Introduction to solvers and algorithms for CFD and Astrophysics

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Italy

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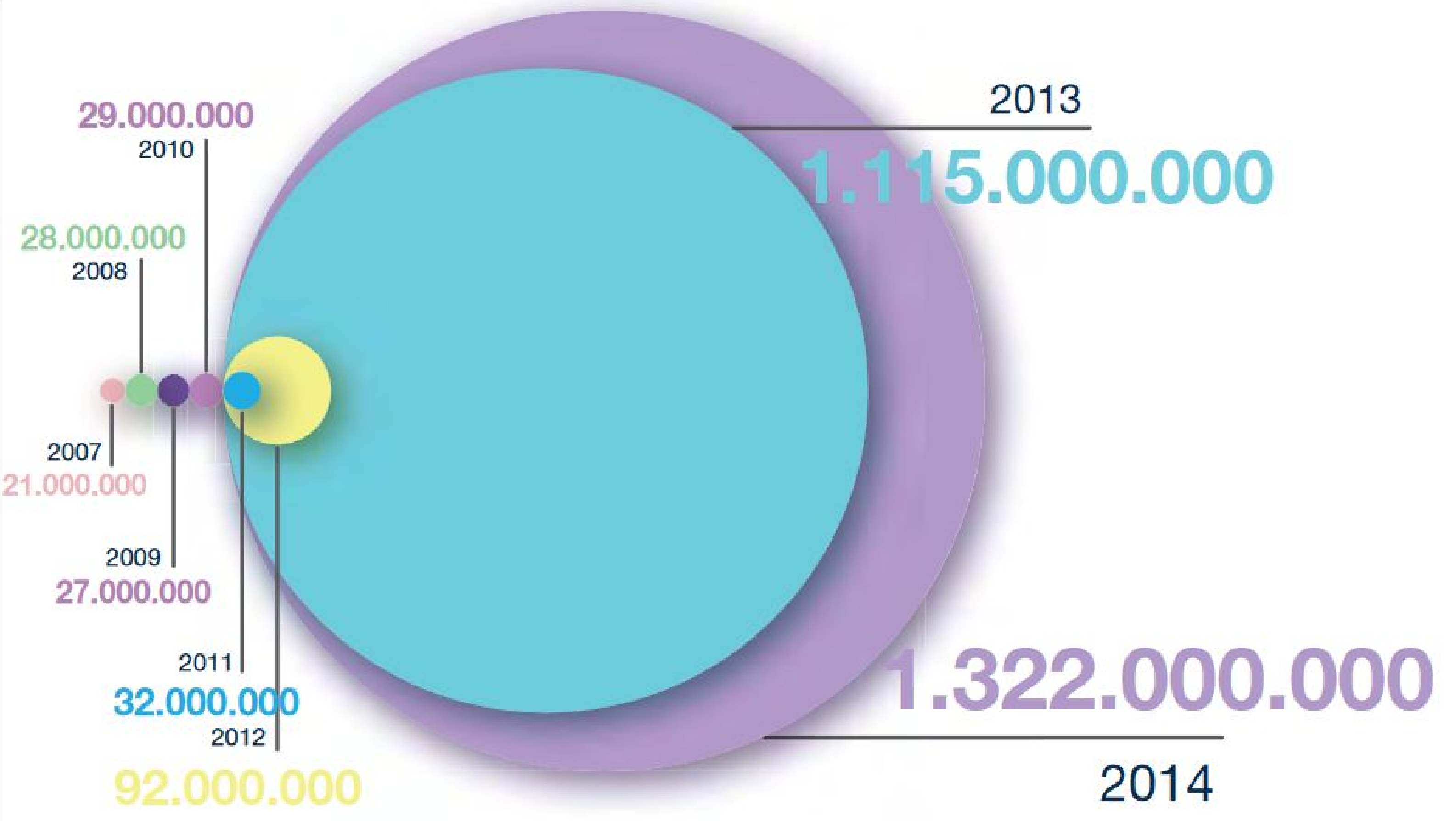
Aim of the workshop

- The aim of this workshop is to present the (most) representative HPC numerical methods used in the fields of Computational Fluid Dynamics (CFD) and Numerical Astrophysics.
- The workshop aims to share the methodologies, numerical methods and their implementation used by the state-of-the-art codes in the HPC environment.
- Key-note lectures will present the challenges of numerically solving Partial Differential Equations (PDE) in problems related to fluid/hydrodynamics, using massively parallel clusters.
- The workshop will focus on state-of the art of the different HPC architecture and the related numerical methods

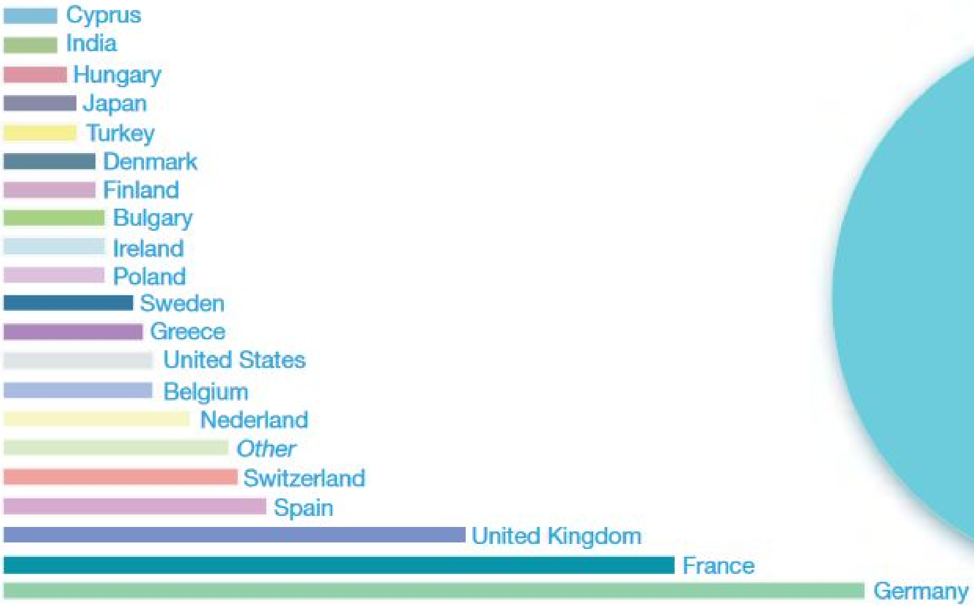
Disclaimer: It is NOT our intent to give a complete survey of the numerical methods used in HPC for the fields of CFD and Numerical Astrophysics. The present workshop shows some of the most used research/community codes granted for access to Tier-0 HPC european (and national) ecosystems in the recent years.

HPC Usage by scientific Sector @ CINECA

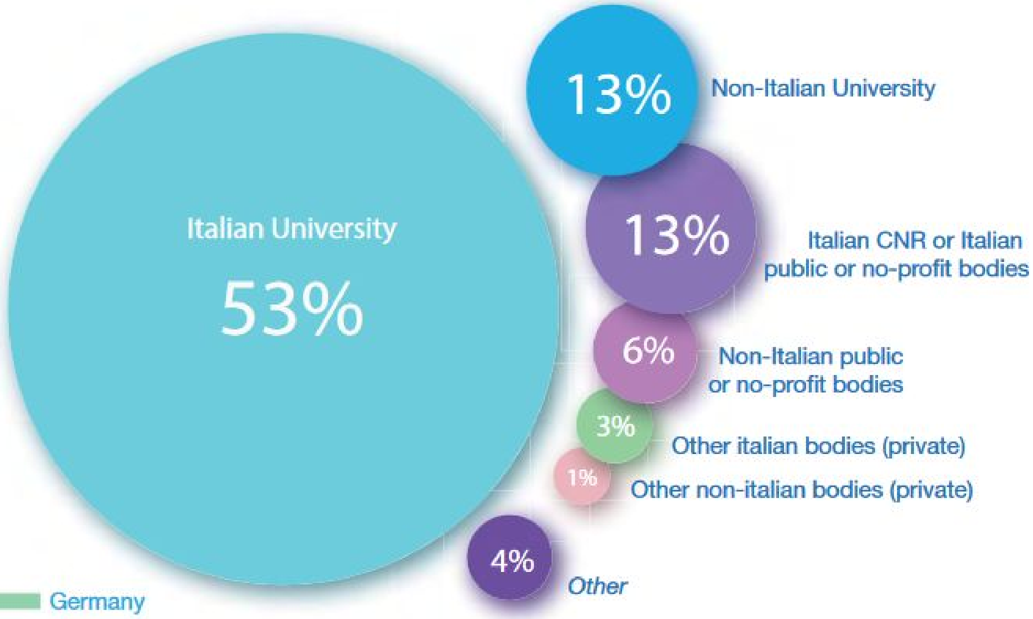
- Scientific computing core hours production



HPC Usage by scientific Sector @ CINECA

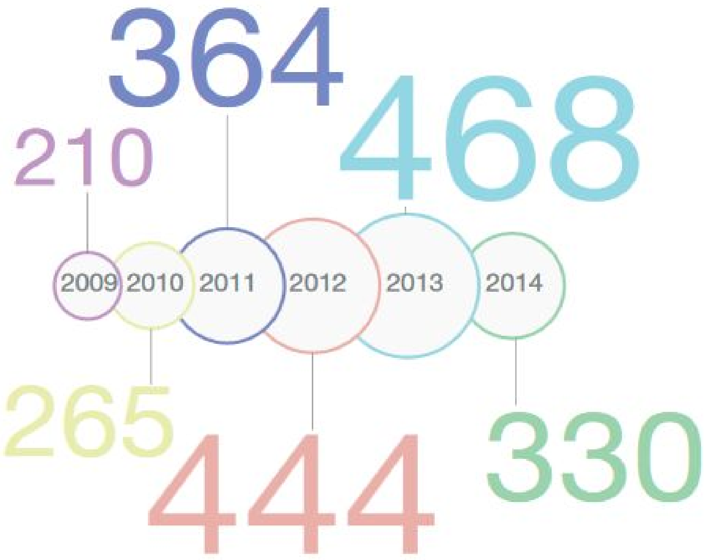


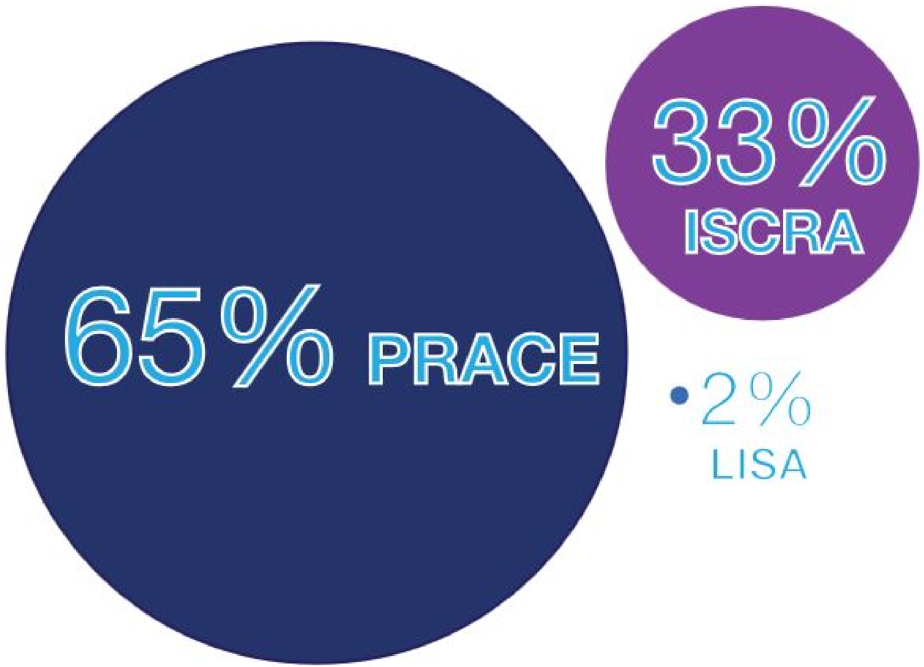
Cineca users with affiliation to foreign entities.



Classification User Institutes

HPC Usage by scientific Sector @ CINECA

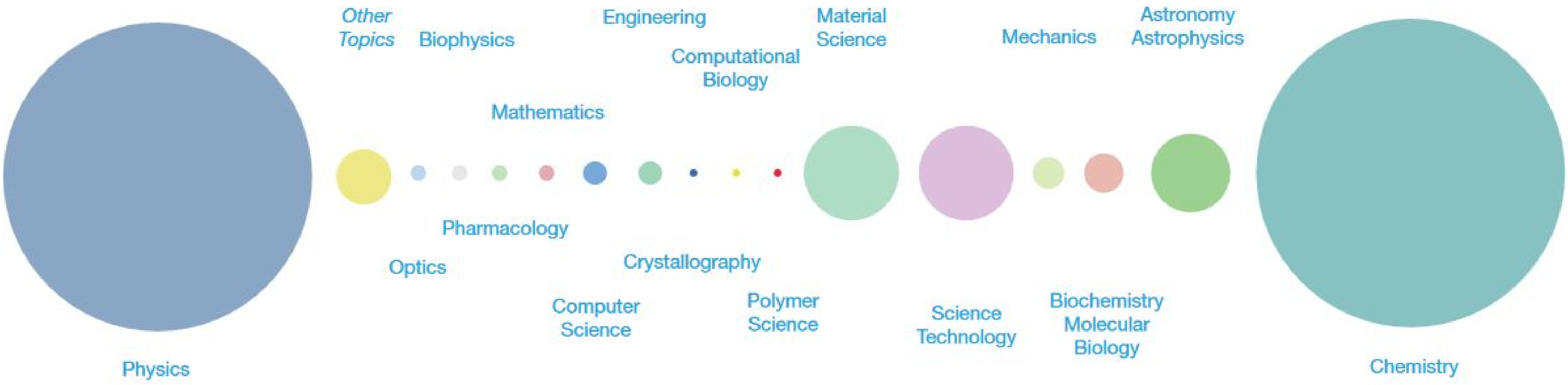




Total number of publications

Allocated resources

HPC Usage by scientific Sector @ CINECA

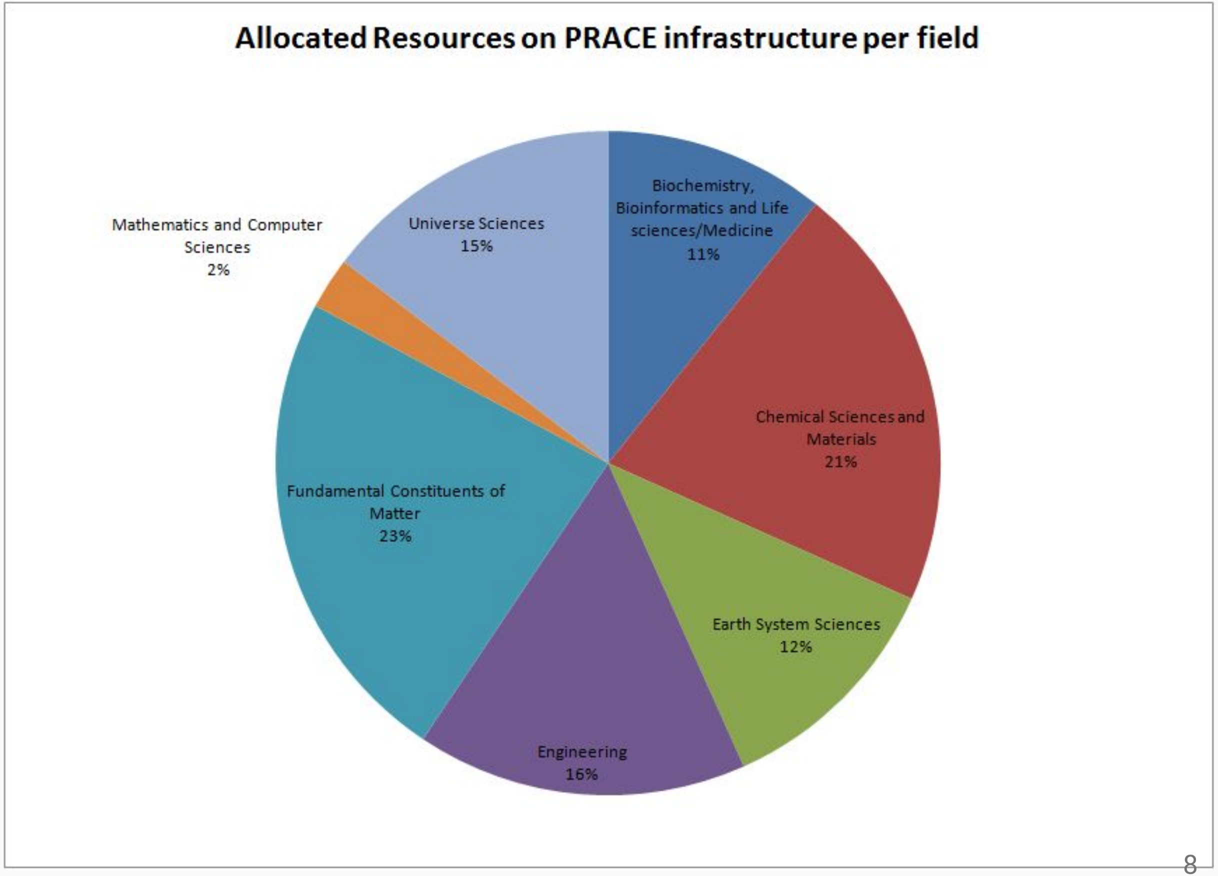


Research areas of the publications mentioning CINECA

HPC Usage by scientific Sector @ PRACE

From Call 1 to Call 13 (2011-now)

- 12 Billions of core hours awarded
- 6 HPC clusters (Now 7)
- 4 hosting members (now 5)
    - CINECA, Italy
    - GENCI@CEA, France
    - BSC, Spain
    - GSC (HLRS, LRZ, JSC), Germany
    - CSCS, Switzerland (starting from call 14)
- 31% ENG + Astro



Overview of Numerical Methods and Algorithms

Layout of following presentations

- Area of research/interest
- Governing Equations
- Numerical Method
- Need for massively parallel clusters
- Implementation in HPC environment and parallelization of the numerical methods
- Use of HPC libraries (if any)
- outcome of HPC grants used (PRACE, ISCRA, etc, etc.)
- future work

Services

Introduction to solvers and algorithms for CFD and Astrophysics

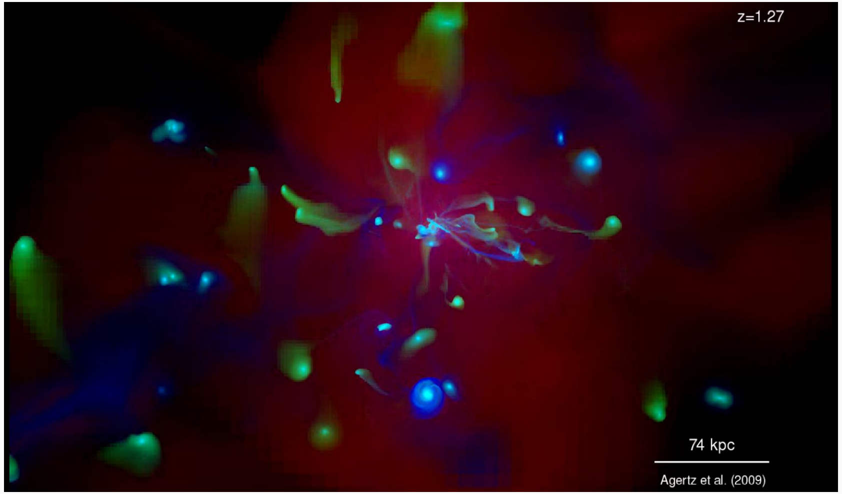
HPC CINECA Infrastructure: State of the art and towards the exascale

Visualizzation of astrophysical and CFD data

Astrophysics

HPC Astrophysical Codes
C. Gheller (CSCS): “The RAMSES codes for computational astrophysics”

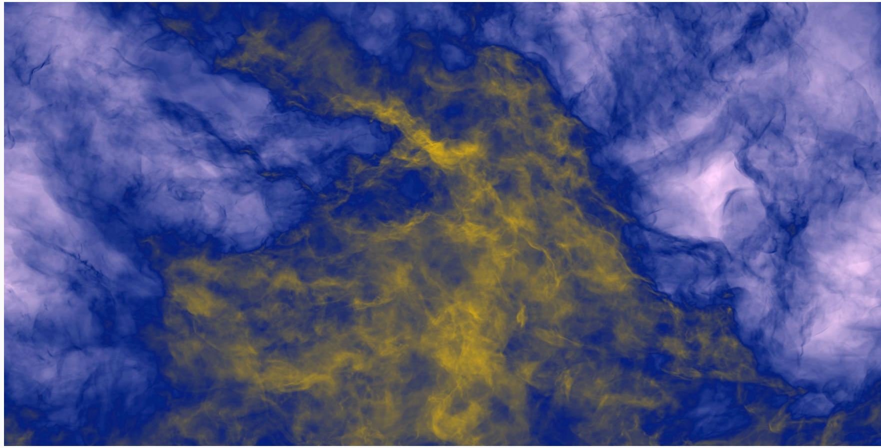
- Name of the codes:RAMSES
- Main Authors: Romain Teyssier (RAMSES)
- Research Area: Cosmology, Galaxy formation, Astrophysics
- Governing Equations: HD, RHD, MHD
- Numerical Method: Various (SPH, PIC, Lagrangian, ….)
- Implementation:
  - Written in F90 and C/C++
  - Parallelization MPI
  - HDF5
  - AMR
- Scalability: excellent weak and strong scaling up to 20-40k



From http://www.ics.uzh.ch

HPC Astrophysical Codes
F.Vazza (UniBO): “Challenges and goals of Eulerian MHD in cosmology”

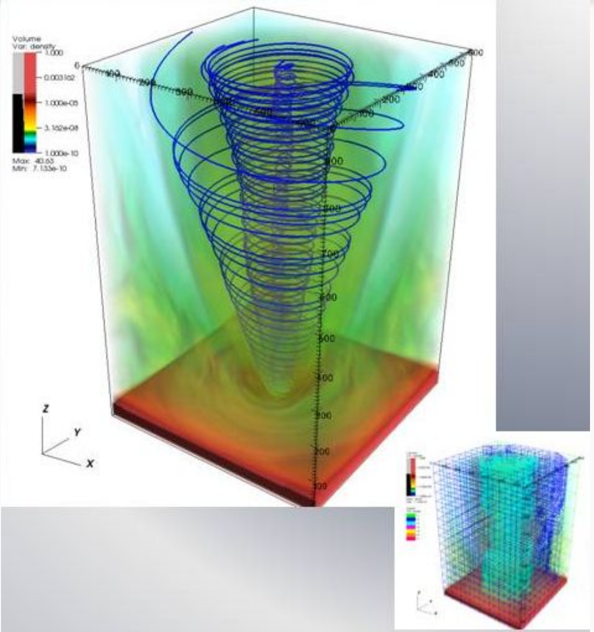
- Name of the codes: ENZO
- Main Authors: Greg Bryan + ENZO collaboration
- Research Area: Cosmology, Galaxy formation, Star formation, Galaxy Clusters
- Governing Equations: HD, MHD, Chemistry, Radiative processes...
- Numerical Method: Various (PPM, PLM, Zeus..)
- Implementation:
  - Written in F90 and C/C++
  - Parallelization MPI
  - HDF5
  - AMR
  - CPU/GPU implementations of HD/MHD
- Scalability: excellent weak and strong scaling up to 20-40k



From http://enzo-project.org/

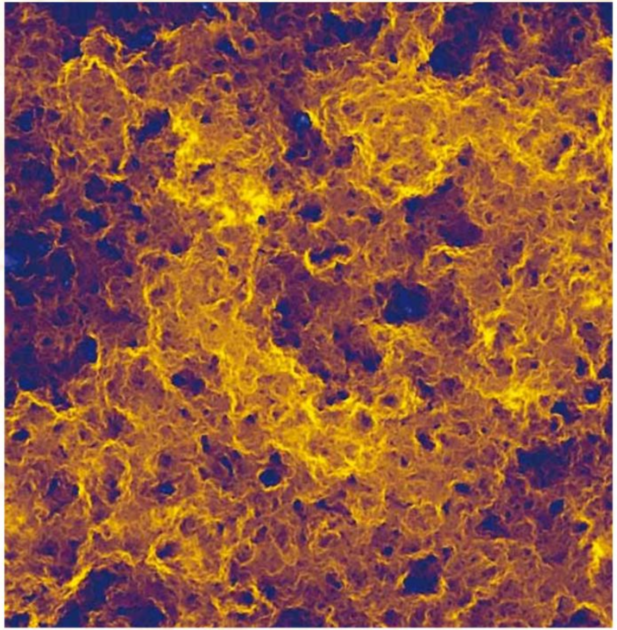
HPC Astrophysics Codes
A. Mignone (UniTO): “The PLUTO Code, an introduction” + “Tutorial on PLUTO”

- Name of the code: PLUTO
- Authors: Mignone, A.; Bodo, G.; Massaglia, S.; Matsakos, T.; Tesileanu, O.; Zanni, C.; Ferrari, A.
- Research Area: Astrophysics/Plasma Physics
- Governing Equations: HD, MHD, RHD, RMHD
- Numerical Method: multi-physics, multi-algorithm modular environment oriented towards the treatment of astrophysical flows in presence of discontinuities
- Implementation:
  - Written in C
  - parallelization pure MPI
  - I/O by HDF5
  - CHOMBO
- Scalability: excellent weak and strong scaling up to 200K cores



HPC Astrophysical Codes
M. Baldi (UniBO): “Numerical methods for standard and non-standard cosmological simulations: The Gadget 3 code”

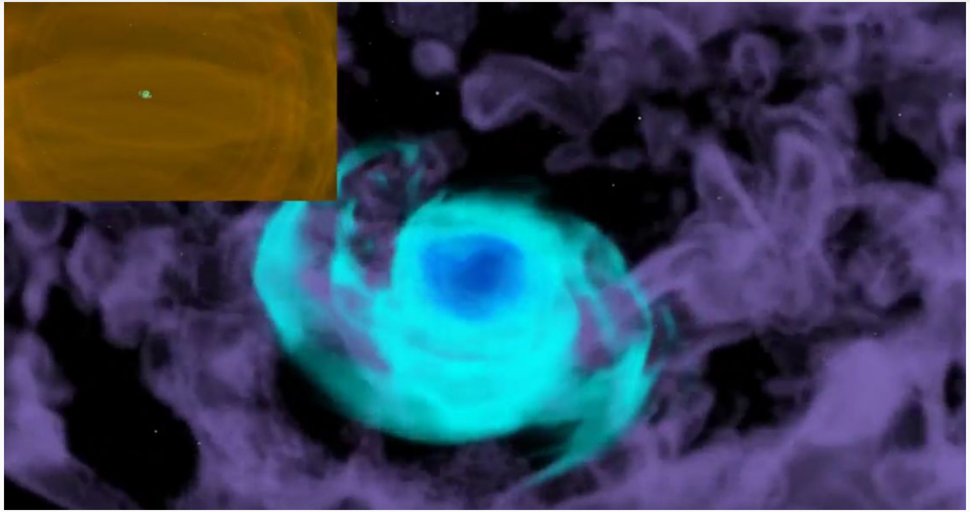
- Name of the code: GADGET 3
- Main Author: Volker Springel
- Research Area: Astrophysics/Cosmology,
- Governing Equations: multi-physics, RHD
- Numerical Method: SPH, Tree-PM
- Implementation:
    - written in C
    - parallelization MPI + OpenMP
    - DFT by FFTW
    - I/O by HDF5
- Scalability: good weak and strong scaling up to 10K-30k cores



© Millenium XXL Project

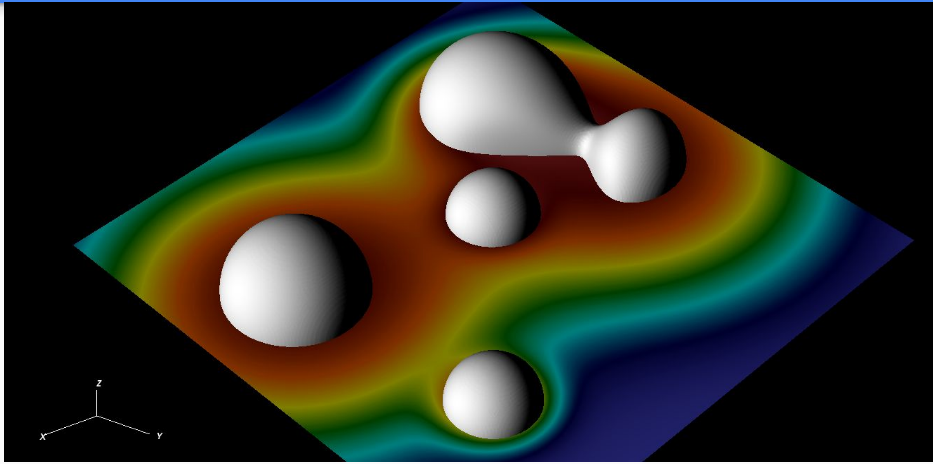
HPC Astrophysical Codes
S. Bernuzzi (UniPR): “Numerical relativity in the gravitational-wave astronomy era”

- Name of the code: BAM
- Main Author/Authors: Bruegmann, B and others
- Research Area: numerical relativty and compact binaries mergers
- Governing Equations: GR + GRHD
- Numerical Method: EULERIAN
- Implementation:
  - Written in C
  - Parallelization: MPI and OpenMP
- Scalability: 8k cores



HPC Astrophysical Codes
B. Giacomazzo: “The Einstein Toolkit: an open framework for Numerical General Relativistic Astrophysics”

- Name of the code: Einstein Toolkit
- Authors: F. Löffler, J. Faber, E. Bentivegna, T. Bode, P. Diener, R. Haas, I. Hinder, B. C. Mundim, C. D. Ott, E. Schnetter, E. Allen, M. Campanelli, and P. Laguna.
- Research Area: Astrophysics, General relativity, Plasma physics
- Governing Equations: GRHD, GRMHD
- Numerical Methods: Various (TVD, PPM, ENO, ePPM, WENO5, MP5, ...)
- Implementation:
  - Written in F90 and C
  - parallelization MP
  - I/O by HDF5
- Scalability: excellent weak and strong scaling up to 10-30k cores



From http://einsteintoolkit.org

HPC CFD code

Useful definiton

In the context of HPC, there are two common notions of scalability:

The first is ***strong scaling***, which is defined as how the solution time varies with the number of processors for a fixed *total* problem size.

The second is ***weak scaling***, which is defined as how the solution time varies with the number of processors for a fixed problem size *per processor*.

HPC CFD Codes: P. Orlandi, A minimal flow unit for turbulence, combustion and astrophysics

- Authors: P. Orlandi, S. Pirozzoli, M. Bernardini
- Research Area: DNS of turbulent low-speed flows. Homogeneous isotropic turbulence, channel and pipe flows (with rotation and roughness elements), passive scalars and inertial particles
- Governing Equations: Incompressible Navier Stokes (DNS)
- Numerical Method: Method-of-lines, two-stage discretization.
  - Spatial discretization on Cartesian staggered grid, Immersed boundary method, second-order FD
  - Time advancement, hybrid third-order Runge-Kutta/Crank-Nicholson scheme
  - Fractional-step: explicit treatment of the convective terms, implicit treatment of the viscous ones
- Implemented in F90, parallelization pure MPI
  - FFTs and tridag systems exploit available libraries (FFTW or IBM ESSL)
- Scalability: excellent weak and strong scaling for channel flow simulations on FERMI

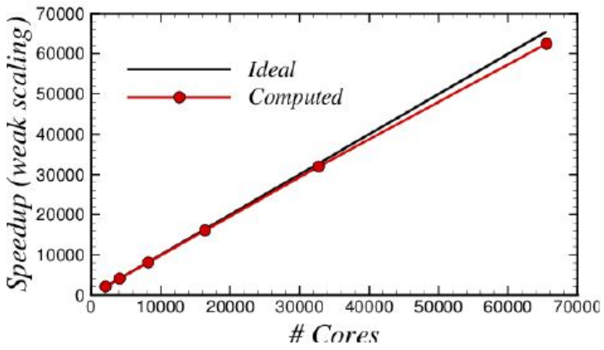


Figure 3: outcome of weak scalability tests

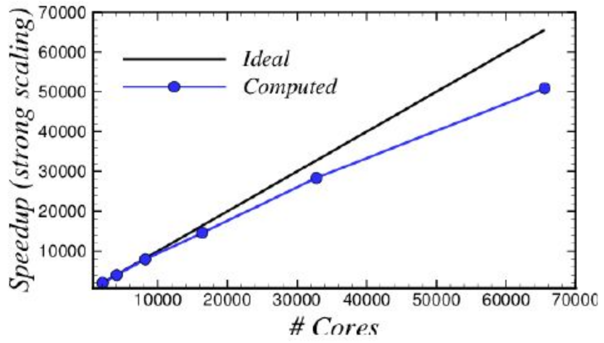
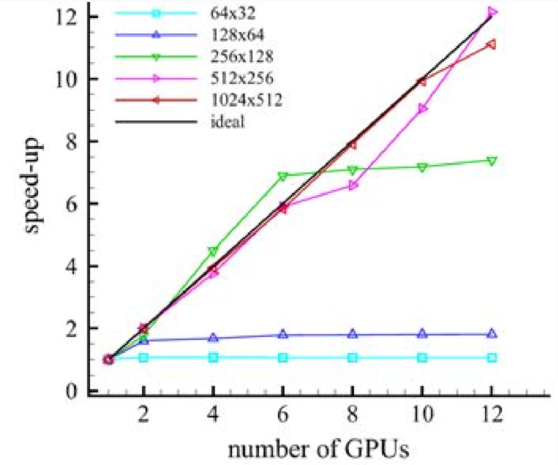
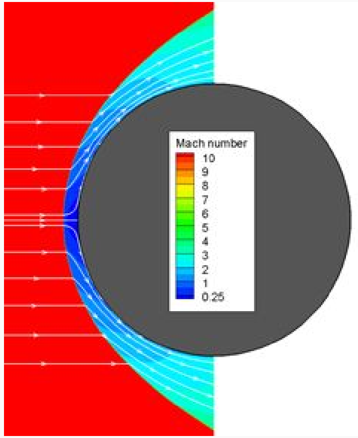


Figure 4: outcome of strong scalability tests.

HPC CFD Codes: F. Bonelli, CFD and state-to-state of hypersonic flows using GPUs

- Authors: Francesco Bonelli, Michele Tuttafesta, Gianpiero Colonna, Luigi Cutrone, Giuseppe Pascazio
- Research Area: hypersonic flows in thermochemical non-equilibrium
- Governing Equations: compressible Navier-Stokes or Euler equations
- Numerical Method: Cell-centered Finite Volume Space discretization on a Multi-block structured mesh, Operator splitting approach, Method-of-lines
  - Space discretization:
    Inviscid flux: Flux Vector Splitting of Steger and Warming or AUSM with MUSCL approach for higher order accuracy;
    Viscous flux: gradients of the primitive variables are evaluated by applying Gauss theorem
  - Time integration: Runge-Kutta scheme up to third order
  - Implemented in CUDA C, parallelization with MPI and CUDA
  - Scalability: excellent strong scaling for mesh larger than 256x128 and excellent weak scaling (computation performed on a GPU cluster available at "Politecnico di Bari")
  - Speed up GPU vs single core CPU: up to 150

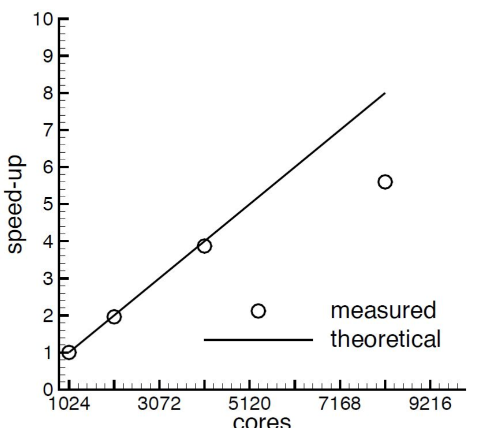


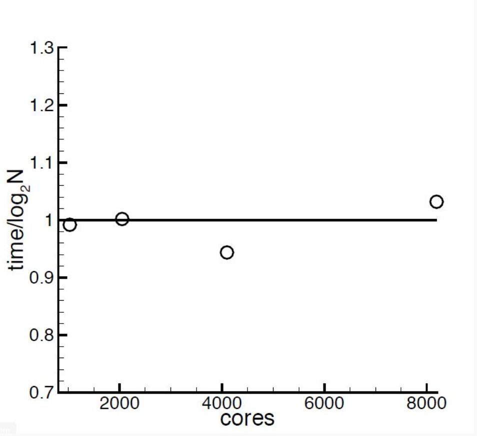


Strong scaling (left) and hypersonic flow over a sphere (right)

HPC CFD codes: P. Gualtieri, Particle-laden turbulent flows: small scale clustering and two-way coupling effects

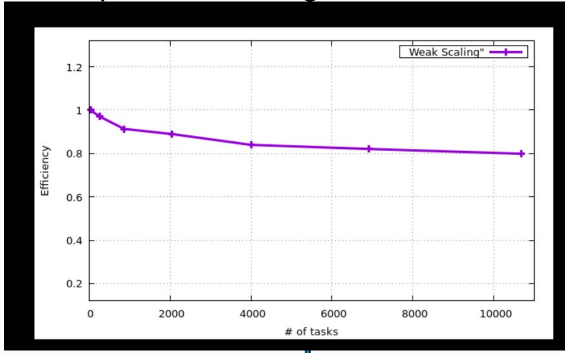
- n_s_trip (Navier Stokes Triperiodic)
- Authors: P. Gualtieri, F. Battista, J.P. Mollicone, C.M. Casciola in collaboration with Giorgio Amati (OpenMP code developed @Caspur) and with Francesco Salvadore (MPI code developed @Cineca)
- Research Area: particle laden turbulent flows, (multi-scale) turbulent transport, two-way coupling effects
- Governing Equations: Incompressible Navier-Stokes equations
- Numerical Method: Method-of-lines
    - Space discretization: Pseudo-spectral
    - Time integration: Low Storage 4th order Runge-Kutta
    - Written in Fortran77 (OpenMP) ; Fortran 90 (MPI)
    - Parallelization: Both OpenMP & MPI
    - Numerical librarires: NCAR and ESSL in the OpenMP version. P3dFFT and FFTW in the MPI version
    - Serial I/O (OpenMP) and MPI-I/O
- Scalability:
    - Strong scaling N=1536^3 Fourier Modes (left
    - Weak scaling (right)

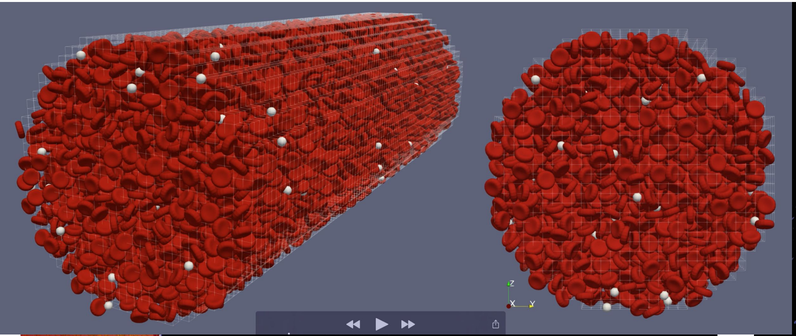


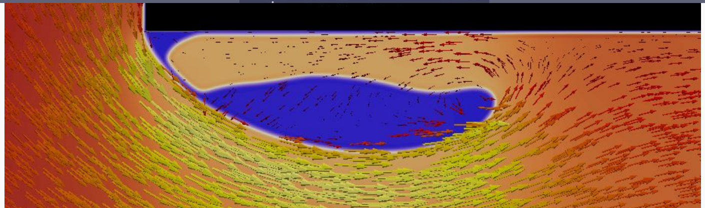


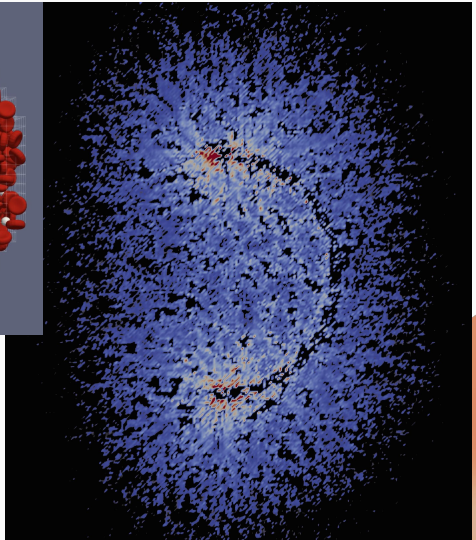
HPC Codes: G. Falcucci: Multi-scale Modeling of complex flows through the Lattice Boltzmann Method

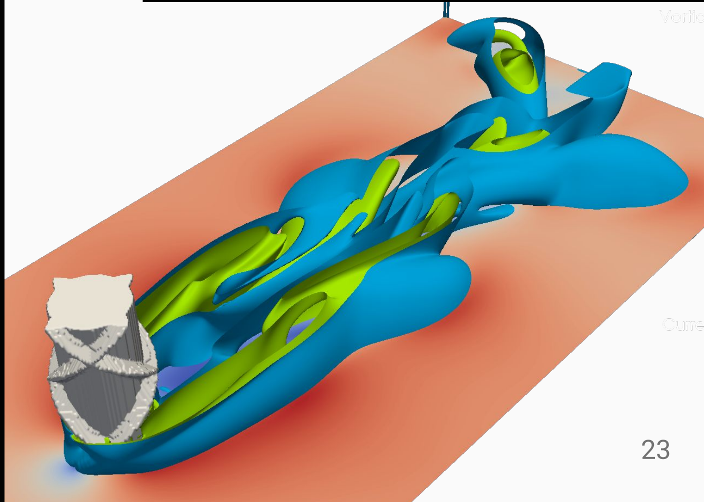
- Authors: G. Falcucci and S. Succi
- Research Area: multi-scale modeling of complex flows, multiphase pseudo-potential, multicomponent/reacting flows, FSI
- Governing Equations: Kinetic Theory
- Numerical Method: Lattice Boltzmann
  - Written in Fortran77 and Fortran90 (+ Python scripting for post-processing)
  - Parallelization: OpenMP and MPI
- Scalability: scalability on hundreds of computational cores (and even more)





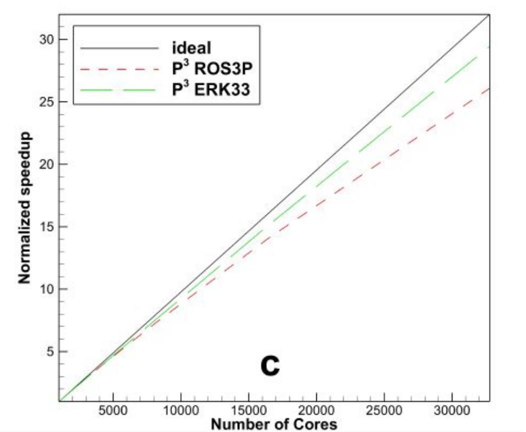






HPC CFD Codes: A. Colombo, Discontinuous Galerkin Methods in HPC

- Authors: F. Bassi, A. Colombo, L. Botti, A. Ghidoni, A. Nigro, A. Crivellini
- Research Area: transonic flows, shock boundary layer interaction (SBLI)
- Governing Equations: from Euler equations to the hybrid RANS-LES approaches, inc. and compressible
- Numerical Method: Discontinuous Galerkin method, MIGALE code
  - The equations of all the implemented flow models are discretized to the same high-order accuracy on hybrid (possibly curved) meshes
  - explicit and implicit high-order (up to order six) time integrators implemented to exploit the high-order discretization both in space and time.
  - based on the SPMD (single process, multiple data) paradigm, MPI paradigm
- Numerical Libraries
  - PETSc library to achieve parallelism
- The scalability of the code MIGALE has been investigated on three different TIER-0 and one TIER-1 facilities: CURIE, HORNET and FERMI
  - Good scalability results for all clusters
  - weak scalability up to 32k cores on FERMI



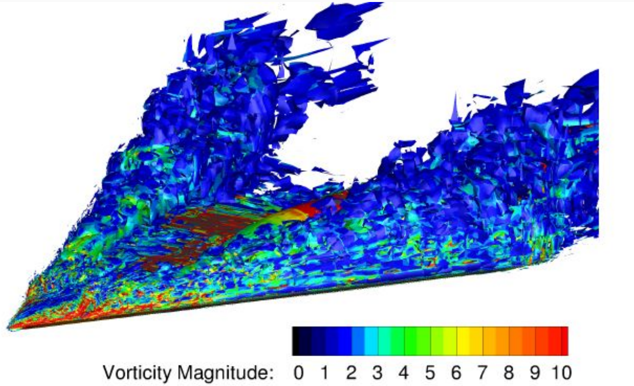


Figure 1: X-LES over the VFE-2 delta wing [1,2]

HPC CFD Codes: OpenFOAM, currente state, perspective and in-situ visualization

- OpenFOAM is become more and more popular in the CFD community
  - OpenFOAM is (aiming to) becoming The open-source community code
    - Third most-used CFD community code by users (after Ansys-Fluent and CD-Adapco-Starccm+), http://www.resolvedanalytics.com/theflux/comparing-popular-cfd-software-packages
    - Fifth most-used CFD code in HPC environment
- Does OpenFOAM can seat in this “round table” of Tier-0 CFD codes?
  - Not yet
- Missing for a “full enabling” on massively parallel clusters (Tier-0 size)
  - Pstream (MPI Library) actually scales reasonably well up to orders of thousands of cores
  - Serial I/O, not MPI
  - Actual sparse matrices storage system (LDU) does not enable any cache-blocking mechanism or efficient vectorization
- Work “done/in progress/ to do” inside the community
  - Modified version of Pstream OpenFOAM available scaling up to order of thousands of cores (done v1606)
  - Implementation of Adios MPI I/O library on-going
  - In-situ visualization with Catalystic
  - CFD4Exascale focuses on the technologies necessary to transition CFD from its current peta-scale performance point towards exascale deployment.

Thank You