Applied Scientific Computing at ICTP in the Era of the AI

Ivan Girotto

March 2026

**USC-C General Assembly**

ABDUS SALAM 100 YEARS

ICTP The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency

unesco United Nations Educational, Scientific and Cultural Organization
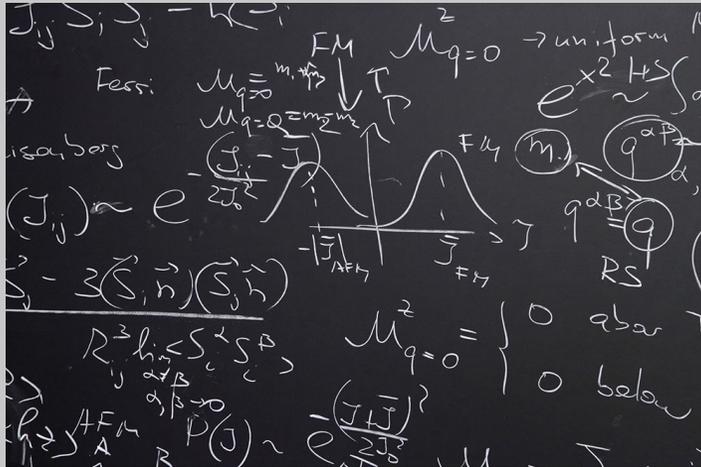
What is ICTP?

- 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.
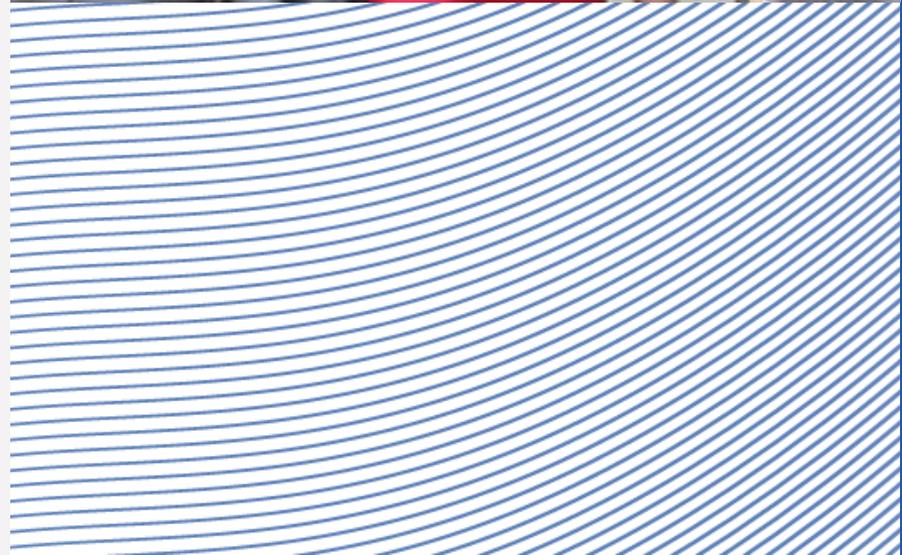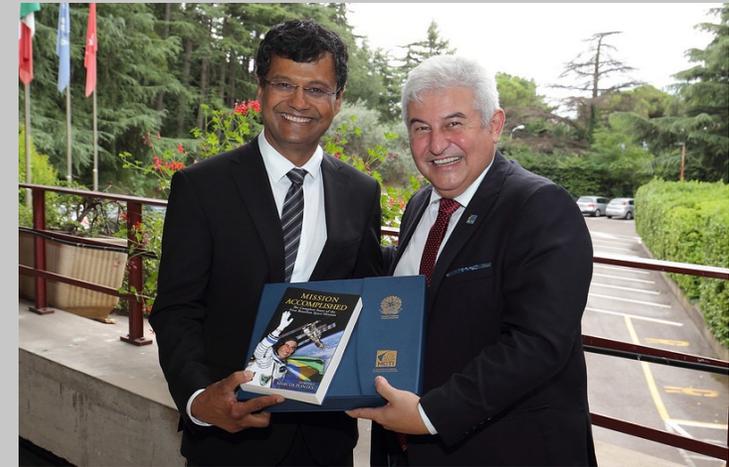
What is ICTP?

Research   **Education**   **Cooperation**

ICTP SCIENTIFIC OUTREACH

ICTP Impact 2024

Legend:

| 04 | ICTP Partner Institutes | ICTP |
17	ICTP Schools, Workshops and Conferences (outside of Trieste)	S
05	ICTP-EAU Affiliated Centres	C
05	ICTP-EAU Networks	N
13	ICTP-EAU Scientific Meetings	M
31	Physics Without Frontiers Activities	P

ICTP: An International Hub for Scientific Networking

- Organises about **60** conferences & workshops each year.

- Welcomes up to more than **5,000** scientists from **150+** nations each year.

- Attracts an additional **1,000–2,000** scientists per year through hosted activities.
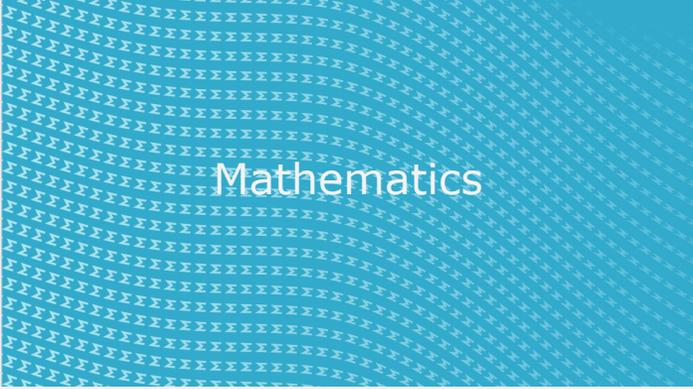
Research Sections
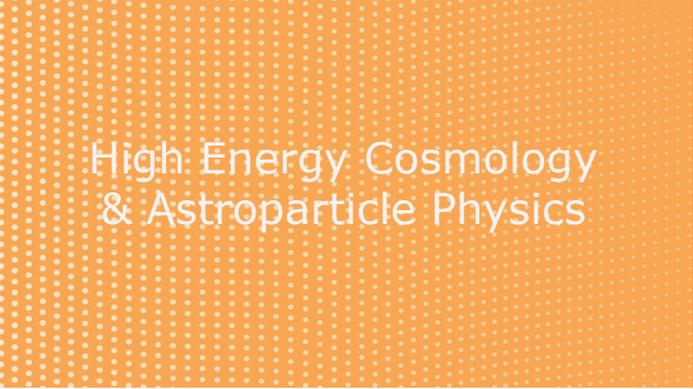
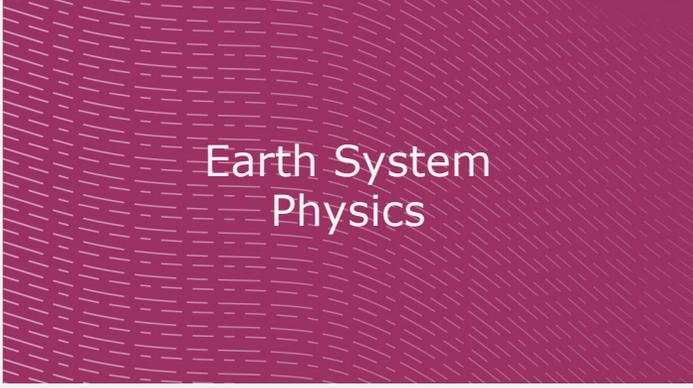High Energy Cosmology & Astroparticle Physics
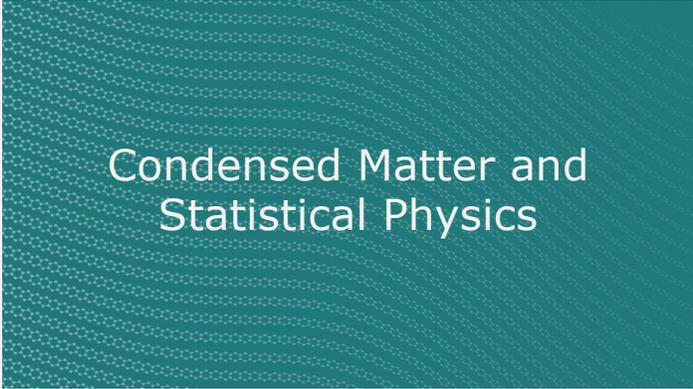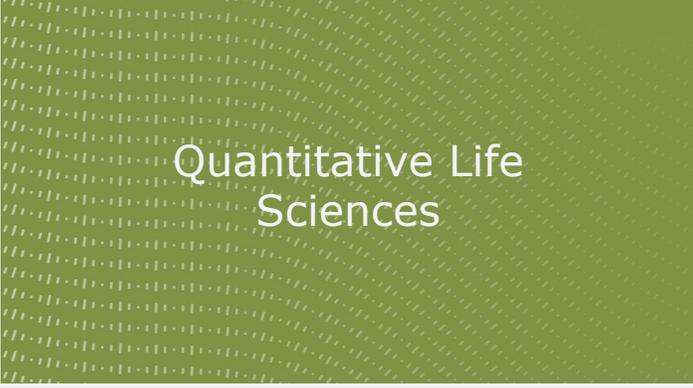
Condensed Matter and Statistical Physics

Mathematics

Science, Technology and Innovation
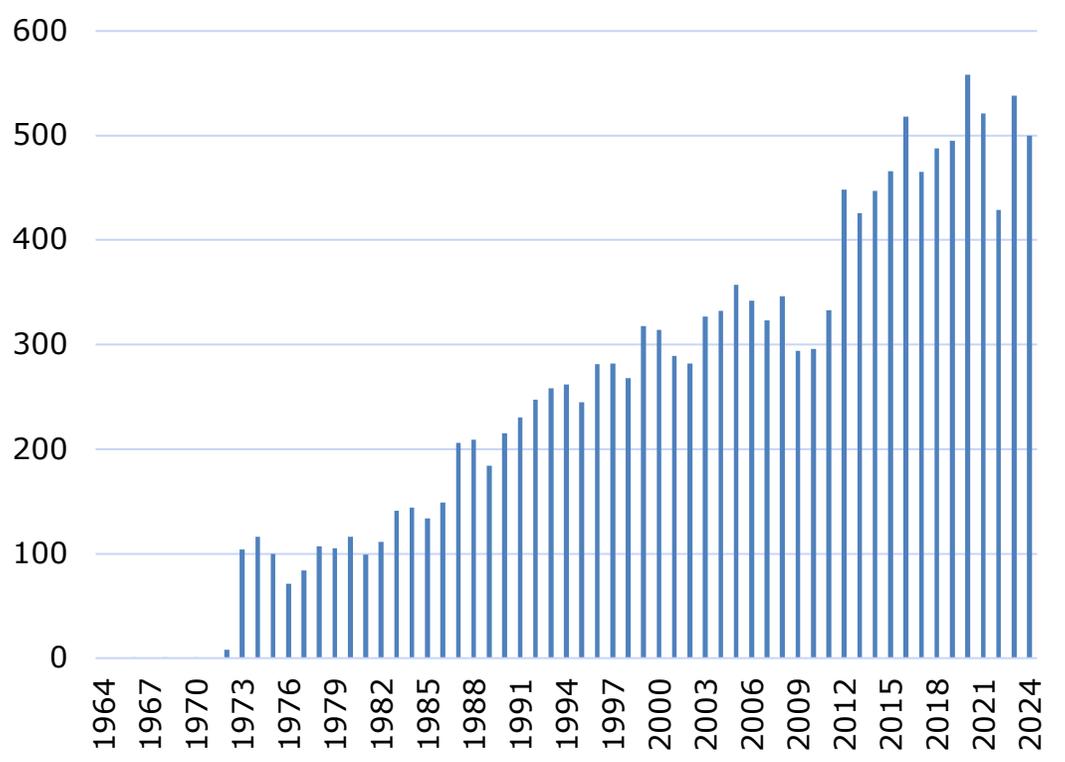
Earth System Physics

Quantitative Life Sciences

Also: Sustainable Energy, Scientific Computing and Medical Physics

RESEARCH AT ICTP

Papers produced within ICTP

Papers listed by final publication year

Citations of ICTP papers
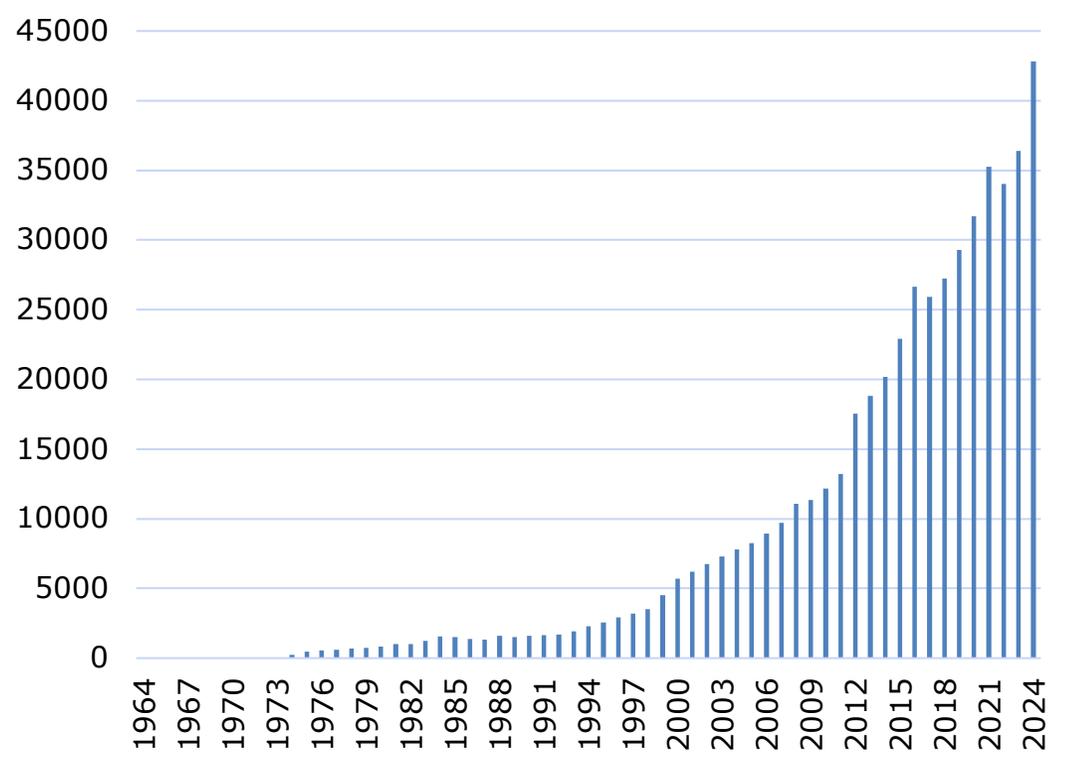
Regional Climate Models

What they are

- Computer programs performing a physical down-scaling over a limited domain region of the Earth

- Numerical discretized equations solved in a full 3D flattened box domain

- High resolution (50km - 1km).

- Limited Area Models

- Driven by a GCM simulation at the domain borders

- Same physical basis as global models.

GLOBAL MODEL — DOWNSCALING High-ressolution regional climate modeling — CONVECTIVE STORMS

Global model
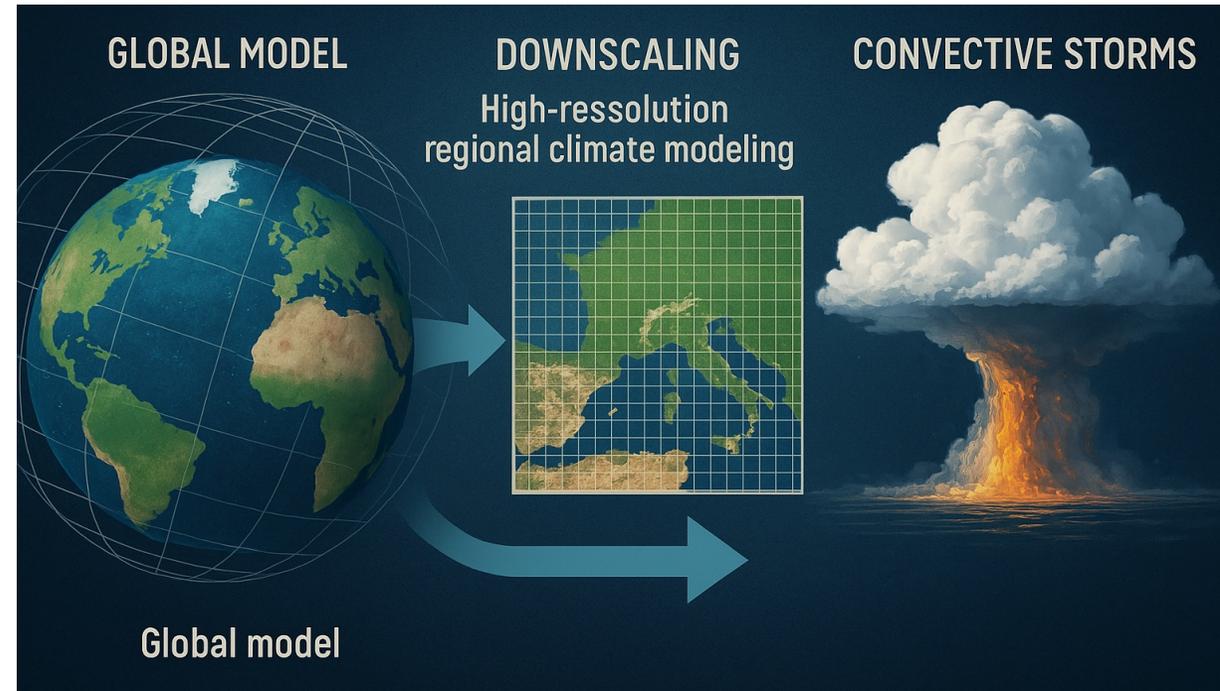
Erika Coppola (head of section) and ESP group @ ICTP

High-Resolution Kilometer-Scale Regional Climate Modeling
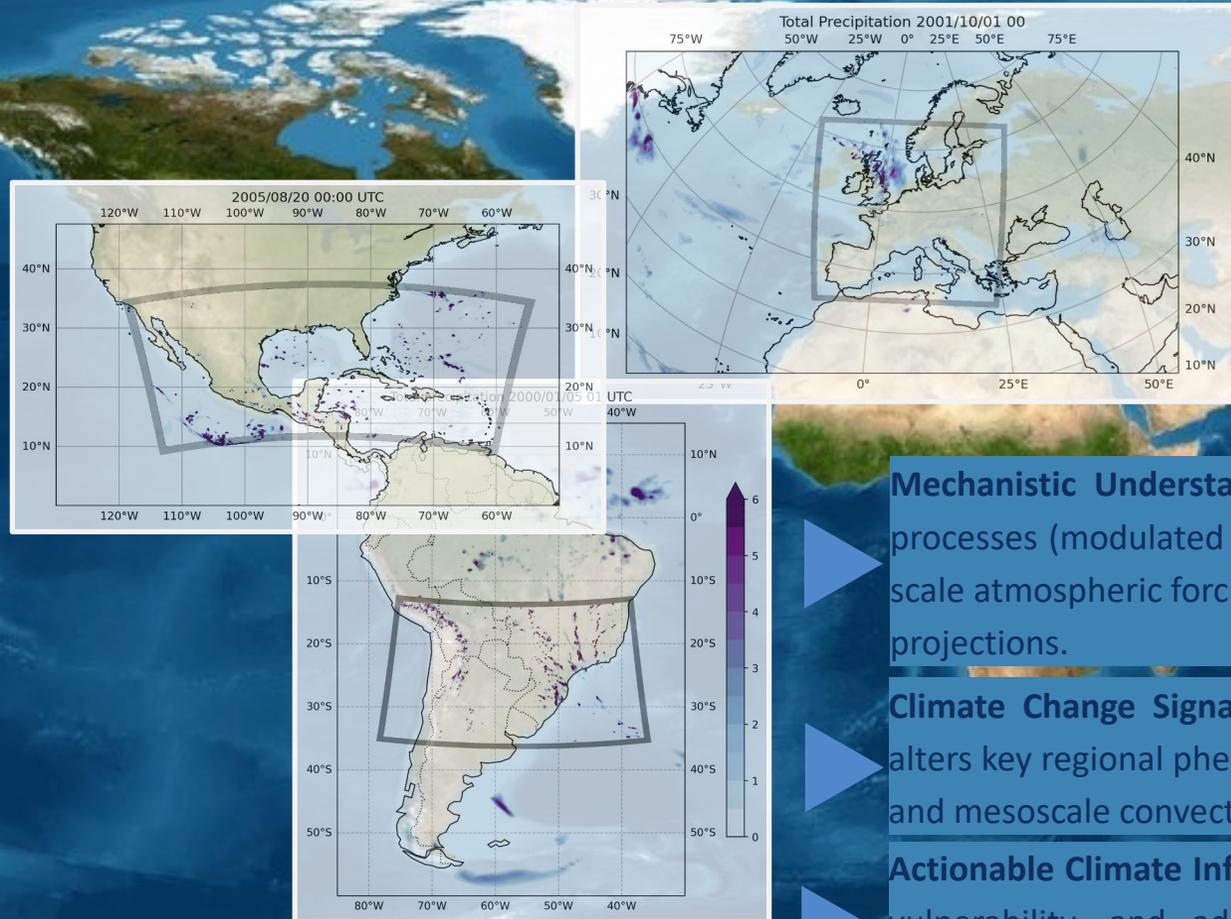
Mechanistic Understanding – To unravel the interactions between fine-scale processes (modulated by topography and land surface heterogeneity) and large-scale atmospheric forcings, which are critical for reducing uncertainties in climate projections.

Climate Change Signal Assessment – To evaluate how global climate change alters key regional phenomena, such as extreme precipitation, convective storms, and mesoscale convective systems, which are poorly resolved in coarser models.

Actionable Climate Information – To generate decision-relevant data for impact, vulnerability, and adaptation assessments, supporting policymakers, urban planners, and stakeholders in climate resilience planning.

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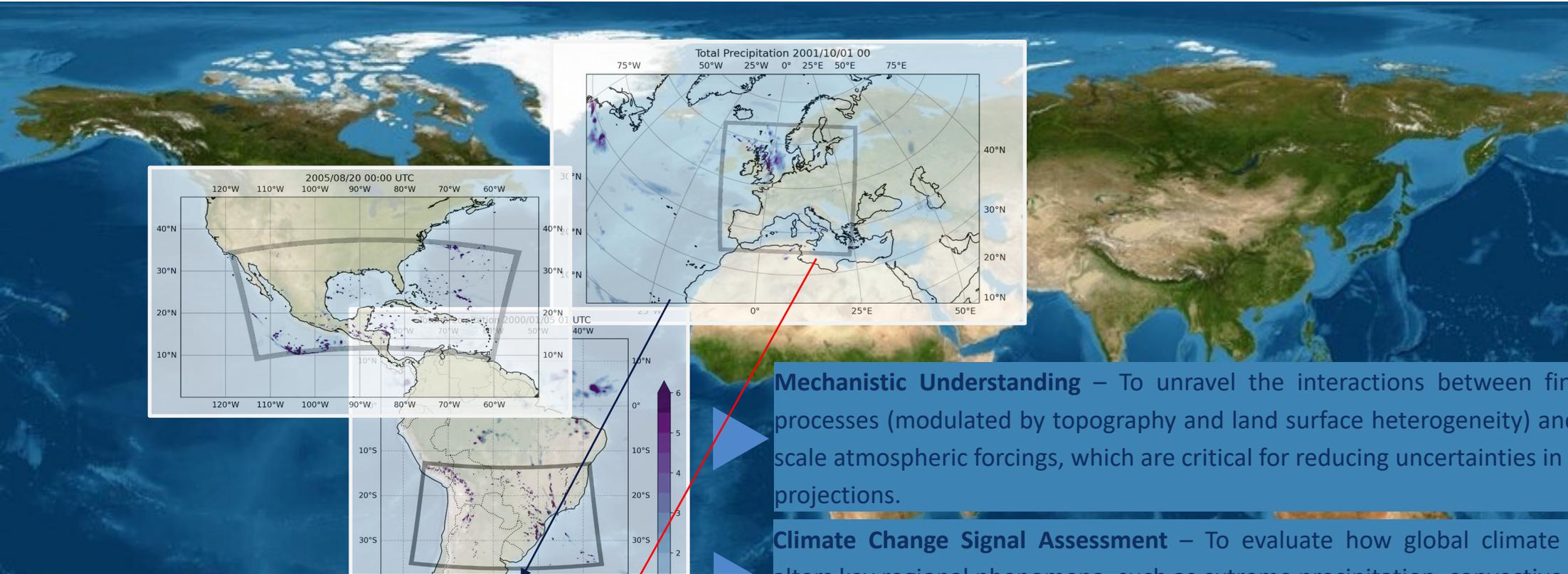# High-Resolution Kilometer-Scale Regional Climate Modeling

Mechanistic Understanding – To unravel the interactions between fine-scale processes (modulated by topography and land surface heterogeneity) and large-scale atmospheric forcings, which are critical for reducing uncertainties in climate projections.

Climate Change Signal Assessment – To evaluate how global climate change alters key regional phenomena, such as extreme precipitation, convective storms, which are poorly resolved in coarser models.

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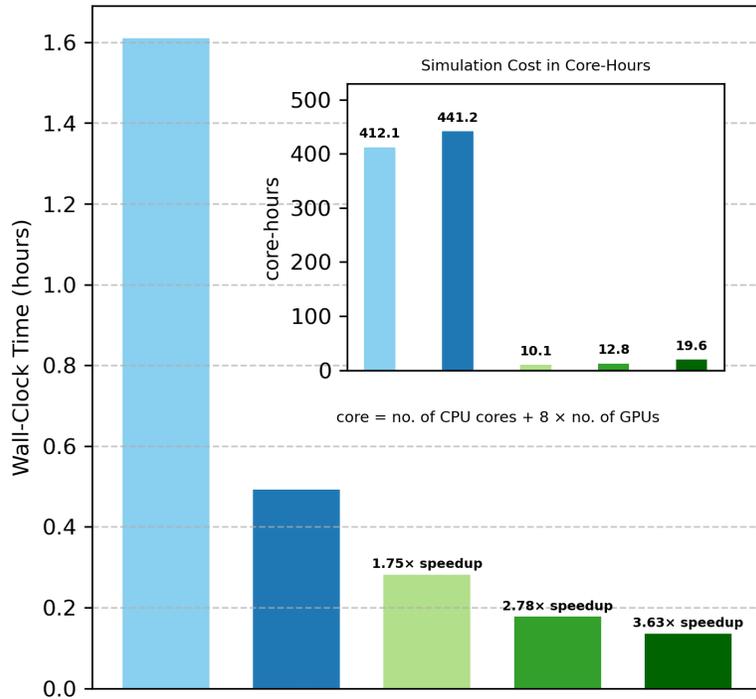
Domain		CPU h per year	Raw output per year (Tb)
EUR	12 km	7500 h	1 T
CP domain		CPU h per year	Raw output per year (Tb)
EUR -	3km	207000 h	8.8

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Enabling of the ICTP RegCM to GPUs

- Need of reducing the computational time for high resolution climate projections
- Optimal exploitation of the new HPC facility available at CINECA: Leonardo

Legend (left chart):
- 8 Booster nodes: 256 CPU cores - 0 GPUs
- 8 DCGP nodes: 896 CPU cores - 0 GPUs
- 1 Booster node: 4 CPU cores - 4 GPUs
- 2 Booster nodes: 8CPU cores - 8 GPUs
- 4 Booster nodes: 16CPU cores - 16 GPUs

Performance of the RegCM5 in RCE configuration on a 512x1024x60 Grid Size.

Simulation Cost in Core-Hours: 412.1, 441.2, 10.1, 12.8, 19.6

core = no. of CPU cores + 8 × no. of GPUs

1.75× speedup, 2.78× speedup, 3.63× speedup

Legend (right chart):
- 2 DCGP nodes: 200 CPU cores - 0 GPUs
- 4 DCGP nodes: 400 CPU cores - 0 GPUs
- 8 DCGP nodes: 800 CPU cores - 0 GPUs
- 1 ACC MN-5 node: 4 CPU cores - 4 GPUs
- 2 ACC MN-5 nodes: 8 CPU cores - 8 GPUs
- 4 ACC MN-5 nodes: 16 CPU cores - 16 GPUs

Performance of the RegCM5-CLM4.5 Coupled Configuration on a 1000x1000x50 Grid for 7 model days.

0.23x, 0.51x, 1.00x, 0.60x, 1.26x, 3.49x

Interdishiplinary effort between ESP group and HPC experts from ICTP, NVIDIA, Master in HPC students (Christian Tica)
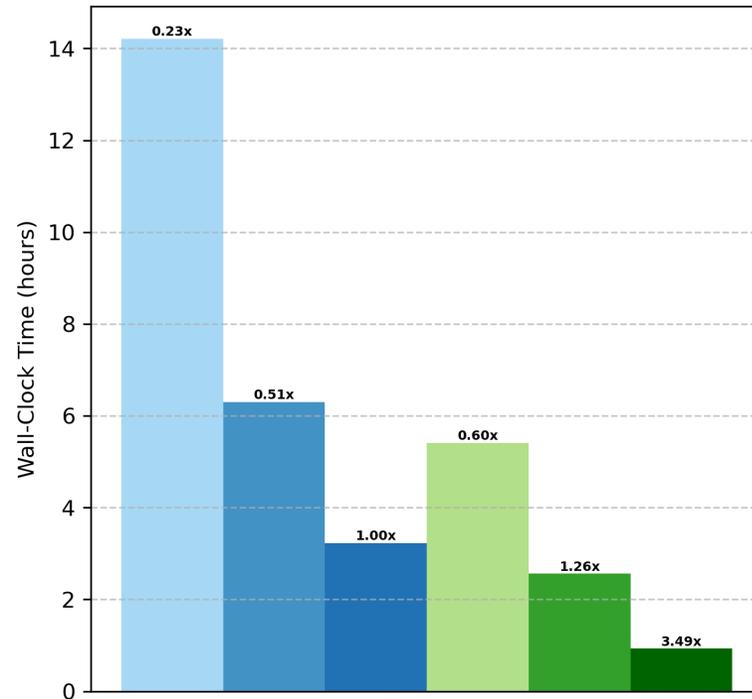
Idea: Use DL to emulate the km-scale climate model for producing very high-resolution precipitation projections

Problem

DOWNSCALING

LOW-RESOLUTION ATMOSPHERIC DATA (HOURLY)

HIGH-RESOLUTION PRECIPITATION (HOURLY)

Model: GNN regressor
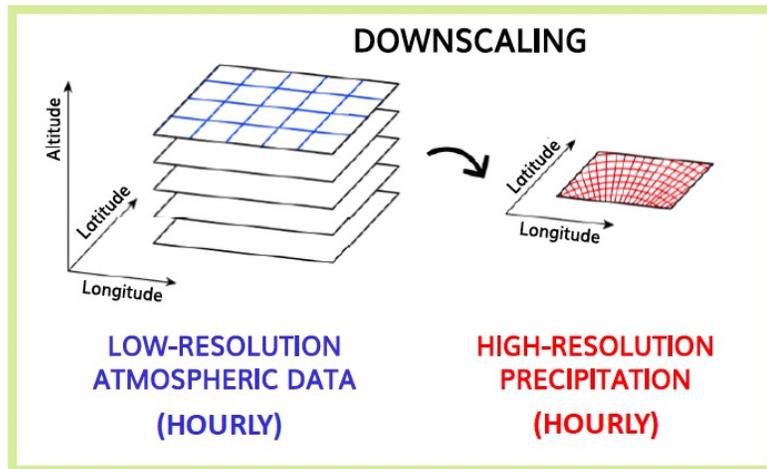
Results

Daily Comparison | ALPS | tasmax | 1975-07-15

Ground Truth (1975-07-15)

Prediction (GNN4CD)

Bias (Pred - GT)
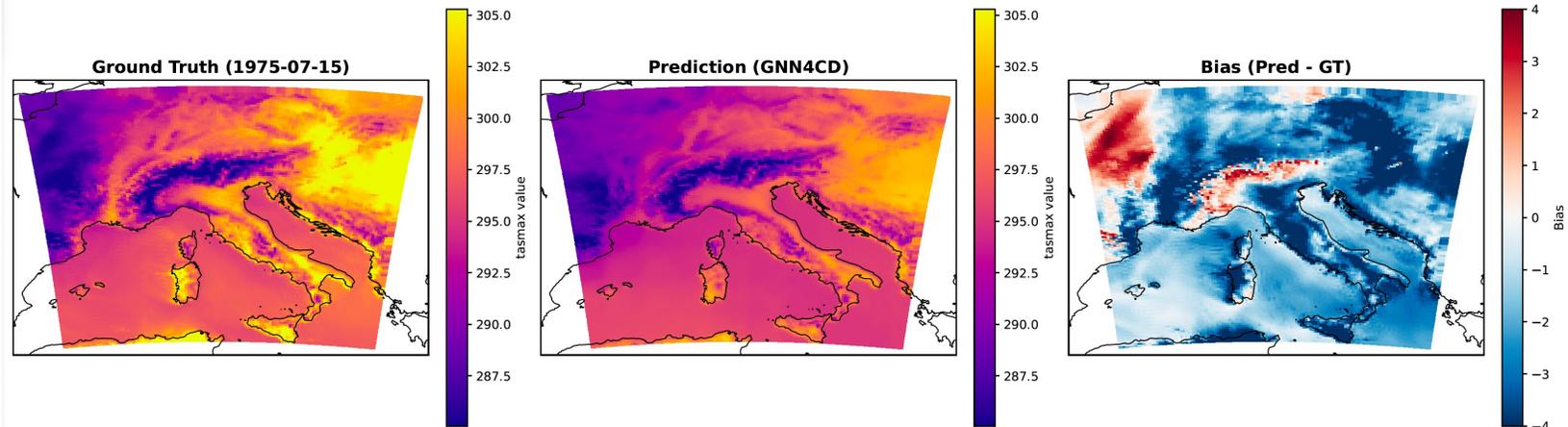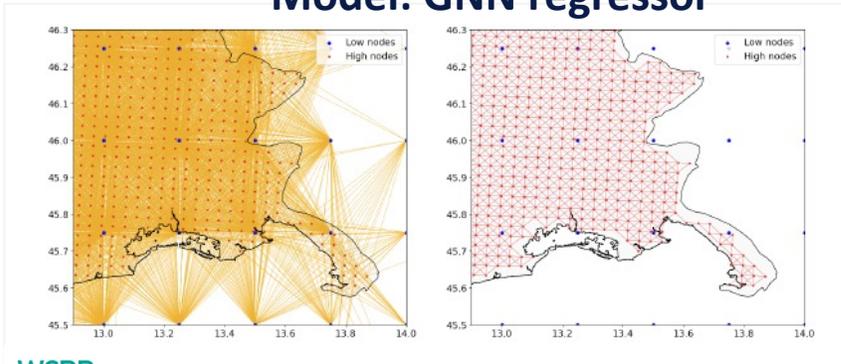
Goal

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

H2020-LC-CLA-2020-2

- The study, which required large computational resources to train the AI algorithms and run the simulations, was made possible by a special early access to Leonardo, a recently established GPU-based facility at CINECA.

- The number of possible atomic arrangements is far too large for traditional simulations. AI made it possible to model larger, more complex systems over longer time scales.

Hybrid Monte Carlo method coupled with deeplearning interatomic potentials to sample the phase space, allowing to treat positional and configurational disorders on an equal footing. The simulations were performed with LAMMPS coupled with DeepMD.

ICTP scientists have applied AI methods to study the microscopic structure of the Earth's inner core, investigating the role played by silicon

Li, Z., Scandolo, S. Short-range order stabilizes a cubic iron alloy in Earth's inner core. *Nat Commun* 16, 7574 (2025). https://doi.org/10.1038/s41467-025-62666-1

Light and materials

Quantum calculations expose hidden chemistry of ice

A collaboration with Giulia Galli's group at UChicago

M. Monti, Y. Jin, G.D. Mirón, A. Kundu, M. Govoni, G. Galli, A. Hassanali, Defects at play: Shaping the photophysics and photochemistry of ice, Proc. Natl. Acad. Sci. U.S.A. 122 (47) e2516805122, https://doi.org/10.1073/pnas.2516805122 (2025).

- Adopted high-level excited-state calculations to explain how ice absorbs and emits light

- By simulating pristine ice and specific defects, the team showed that imperfections in the crystal strongly control absorption, emission and photochemical pathways. The researchers could isolate one defect at a time (impossible experimentally) and identify a distinct optical "fingerprint" for each case

- The work gives a quantum-level picture of how light interacts with ice, with implications for atmospheric chemistry, planetary surfaces and other icy environments

Fluorescence can emerge from non-aromatic amino-acid crystals

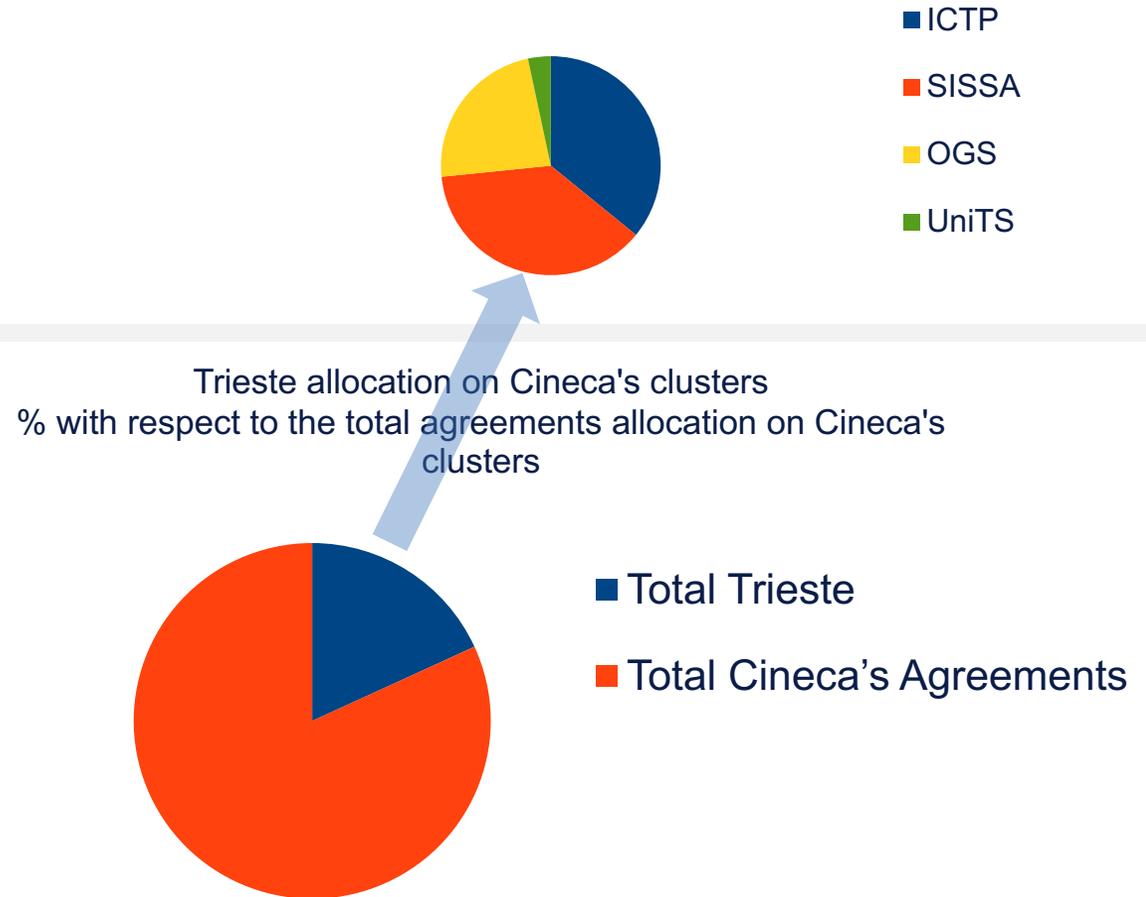**HyBOP (Hydrogen-Bond Networks as Optical Probes)**

- High-level excited-state simulations explain why subtle structural changes can turn light emission on or off in cysteine crystals

- The team found that crystals grown in light water and heavy water adopt different structures. In the fluorescent form, vibrations are more constrained, giving the system time to emit light instead of losing the energy non-radiatively.

- The study shows how molecular packing and hydrogen-bond networks can create new optical behavior in simple organic assemblies, opening a route to bio-inspired fluorescent materials and probes

- Excited-state calculations were needed to follow how the crystal moves after absorbing light and to distinguish photon emission from ultrafast internal conversion

D. Banerjee, S. Chibh, O.S. Tiwari, G.D. Mirón, M. Monti, H.R. Yakir, S. Pawar, D. Fixler, L.J.W. Shimon, E. Gazit, A. Hassanali, *Angew. Chem. Int. Ed.* 2025, 64, e202505331 https://doi.org/10.1002/anie.202505331

What does ICTP need?

Distribution of Trieste's allocation on Cineca's clusters

- **50-100M core-hours per year**

- **a growing trend**
  - **more grants (i.e. ISCRA, EuroHPC)**

- **more access to recourses worlwide**

- **4PB current storage occupation**

■ ICTP
■ SISSA
■ OGS
■ UniTS

Trieste allocation on Cineca's clusters
% with respect to the total agreements allocation on Cineca's clusters

■ Total Trieste
■ Total Cineca's Agreements

It's much more!! No ISCRA, no INAF, etc...

New Strategy, New Priorities

A. **International Science Alliance**
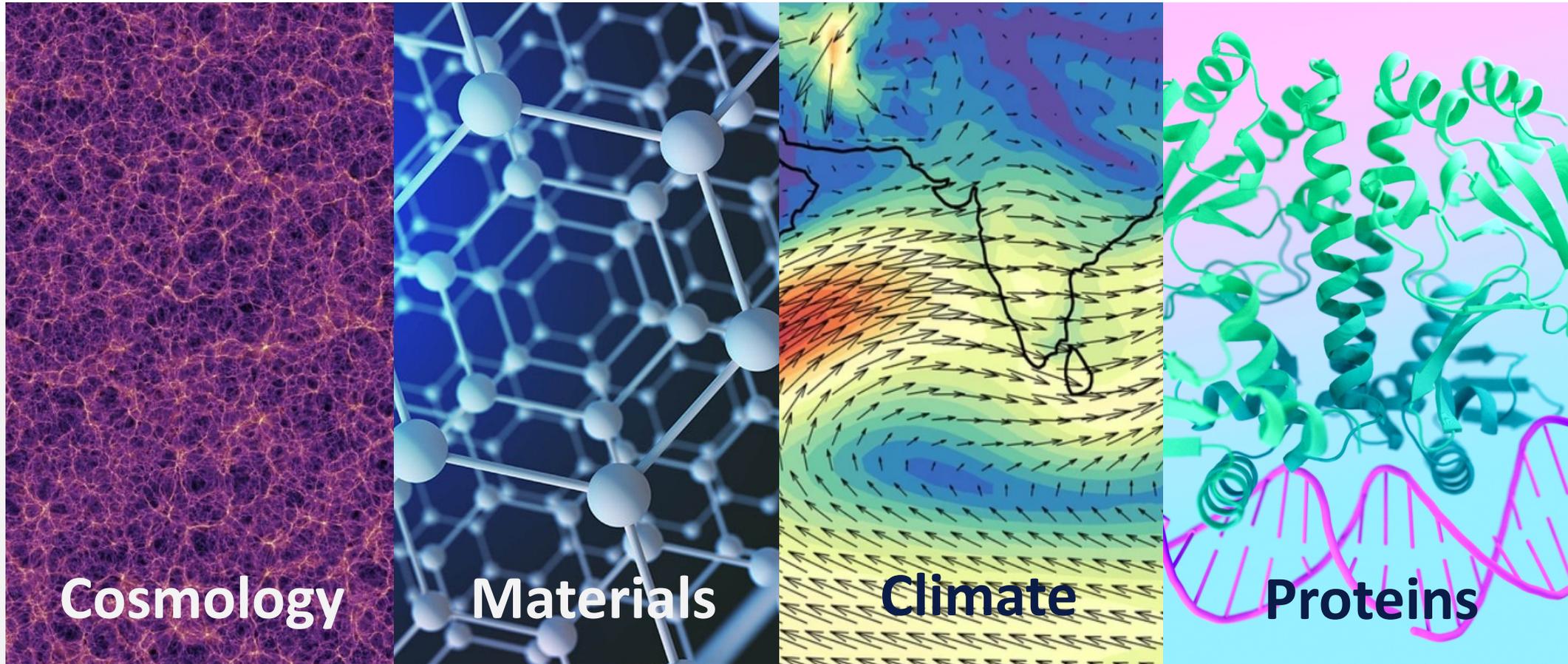*A new paradigm with more equal partnerships.*

B. **International Consortium for Scientific Computing**
Open Computing an essential ingredient of Open Science.

C. **ICTP Core**
A strong core to remain globally credible and effective.

The role of computing in science

Cosmology

Materials

Climate

Proteins

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

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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

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ICOMP's objectives
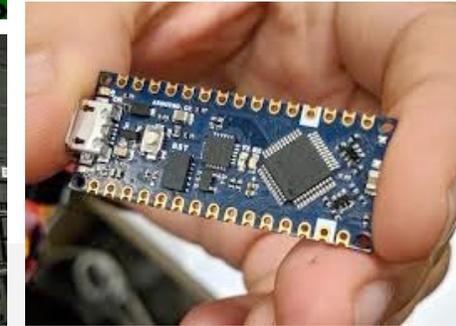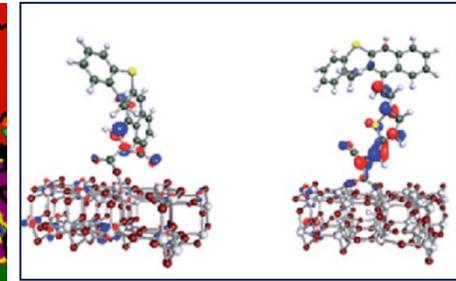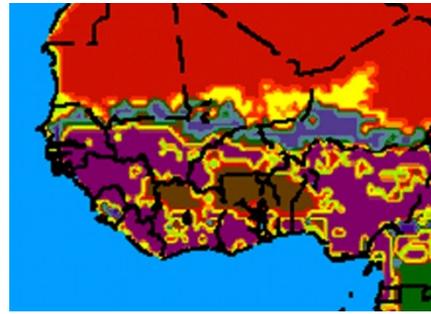
The **International Consortium for Scientific Computing** aims at:

- ✓ 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)

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

[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

IBM-ICTP Collaboration
Prizes and advanced schools
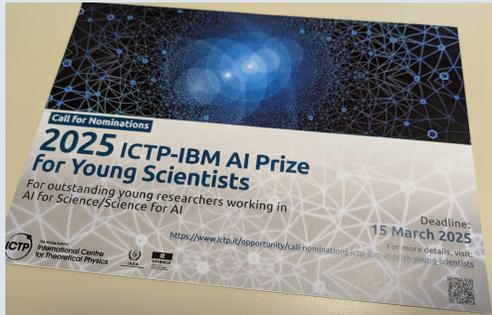
Annual prize for **outstanding young researchers working in AI for science / science for AI**

Prize ceremony at ICTP in summer 2026 **on the occasion of the school on applied 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

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

Access to computational resources for African-based researchers

52 proposals from 13 countries!!!

With support from:

CECAM - in partnership with ICTP and with the support of CINECA, and CSCS - announces the first call for assignment of HPC resources to African-based scientists in the areas of materials (soft and hard) and bio simulations.

Deadline for submission of the proposals: October 31, 2025.

All applications must be submitted via the form accessible from the CECAM website. You will need to be a registered user on the website to submit.

For more information and technical assistance with registration and submission, write to helpdesk@cecam.org with subject Name_Surname_CompAf_Info.

What we offer:

1. Access to high-end computational resources in the range 200.000 to 500.000 core hours per project.
2. Technical assistance with code installation (if necessary) and management of the allocated resources.
3. Visibility of results via sponsored participation to a CECAM Flagship when appropriate.

What we expect:

1. A clear scientific plan that includes the added value of the proposed calculations in the field.
2. Precise and documented justification of the amount of requested resources.
3. Description of the software to be used.
4. Plan for use of the resources (code development, preliminary runs, production runs...)
5. A detailed description of previous experience in using computational resources.
6. Periodic reporting on use of resources.
7. Use of the resources within one year from assignation. At the 8-month mark from the start of the project, a review of the progress will be performed. At this time, additional resources can be requested if properly justified.

Who can apply:

Post-doctoral fellows, researchers, and professors in African based research institutions.

The selection process:

Proposals submitted via the link below will be reviewed by an international panel of experts. Crucial assessment criteria include the scientific interest of the topic, previous computational expertise of the PI, clarity of the plan and timeline for the calculations, and appropriate justification of the requested resources.

Similar initiative to enable projects on climate modeling for scientists from Africa ongoing ICTP/UM6P/Cambridge

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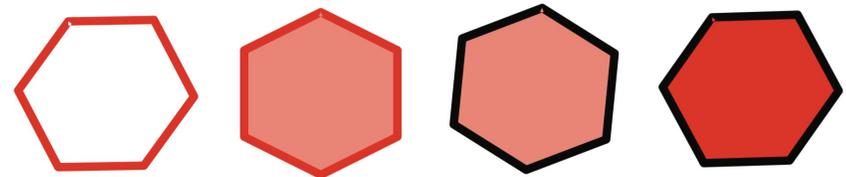
2026 MARVEL/ICTP College on
Computational Materials Science
(~250 students, 200 KEuro from MARVEL)

ICTP co-founds "AI Alliance" for responsible AI

The AI Alliance

A community of technology creators, developers and adopters collaborating to advance safe, responsible AI rooted in open innovation.

Founding Members and Collaborators*

- Universities
- Startups & Enterprises
- Science Organizations & Non-profits

Total annual R&D funding represented

>$80B

Students supported by these academic institutions
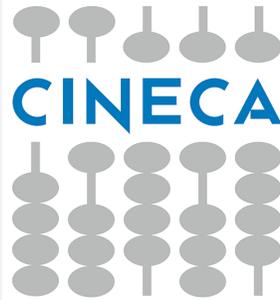
>400,000

Total staff members

>1,000,000

U.S. - Indiana
- University of Notre Dame

U.S. - Ohio
- Cleveland Clinic

U.S. - Connecticut
- Yale University

U.S. - New Hampshire
- Dartmouth

Germany
- TU Munich

Japan
- Keio University
- The University of Tokyo
- Fenrir Inc.
- SB Intuitions (Softbank subsidiary)
- Sakana AI
- Sony Group

U.S. - Massachusetts
- Mass Open Cloud Alliance

UK
- Imperial College of London
- Stability AI

Bulgaria
- Institute for Computer Science, Artificial Intelligence and Technology

U.S. - California
- UC Berkeley's College of Computing, Data Science, and Society
- Aitomatic
- AMD
- Anyscale
- Cerebras
- Intel
- LangChain
- LlamaIndex
- Meta
- Roadzen
- ServiceNow
- Together AI
- Linux Foundation
- MLCommons
- Partnership on AI

U.S. - Illinois
- University of Illinois Urbana-Champaign

Switzerland
- CERN
- Ecole Polytechnique Fédérale de Lausanne
- ETH Zurich

U.S. - Texas
- University of Texas at Austin
- Dell Technologies
- OpenTeams
- Oracle
- Quansight
- NumFOCUS

U.S. - Washington D.C.
- National Aeronautics and Space Administration*

Israel
- Hebrew University

Vietnam
- FPT Software

U.S. - New York
- Cornell University
- NYU
- Rensselaer Polytechnic Institute
- IBM
- Hugging Face
- Simons Foundation & Flatiron Institute

Italy
- International Centre for Theoretical Physics

U.A.E.
- Mohamed bin Zayed University of Artificial Intelligence

Singapore
- A*STAR

U.S. - Virginia
- National Science Foundation*

U.S. - North Carolina
- Red Hat

India
- IIT Bombay

Australia
- Fast.ai

Partners (so far)

Applied Scientific Computing at ICTP
(in the Era of the AI)

- Modern research at ICTP combines established simulation methodologies with emerging AI-driven modelling approaches to study physical interactions across temporal and spatial scales that remain challenging even for today's most advanced high-performance computing infrastructures

- As the cost and complexity of advanced technologies continue to rise, ICTP increasingly relies on access to distributed computational resources provided by partners worldwide

- At the same time, the rapid integration of AI methodologies has significantly expanded the demand for computational resources within the ICTP scientific community

- In this context, ICOMP represents ICTP's strategic initiative to develop international partnerships that address this growing demand. The programme aims both to enable scientists from developing countries to conduct research on world-class computing infrastructures and to foster sustainable computational ecosystems that help bridge the technological gap between developing and developed countries, thereby empowering the global scientific community to pursue transformative discoveries

Thank you!