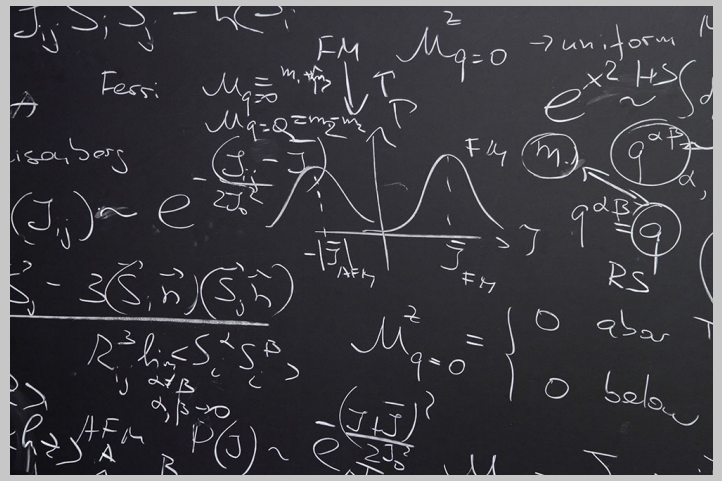
unesco United Nations Educational, Scientific and Cultural Organization

What is ICTP?

- Founded in 1964 by Nobel Laureate Abdus Salam to enhance international cooperation through science.
- Combines world class research with a unique global mission of building science capacity in the developing world.
- Governed by tripartite agreement between Italy UNESCO and IAEA.

What is ICTP?

Research



Education

Cooperation

Research Sections

High Energy Cosmology & Astroparticle Physics

Condensed Matter and Statistical Physics

Mathematics

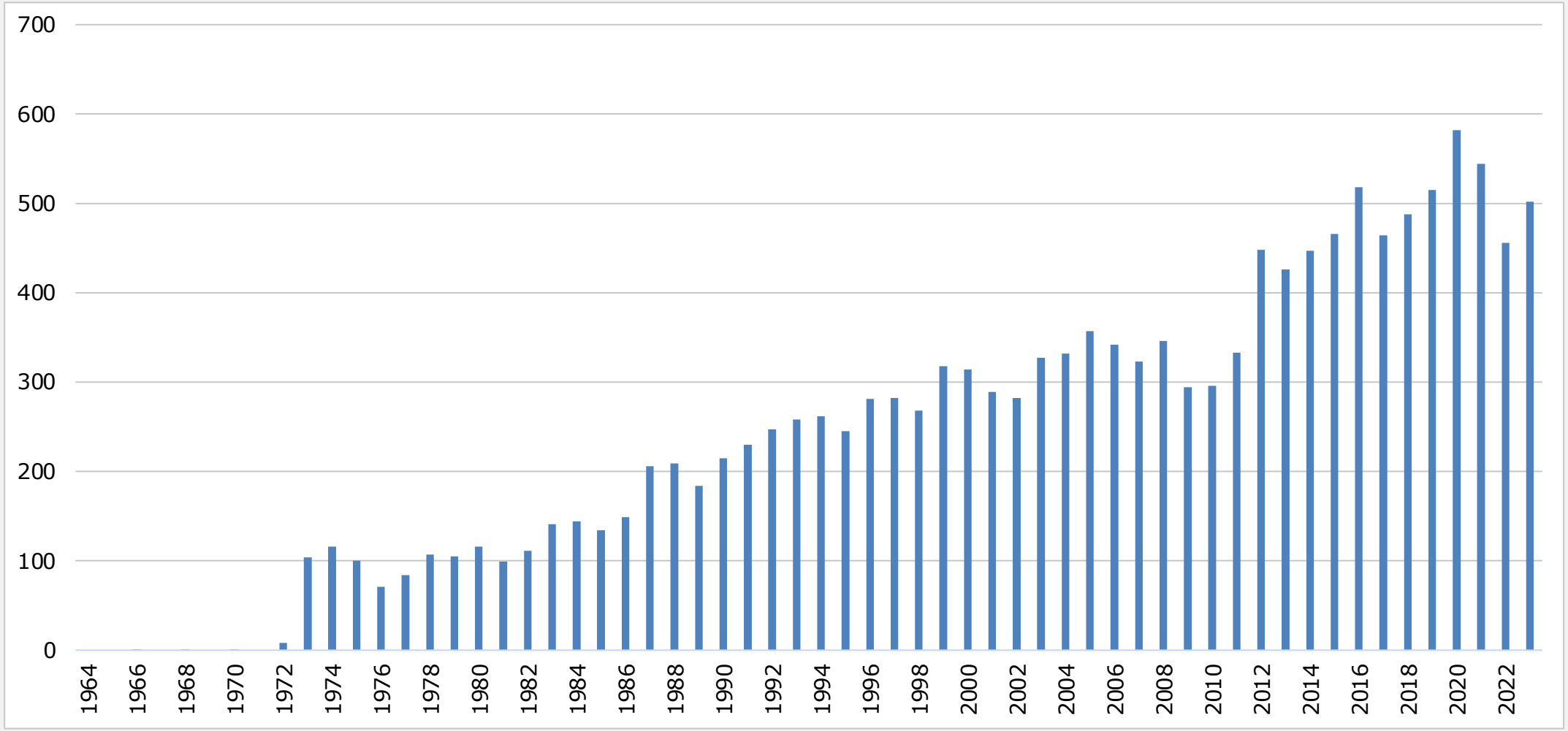
Science, Technology and Innovation

Earth System Physics

Quantitative Life Sciences

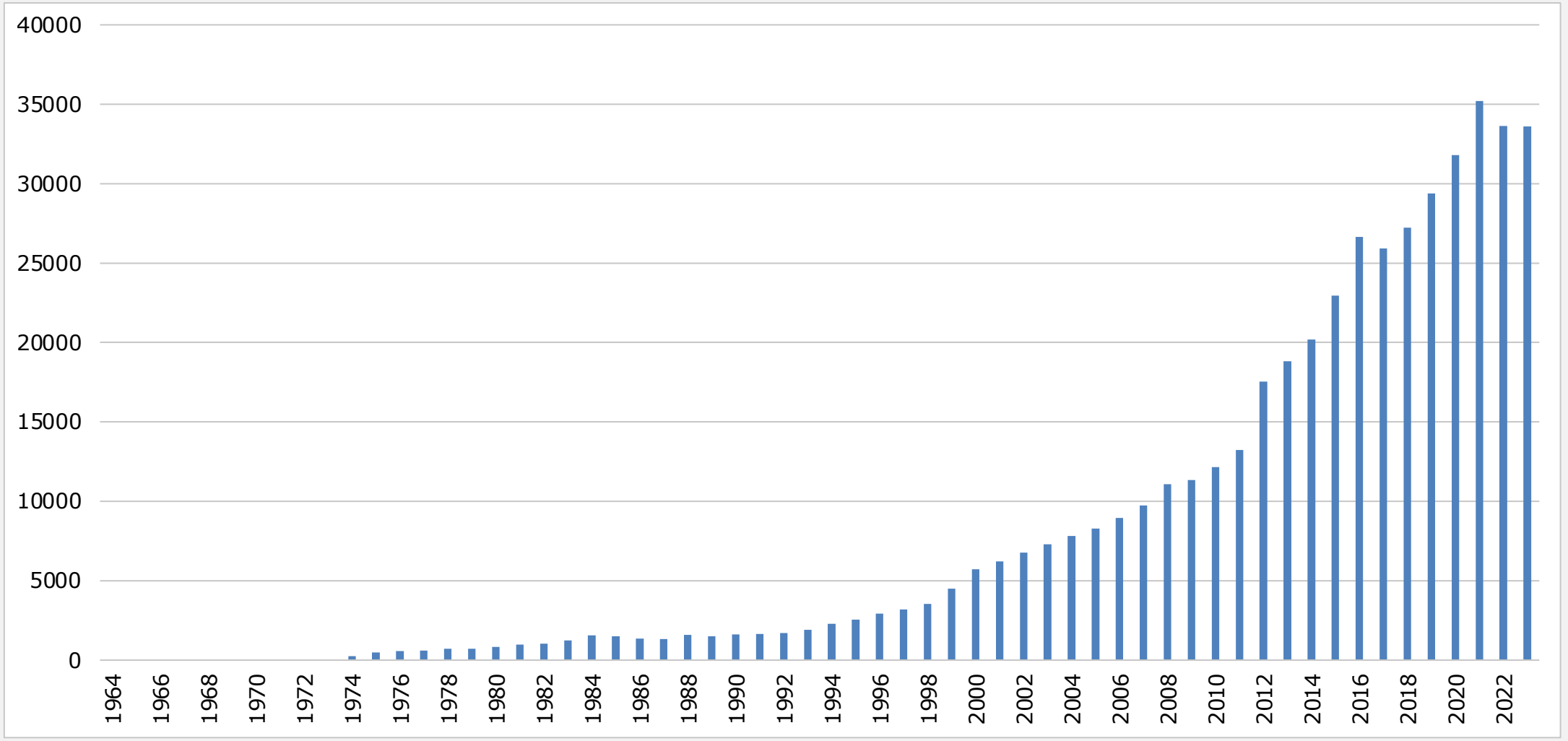
Also: Sustainable Energy and High Performance Computing

Papers produced within ICTP



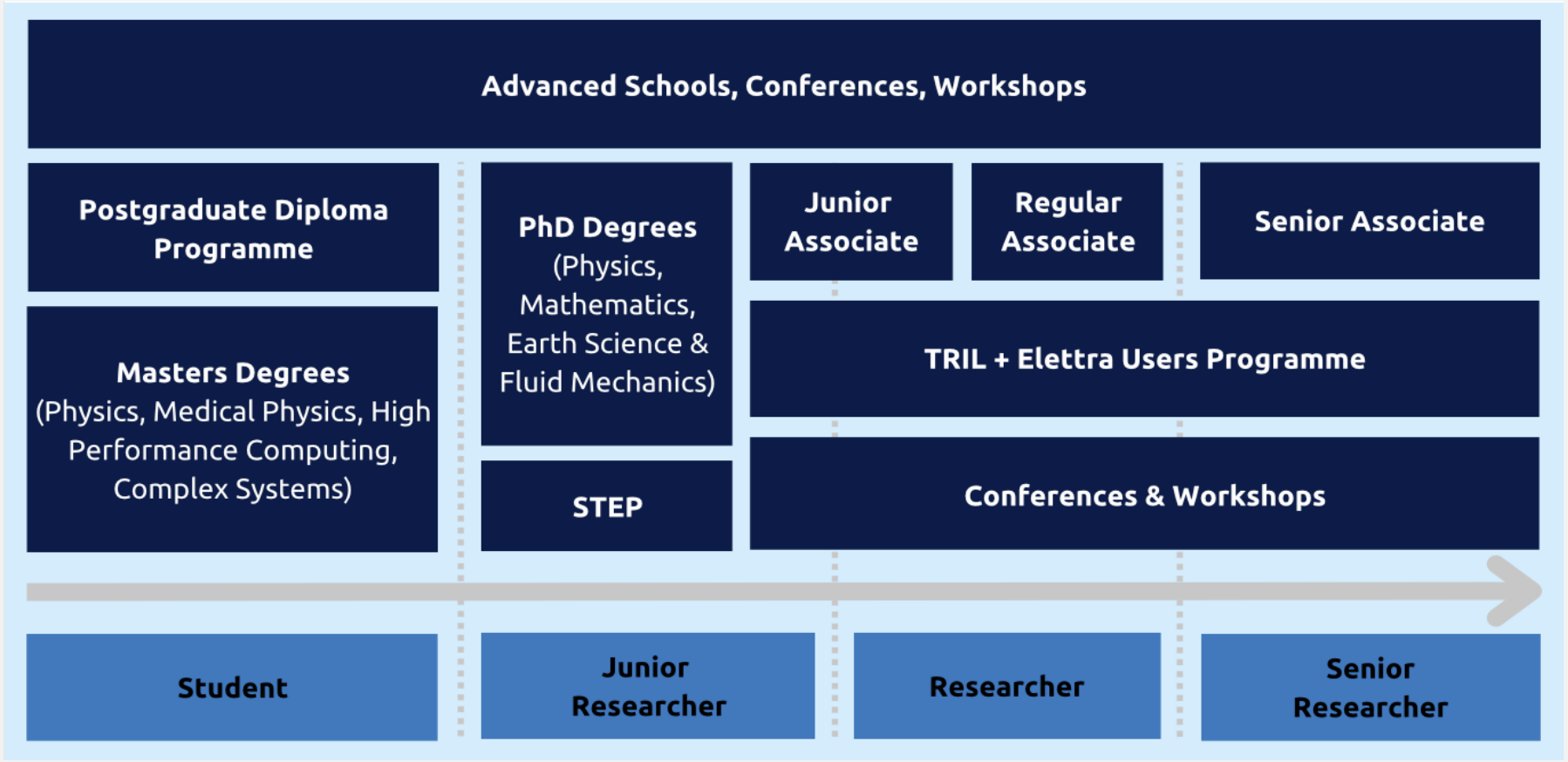
Papers listed by final publication year

Citations of ICTP papers



ICTP Programmes:

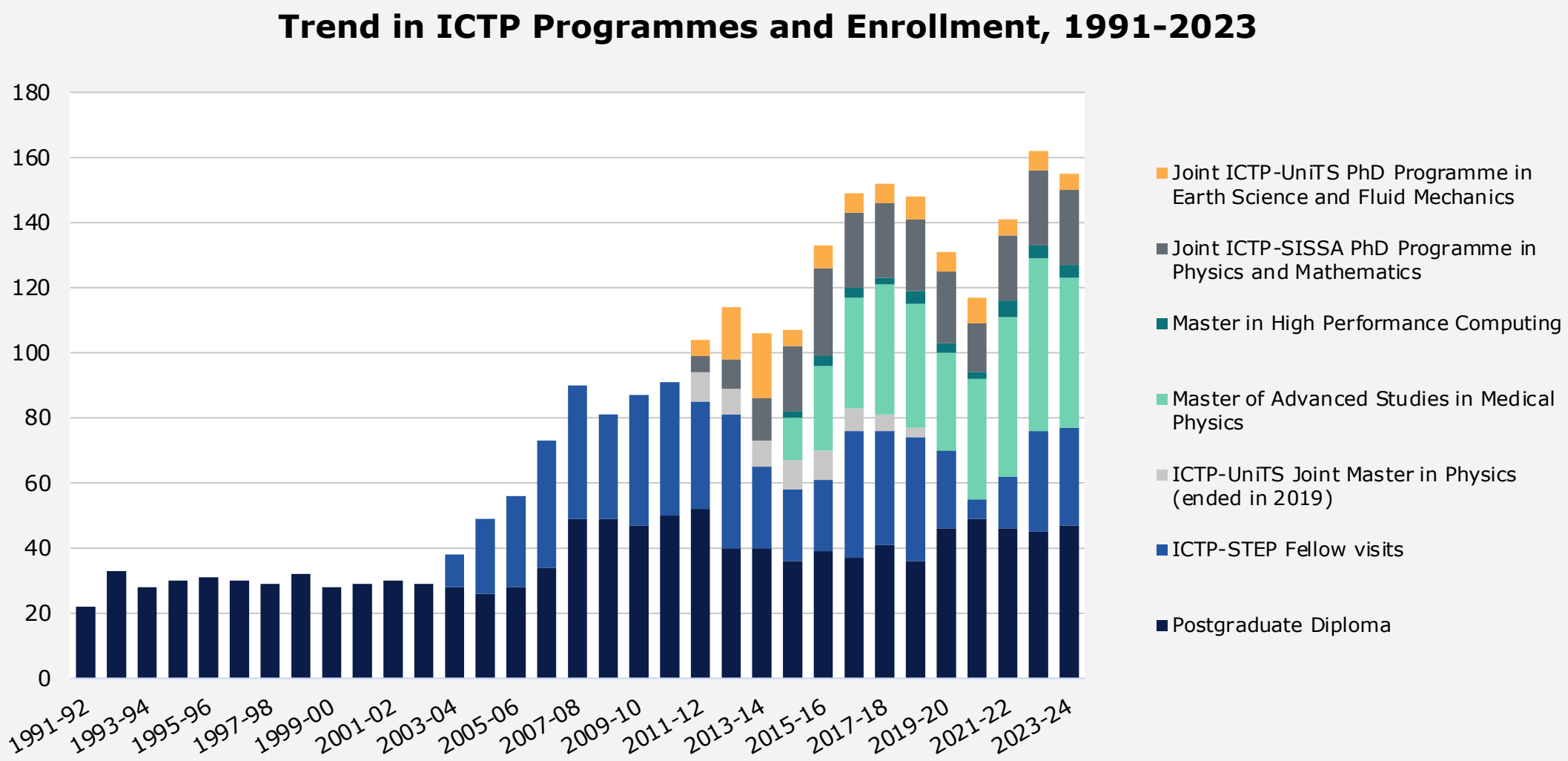
Supporting Scientists in all Stages of their Careers



ICTP Degree Programmes

- PhD in Physics (with University of Trieste)
- PhD in Physics and Mathematics (with SISSA)
- PhD in Earth Science and Fluid Mechanics (with University of Trieste)
- Masters in Medical Physics (with University of Trieste)
- Masters in High Performance Computing (with SISSA)
- Master of Complex Systems (with consortium of European universities)

ICTP Degree Programmes as of 2023



ICTP's Postgraduate Diploma Programme:
Preparing Young Scholars for PhD Studies

Since 1991:

- **1000+** Diploma graduates
- More than **75%** earned or working toward PhDs

Master of Advanced Studies in Medical Physics:

Training Professionals for the Developing World

2023/2024:

46 students

from **33** countries

33% female students

25% of students funded by IAEA

Master in
High Performance Computing

www.mhpc.it | info@mhpc.it

SISSA

The Abdus Salam
International Centre
for Theoretical Physics

A SPECIALIST IN MHPC… WHY?

- ADVANCED HPC HAS BECOME A KEY TOOL BOTH IN ACADEMIA AND IN INDUSTRY
- **HW/SW COMPLEXITY**
- PLANNING/EXPLOITING NEW HPC SYSTEM
- **BIG DATA ISSUES**
- NEW APPROACHES OF DATA ACCESS AND MANAGEMENT
- **STRONG NEED OF PROFESSIONALS TO EFFICIENTLY SOLVE LARGE COMPUTATIONAL PROBLEMS**

MHPC STRENGHTS

- HIGH DEMAND FOR PROFESSIONALS IN HPC
- **STRONG CONNECTION WITH INSTITUTIONS AND COMPANIES**
- ICTP AND SISSA: STIMULATING RESEARCH AND WORK ENVIRONMENT
- **"SISTEMA TRIESTE": 30 RESEARCH AND HIGH TRAINING CENTERS**

MHPC IN NUMBERS

- **11 EDITIONS**
- More than 100 ADMITTED STUDENTS
- **MORE THAN 20% OF THEM ARE WOMEN**
- 87,5% OF OUR STUDENTS HAD A SCHOLARSHIP
- **94% OF OUR ALUMNI FINDS JOBS WITHIN 1 YEAR (reversed trend after 5 years):**
  - 66% ACADEMIA
  - 34% INDUSTRY

COURSES: SOME EXAMPLES

- **FOUNDATION OF HPC**
- INTRODUCTION TO PARALLEL COMPUTING
- **ADVANCED PROGRAMMING**
- PARALLEL FFT
- **DATA STRUCTURES AND SORTING & SEARCHING**
- SCIENTIFIC DATA MANAGEMENT
- **ADVANCED COMPUTER ARCHITECTURES & OPTIMIZATIONS**
- THE FINITE ELEMENT METHOD USING DEAL.II
- **MACHINE LEARNING**

Master in High Performance Computing

THE MHPC STRUCTURE

FIRST PART

INTRODUCTION: HPC & PROGRAMMING

6 MONTHS

SECOND PART

HPC ALGORITHMS FOR SCIENCE&TECH

3 MONTHS

THIRD PART

THESIS PROJECT

6-9 MONTHS

The Abdus Salam International Centre for Theoretical Physics

SISSA

ICTP SUPPORTED PARTICIPANTS @ MHPC

1 — 7

Out of the 30 supported students (30% females) from 18 countries about 40% have found a position in industry, 60% in public research (including HPC centers)

2014 - 2024

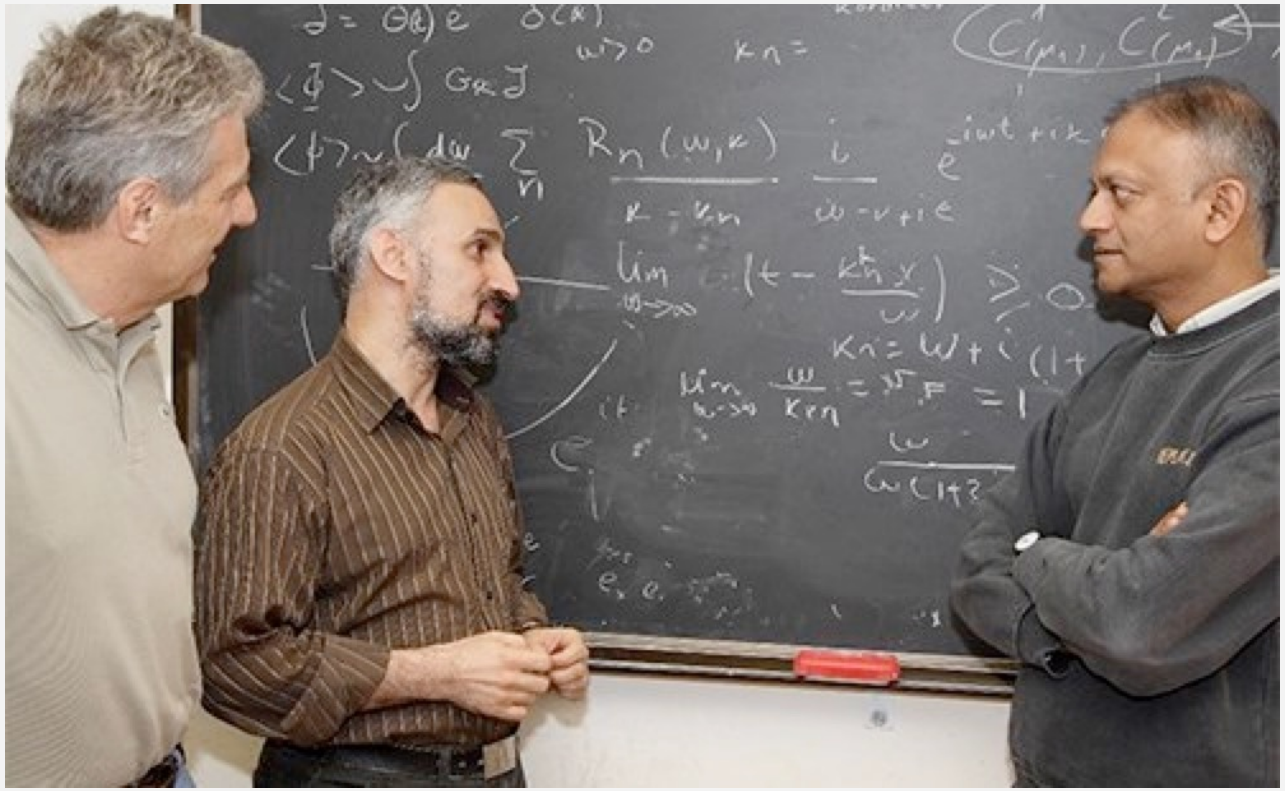
OUR PARTNERS

MHPC

NEW AREA

Associates Programme: Working Together at ICTP

- **3,000+** Associates since 1964
- 6 year term, visits to IAEA to collaborate with ICTP Scientists
- Simons Associates may also bring a student



ICTP: An International Hub for Scientific Networking

- Organises more than **60** conferences & workshops each year.
- Welcomes up to more than **6,000** scientists from **150+** nations each year.
- Attracts an additional **1,000-2,000** scientists per year through hosted activities.

TRAINING AT ICTP

ICTP Visiting Scientists:
Where do they come from?

SINCE 1970:

More than

180,000

visits

from scientists from **188** countries around the world

IN 2023:

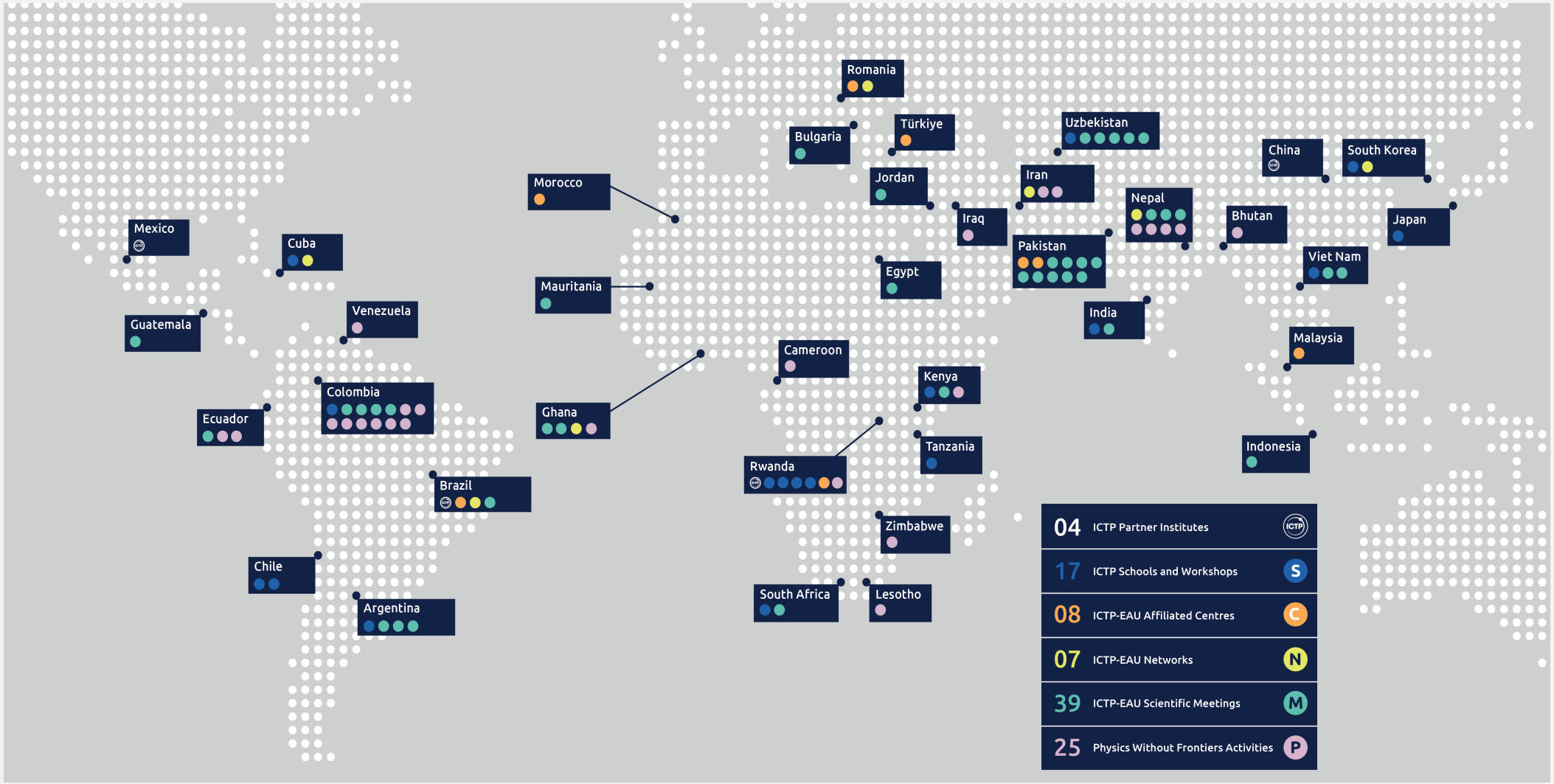
32%

of visitors were women

59%

of visitors were from developing and least-developed countries

ICTP Impact 2023



ICTP Success Stories

Freddy Cachazo,Venezuela
Diploma Alumni (1996-97)

- Recipient, 2014 New Horizons Prize
- Gribov Medallist 2009
- Dyson Chair, Perimeter Institute

Zohra Ben Lakhdar, Tunisia
ICTP Associate

- Recipient, 2005 L'Oreal-UNESCO Award for Women in Science
- Founding member, Tunisian Physics Society and Tunisian Astronomy Society
- Professor of Physics, Tunis El Manar University

Narayan Adhikari, Nepal
Diploma Alumni (1997-98)

- ICTP Regular Associate 2008-15
- ICTP Senior Associate 2018-23
- Research group leader, Tribhuvan University, Nepal

"Over the years, ICTP has left a deep legacy in performing and promoting outstanding fundamental scientific research. In particular, it has had a major impact supporting science in developing countries."

STEPHEN HAWKING

UNIVERSITY OF CAMBRIDGE

“Much good emanates from ICTP. Salam's vision of a facility that couples the doing of first-rate research with advanced scientific training has been overwhelmingly vindicated and validated.”

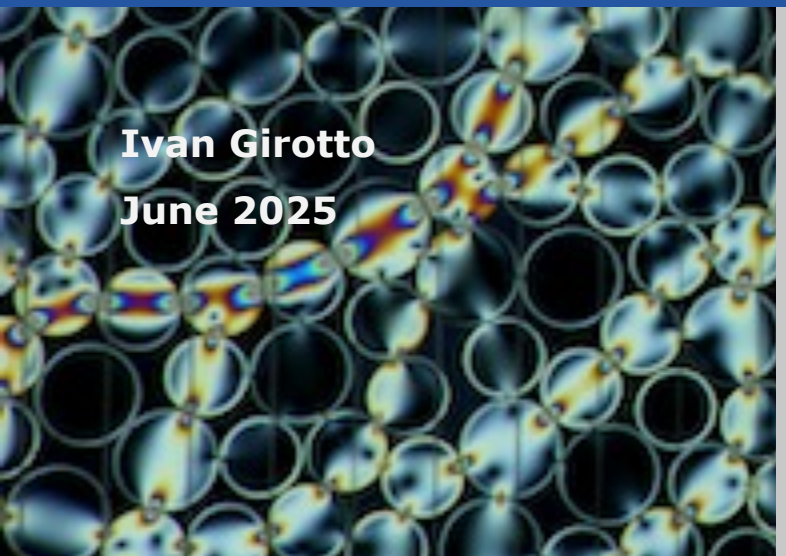
DAVID GROSS

NOBEL LAUREATE IN PHYSICS 2004 AND DIRECTOR OF THE KAVLI INSTITUTE FOR THEORETICAL PHYSICS

ICOMP:

An International Consortium for Scientific Computing

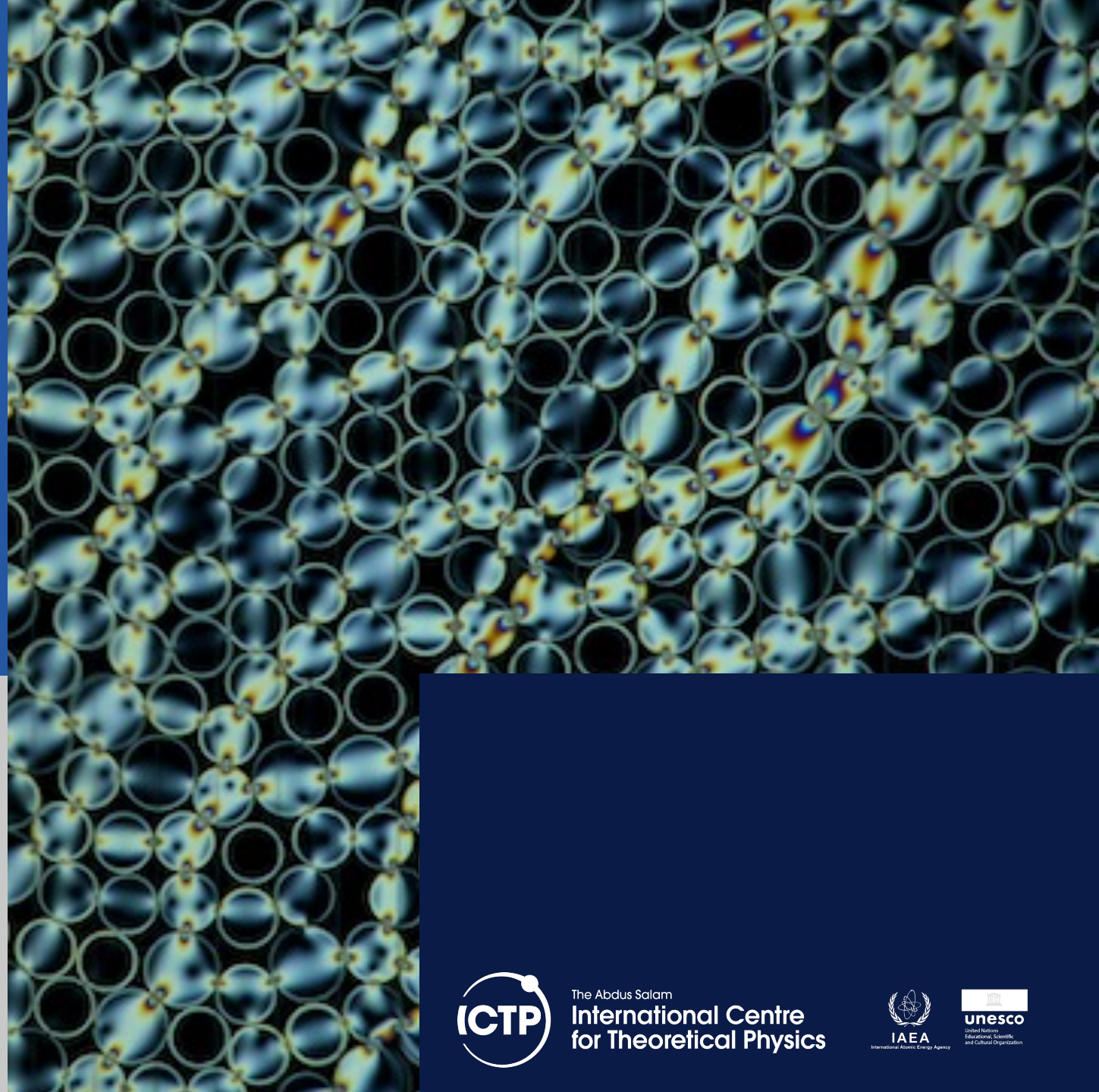
A. Hassanali, E. Coppola, R. Gebauer, J. Barbier,
I. Girotto, S. Di Gioia, S. Scandolo



Ivan Girotto

June 2025

ICTP 1964–2024

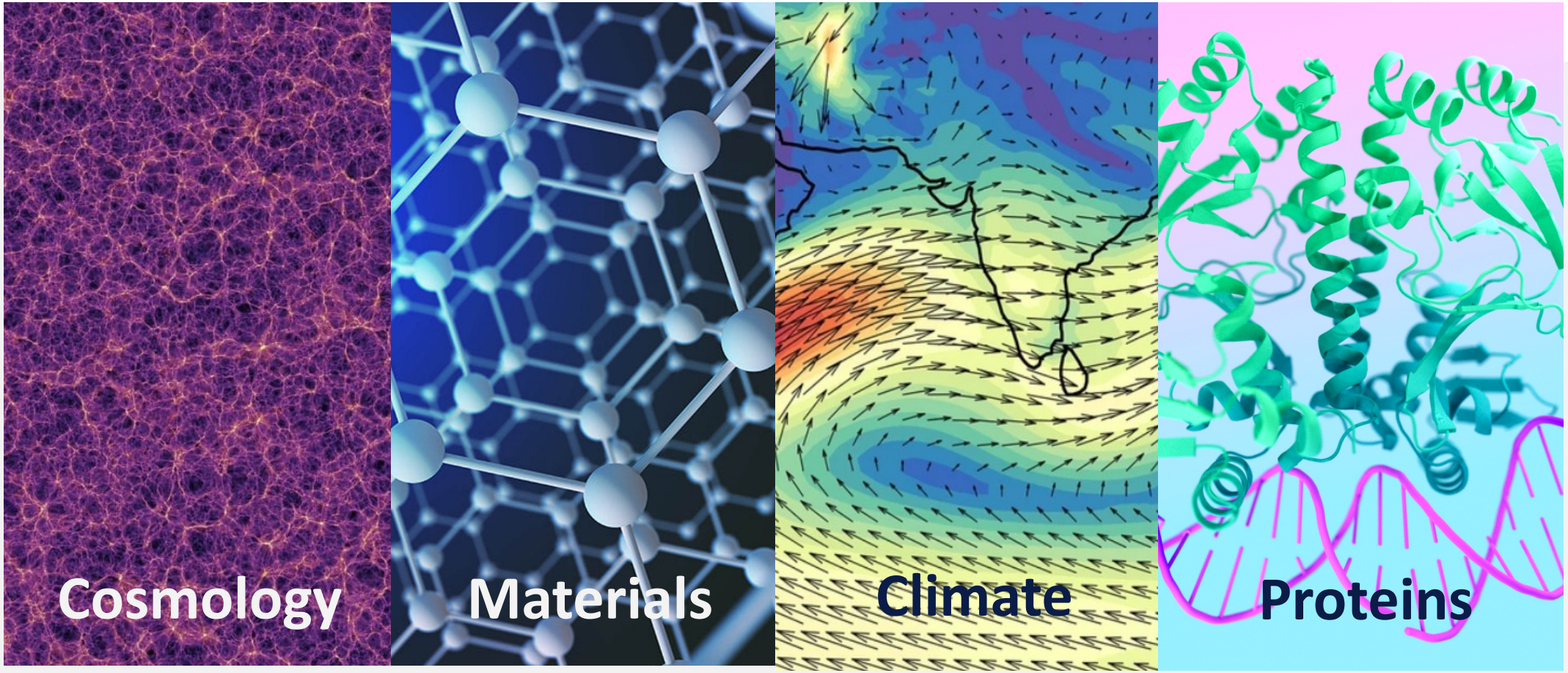


The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency

unesco United Nations Educational, Scientific and Cultural Organization

The role of computing in science



Computational activities at ICTP

Research and training

Research in

- ❑ **Climate and Earth modeling (ESP)**
- ❑ **Energy, Biochemistry, Quantum Information (CMSP)**
- ❑ **Fundamentals of AI (QLS)**
- ❑ **"Edge" computing (STI)**

+ High-Performance Computing support team

The role of ICTP

Fostering science globally

Daniel's dream:
use AI to design new drugs from medicinal plants

Challenges:

- Lack of international collaborations & research ecosystems
- Limited «human capacity» in emerging fields (AI, Data Science, Quantum computing)
- Computational infrastructures (Africa's only facility in Top500 is 356th)
- Growing «divide» between developed and developing world

The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency

unesco United Nations Educational, Scientific and Cultural Organization

ICTP 1964–2024

International Symposium

The Future of Scientific Computing: A Global Perspective | (smr 4028)

27 May 2024

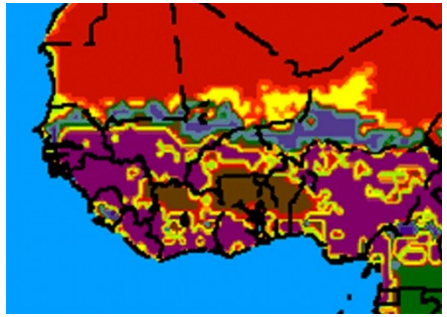
An ICTP 60th Anniversary Event

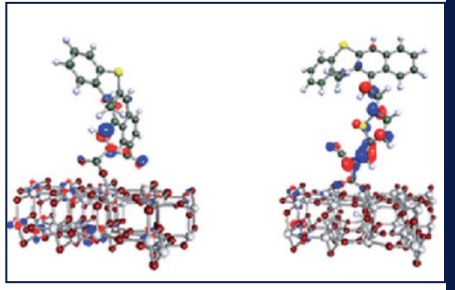
Launch of an *International Consortium for Scientific Computing* "ICOMP"

27/May/2024

Trieste, Italy

ICOMP's objectives





The **International Consortium for Scientific Computing** aims at:

- ✓ Creating a shared platform to seize the opportunities offered by new algorithms (ML, AI, BigData) and new hardware architectures
- ✓ Offering access to large-scale computational facilities
- ✓ Strengthening training programs and tie them to scientific collaborations & access to computer time
- ✓ Tackling selected scientific grand challenges (with impact on SDGs)

INTERNATIONAL CONSORTIUM FOR SCIENTIFIC COMPUTING

Building global capacity in scientific computing

[31 Mar – 4 Apr] Workshop on TinyML for Sustainable Development *(in Malawi)*

[5-16 May] Summer School on Theory, Mechanisms and Hierarchical Modelling of Climate Dynamics: Artificial Intelligence and Climate Modelling

[5-9 May] Conference on Mixing Times between Probability, Computer Science and Statistical Physics

[30 Jun – 11 July] Magurele Summer School for Computing in a Rapidly Evolving Society: Parallel Algorithms and Optimizations

[3-4 July] How creative is Generative AI? Perspectives from Science and Philosophy

[7-9 July] Youth in High-Dimensions: Recent Progress in Machine Learning, High-Dimensional Statistics and Inference

[11-18 July] Advanced School on Foundation Models for Scientific Discovery

[8-19 Sept] Advanced School on High-Performance Computing and Applied AI for High-Resolution Regional Climate Modeling (*at UM6P Benguerir, Morocco*)

[27 Oct – 7 Nov] School on Detector Signal Processing and Machine Learning for Scientific Instrumentation and Reconfigurable Computing

INTERNATIONAL CONSORTIUM FOR SCIENTIFIC COMPUTING

IBM-ICTP Collaboration

Prizes and advanced schools

Annual prize for **outstanding young researchers working in AI for science / science for AI**

Prize ceremony at ICTP on **10 July 2025 on the occasion of two schools on AI, sponsored by IBM**

“Richard Feynman Prize in Quantum Computing”

Prize ceremony at ICTP in summer **2026**, **on the occasion of a school on QC, also sponsored by IBM**

"Democratizing" access to computational resources

cecam
Centre Européen de Calcul Atomique et Moléculaire

Agreement with CECAM/EPFL to provide African scientists with computational resources made available by European Supercomputing Centers:

- ✓ CSCS – Switzerland
- ✓ CINECA – Italy
- ✓ Vega – Slovenia
- ✓ Jülich – Germany

UM6P University Mohammed VI Polytechnic

[In progress]
Collaboration with EU, CINECA, and Morocco for the establishment of an *AI factory* at UM6P in Benguerir (40 MEuro, of which 1 MEuro to ICTP for training and research collaborations)

Other ICOMP highlights

✓Agreements with South Africa and Brazil for mobility and joint activities

✓ ICTP joined GESDA's Open Quantum Institute

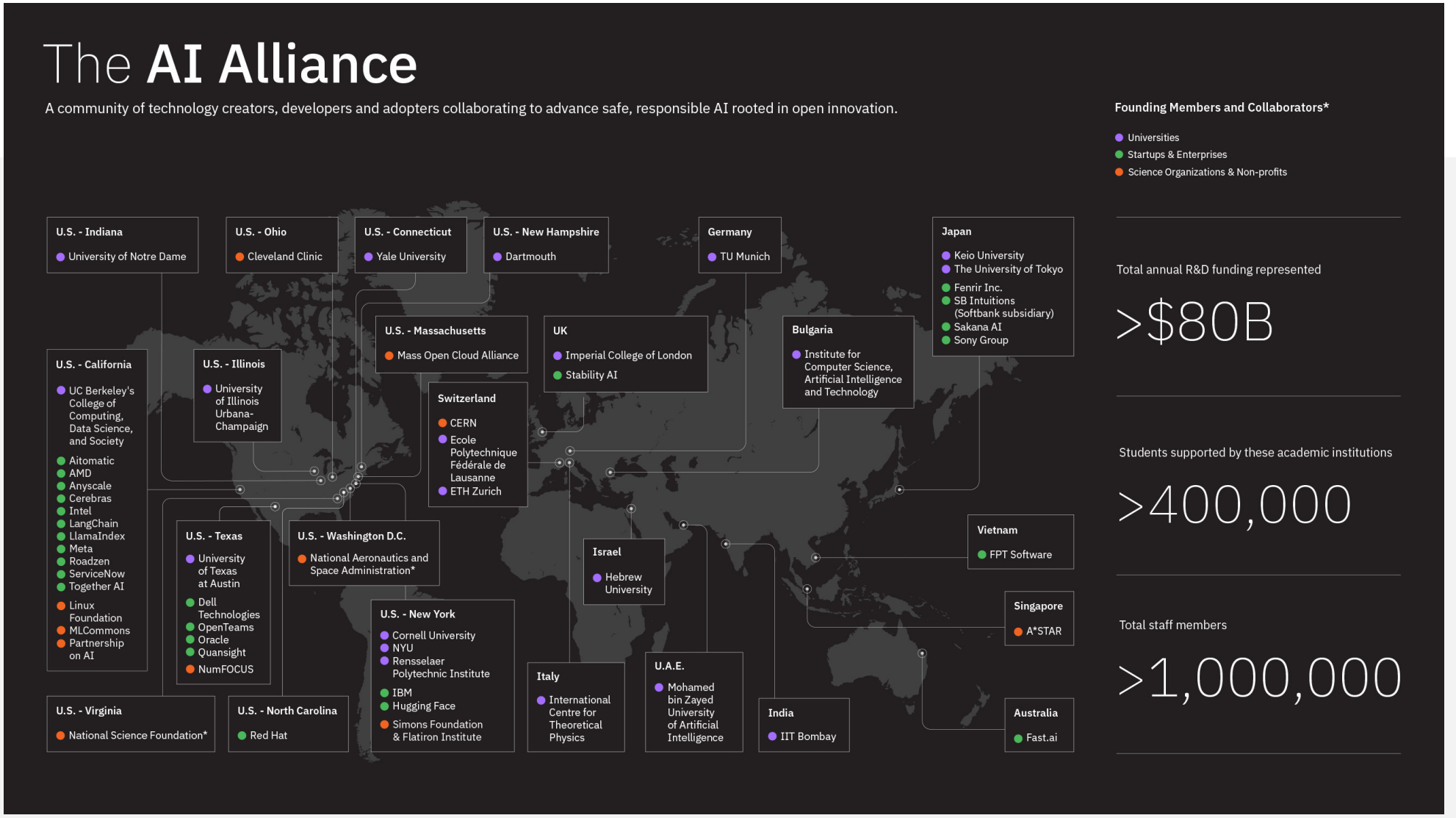
[April 2025]
ICTP joins *AgorAI*, a private-public partnership led by Generali, for R&D in AI and Data Science, with five academic partners and Fincantieri, illycaffè, Goldman Sachs, Deloitte, and Google.
Expected budget: ~10 MEuro/year

MARVEL

NATIONAL CENTRE OF COMPETENCE IN RESEARCH

2026 MARVEL/ICTP College on Computational Materials Science
(~250 students, 200 KEuro from MARVEL)

ICTP co-founds "AI Alliance" for responsible AI



Partners (so far)

SISSA
Scuola Internazionale Superiore di Studi Avanzati

NITheCS
National Institute for Theoretical and Computational Sciences

cecam
Centre Européen de Calcul Atomique et Moléculaire

CINECA

CHPC
CENTRE FOR HIGH PERFORMANCE COMPUTING

CSCS

QUANTINUUM

IBM

ICSC
Centro Nazionale di Ricerca in HPC, Big Data and Quantum Computing

MARVEL

BSC
Barcelona Supercomputing Center
Centro Nacional de Supercomputación

gesda

The AI Alliance

science & innovation
Department:
Science and Innovation
REPUBLIC OF SOUTH AFRICA

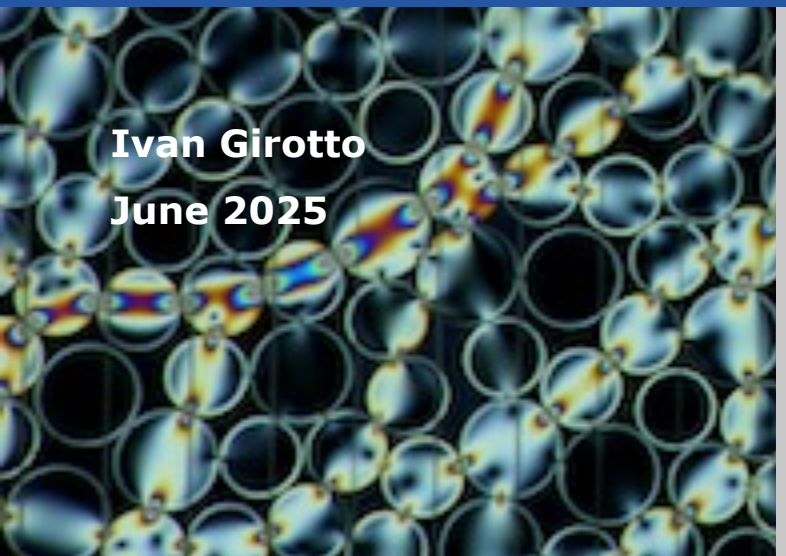
MINISTÉRIO DA CIÊNCIA, TECNOLOGIA E INOVAÇÃO

GOVERNO FEDERAL
BRASIL
UNIÃO E RECONSTRUÇÃO

CNPq
Conselho Nacional de Desenvolvimento Científico e Tecnológico

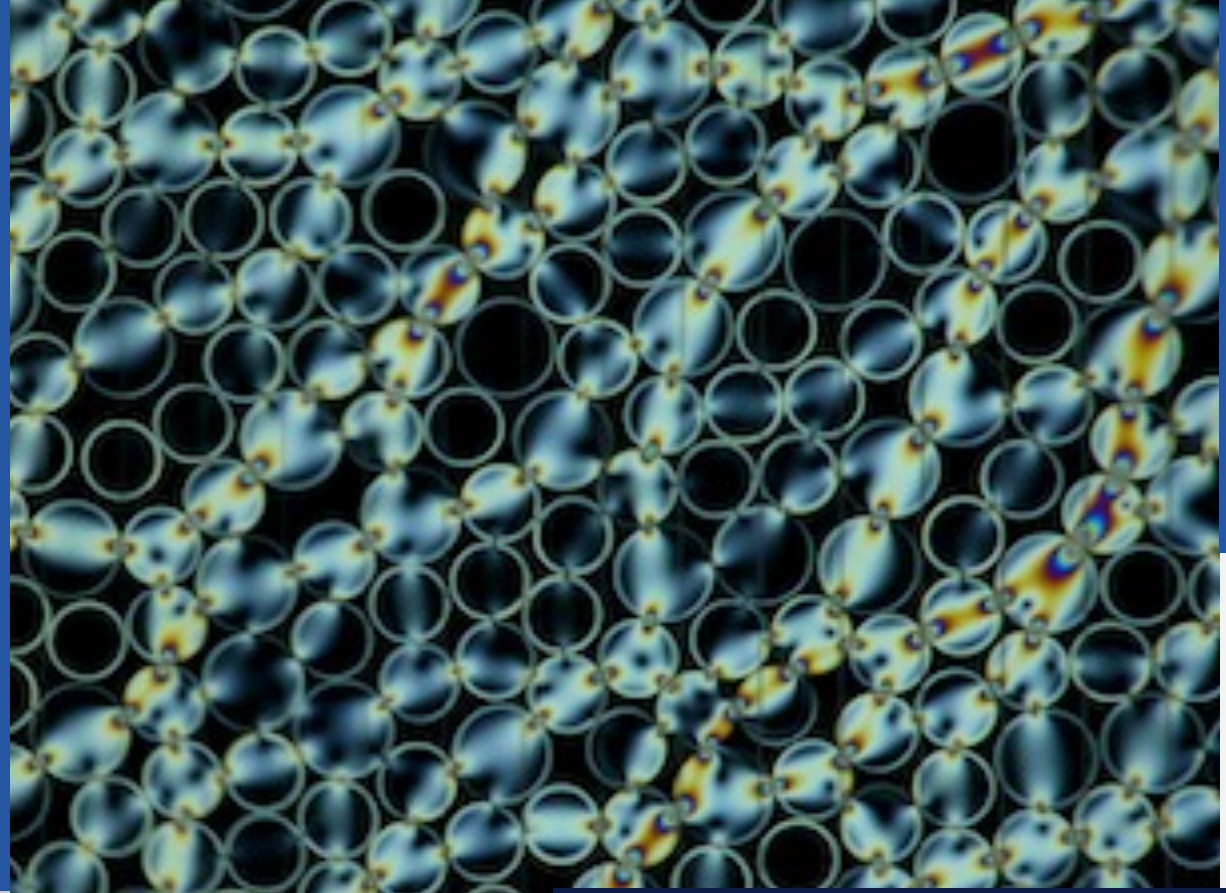
OQI
Open Quantum Institute

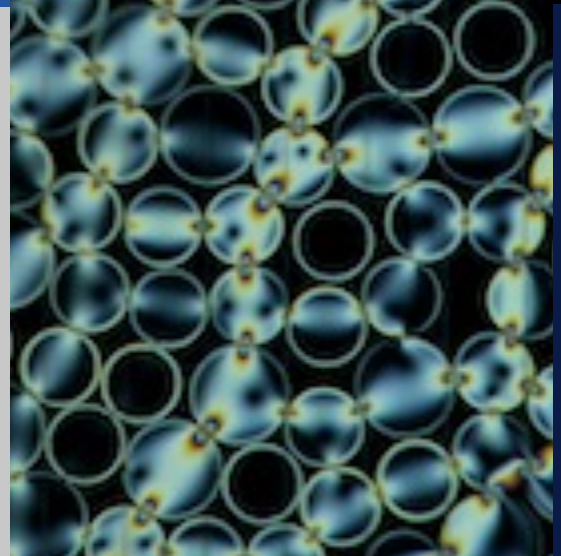
HPC 101



Ivan Girotto

June 2025





The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency

unesco United Nations Educational, Scientific and Cultural Organization

Why use Computers in Science?

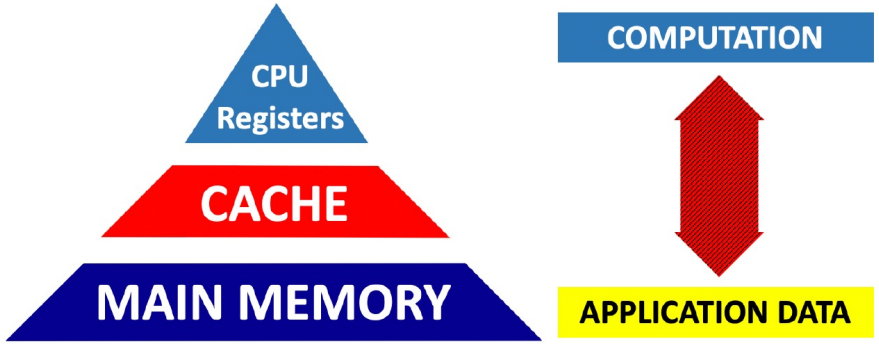
- Use complex theories without a closed solution: solve equations or problems that can only be solved numerically, i.e. by inserting numbers into expressions and analyzing the results
- Do “impossible” experiments: study (virtual) experiments, where the boundary conditions are inaccessible or not controllable
- Benchmark correctness of models and theories: the better a model/theory reproduces known experimental results, the better its predictions

What is High-Performance Computing (HPC)?

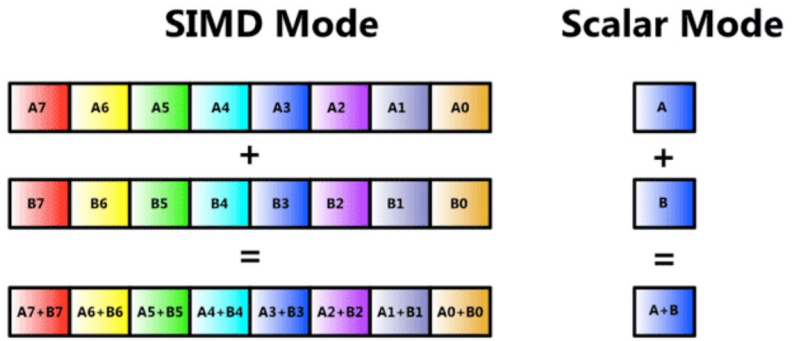
- Not a real definition, depends from the prospective:
  - HPC is when I care how fast I get an answer
  - HPC is when I foresee my problem to get bigger and bigger
- Thus HPC can happen on:
  - A workstation, desktop, laptop, smartphone!
  - A supercomputer
  - A Linux Cluster
  - A grid or a cloud
  - Cyberinfrastructure = any combination of the above
- HPC means also High-Productivity Computing

Key features of modern CPUs

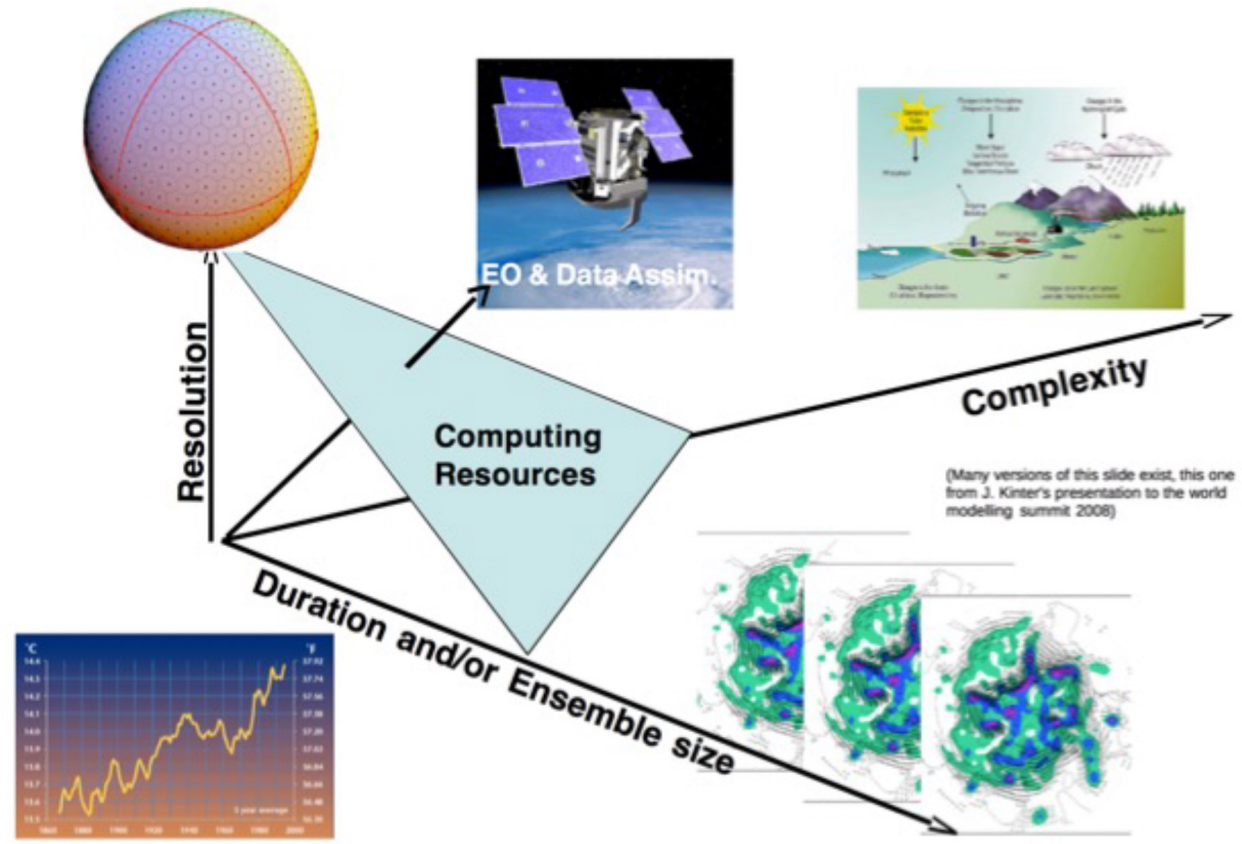
- Efficient data memory access patterns are crucial to best performances
  - design and development of computer algorithms that maximize data locality in time and space (data distance)

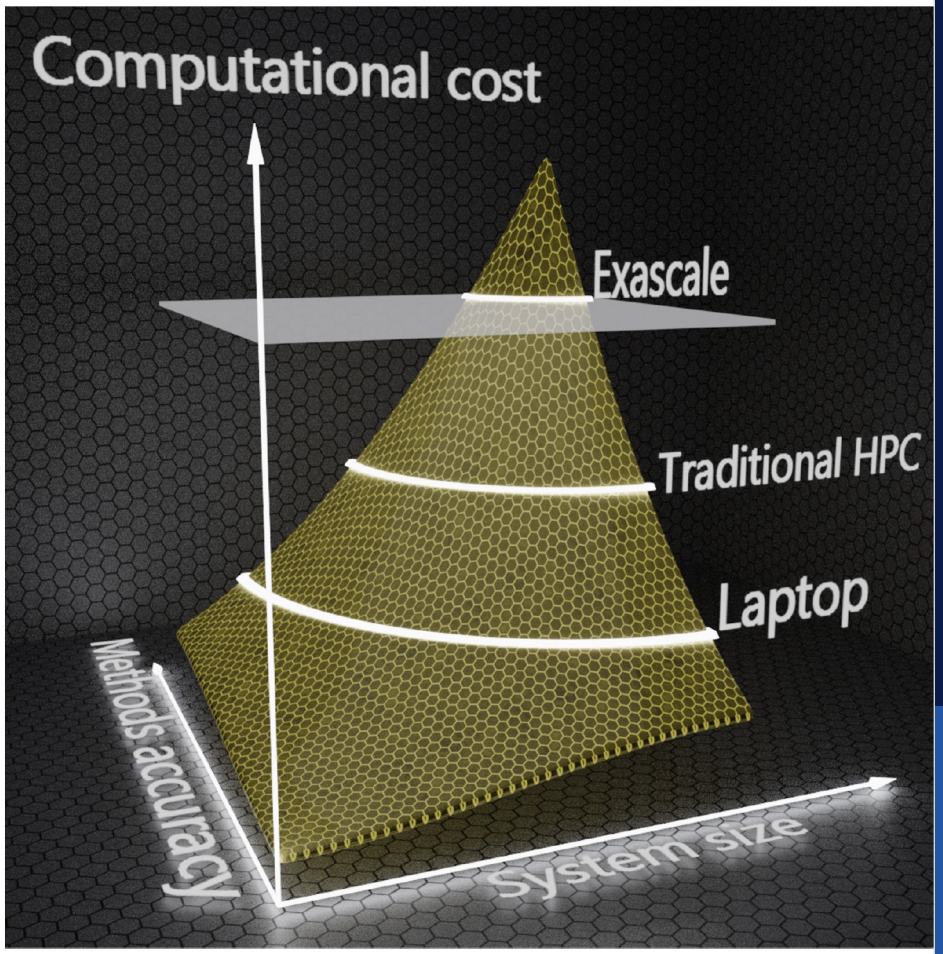


- Modern CPUs are equipped with vector registers and ALUs capable of multiple concurrent operations on multiple data
  - vectorization is aided by compilers, but requiring design and development of computer codes that maximize simple operations on contiguous data of the same type



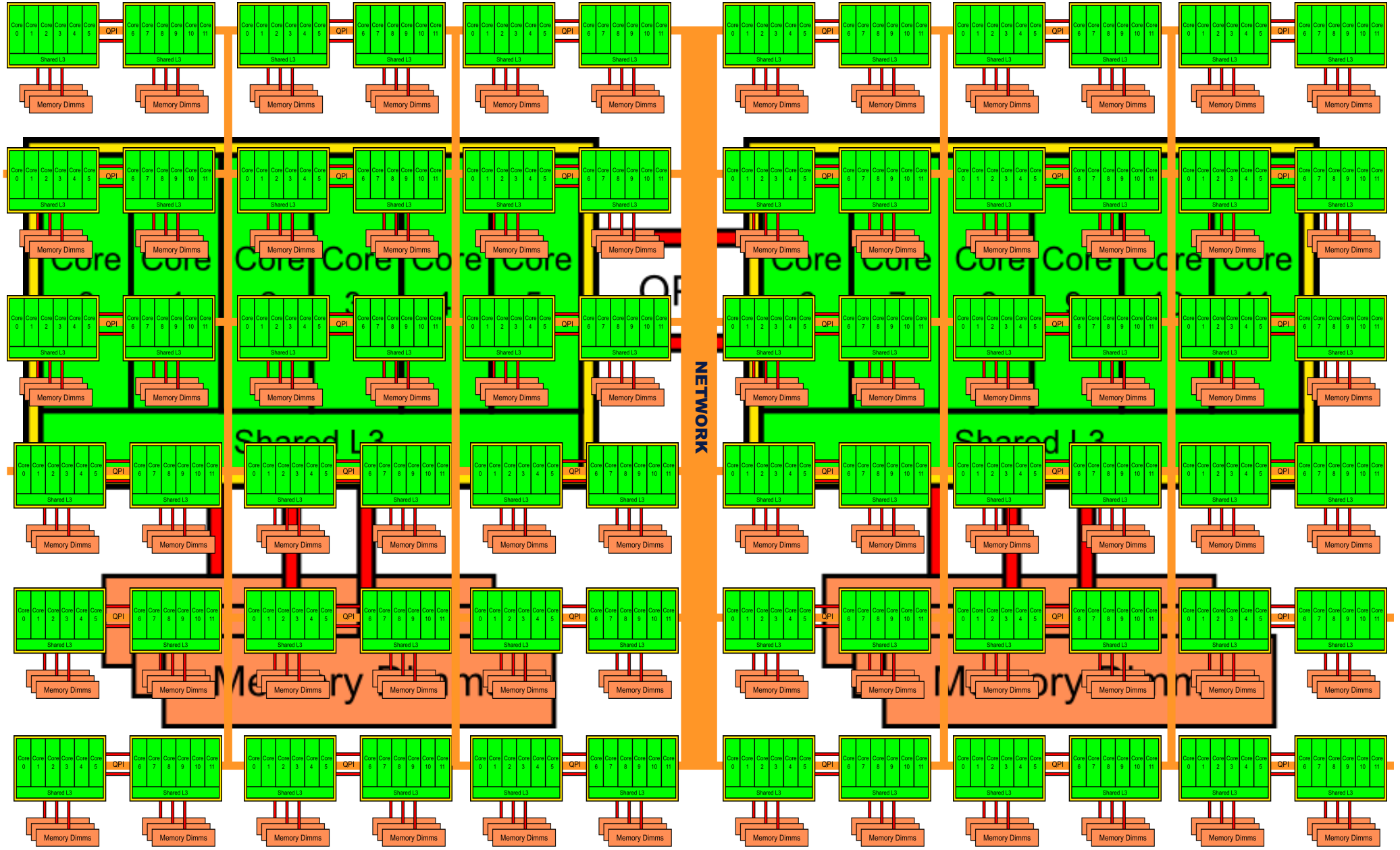
- When all CPU component work at maximum speed that is called *peak of performance* (Floating point operations per seconds FLOP/s)
  - Tech-spec normally describe the theoretical peak
  - Benchmarks measure the real peak
  - Applications show the real performance value
- Real performance are also mostly related to the memory bandwidth (GBytes/s)


EO & Data Assim.
Resolution
Computing Resources
Complexity
Duration and/or Ensemble size
(Many versions of this slide exist, this one from J. Kinter's presentation to the world modelling summit 2008)

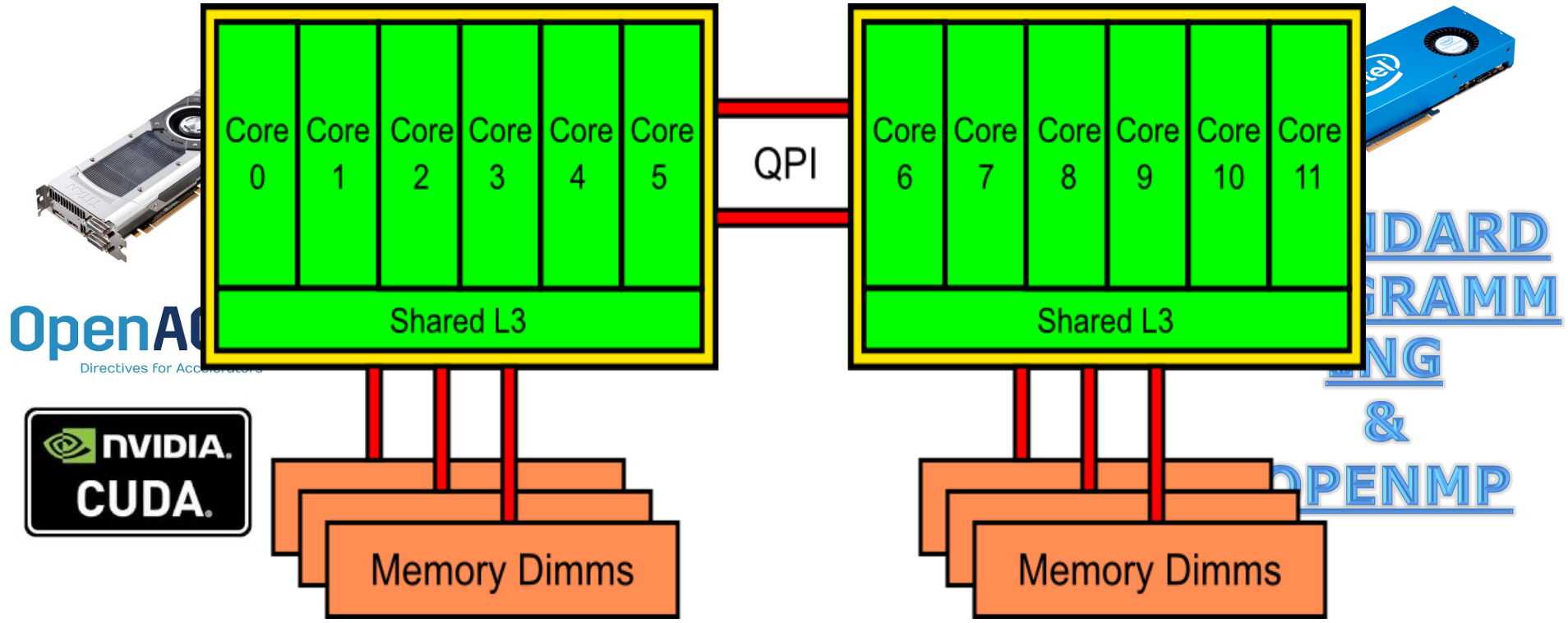

Computational cost
Exascale
Traditional HPC
Laptop
Methods accuracy
System size

Why would HPC matter to you?

- Scientific computing is becoming more important in many research disciplines
- Problems become more complex, thus need complex software and teams of researchers with diverse expertise working together
- HPC hardware is more complex, application performance depends on many factors
- Technology is also for increasing competitiveness
- HPC knowledge is an opportunity


NETWORK

Multiple Socket CPUs + Acceleretors



Design of Parallel Algorithm

- A serial algorithm is a sequence of basic steps for solving a given problem using a single serial computer
- Similarly, a parallel algorithm is a set of instruction that describe how to solve a given problem using multiple (>=1) parallel processors
- The parallelism add the dimension of concurrency. Designer must define a set of steps that can be executed simultaneously!!!
- Identify portions of the work that can be performed concurrently
- Mapping the concurrent pieces of work onto multiple processes running in parallel
- Distributing the input, output and intermediate data associated within the program
- Managing accesses to data shared by multiple processors
- Synchronizing the processors at various stages of the parallel program execution

Scalability

- When we want consider the scalability of our problem we are interested in two main features:
  - how much faster do we go increasing the number of processes for a fixed problem size (strong scaling)
  - how does the application behave if we increase the problem size keeping the workload fixed per processors

How do we evaluate the improvement?

- We want estimate the amount of the introduced overhead => $T_o = n_{pes}T_P - T_S$
- But to quantify the improvement we use the term **Speedup**:

$$S_P = \frac{T_S}{T_P}$$

Type of Parallelism

- **Functional (or task) parallelism**:

different people are performing different task at the same time

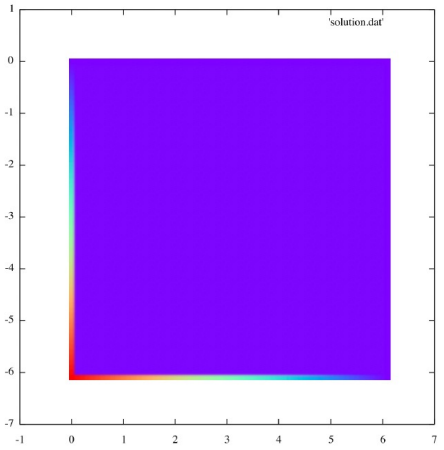
- **Data Parallelism**:

different people are performing the same task, but on different equivalent and independent objects

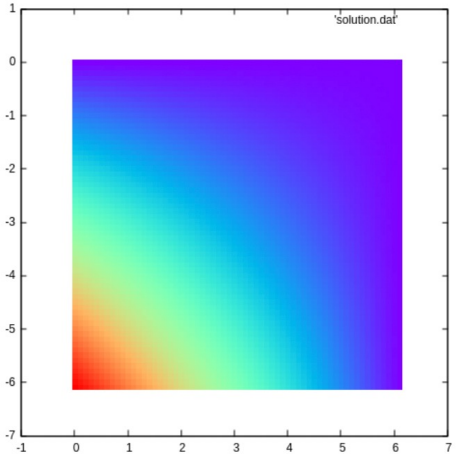
Process Interactions

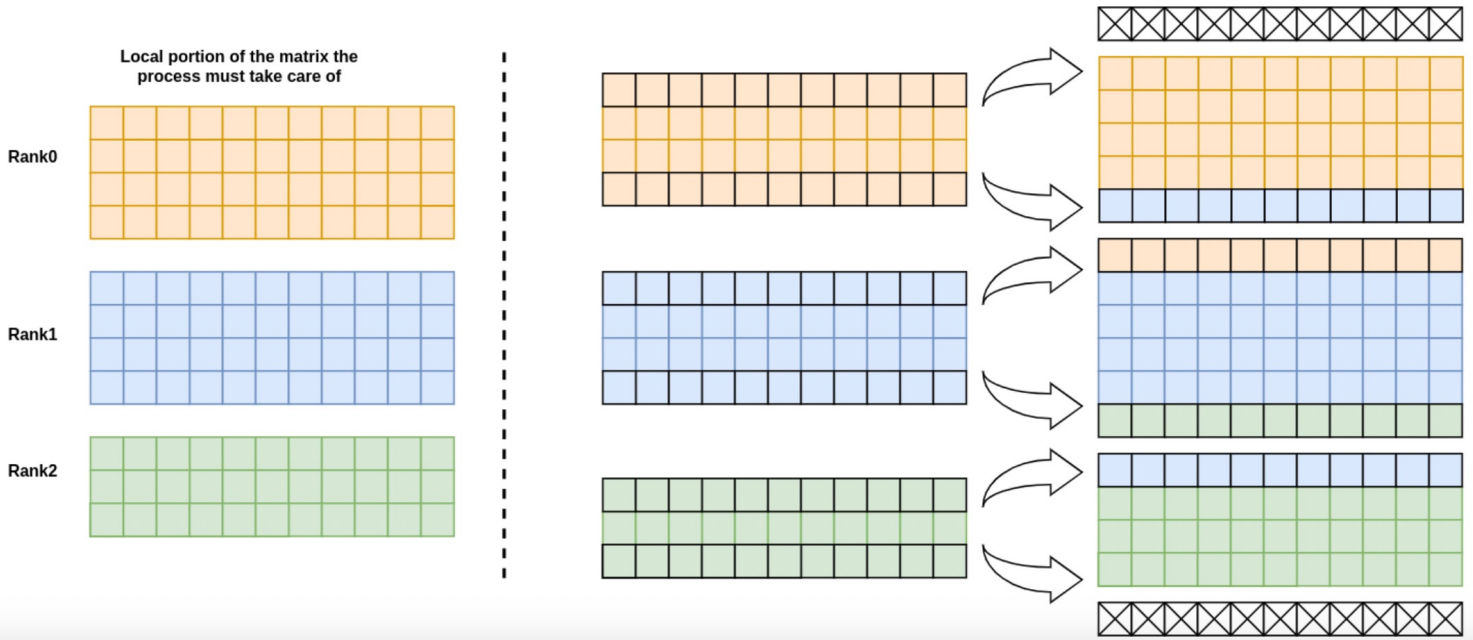
- The effective speed-up obtained by the parallelization depend by the amount of overhead we introduce making the algorithm parallel
- There are mainly two key sources of overhead:
    1. Time spent in inter-process interactions (**communication**)
    2. Time some process may spent being idle (**synchronization**)

Parallel Efficiency: Jacoby example



$$\frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} = 0$$



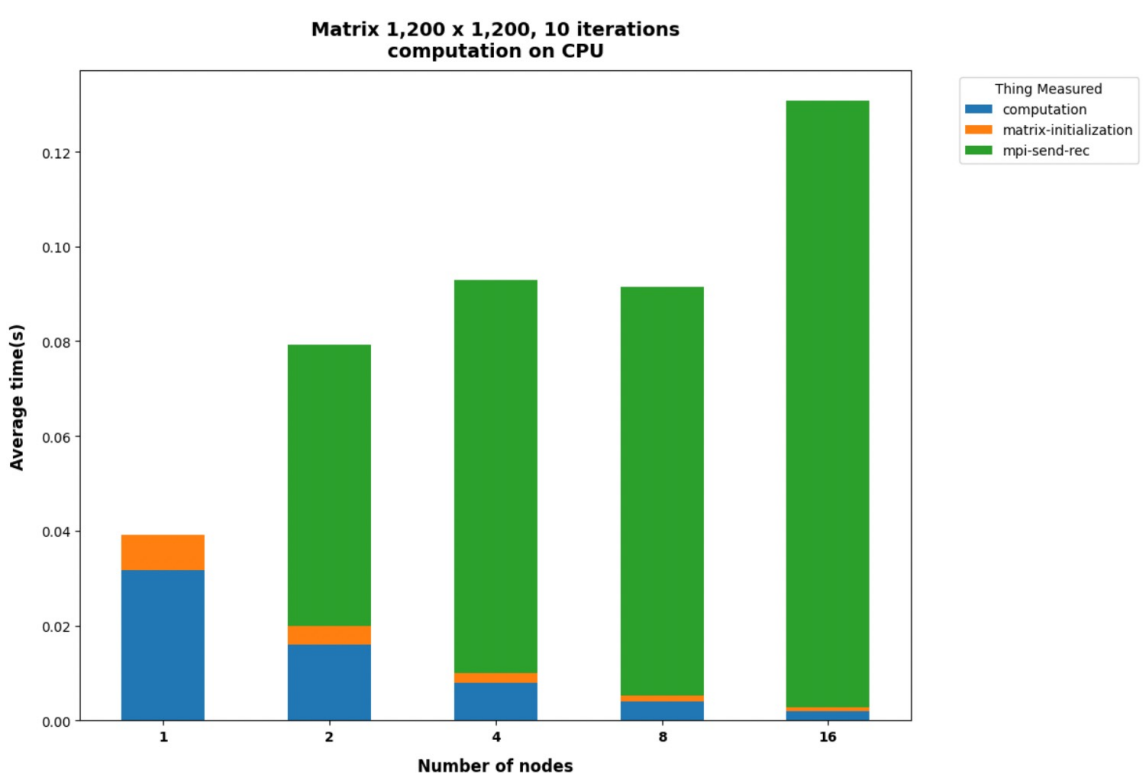


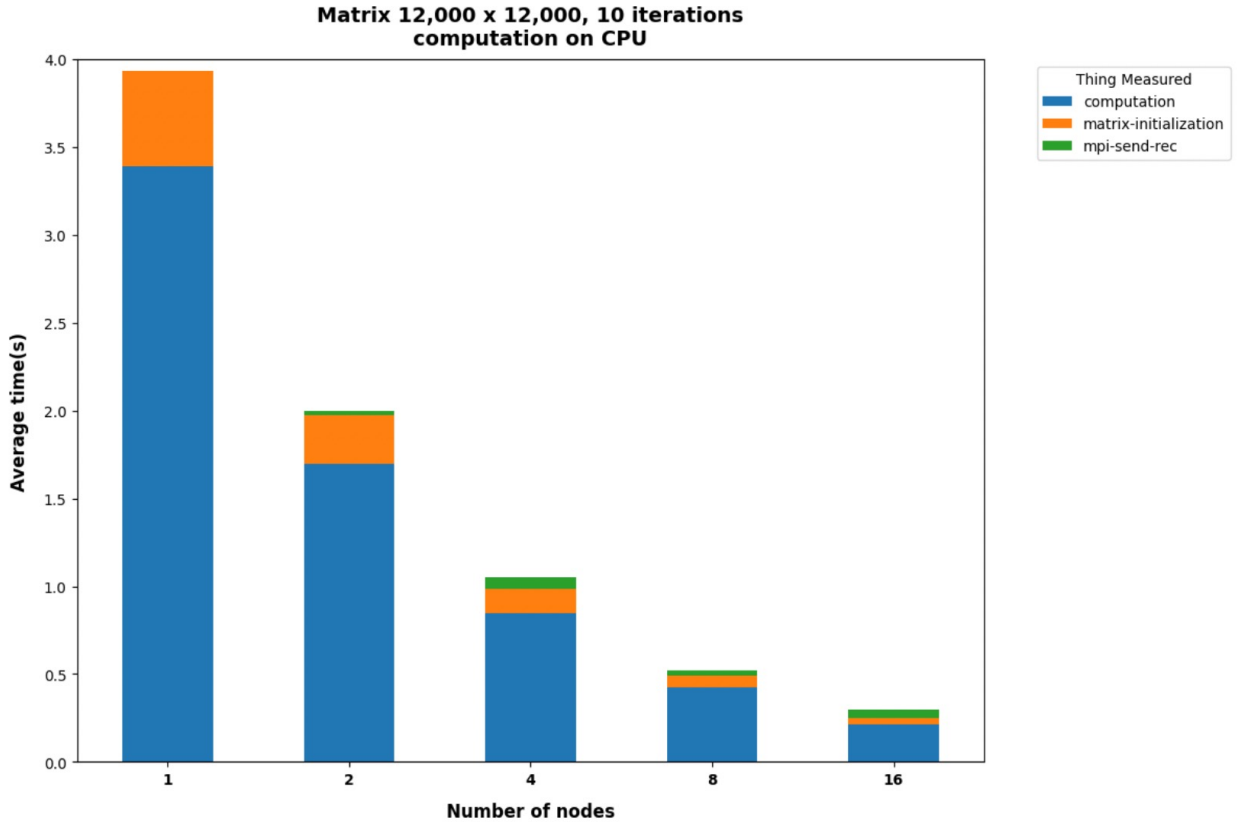
$$V_{i,j}^{new} = 0.25(V_{i+1,j} + V_{i-1,j} + V_{i,j+1} + V_{i,j-1})$$

0	0	0	0	0	0	0	0	0	0	0
10										0
20										0
30			$V_{i+1,j}$							0
40		$V_{i,j-1}$	$V_{i,j}$	$V_{i,j+1}$						0
50			$V_{i-1,j}$							0
60										0
70										0
80										0
90										0
100	90	80	70	60	50	40	30	20	10	0

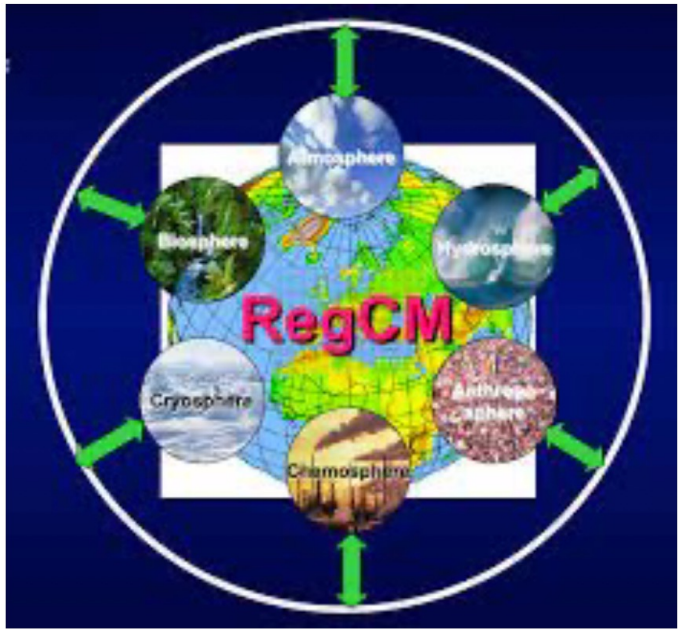
Figure 1: A diagram of the Jacobi Relaxation for Solving the Laplace's Equation on an evenly spaced 9x9 grid with the boundary conditions outlined in the text above.

Parallel Efficiency: Jacoby example





High-performance codes



FFTW

OpenFOAM®

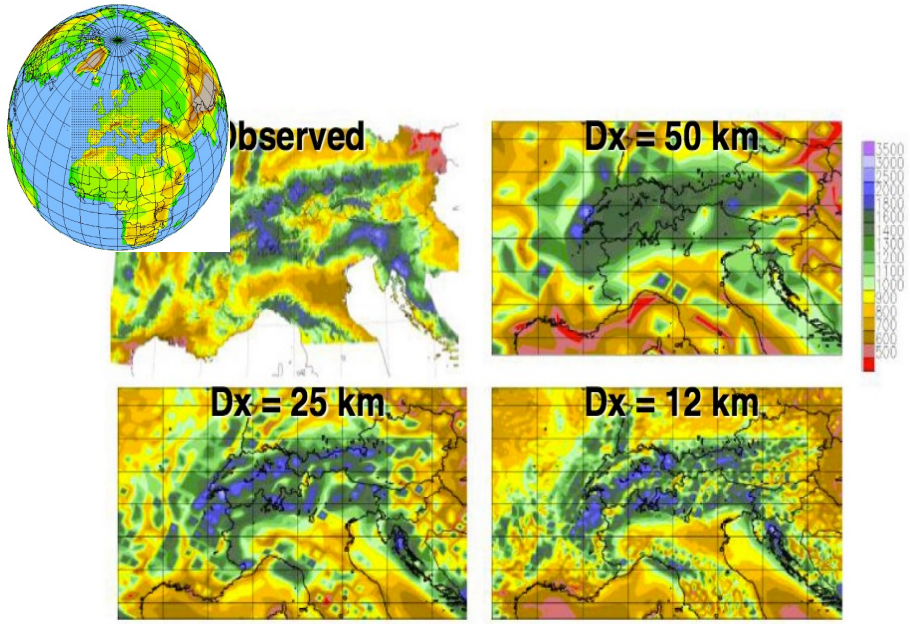
Yambo

QUANTUMESPRESSO

OpenBLAS

LAMMPS
Large-scale Atomic/Molecular Massively Parallel Simulator

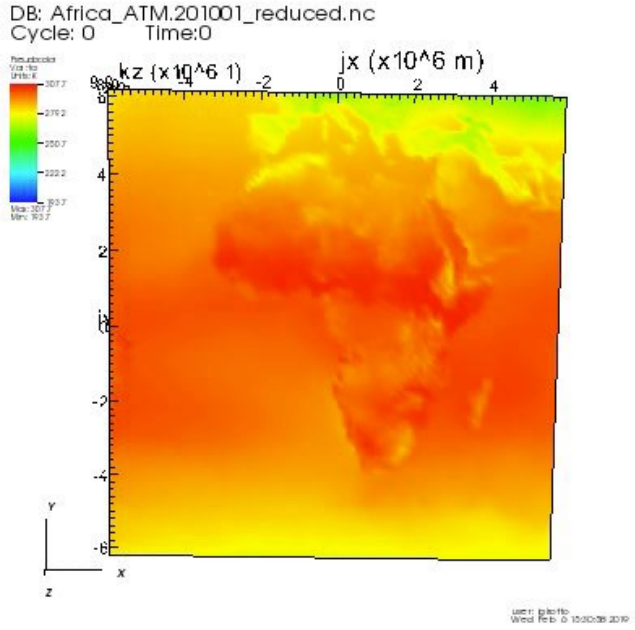
Large Scale Computer Simulations @ ICTP



- ICTP contributes to the IPCC report
- The RegCM code is developed and maintained by the ESP group @ ICTP
- The model is performed on several domains covering most of the world's land

[…] for Europe, we plan to run seven 140 year simulations. Each month of simulation, with 500 processors, is expected to take about 2.9 hours of compute time and produce 60GB of raw output files

The on-going simulations, planned to end in early 2020, is expected to finally require about 100M cpu-h and approximately 2PB of data will be publicly made available

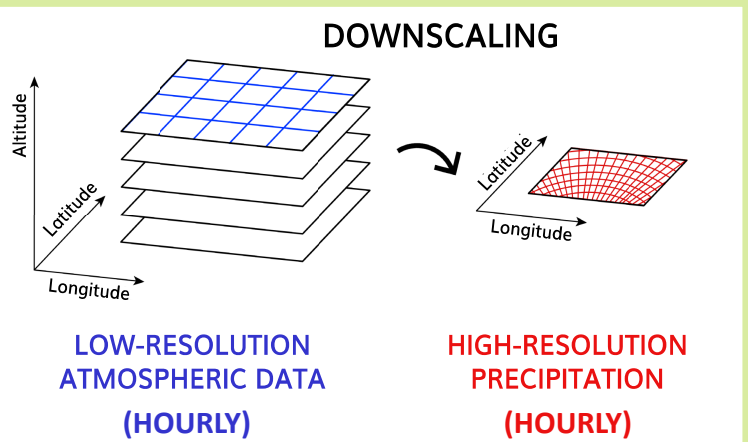


DL 4 Climate @ICTP (P.I. E. Coppola, collaborator: S. Di Gioia)

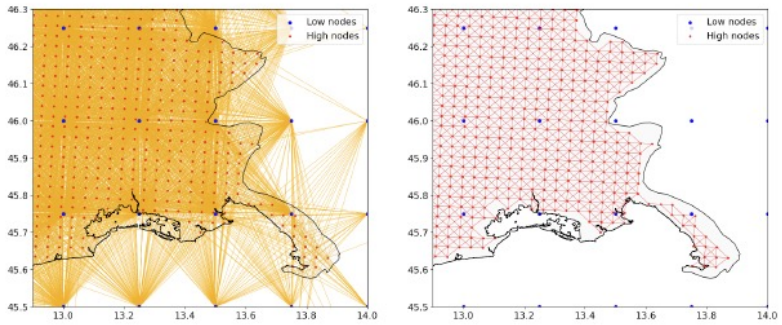
Blasone V., Coppola E., Sanguinetti G., Arora V., Di Gioia S., and Bortolussi L.
A deep learning framework to efficiently estimate precipitation at the convection permitting scale. In ICLR 2024 Workshop on Tackling Climate Change with Machine Learning, 2024.

Idea: Use DL to emulate the km-scale climate model for producing very high-resolution precipitation projections

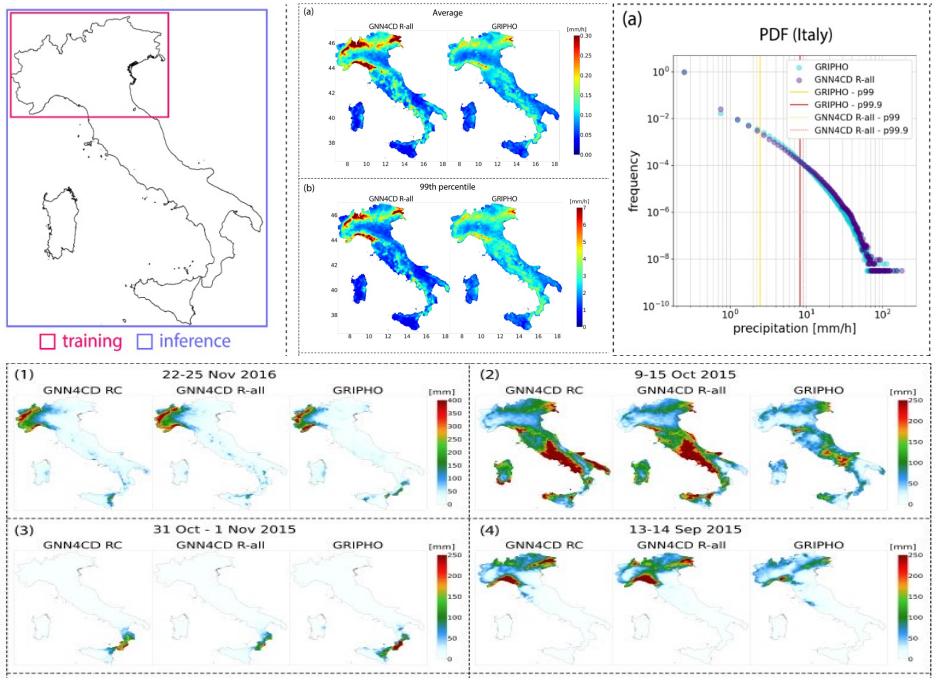
Problem



Model: GNN regressor



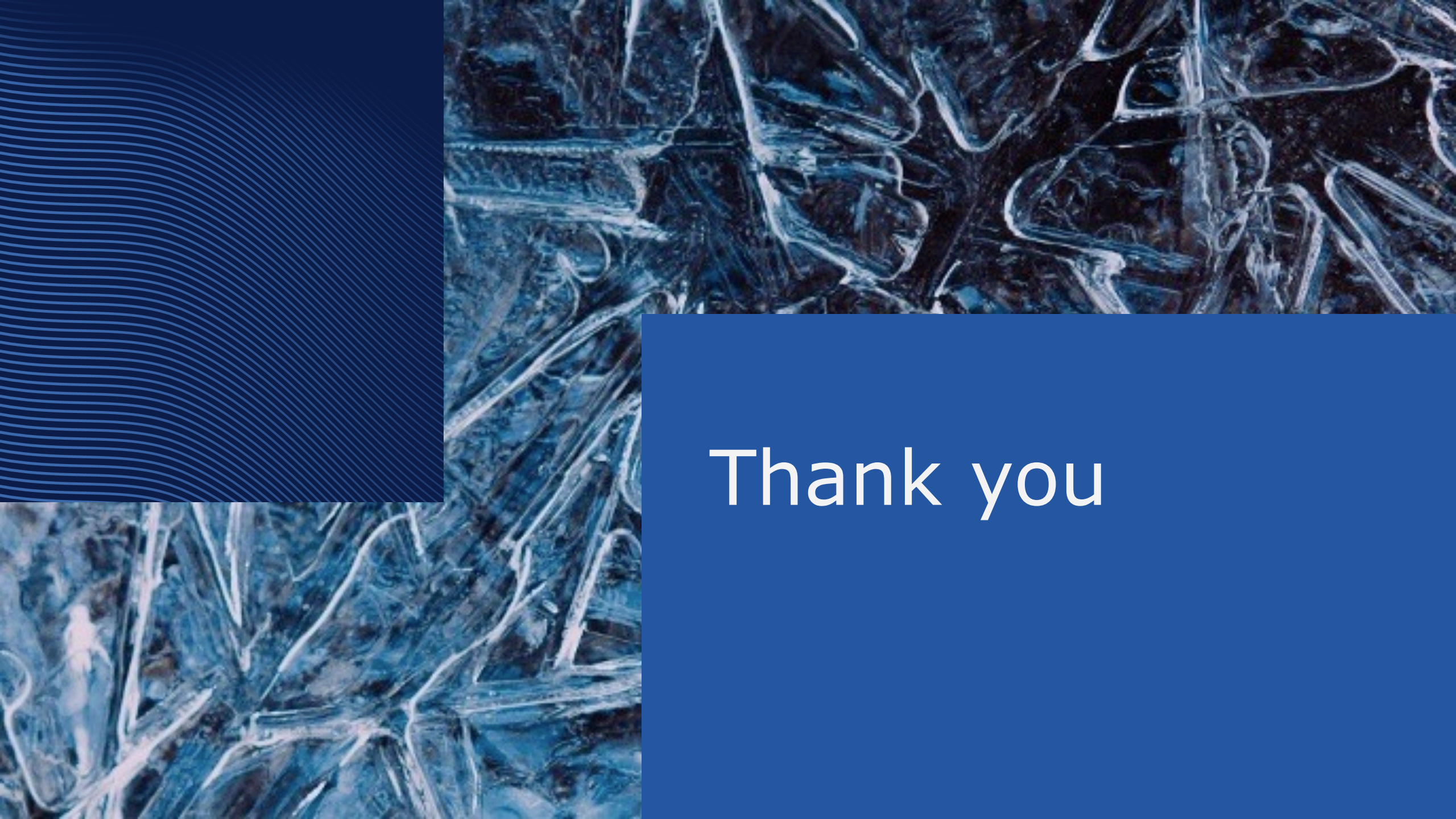
Results



Goal

increase the ensemble size of high-resolution regional climate projections with computationally cost/energy efficient solutions

H2020-LC-CLA-2020-2



Thank you