Introduction & HPC

Ivan Girotto – igirotto@ictp.it

HPC Applications Specialist

International Centre for Theoretical Physics (ICTP)

The Abdus Salam
International Centre
for Theoretical Physics

United Nations
Educational, Scientific and
Cultural Organization

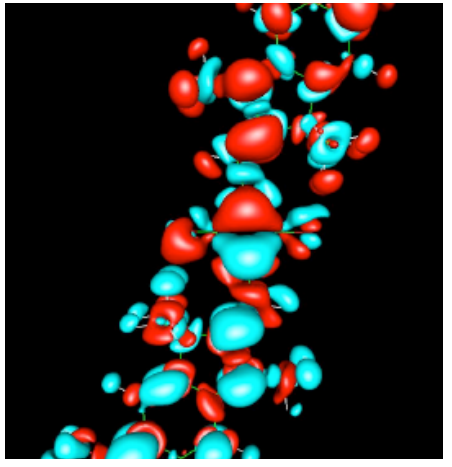
IAEA
International Atomic Energy Agency

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.

Research at ICTP

42 Scientists (P-staff)
65 Postdocs
40 PhD students
22 Long-term visitors
[from 43 countries / 56% developing]



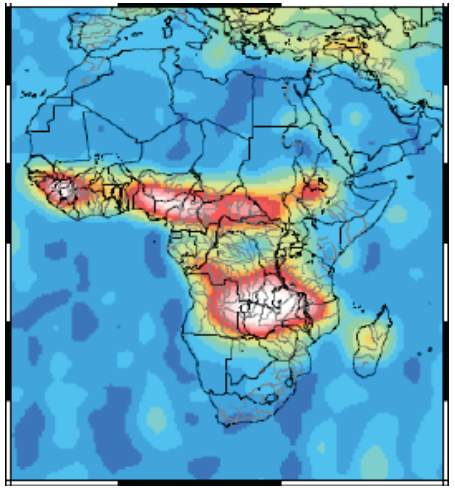
- ✓ 500+ papers/year (74% in Q1 journals)
- ✓ 32,000 citations/year
- ✓ 5 ERC Grant holders

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

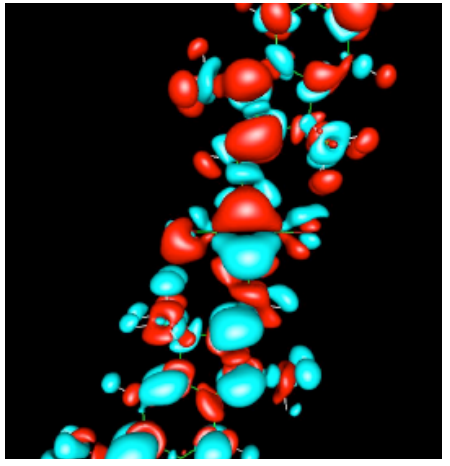
Computational cluster: ~3000 cores + GPUs

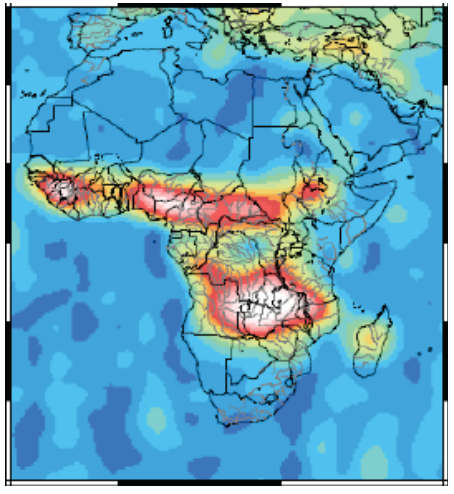


Research at ICTP

Core Research Areas

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

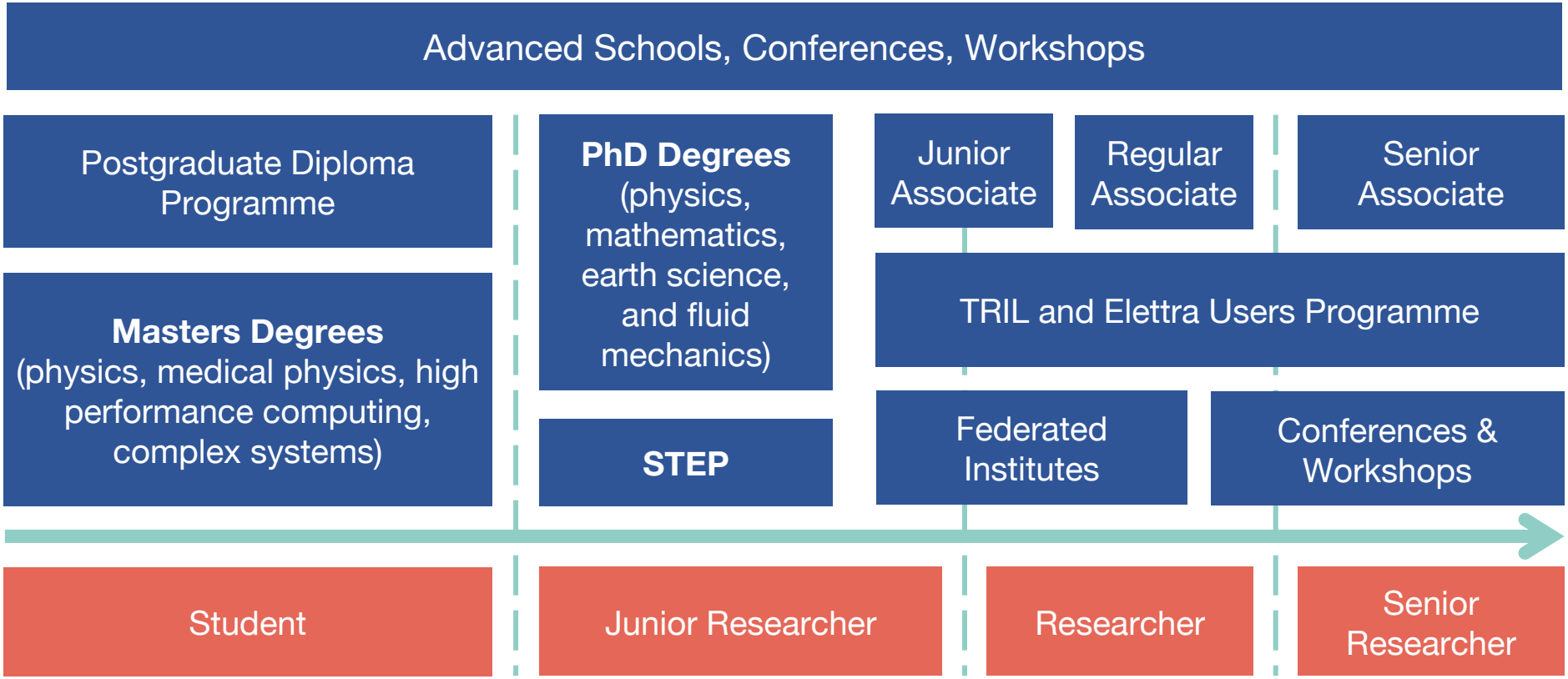




Special initiatives

- "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

ICTP Programmes

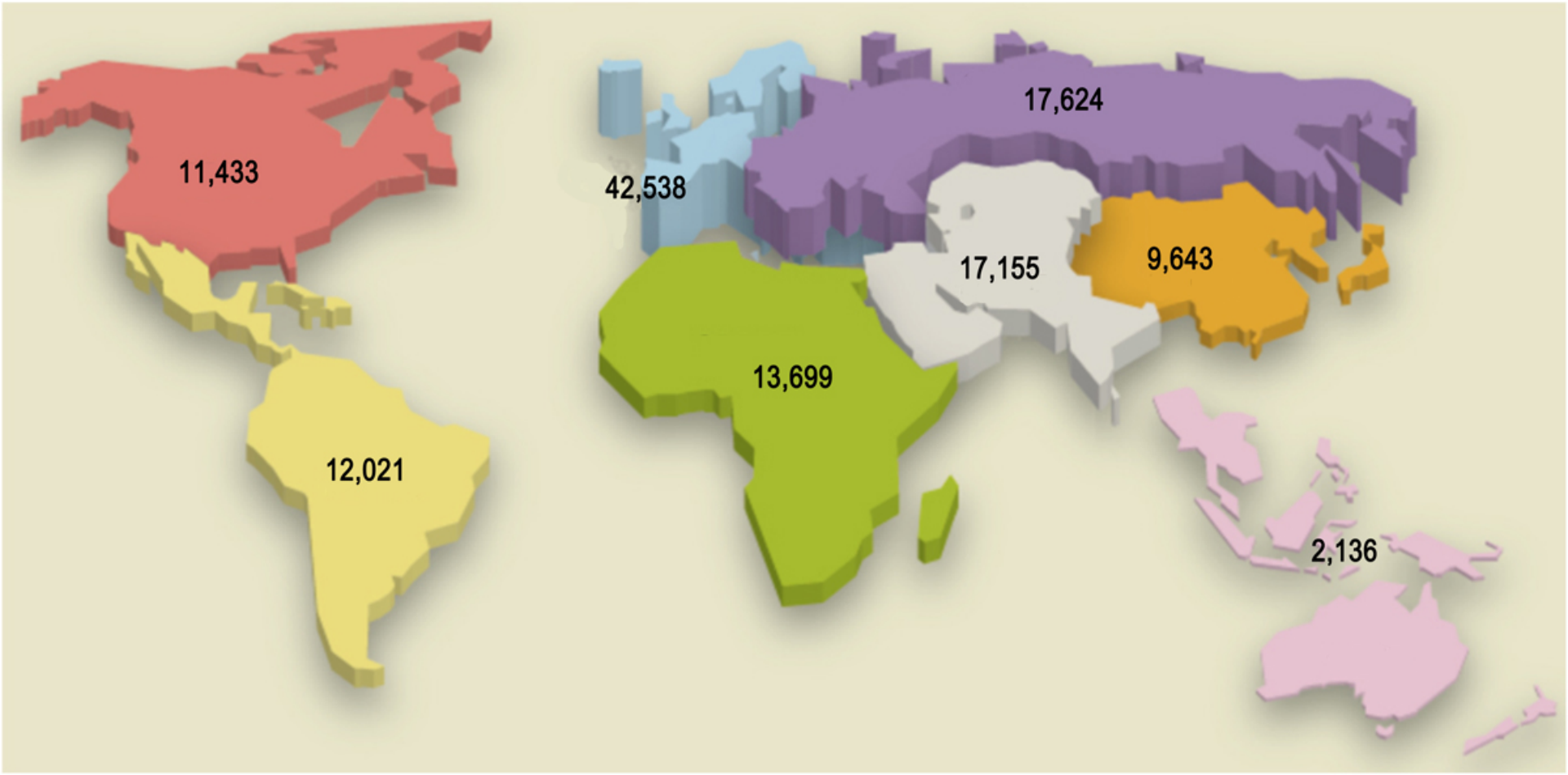


ICTP supports scientists from developing world throughout their career who in turn educate several younger scientists in their home country.

This multiplier effect is the strength of ICTP.

ICTP Visiting Scientists

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



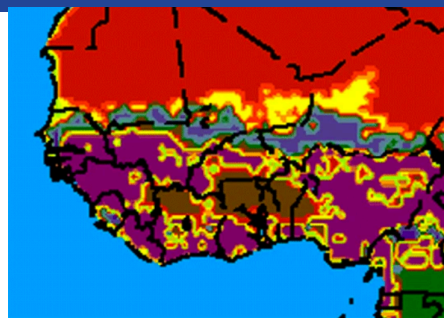
An International Consortium for Scientific Computing

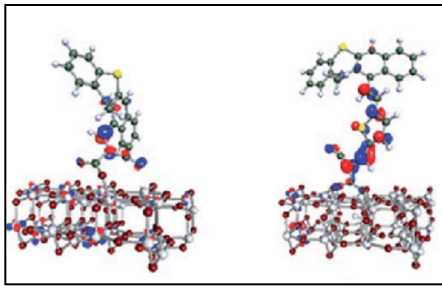
Challenges:

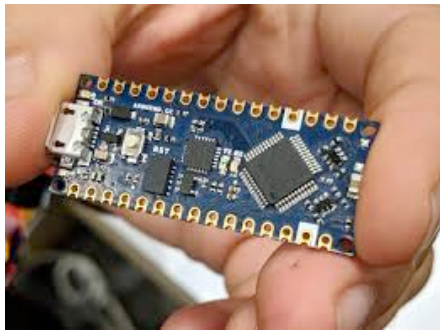
- Growing «divide» developed/developing world
- Lack of international collaborations & research ecosystems
- Scarce «human capacity»
- HPC infrastructures (Africa's top facility 182th in Top500)

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

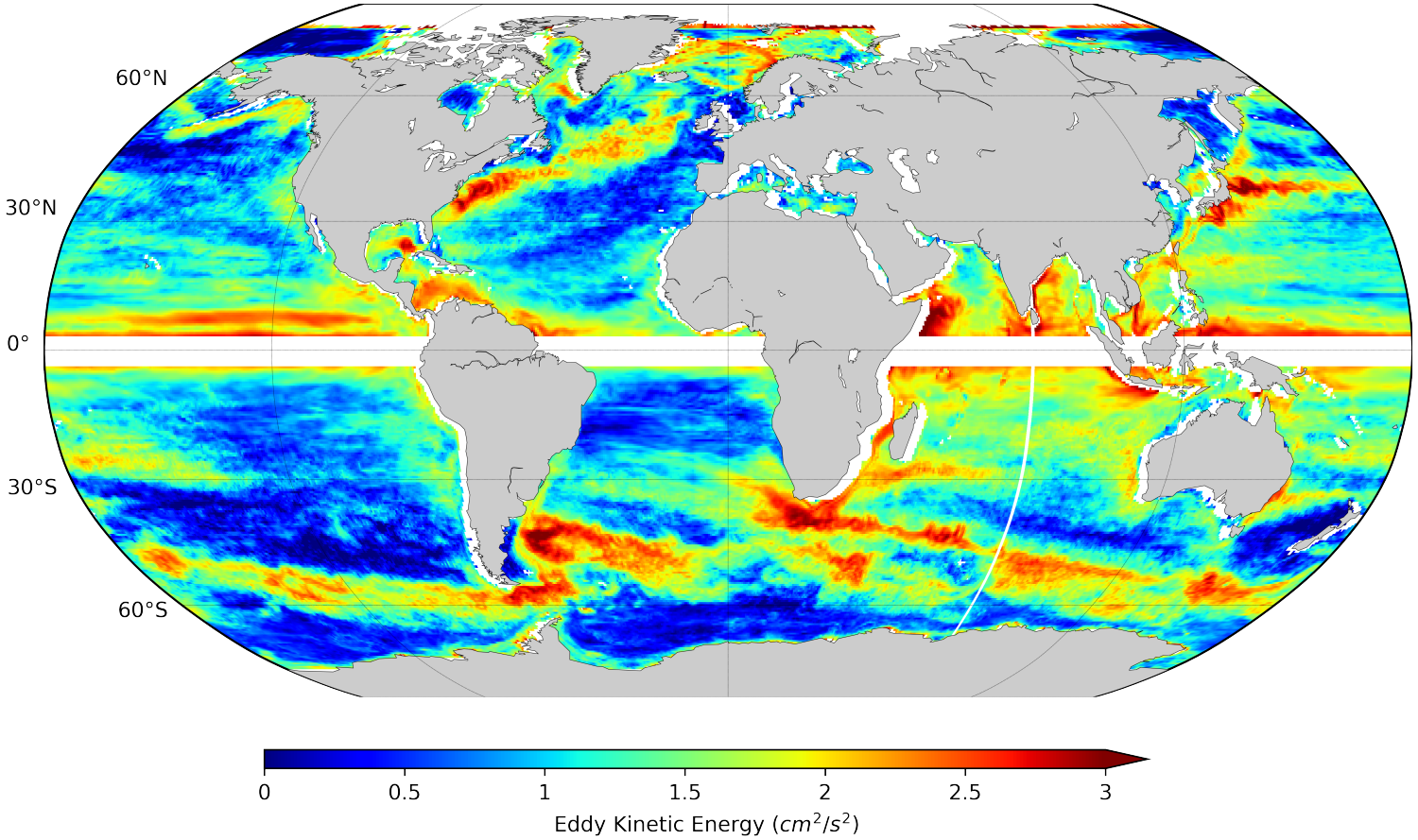
Impact of Using Computer is Science

- **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

*** from EU Digital Single Market Blog by Roberto Viola, Director-General, DG Communications Networks, Content and Technologies and Robert-Jan Smits, Director-General, DG Research and Innovation**

Large Scale Computer Simulations @ ICTP

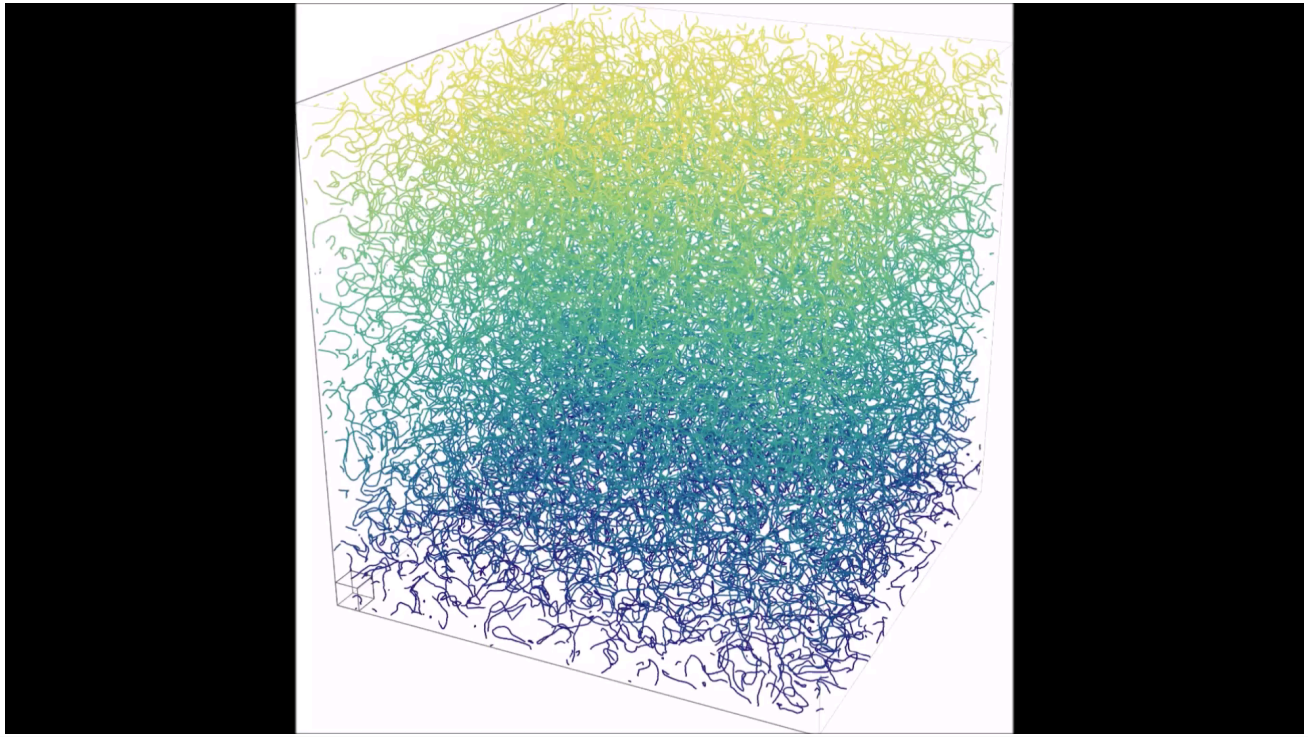
GFDL/MOM global ocean model as part of the international program FAFMIP. Simulations runs on 2400 cores (~50 nodes) on the SKL partition



*** Courtesy of Dr. Ricardo Farneti (ESP group)**

Large Scale Computer Simulations @ ICTP

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 Gorghetto, Edward Hardy, Giovanni Villadoro

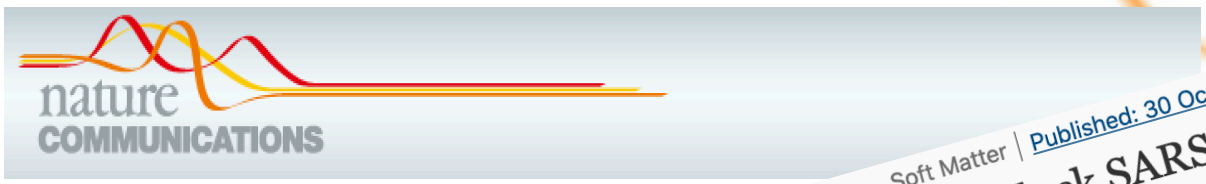
Large Scale Computer Simulations @ ICTP

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 locali
in a two-dimensional metal-org

M. Corva[1,2], A. Ferrari[1,5], M. Rinaldi[1], Z. Feng[1,6], M. Roiaz[3], C. Ramesh
M. Dell'Angela[2], G. Pastore[1], G. Comelli[1,2], N. Seriani[4] & E. Vesselli[1,

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 Goliaei, Ivan Girotto, Ricardo Franklin-Mergarejo, Oriol Güell, Ali Hassanali & Édgar Roldán
...rantini[1,2],

Large Scale Computer Simulations @ ICTP

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 ☆

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

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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)

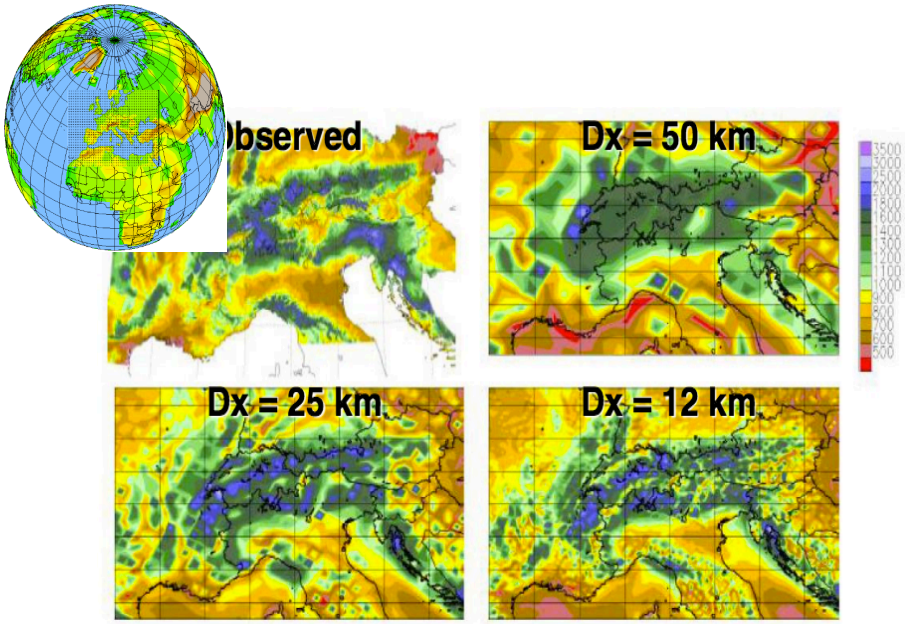
PHYSICAL REVIEW LETTERS

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

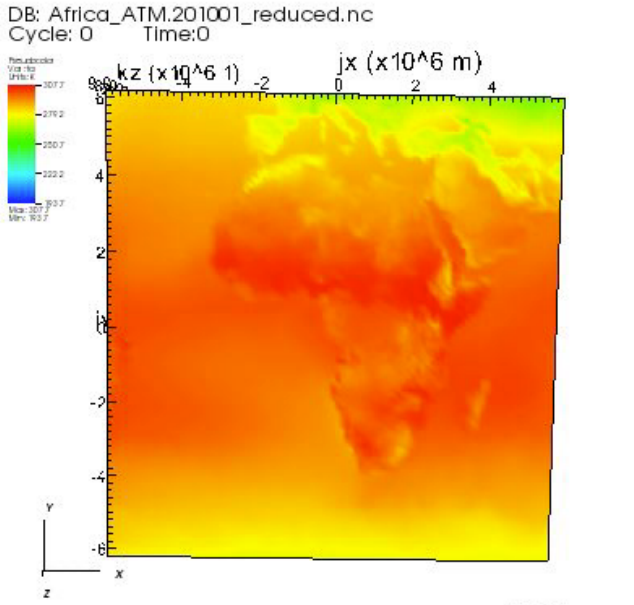
Large Scale Computer Simulations @ ICTP



- 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

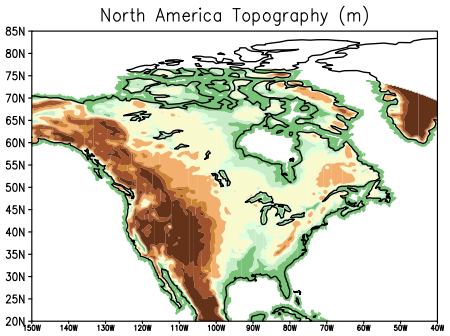
[…] for Europe, we plan to run seven 140 year simulations. Each month of simulation, with 500 processors, is expected to take about 2.9 hours of compute time and produce 60GB of raw output files

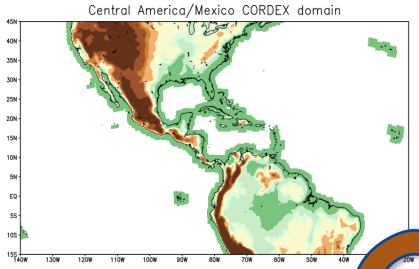
The on-going simulations, planned to end in early 2020, is expected to finally require about 100M cpu-h and approximately 2PB of data will be publicly made available

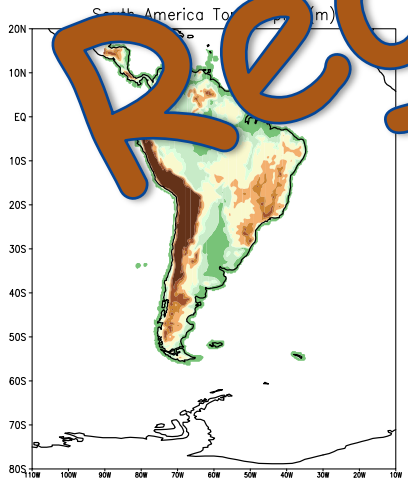


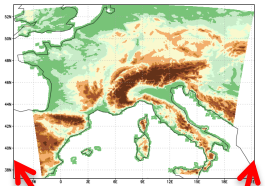
RegCM4.7 tested domain available and long scenario simulations available

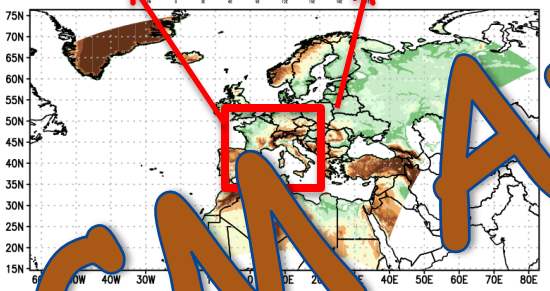
*** Courtesy of Dr. Erika Coppola (ESP group)**

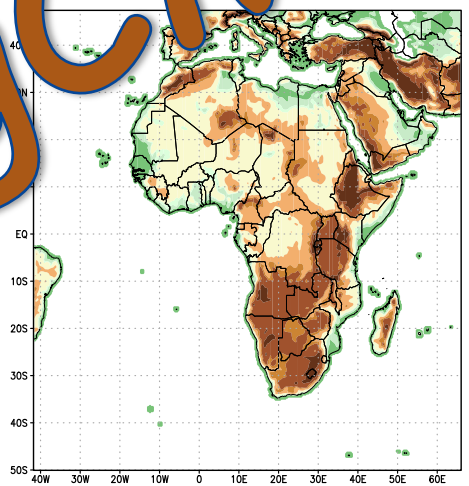


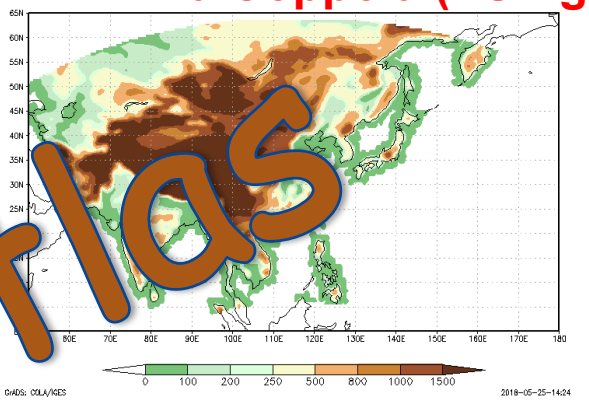


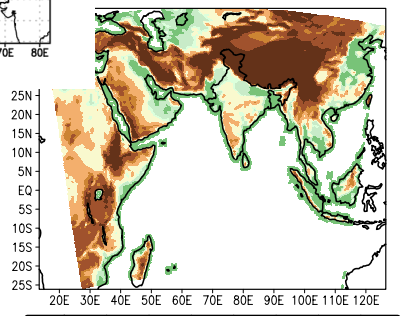


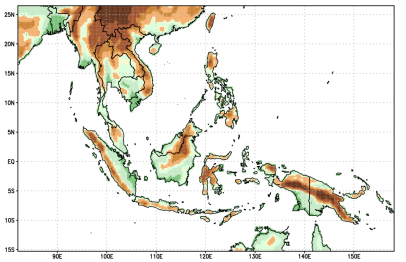


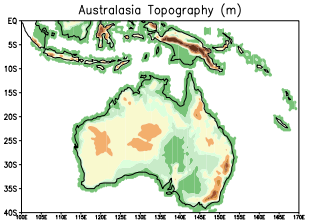


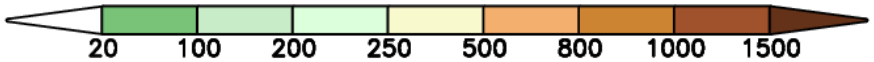












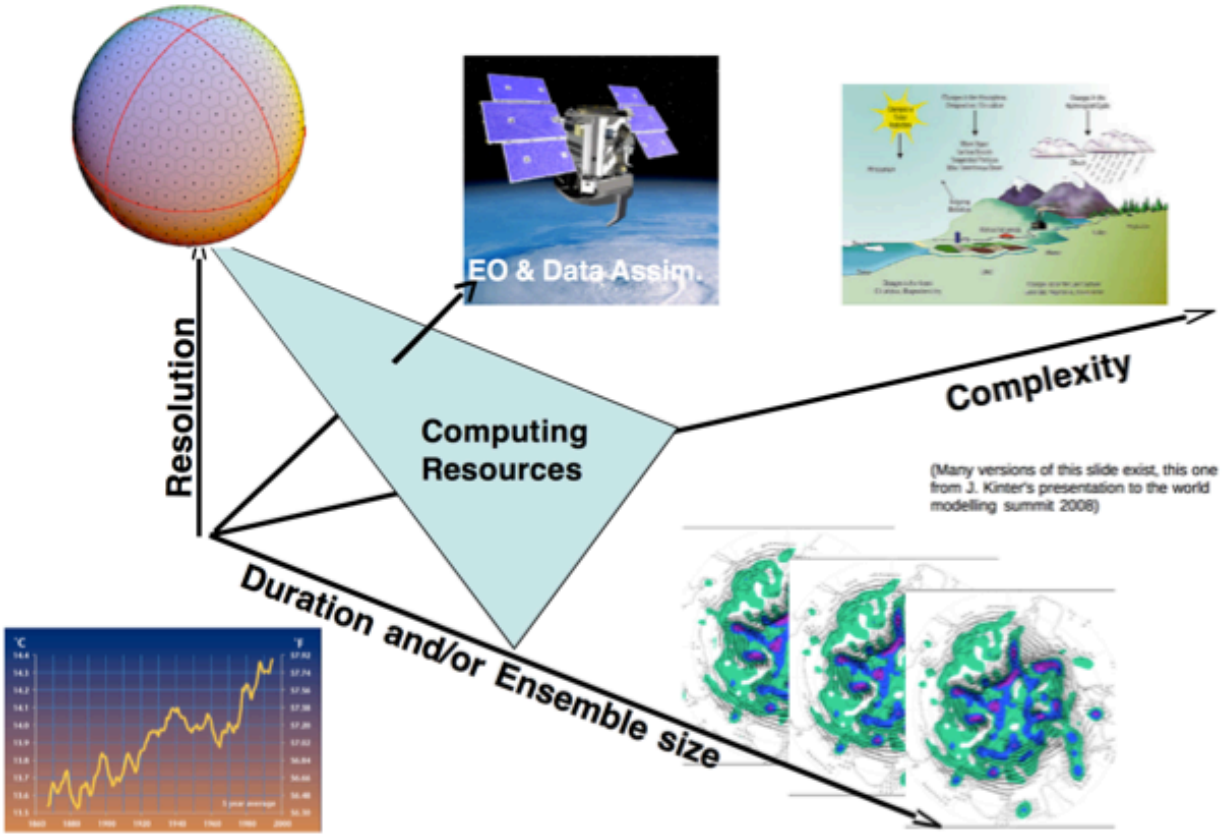
RegCM Atlas

The Abdus Salam International Centre 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 …

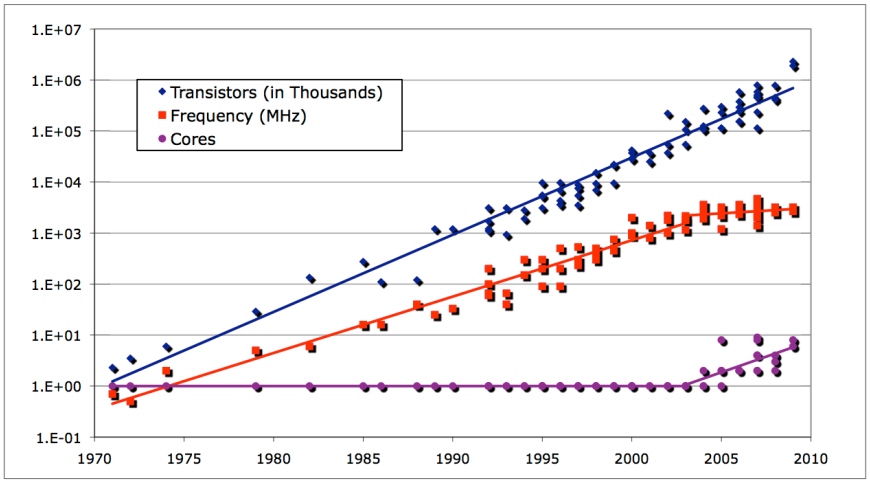


Why would HPC matter to you?

- 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

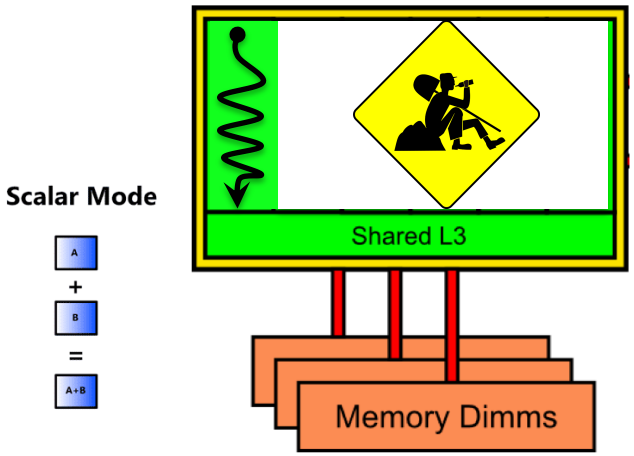
Collateral Consequences /1

- Growing of computer capability is achieved increasing computer complexity



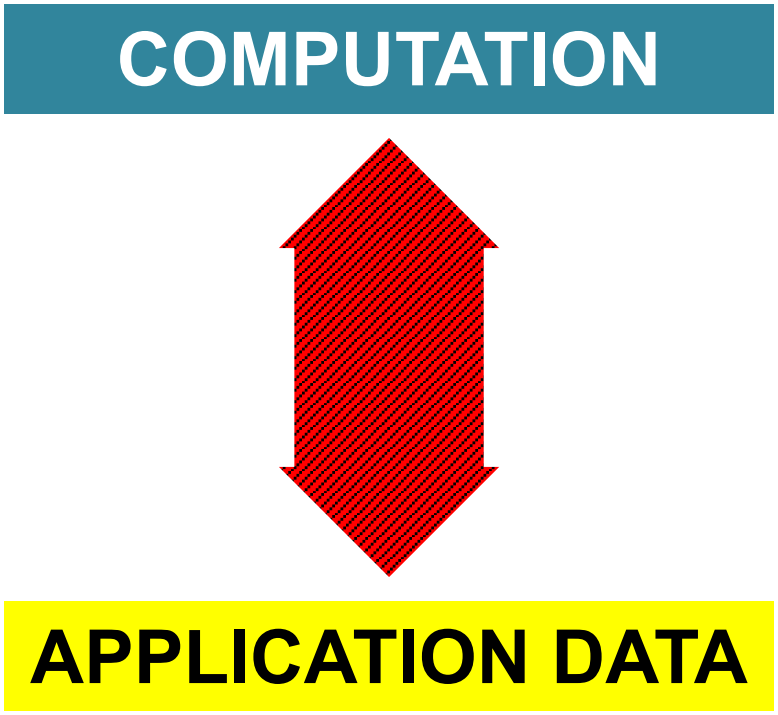
- CPU power is measured in number of floating point operations x second (FLOPs)
  - FLOPS = #cores x clock freq. x (FLOP/cycle)

#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



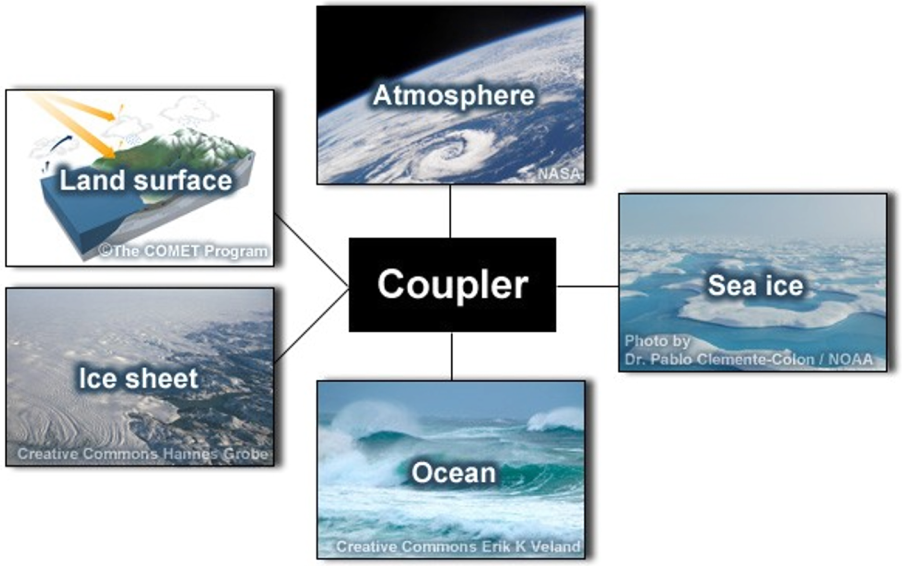
Collateral Consequences /2

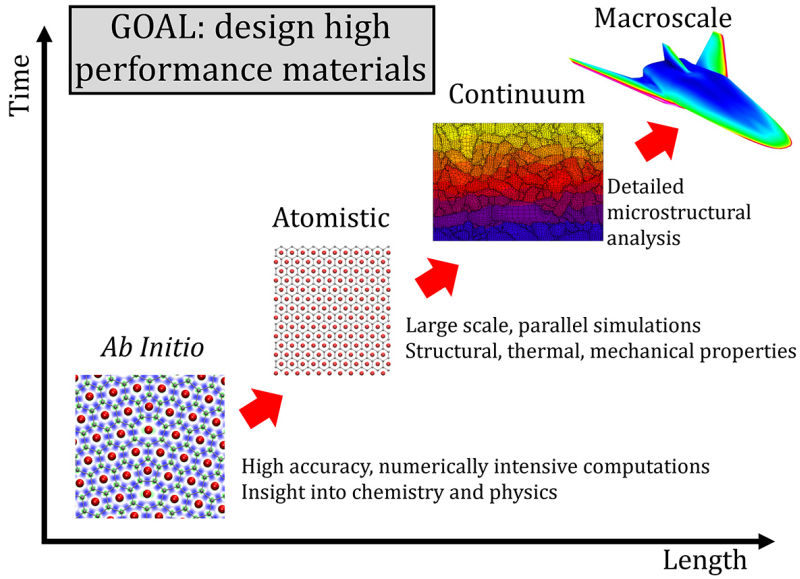
- When all CPU component work at maximum speed that is called *peak of performance*
  - Tech-spec normally describe the theoretical peak
  - Benchmarks measure the real peak
  - Applications show the real performance value
- CPU performance is measured FLOP/s
- But the real performance is in many cases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



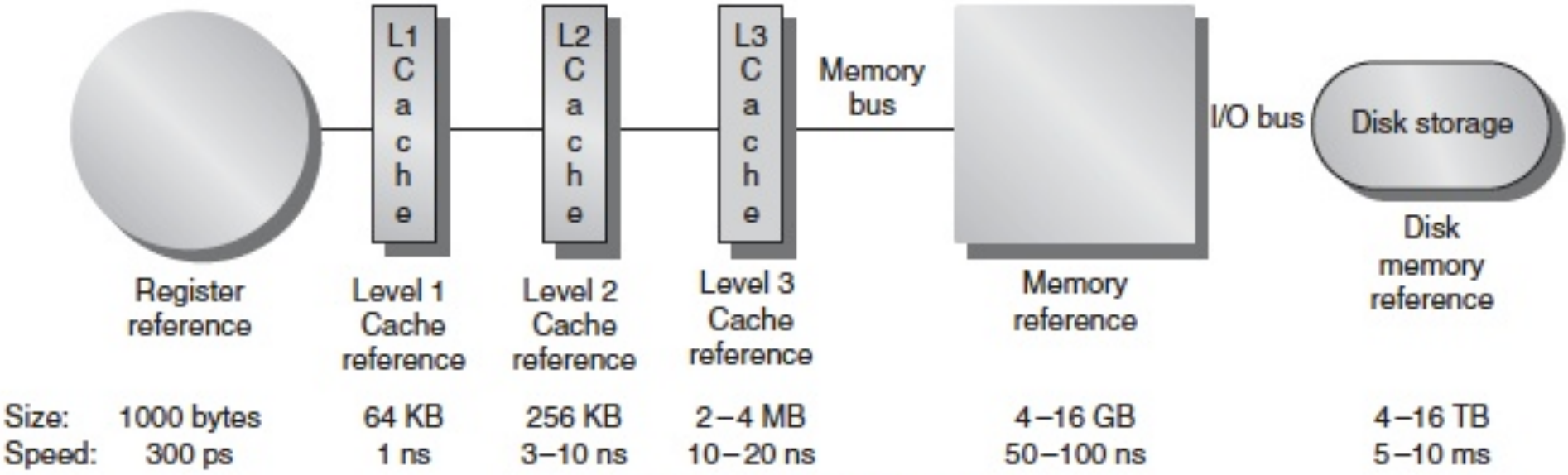
Collateral Consequences /2

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

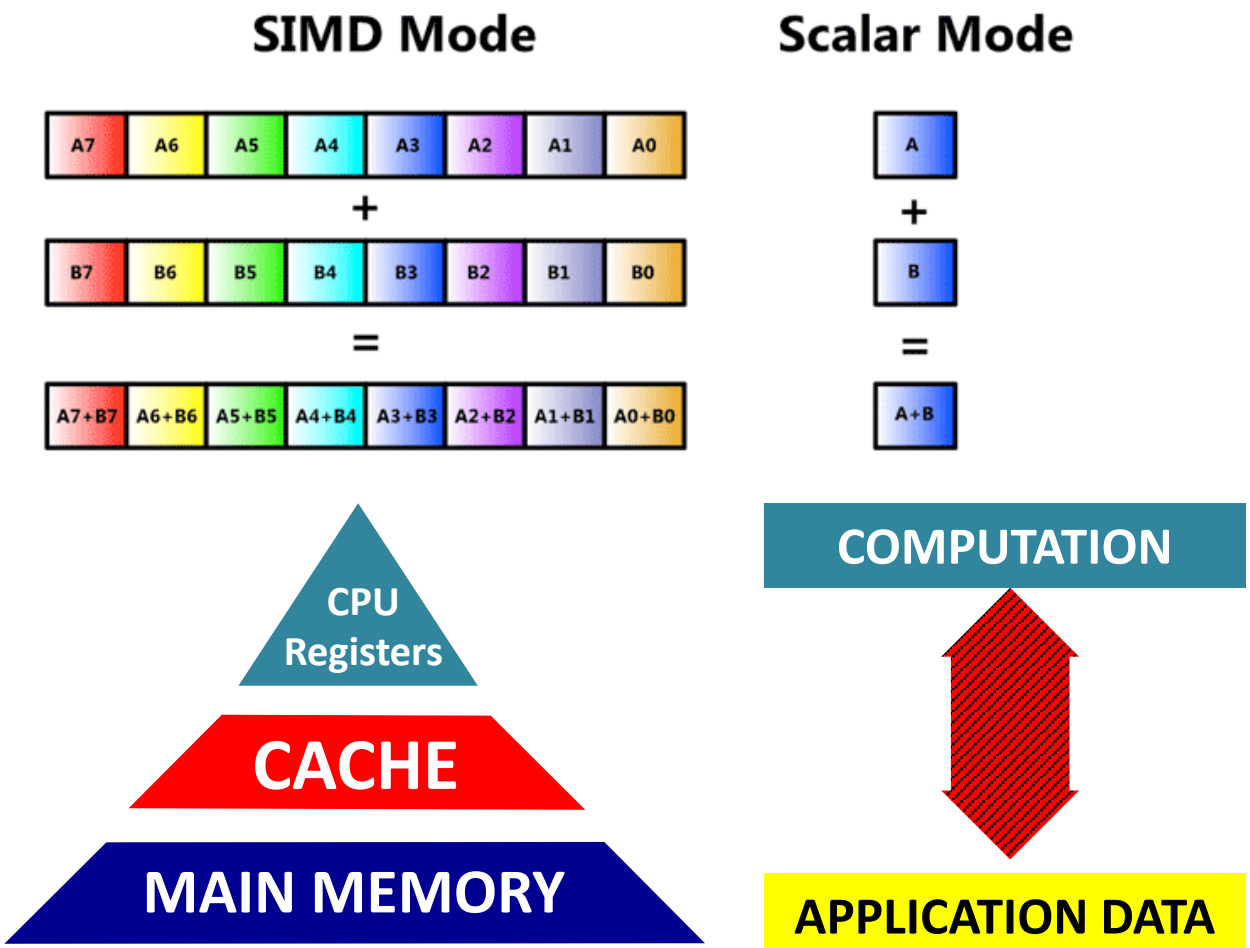




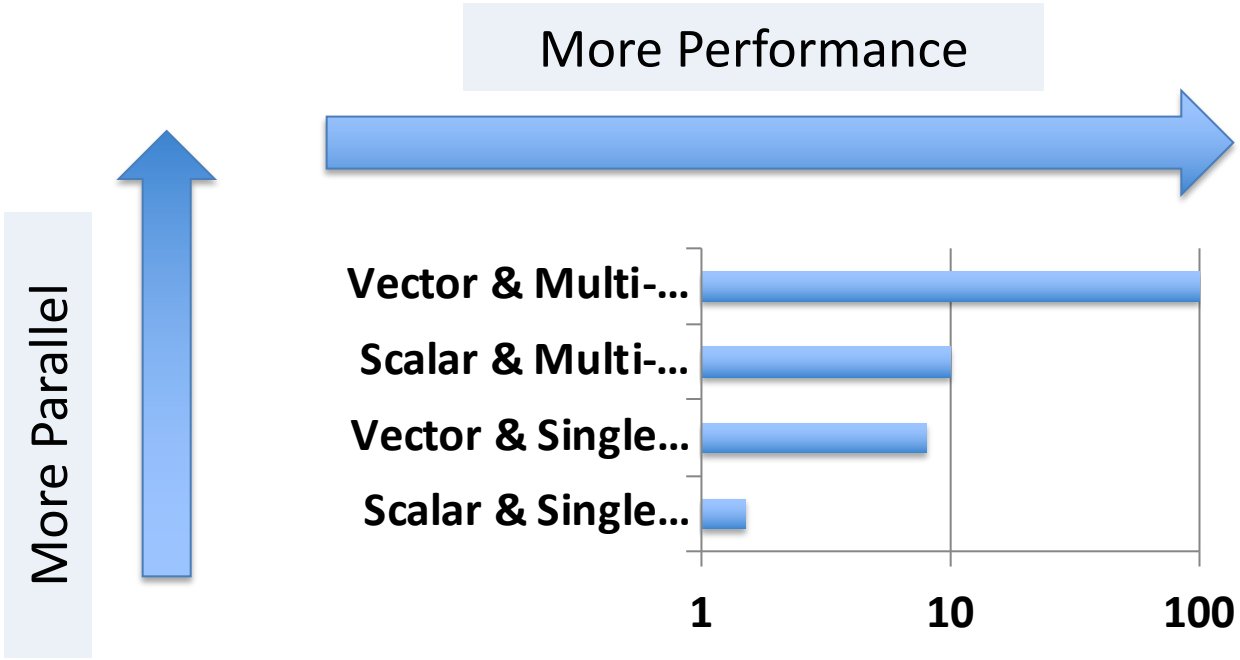
https://www.nas.nasa.gov/SC14/demos/demo26.html#prettyPhoto

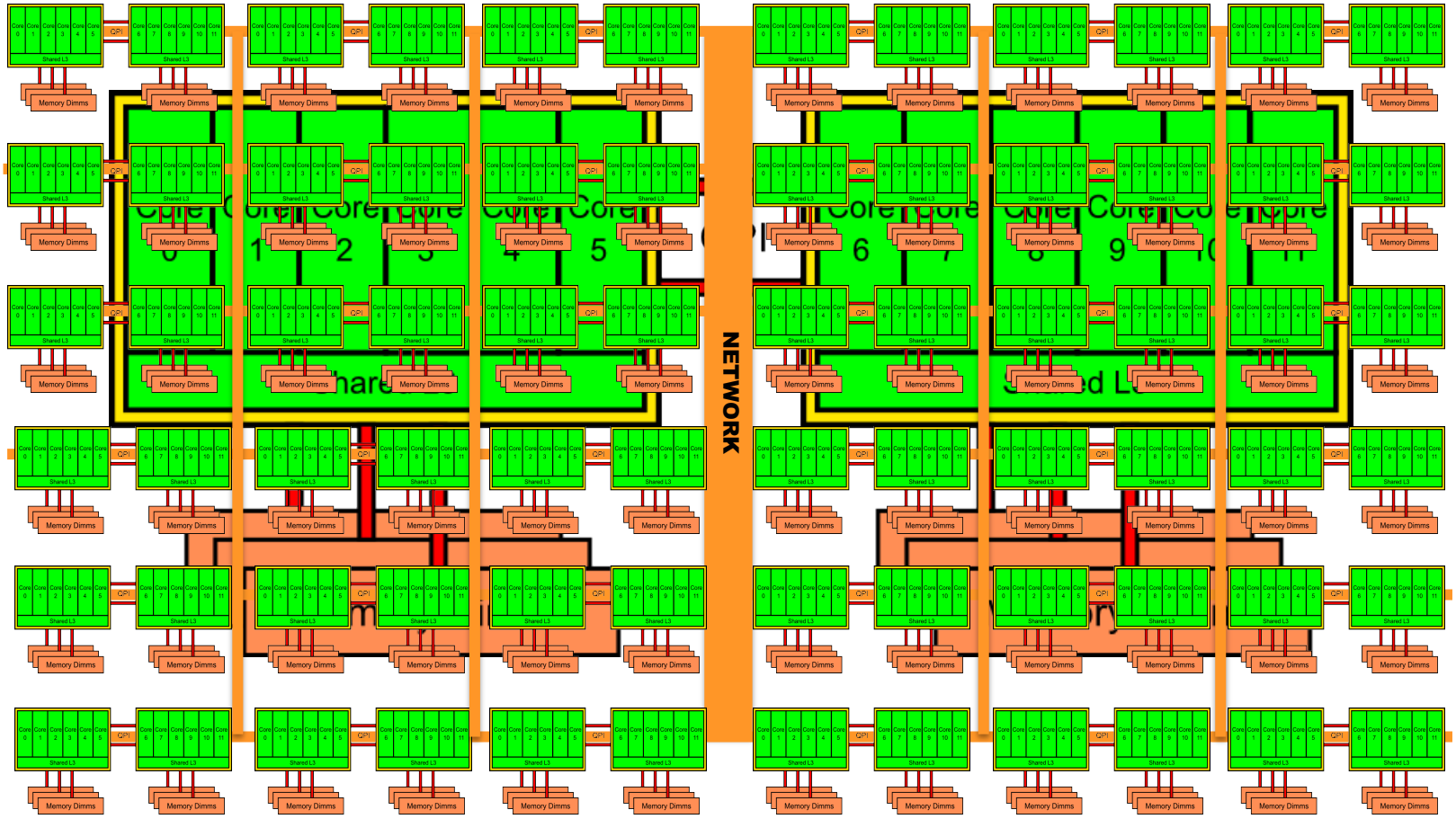


(a) Memory hierarchy for server

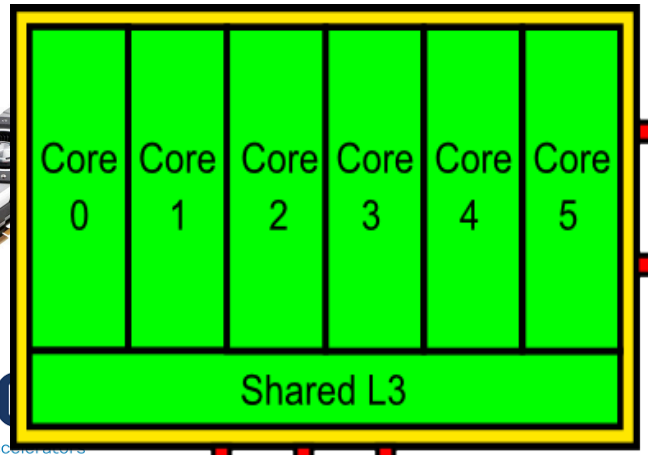

SIMD Mode
Scalar Mode
A7 A6 A5 A4 A3 A2 A1 A0
+
B7 B6 B5 B4 B3 B2 B1 B0
=
A7+B7 A6+B6 A5+B5 A4+B4 A3+B3 A2+B2 A1+B1 A0+B0
A
+
B
=
A+B
CPU Registers
CACHE
MAIN MEMORY
COMPUTATION
APPLICATION DATA

Threading and Vectorization




NETWORK
Memory Dimms
QPI
Shared L3

Multiple Socket CPUs + Acceleretors



OpenAC
Directives for Acc

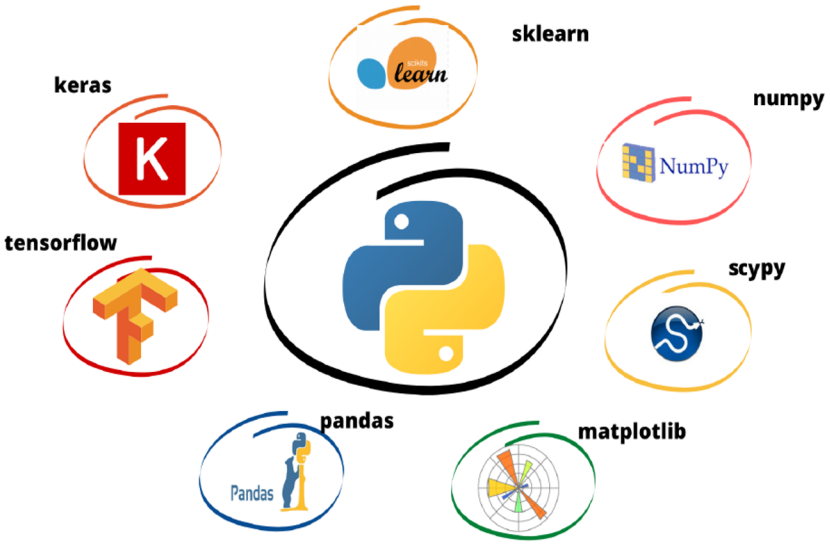
NVIDIA CUDA

NDARD
AMMING
&
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



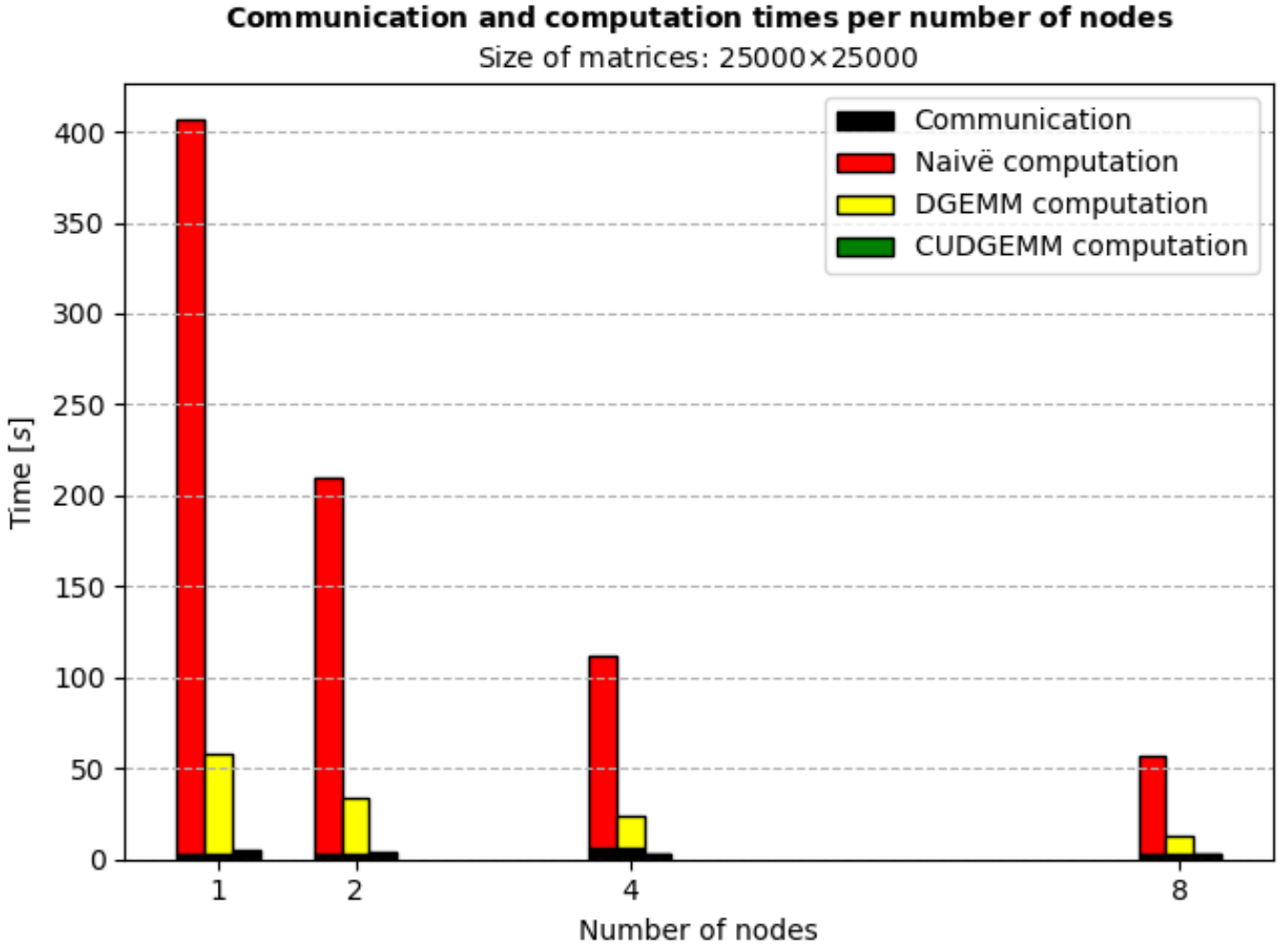
FFTW

OpenFOAM®

QUANTUMESPRESSO

OpenBLAS

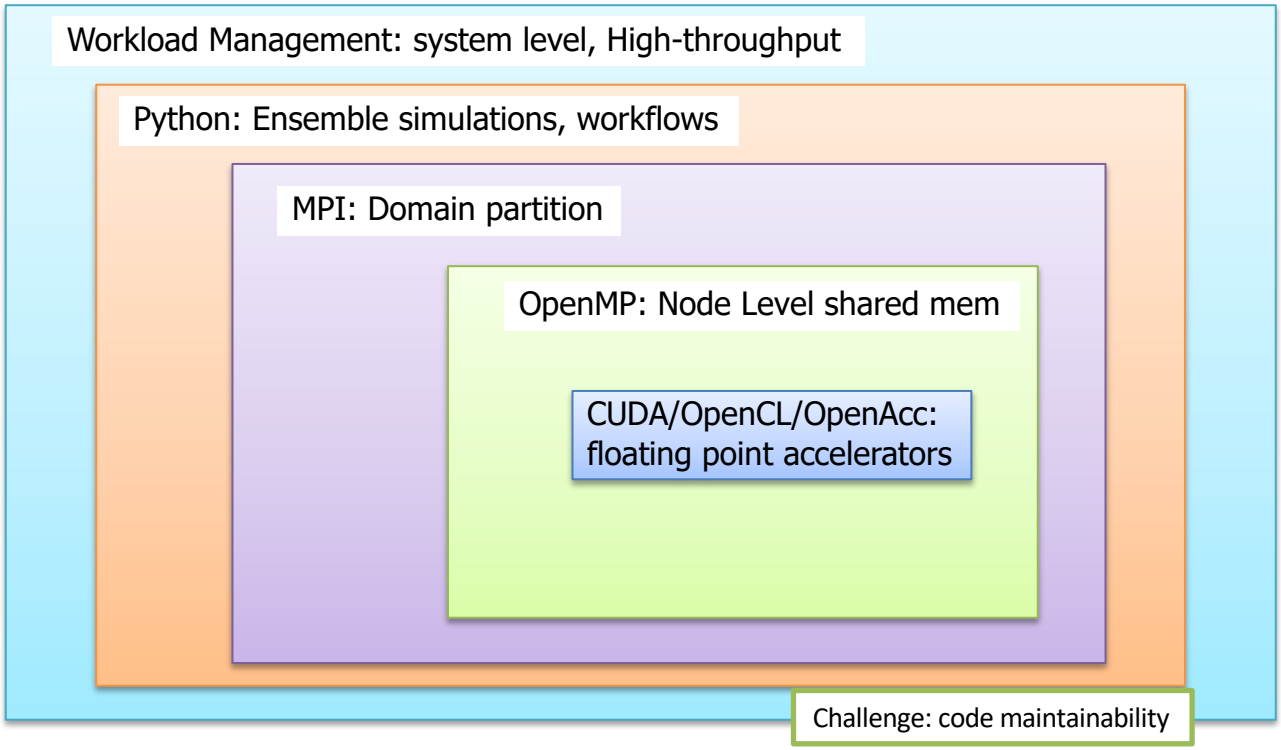
LAMMPS
Large-scale Atomic/Molecular Massively Parallel Simulator


Communication and computation times per number of nodes
Size of matrices: 25000×25000
Communication
Naivë computation
DGEMM computation
CUDGEMM computation
Time [s]
0
50
100
150
200
250
300
350
400
1
2
4
8
Number of nodes

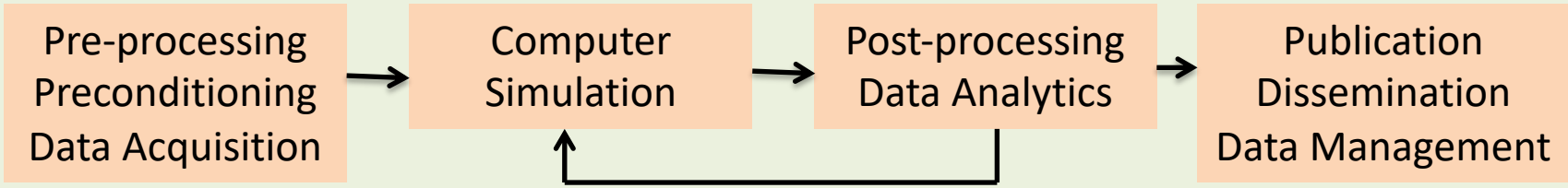
Scalability

- 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



HPC INFRASTRUCTURE



Scientists/Application Developers/End Users

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**:

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

The MHPC in pills: www.mhpc.it

- 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

MHPC
Master in High Performance Computing

Background Requirements

- 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

The Curricula : www.mhpc.it

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

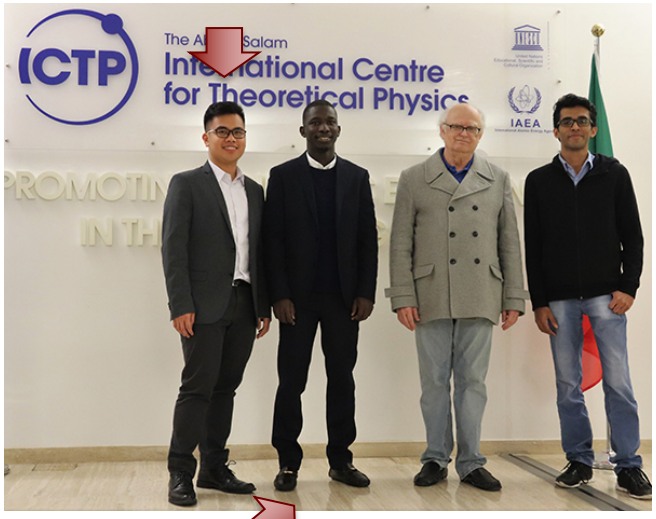
HPC Training Scholarship Winners

Alejandra Foggia
& Rajat Panda
CMSP group @ ICTP

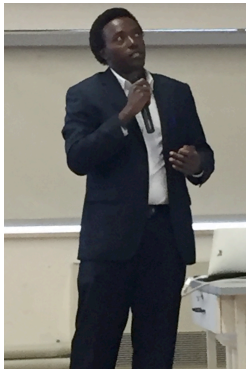
Muhammad Owais, Pakistan
Junior Research Engineer
BSC-CNS (Spain)

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

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)



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

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

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

Fernando Posada, Colombia
Assistant Professor
Temple University (USA)

Other Programs

The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

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, NRCPC 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

READ THE USER GUIDE!!

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
------------------------------ /leonardo/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

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

------------------------------------------------------------------------------ /leonardo/prod/opt/modulefiles/base/archive ------------------------
fake/1.0

------------------------------------------------------------------------------ /leonardo/prod/opt/modulefiles/base/libraries ----------------------
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--
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--
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                               netlib-scalapack/2.2.0--openmpi--4.1.4--gcc--11.3.0

------------------------------------------------------------------------------ /leonardo/prod/opt/modulefiles/base/tools --------------------------
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

------------------------------------------------------------------------------ /leonardo/prod/opt/modulefiles/base/compilers ----------------------
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
```