



Introduction & HPC

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HPC Applications Specialist
International Centre for Theoretical Physics (ICTP)



The Abdus Salam
**International Centre
for Theoretical Physics**





Mission - An institute run by scientists for scientists

- Foster the growth of advanced studies and research in physical and mathematical sciences, especially in support of excellence in developing countries.
- Develop high-level scientific programmes keeping in mind the needs of developing countries, and provide an international forum of scientific contact for scientists from all countries.
- Conduct research at the highest international standards and maintain a conducive environment of scientific inquiry for the entire ICTP community.
- Thanks to the generous funding from the Italian Government, UNESCO and the IAEA, ICTP has been able to initiate and implement various schemes of support and assistance to scientists from developing countries.

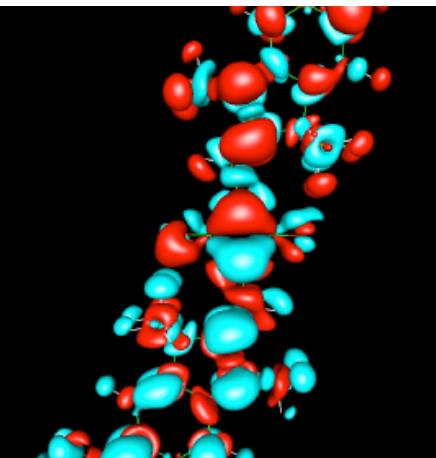
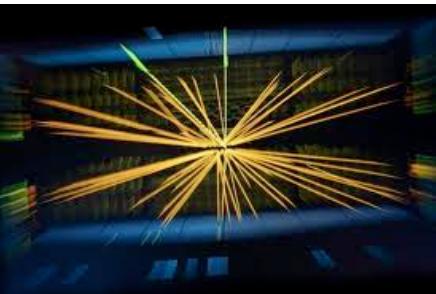
42 Scientists (P-staff)

65 Postdocs

40 PhD students

22 Long-term visitors

[from 43 countries / 56% developing]



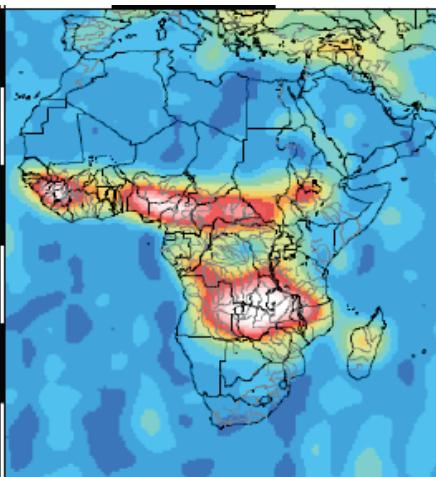
- ✓ 500+ papers/year (74% in Q1 journals)
- ✓ 32,000 citations/year
- ✓ 5 ERC Grant holders

Joint Institutes:

- Institute for the Fundamental Physics of the Universe (IFPU)
- Institute for Geometry and Physics (IGAP)
- Trieste Institute for Quantum Technologies (TQT)

Library: 64,000 books, 3,500 e-journals

Computational cluster: ~3000 cores + GPUs

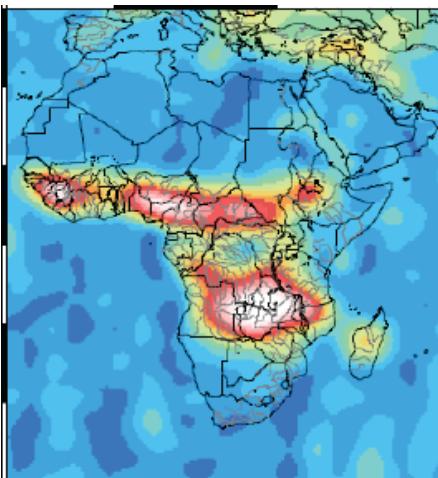
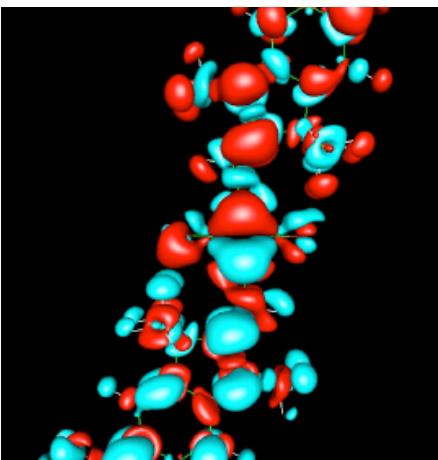


Core Research Areas

- High-Energy, Cosmology and Astroparticle Physics
- Condensed Matter and Statistical Phys.
- Mathematics
- Quantitative Life Sciences
- Earth System Physics

Special initiatives

- “Science, Technology & Innovation”
 - Science for Cultural heritage (x-ray tomography etc)
 - ICT for Development (wireless, Internet of things)
 - Fast detectors / FPGA
 - Ionospheric Physics
- High Performance Computing
- Materials for Renewable Energy



Advanced Schools, Conferences, Workshops

Postgraduate Diploma
Programme

PhD Degrees
(physics,
mathematics,
earth science,
and fluid
mechanics)

Junior
Associate

Regular
Associate

Senior
Associate

Masters Degrees
(physics, medical physics, high
performance computing,
complex systems)

STEP

TRIL and Elettra Users Programme

Federated
Institutes

Conferences &
Workshops

Student

Junior Researcher

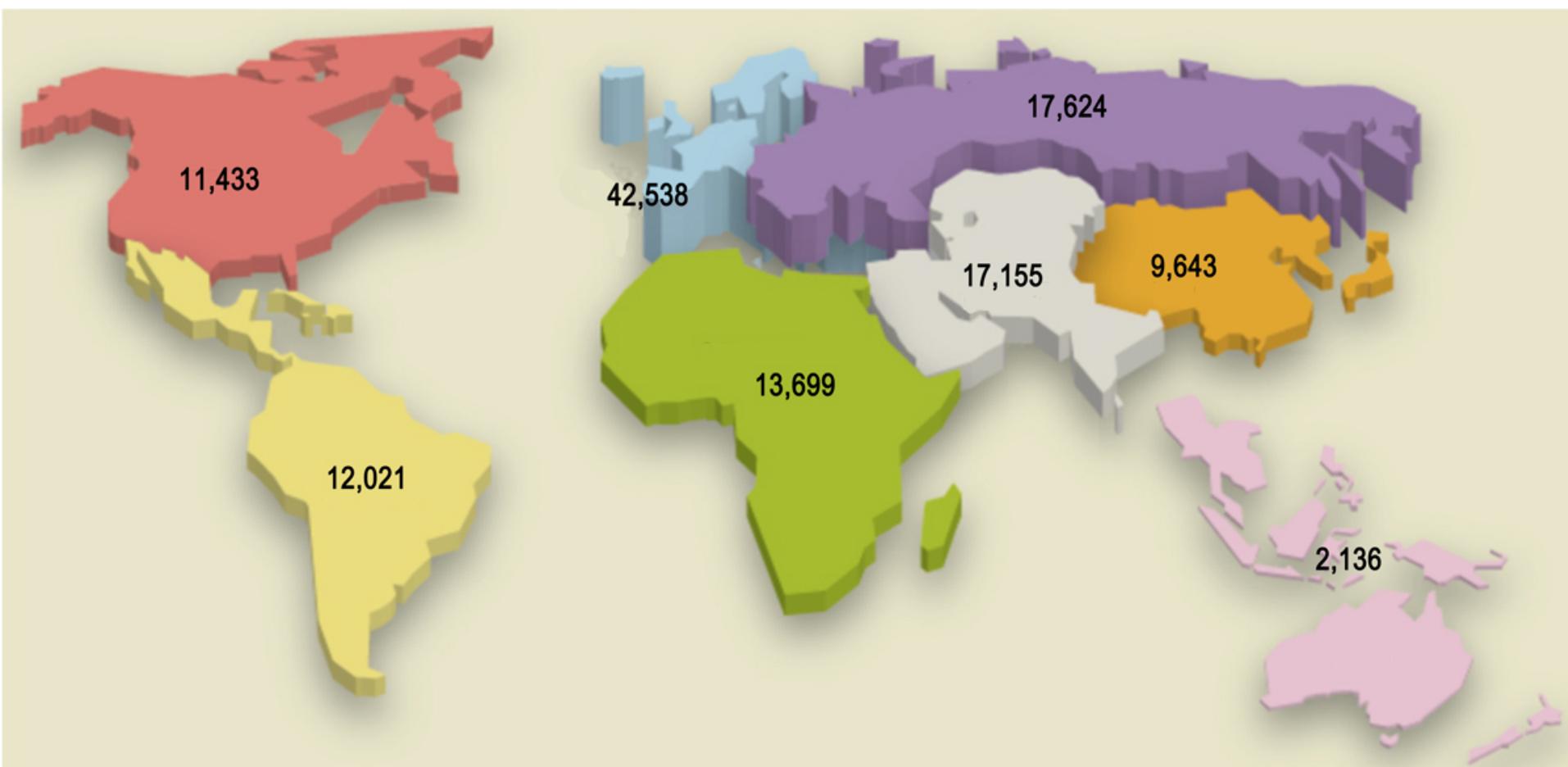
Researcher

Senior
Researcher

ICTP supports scientists from developing world throughout their career
who in turn educate several younger scientists in their home country.

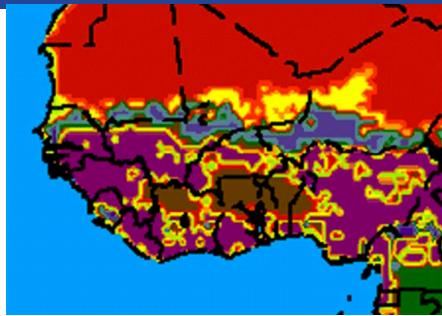
This multiplier effect is the strength of ICTP.

- More than 180,000 scientific visits since 1970
- 190 countries represented
- 27% of ICTP visiting scientists are women
- 4 Partner Institutes



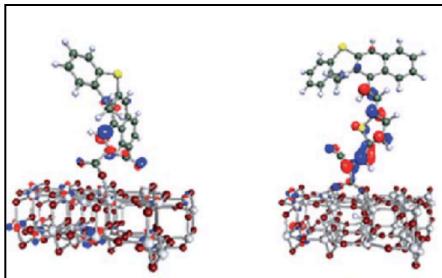
Challenges:

- Growing «divide» developed/developing world
- Lack of international collaborations & research ecosystems
- Scarce «human capacity»
- HPC infrastructures (Africa's top facility 182th in Top500)



The **International Consortium for Scientific Computing** will:

- ✓ Create a **shared platform** to seize the opportunities offered by new algorithms (ML, AI, BigData) and new hardware architectures
- ✓ Offer **access** to large-scale HPC resources
- ✓ Strengthen **training** programs and tie them to scientific **collaboration** & access to computer time
- ✓ Tackle selected scientific grand challenges (especially with impact on SDGs)





ICTP Scientific Calendar

- Schools, Conferences, Workshops around the year
- Half of them on subjects related to main research areas (core)
- The rest on many subjects:
medical physics, optics, nano physics, plasma physics, electronics, high performance computing, biophysics, satellite navigation, science dissemination and e-learning, m-science, entrepreneurship, nuclear physics (IAEA), teacher training, 3-D Printing, etc...
- <http://www.ictp.it/scientific-calendar.aspx>



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

Impact of Using Computer is Science

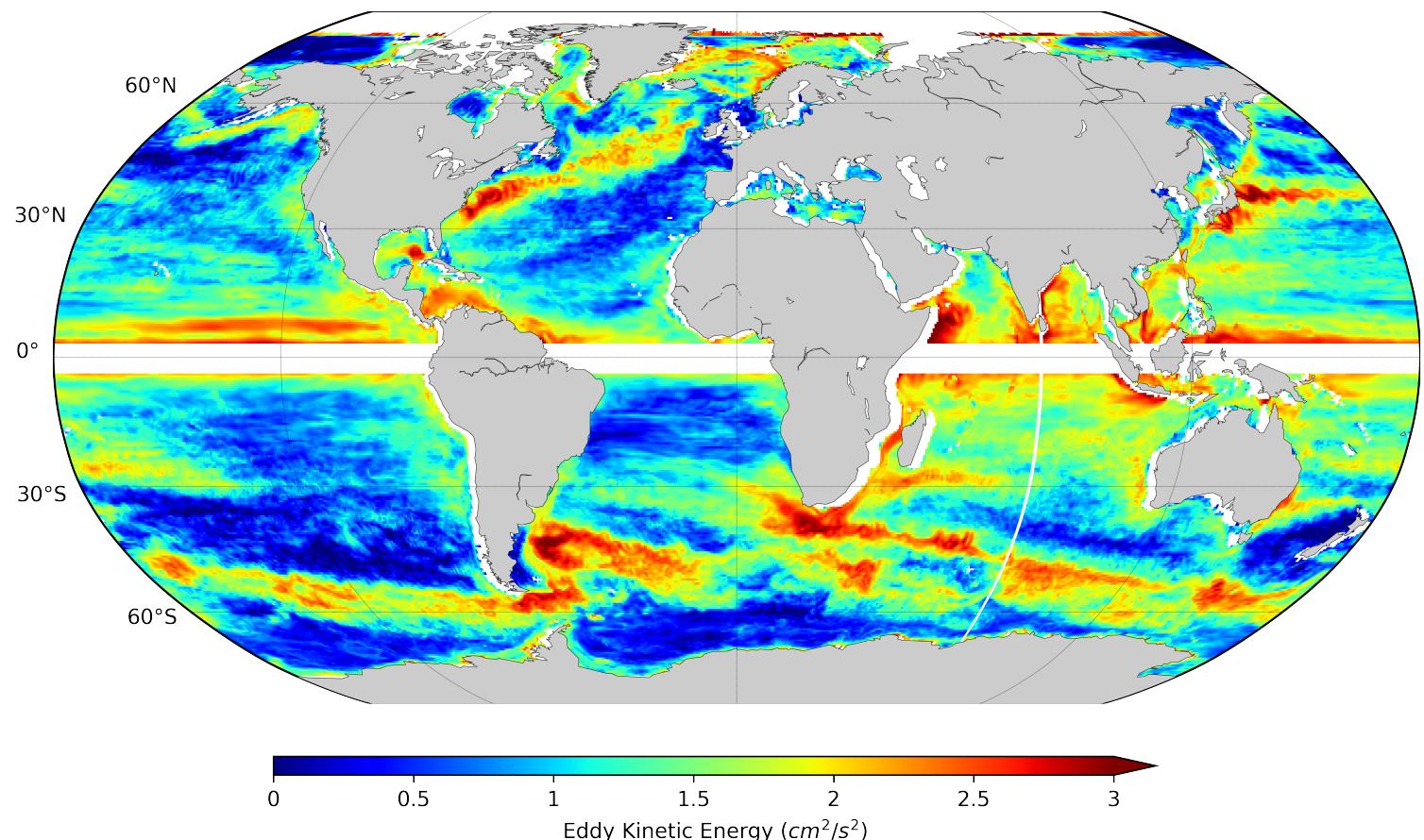


- **A more competitive industry**
 - We could never have designed the world-beating Airbus A380 without HPC
 - Thanks to HPC-based simulation, the car industry has reduced the time for developing new vehicle platforms from 60 months to 24
- **Direct benefits to our health**
 - One day of supercomputer time was required to analyse 120 billion nucleotide sequences, narrowing down the cause of a baby's illness to two genetic variants. Thanks to this, effective treatment was possible and the baby is alive and well 5 years later
- **Better forecasting**
 - Severe weather costs 150.000 lives and €270 billion in economic damage in Europe between 1970 and 2012
- **Making possible more scientific advances**
 - Supercomputing is needed for processing sophisticated computational models able to simulate the cellular structure and functionalities of the brain
- **More reliable decision-making**
 - The convergence of HPC, Big Data and Cloud technologies will allow new applications and services in an increasingly complex scenario where decision-making processes have to be fast and precise to avoid catastrophes

Large Scale Computer Simulations @ ICTP

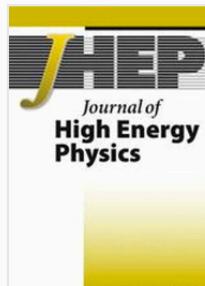
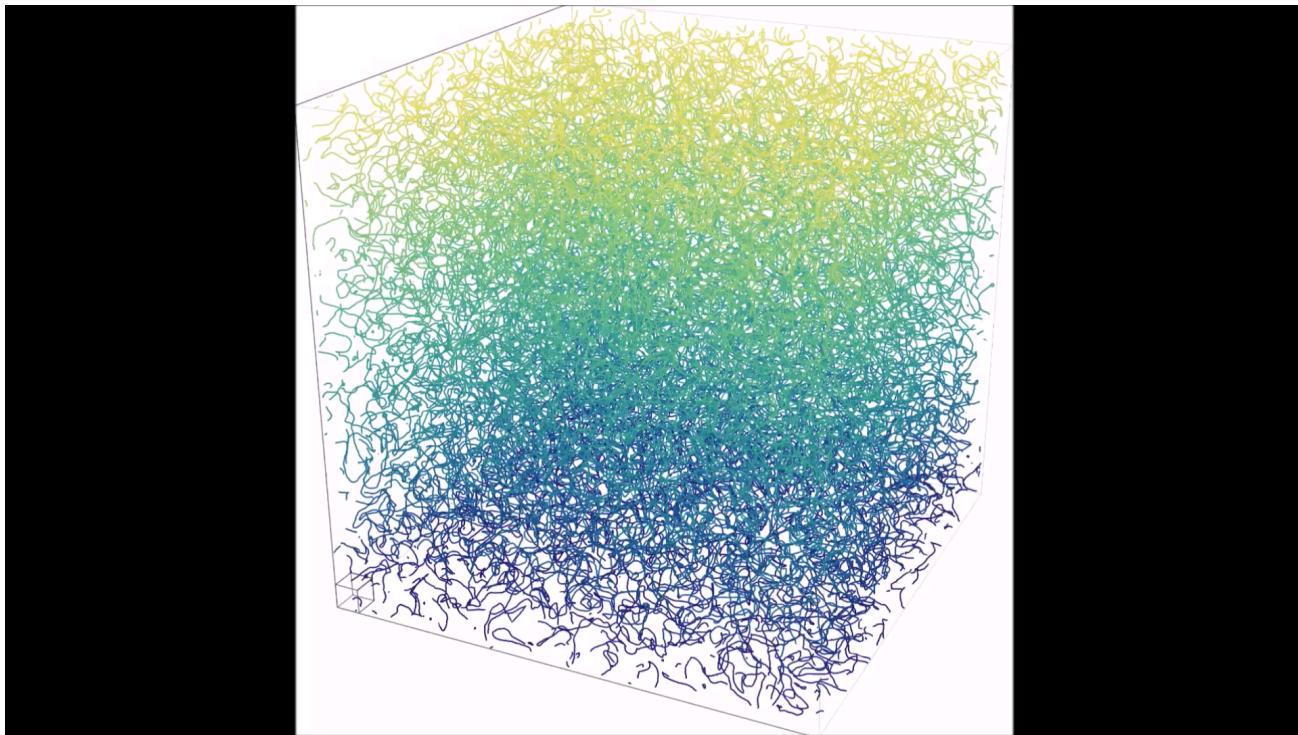


GFDL/MOM global ocean model as part of the international program FAFMIP. Simulations runs on 2400 cores (~50 nodes) on the SKL partition



* Courtesy of Dr. Ricardo Farneti (ESP group)

Solving numerically a wave-like PDE on a large 3d grid (up to 4096^3)



[Journal of High Energy Physics](#)

July 2018, 2018:151 | [Cite as](#)

Axions from strings: the attractive solution

Authors

[Authors and affiliations](#)

Marco Gorgetto, Edward Hardy, Giovanni Villadoro 

Understanding the electrochemical double layer at the hematite/water interface: A first principles molecular dynamics study

Cite as: J. Chem. Phys. **150**, 041707 (2019); <https://doi.org/10.1063/1.5047930>

Submitted: 10 July 2018 . Accepted: 06 September 2018 . Published Online: 29 November 2018

Kanchan Ulman, Emiliano Poli , Nicola Seriani, Simone Piccinin , and Ralph Gebauer

heavy ab-initio MD calculations!!



ARTICLE

DOI: 10.1038/s41467-018-07190-1

OPEN

Vibrational fingerprint of localized interactions in a two-dimensional metal-organic framework

M. Corva^{1,2}, A. Ferrari^{1,5}, M. Rinaldi¹, Z. Feng^{1,6}, M. Roia^z³, C. Ramesh¹, M. Dell'Angela², G. Pastore¹, G. Comelli^{1,2}, N. Seriani⁴ & E. Vesselli^{1,2}

Regular Article – Soft Matter | Published: 30 October 2021

Phospholipids dock SARS-CoV-2 spike protein via hydrophobic interactions: a minimal in-silico study of lecithin nasal spray therapy

Muhammad Nawaz Qaisrani, Roman Belousov, Jawad Ur Rehman, Elham Moharramzadeh Golaei, Ivan Girotto, Ricardo Franklin-Mergarejo, Oriol Güell, Ali Hassanali  & Édgar Roldán 



Diagonalization of really big matrixes!



Computer Physics Communications

Volume 235, February 2019, Pages 477-488



Massively parallel implementation and approaches to simulate quantum dynamics using Krylov subspace techniques ★

arXiv.org > cond-mat > arXiv:1902.09236

Condensed Matter > Strongly Correlated Electrons

Marlon Brenes ^{a, b}✉, Vipin Kerala Varma ^{a, c, d, e}, Antonello Scardicchio ^{a, f}, Ivan Girotto ^{a, g, h}

✉ Show more

<https://doi.org/10.1016/j.cpc.2018.08.010>

Get rights and content

Non-Abelian symmetries and disorder: a broad non-ergodic regime and anomalous thermalization

I. V. Protopopov, R. K. Panda, T. Parolini, A. Scardicchio, E. Demler, D. A. Abanin

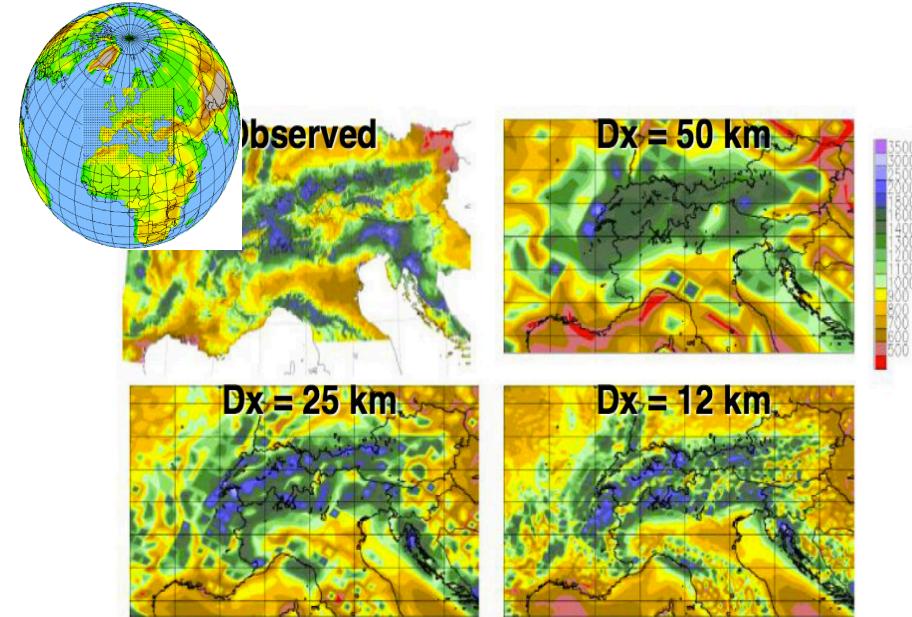
(Submitted on 25 Feb 2019)

PHYSICAL REVIEW LETTERS

Many-Body Localization Dynamics from Gauge Invariance

Marlon Brenes, Marcello Dalmonte, Markus Heyl, and Antonello Scardicchio
Phys. Rev. Lett. **120**, 030601 – Published 19 January 2018

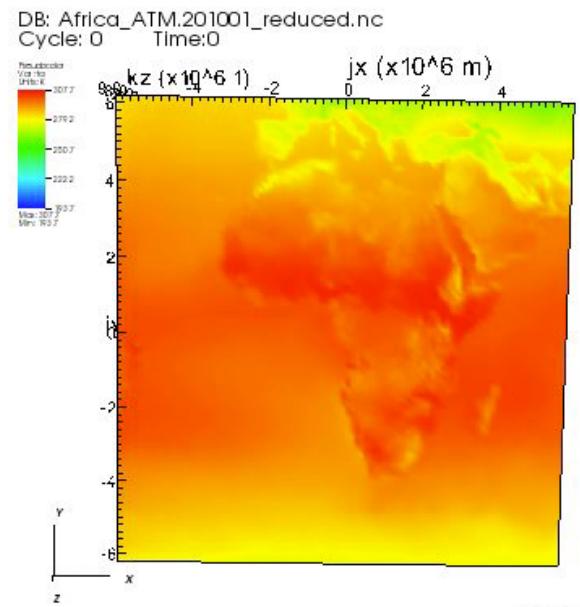
Large Scale Computer Simulations @ ICTP



- 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

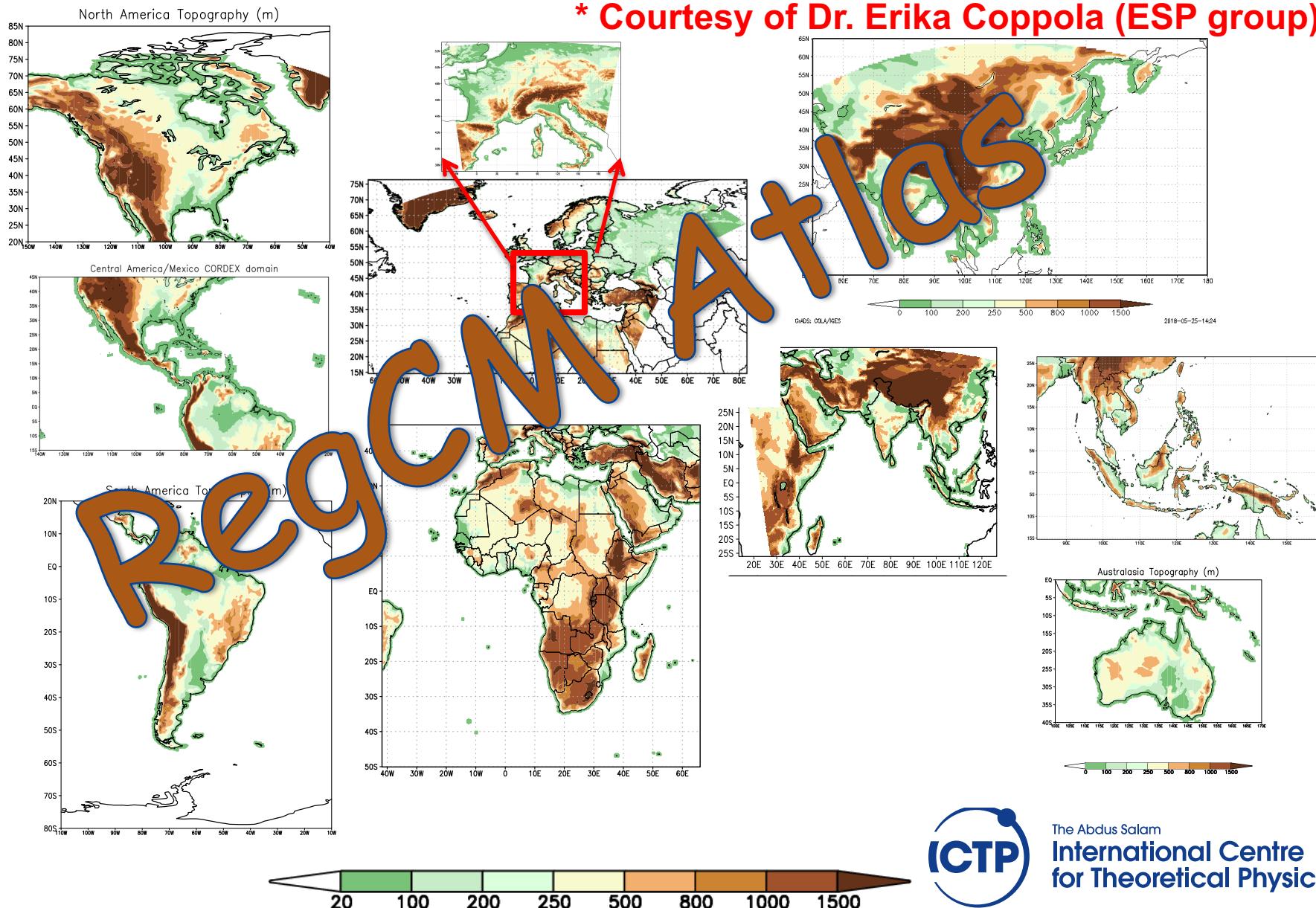
[...] for Europe, we plan to run seven 140 year simulations. Each month of simulation, with 500 processors, is expected to take about 2.9 hours of compute time and produce 60GB of raw output files

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



RegCM4.7 tested domain available and long scenario simulations available

* Courtesy of Dr. Erika Coppola (ESP group)



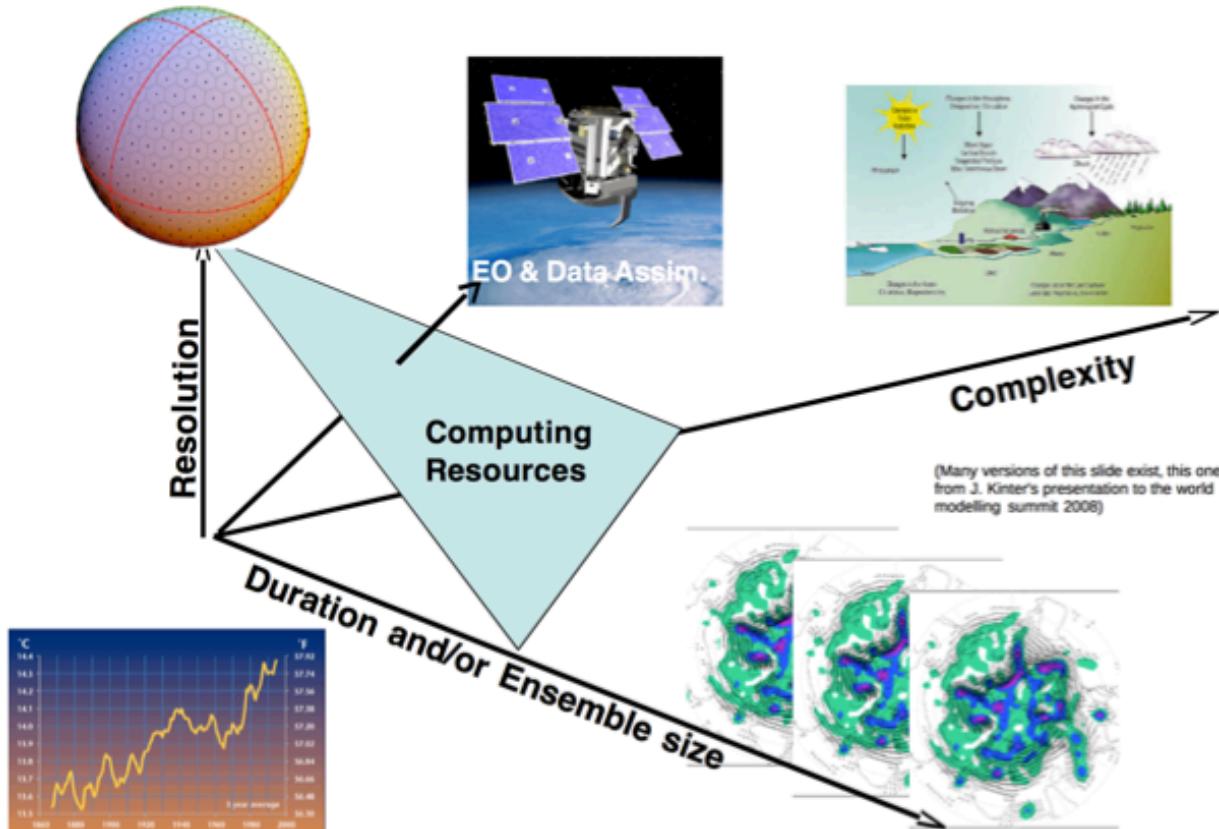
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for Theoretical Physics



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**

More & More Computing ...



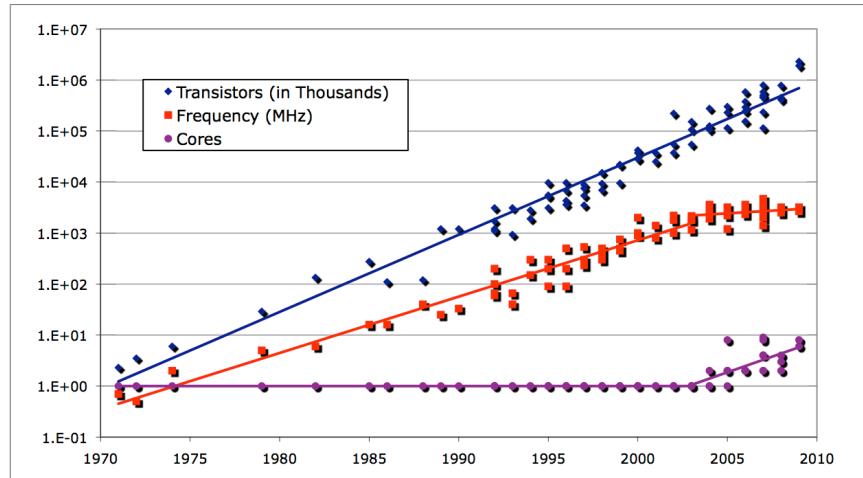


Why would HPC matter to you?

- 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

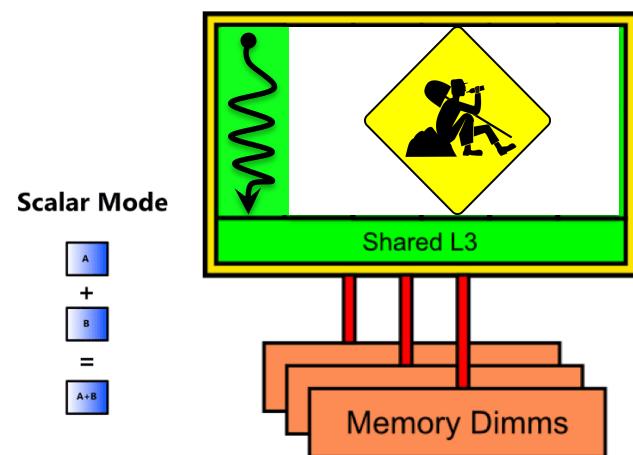
Collateral Consequences /1

- Growing of computer capability is achieved increasing computer complexity



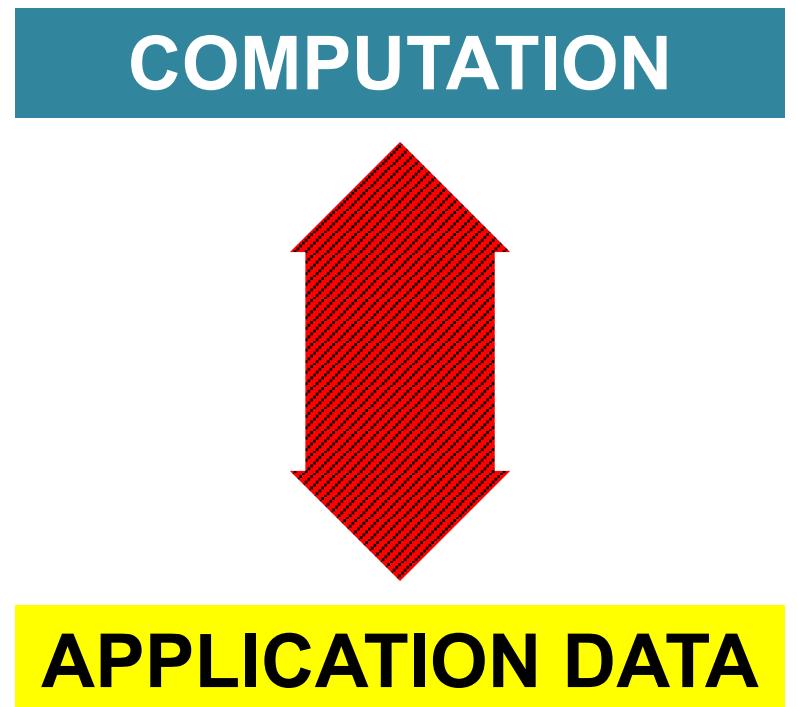
- CPU power is measured in number of floating point operations x second (FLOPs)
 - $\text{FLOPS} = \# \text{cores} \times \text{clock freq.} \times (\text{FLOP/cycle})$

#cores	Vector Length	Freq. (GHz)	GFLOPs
1	1	1.0	1
1	16	1.0	16
10	1	1.0	10
10	16	1.0	160



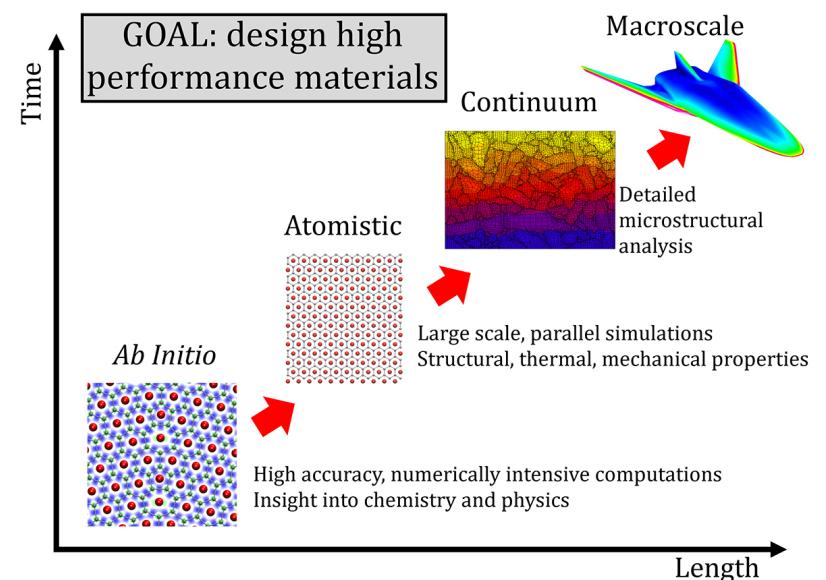
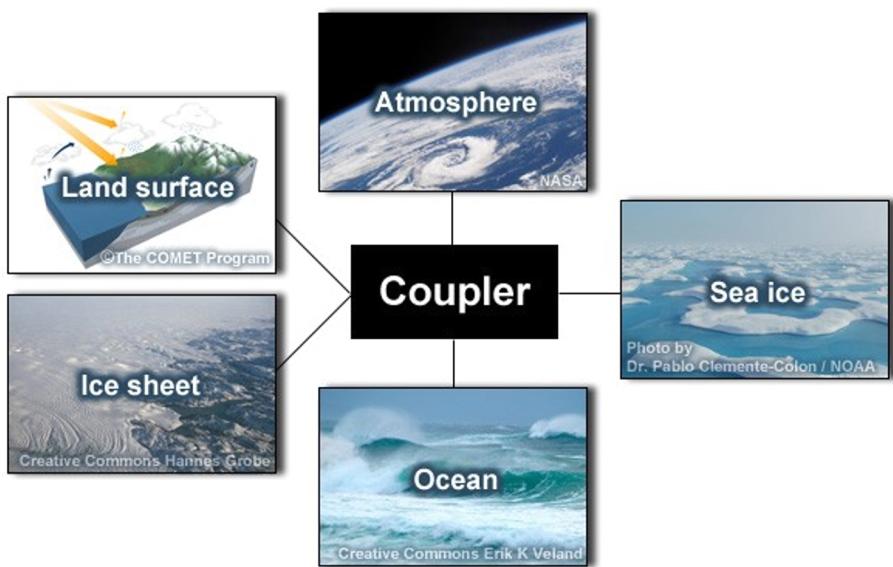
Collateral Consequences /2

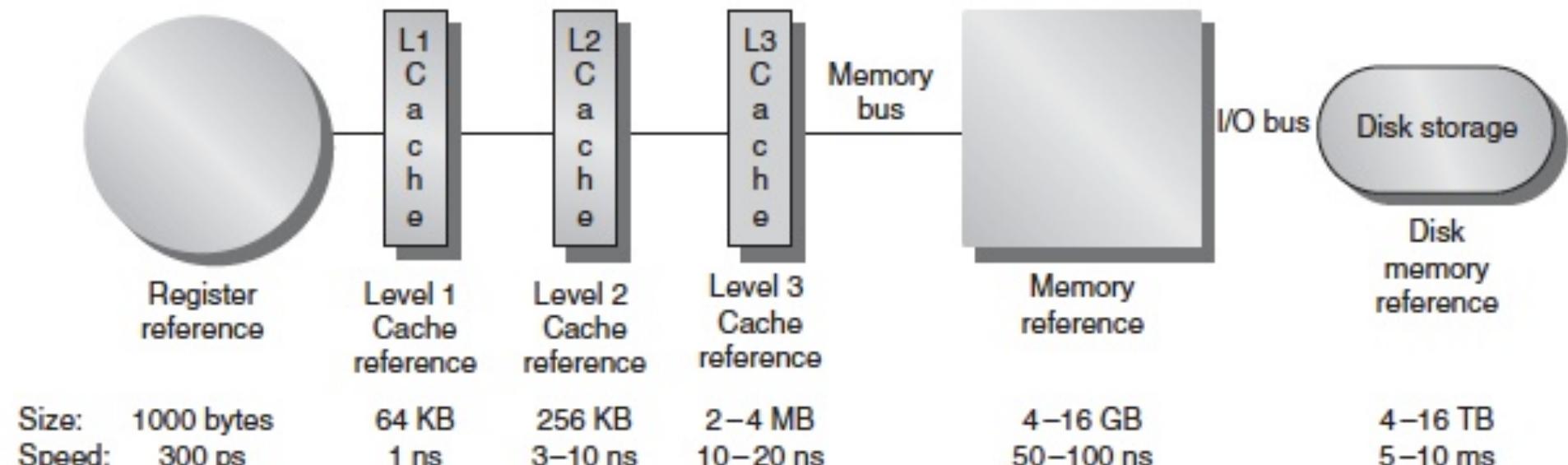
- When all CPU component work at maximum speed that is called *peak of performance*
 - Tech-spec normally describe the theoretical peak
 - Benchmarks measure the real peak
 - Applications show the real performance value
- CPU performance is measured FLOP/s
- But the real performance is in many cases mostly related to the memory bandwidth (Bytes/s)
- The way data are stored in memory is a key-aspect for high performance



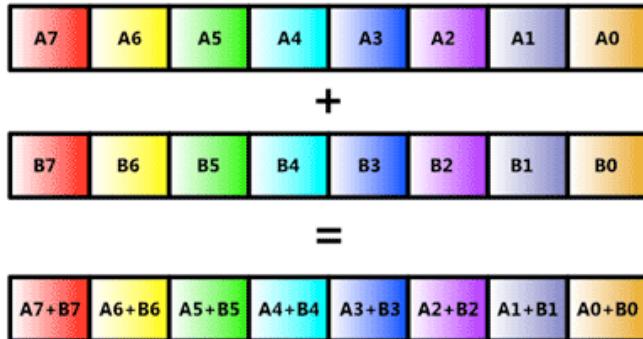
Collateral Consequences /2

- Complexity of physical models is directly proportional to the software complexity
- Number of operations as well as the size of the problem (data) grows extremely quickly when increasing the size of a 3D (multidimensional) domain





SIMD Mode



Scalar Mode

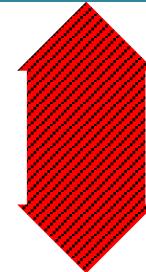
$$\begin{array}{c}
 \boxed{\text{A}} \\
 + \\
 \boxed{\text{B}} \\
 = \\
 \boxed{\text{A}+\text{B}}
 \end{array}$$

CPU
 Registers

CACHE

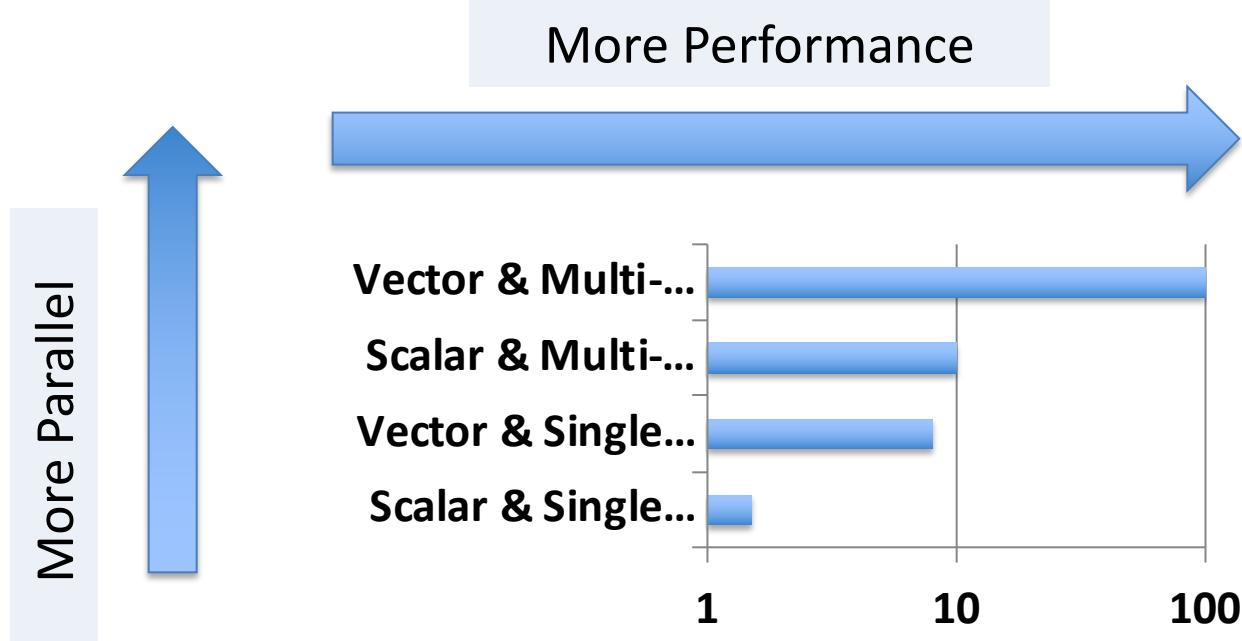
MAIN MEMORY

COMPUTATION



APPLICATION DATA

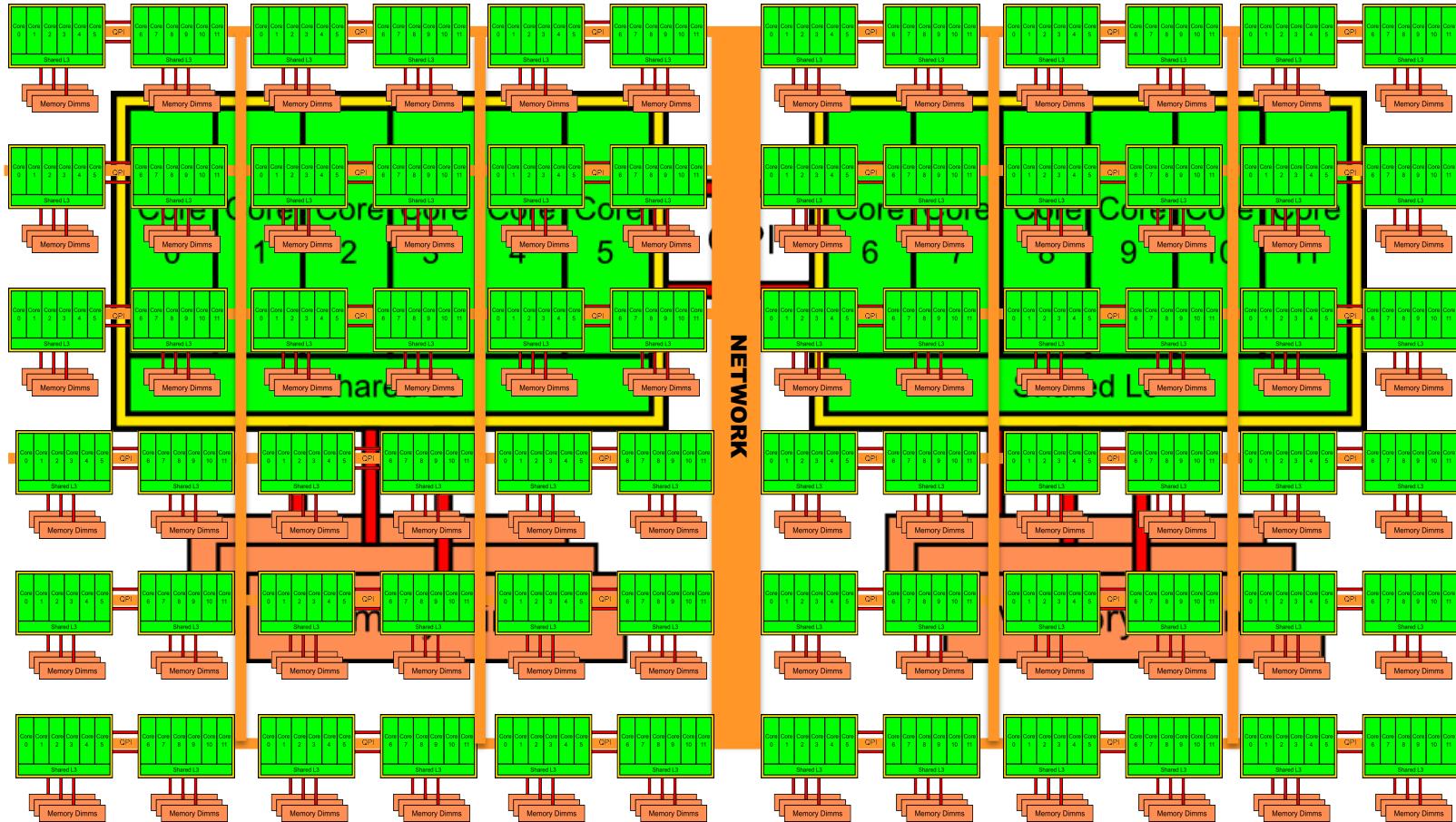
Threading and Vectorization



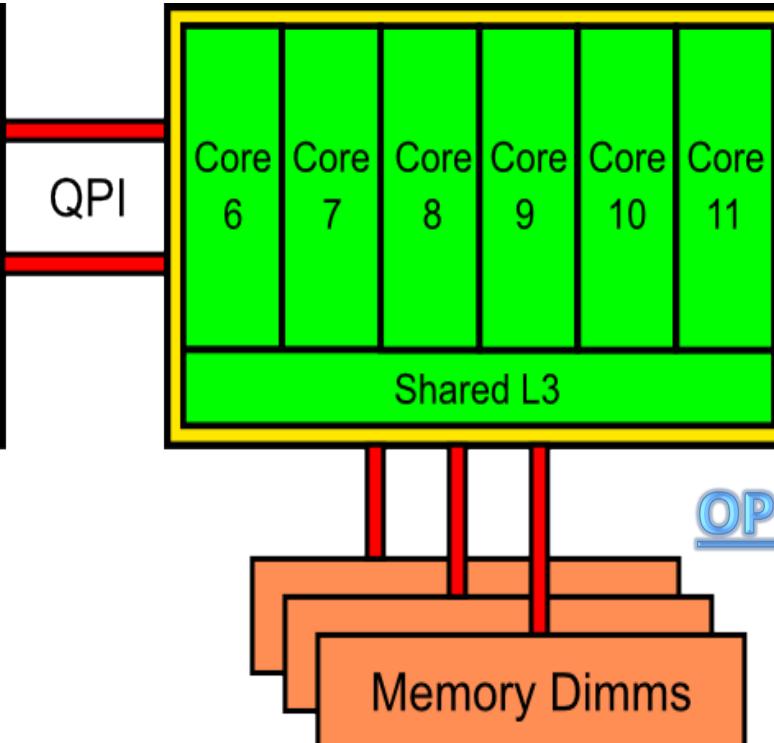
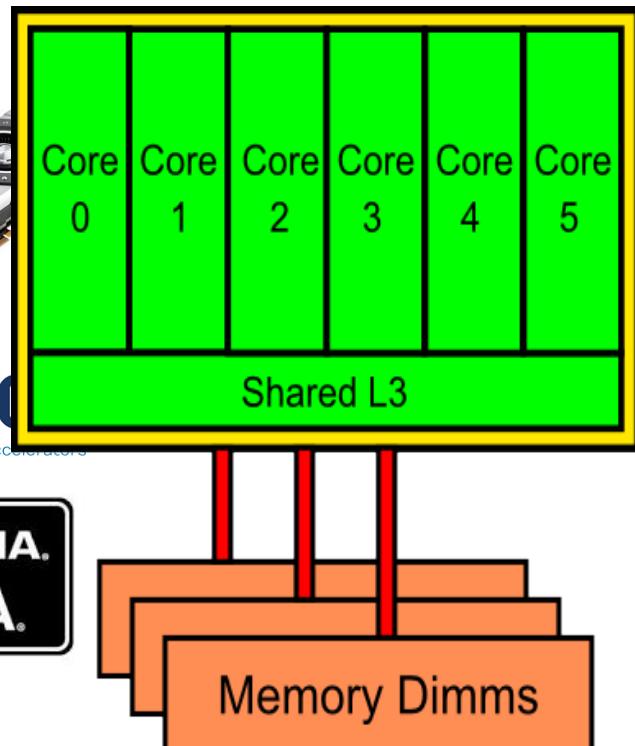


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Multiple Socket CPUs + Accelerators



OpenAC

Directives for Accelerators



STANDARD
PROGRAMMING

&

OPENMP

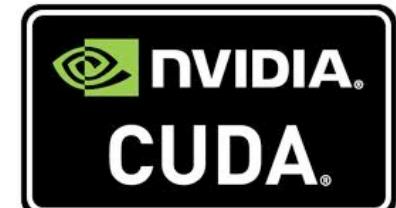
STANDARD
PROGRAMMING

&

OPENMP

Programming Parallel Paradigms

- Are the tools we use to express the parallelism for on a given architecture
- They differ in how programmers can manage and define key features like:
 - parallel regions
 - concurrency
 - process communication
 - synchronism



High-performance codes



FFTW

Open ∇ FOAM®

Yambo.®



QUANTUM ESPRESSO

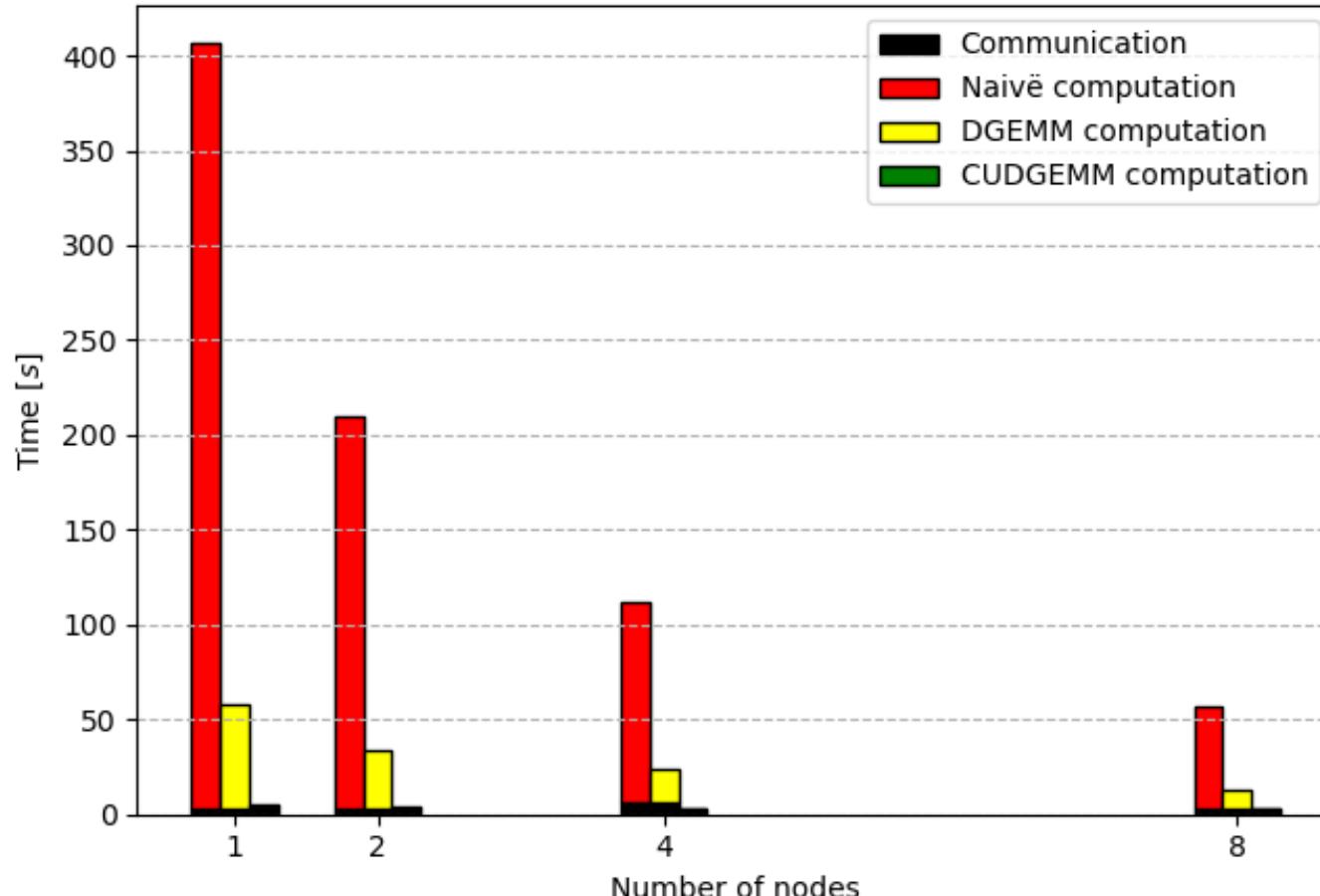
OpenBLAS



LAMMPS
Large-scale Atomic/Molecular
Massively Parallel Simulator

Communication and computation times per number of nodes

Size of matrices: 25000×25000



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

Complexity of software

Workload Management: system level, High-throughput

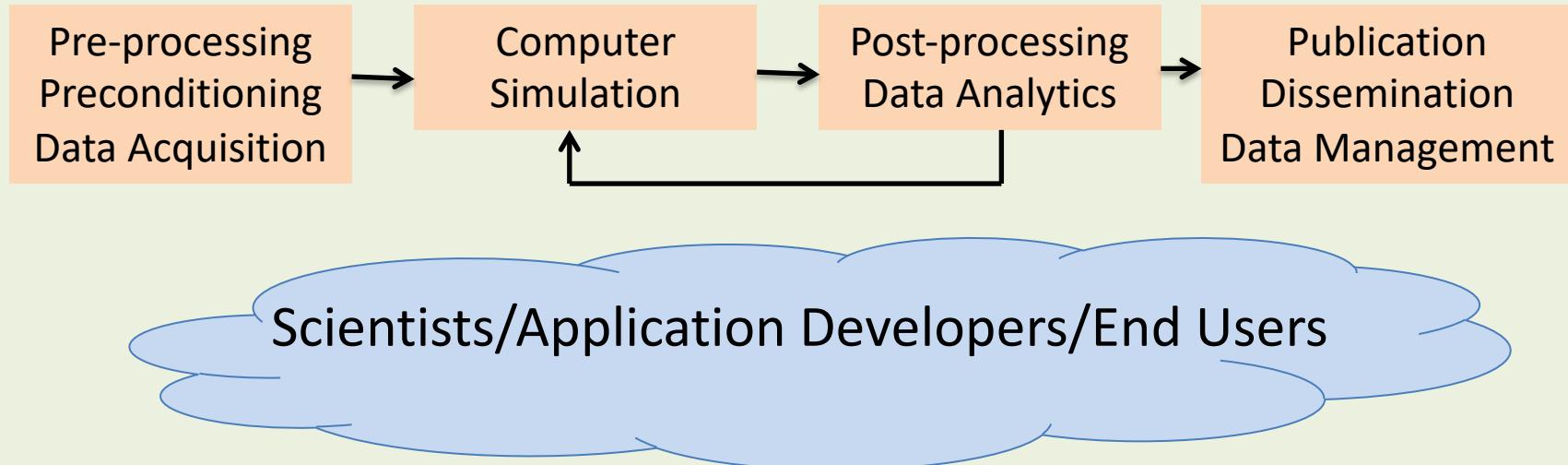
Python: Ensemble simulations, workflows

MPI: Domain partition

OpenMP: Node Level shared mem

CUDA/OpenCL/OpenAcc:
floating point accelerators

Challenge: code maintainability



SW Workflow & Parallel Applications

Compilers/Libraries/Debugging & Profiling

HW/Resource Management/File System/...

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**:

$$S_p = \frac{T_s}{T_p}$$

- High-level educational program, beyond M.Sc.
- Intensive training aimed to build knowledge in solving complex problems with an HPC approach
- Innovative, hands-on based training
- 15 students x year
- since the first edition 100% employees after the program

- Candidates must have some experience in programming and a competence in at least one of the languages between C, C++ and/or Fortran
 - Python knowledge is a plus
- A sound knowledge of Linux operating system
- Master level of a scientific degree is required
- No prior HPC knowledge is assumed
- Enthusiasm is a must

1 year program divided in 6-8 months courses and 6 month project (some overlap)

Mandatory

- Scientific Programming Environment
- Introduction to Computer Architectures for HPC
- Object Oriented Programming
- Parallel Programming
- Introduction to Numerical Analysis
- Advanced Computer Architectures and Software Optimizations
- Parallel Data Management and Data Exchange
- High Performance Computing Technology
- Best Practices in Scientific Computing

Optional Choice

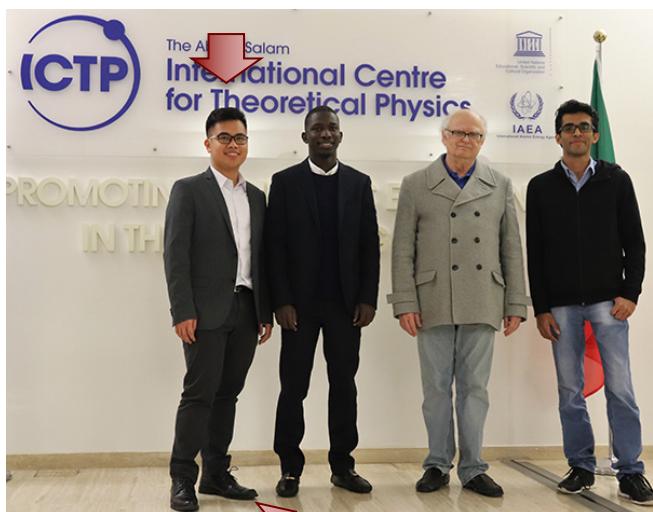
- Data Structures & Sorting and Searching Electronic structure: from blackboard to source code
- The Finite Element Method Using deal.II
- Reduced Basis Methods Fast Fourier Transforms in Parallel and Multiple Dimensions
- Cluster Analysis
- Monte Carlo methods
- Supervised & Unsupervised Machine Learning
- Machine Learning
- Deep Learning
- Approximation and interpolation of simple and complex functions
- Spatial locality algorithms
- Lattice Boltzmann
- Molecular dynamics

HPC Training Scholarship Winners



Alejandra Foggia
& Rajat Panda
CMSP group @ ICTP

James Vance, Philippines
PhD Student
Johannes Gutenberg University Mainz and the Max Planck Institute for Polymer Research(Ghana)



Elliot Menkha, Ghana
Last Month PhD in "Computational Chemistry"
Kwame Nkrumah University of Science and Technology (Ghana)



Anoop Chandran, India
PhD Student
Institute for Advanced Simulation, Julich (Germany)



Muhammad Owais, Pakistan
Junior Research Engineer
BSC-CNS (Spain)



Marlon Brenes Navarro, Costa Rica
PhD Student
Trinity College Dublin (Ireland)



Michael O. Atambo, Kenia
Last month PhD in "Physics and Nanosciences"
CNR-NANO (Italy)



Jimmy Aguilar Mena, Cuba
PhD Student
BSC-CNS (Spain)

Fernando Posada, Colombia
Assistant Professor
Temple University (USA)

Other Programs



Latin American Introductory School to Parallel Programming and Parallel Architecture for High Performance Computing

12 - 23 February 2018
CINVESTAV and ININ, Ocoyoacac, Mexico

The School has the goal of teaching participating scientists about modern computer hardware and programming to provide a foundation for future computational research using High Performance Computing (HPC). Participants will go through an intensive programme with a focus on practical skills.

Description:
School participants will learn to improve the efficiency of their research codes, and to parallelize them. Lectures on a selection of technical aspects of modern HPC hardware will be followed with introductions to widely used parallel programming tools and libraries. In addition, hands-on sessions will allow participants to practice on small example problems of general scientific interest. Example topics will cover numerical methods and parallel strategies, as well as data management. The programme, specifically designed for the needs of scientists using writing, or modifying HPC-relevant features in widely used scientific software for fundamental HPC-relevant features in widely used scientific software for high-performance computing.

How to apply:
Online application: <http://indra.snsi.ipt.ac.mx/event/1344>
Female scientists are encouraged to apply.

Grants:
A number of grants are available to support the participation of young researchers from South America in attending the School. Applications for grants should be submitted by 15 January 2018.

Deadline:
26 November 2017

Search: Search in Conferences:
Overview
Programme
Speakers
Apply here



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ING
.HE EXASCALE
TRANSITION

Joint WASCAL-ICTP Hands-on workshop on HPC technology for Climate Sciences I (smr 3689)

Starts 3 May 2022
Ends 13 May 2022
Central European Time

During this hands-on workshop, IT/HPC admins and climate change scientists will be trained on how to make effectively operational and remotely accessible HPC technology, and how to use the computational resources of operational HPC systems in West Africa (WA) to compute climate models and run simulations. This activity will also ease the creation of HPC community in WA.

Topics:

- HPC IMPORTANCE, DESIGN, PURCHASE, AND INSTALLATION PROCESSES: e.g. HPC Facilities for scientific challenges in Climate modeling
- HPC TECHNOLOGY & ADMINISTRATION: Fundamentals of Computer Architecture and programming, Raking and building HPC clusters
- HPC NETWORK AND SYSTEM ADMINISTRATION (HDFS/NETCDF) and programming, storage, data formats (HDFS/NETCDF)
- HPC SYSTEM COMMON USAGE AND OPERATIONS: e.g. Hands-on work on queue systems, common and submit jobs on HPC clusters, Hands-on work on REGCM, compiling software and submit jobs on HPC clusters, Hands-on work on RECM, WRF

Contact: smr3689@ictp.it
Online forum: <http://smr3689.itsmtp.it/>

The CODATA-RDA
Research Data Science Advanced **ICTP** Workshops on Bio-informatics, Climate Data Sciences, Extreme Sources of Data and Internet of Things(IoT)/Big-Data Analytics

19 - 23 August 2019
Trieste, Italy

During this activity several applied/thematic workshops on Data Science run in parallel.

Extended Topics list:

- **Bioinformatics:** This workshop focuses on bio-workflows using NGSI Data Topics including access to NGSI data analysis. Participants should have some familiarity with language
- **IoT and Big Data Analytics:** deal with amounts of data produced by appliances and other electronic processes and tools available in the cloud. Installation and corporate environments
- **Cloud Computing:** Cloud Computing is a model for delivery of computing power, storage, and other services over a network

Organizers:
Bello DIALLO (WASCAL), Kwareme HACIENE (WASCAL), Kehinde OGUNJEBI (WASCAL), Edem PEDANCU (ICTP), Graziano GULIANI (ICTP), Mary-Jane SULE (ICTP), Clement Ohene (ICTP)

Co-sponsors:
WASCAL

7th Workshop on Collaborative Scientific Software Development

4 - 10 May 2019

performance Computing 'ation with LAMMPS

Bogor, 3 - 6 September 2018

Sunday, 10 March 2019

<http://smr3689.itsmtp.it/>

Invitation
We invite young scientists and engineers, post-graduate students from all South-East Asian countries who (already or plan to) work with Molecular Dynamics. The school will be conducted in English and hence participants should have an adequate working knowledge of this language. The participants are also required to already be familiar basic knowledge of Molecular Dynamics. The number of participants is limited to around 25 persons from local and 6-10 persons from regional region. There is no registration fees for all participants. All participants will be provided with lunch and snacks during the workshop. We do not cover lodging and accommodation costs for local participants. All travel and local accomodation support will be provided to selected participant from ASEAN Countries.

Registration
Registration can be made through Registration tab in this webpage no later than 31 July 2018.

Contact
Disseminating Unit (c.p. Indra Sakti/Ana Harlina/Rifki Sadikin)
Institute for Informatics
Indonesian Institute of Sciences
Phone (Office) +62-22-2504711; +62-21-87917216 (ext 112)
Fax : +62-22-2504712;
Email: informatica@mail.iipi.go.id

OPI - Organisasi Profesi Ilmiah Indonesia

MaX posted!!!



Rank	System	Cores	Rmax [PFlop/s]	Rpeak [PFlop/s]	Power [kW]
1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
4	Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
5	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096
6	Sierra - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94.64	125.71	7,438
7	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPCC National Supercomputing Center in Wuxi China	10,649,600	93.01	125.44	15,371
8	Perlmutter - HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE DOE/SC/LBNL/NERSC United States	761,856	70.87	93.75	2,589
9	Selene - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	555,520	63.46	79.22	2,646
10	Tianhe-2A - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000, NUDT National Super Computer Center in Guangzhou China	4,981,760	61.44	100.68	18,482



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ssh \$USER@login.leonardo.cineca.it



```
srun --nodes=10 --ntasks-per-node=4 --cpus-per-task=8 -A  
ICT23_SMR3872 --time 01:00:00 --gres=gpu:4 --mem=490000MB -p  
boost_usr_prod --pty /bin/bash  
[igirotto@lrdn0001 ~]$ mpirun ./myprog.x
```





```
[igirotto@login07 ~]$ module avail
/leandro/prod/spack/03/install/0.19/linux-rhel8-icelake/gcc-8.5.0/environment-modules-5.2.0-rz47odw4phlhzhhbz7b65nv
dot module-git module-info modules null use.own

profile/archive profile/base profile/candidate profile/chem-phys profile/deeplrn profile/lifesc profile/meteo profile/spoke7
----- /leandro/prod/opt/modulefiles/profiles -----
fake/1.0

----- /leandro/prod/opt/modulefiles/base/archive -----
adios/1.13.1--openmpi--4.1.4--gcc--11.3.0          hdf5/1.12.2--gcc--11.3.0-threadsafe           netlib-scalapack/2.2.0--openmpi--4.1.4-
adios/1.13.1--openmpi--4.1.4--nvhpc--23.1        hdf5/1.12.2--openmpi--4.1.4--gcc--11.3.0       netlib-xblas/1.0.248--gcc--11.3.0
blitz/1.0.2--gcc--11.3.0                         hdf5/1.12.2--openmpi--4.1.4--nvhpc--23.1      openblas/0.3.21--gcc--11.3.0
boost/1.80.0--gcc--11.3.0                         intel-oneapi-mkl/2022.2.1                   openblas/0.3.21--nvhpc--23.1
boost/1.80.0--openmpi--4.1.4--gcc--11.3.0         intel-oneapi-mpi/2021.7.1                  openmpi/4.1.4--gcc--11.3.0-cuda-11.8
boost/1.80.0--openmpi--4.1.4--nvhpc--23.1        intel-oneapi-tbb/2021.7.1                  openmpi/4.1.4--nvhpc--23.1-cuda-11.8
cgal/5.4.1--gcc--11.3.0                          libmatheval/1.1.11--gcc--11.3.0             parallel-netcdf/1.12.3--openmpi--4.1.4-
cgal/5.4.1--openmpi--4.1.4--gcc--11.3.0          libszip/2.1.1--gcc--11.3.0                  parallel-netcdf/1.12.3--openmpi--4.1.4-
cineca-hpyc/2023.05                            magma/2.6.2--gcc--11.3.0-cuda-11.8          parmetis/4.0.3--openmpi--4.1.4--gcc--11
cudnn/8.4.0.27-11.6--gcc--11.3.0                metis/5.1.0--gcc--11.3.0                   parmetis/4.0.3--openmpi--4.1.4--nvhpc--23
cutensor/1.5.0.3--gcc--11.3.0                  nccl/2.14.3-1--gcc--11.3.0-cuda-11.8        petsc/3.18.1--openmpi--4.1.4--gcc--11.3
elpa/2021.11.001--openmpi--4.1.4--gcc--11.3.0-cuda-11.8    netcdf-c/4.9.0--gcc--11.3.0                 petsc/3.18.1--openmpi--4.1.4--nvhpc--23
fftw/3.3.10--gcc--11.3.0                         netcdf-c/4.9.0--openmpi--4.1.4--gcc--11.3.0   petsc/3.18.1--openmpi--4.1.4--nvhpc--23
fftw/3.3.10--openmpi--4.1.4--gcc--11.3.0          netcdf-c/4.9.0--openmpi--4.1.4--nvhpc--23.1   petsc/3.19.0--openmpi--4.1.4--gcc--11.3
fftw/3.3.10--openmpi--4.1.4--nvhpc--23.1          netcdf-fortran/4.6.0--gcc--11.3.0            proj/8.2.1--gcc--11.3.0
gdal/3.5.3--gcc--11.3.0                         netcdf-fortran/4.6.0--openmpi--4.1.4--gcc--11.3.0 slate/2022.07.00--openmpi--4.1.4--gcc--11.3
gsl/2.7.1--gcc--11.3.0                           netcdf-fortran/4.6.0--openmpi--4.1.4--nvhpc--23.1 zlib/1.2.13--gcc--11.3.0
hdf5/1.12.2--gcc--11.3.0

----- /leandro/prod/opt/modulefiles/base/libraries -----
anaconda3/2022.05 git-lfs/3.1.2          intel-oneapi-vtune/2022.4.1          ncview/2.1.8--openmpi--4.1.4--gcc--11.3.0      snakemake/6.15.1 t
cmake/3.24.3   git/2.38.1           jube/2.4.3                     ninja/1.11.1                               spack/0.19.1-d71 \v
curl/7.79.0    git/2.38.1--nvhpc--23.1 maven/3.8.4                    openjdk/11.0.17_8                           superc/2.0
emacs/28.2     gnuplot/5.4.3--gcc--11.3.0 nco/5.0.1--openmpi--4.1.4--gcc--11.3.0      singularity/3.8.7                           texinfo/6.5

----- /leandro/prod/opt/modulefiles/base/tools -----
cuda/11.8      intel-oneapi-compilers/2023.0.0    nvhpc/22.3    perl/5.36.0--gcc--8.5.0    perl/5.36.0--nvhpc--23.1    python/3.10.8--gcc--11.3.0
gcc/11.3.0     llvm/15.0.4--gcc--11.3.0-cuda-11.8    nvhpc/23.1    perl/5.36.0--gcc--11.3.0    python/3.10.8--gcc--8.5.0
```