Introduction to solvers and algorithms for CFD and Astrophysics

M. Guarrasi, I. Spisso
SuperComputing Application and Innovation Department
CINECA, Italy

02 November 2016
Casalecchio di Reno
Italy

Table of contents

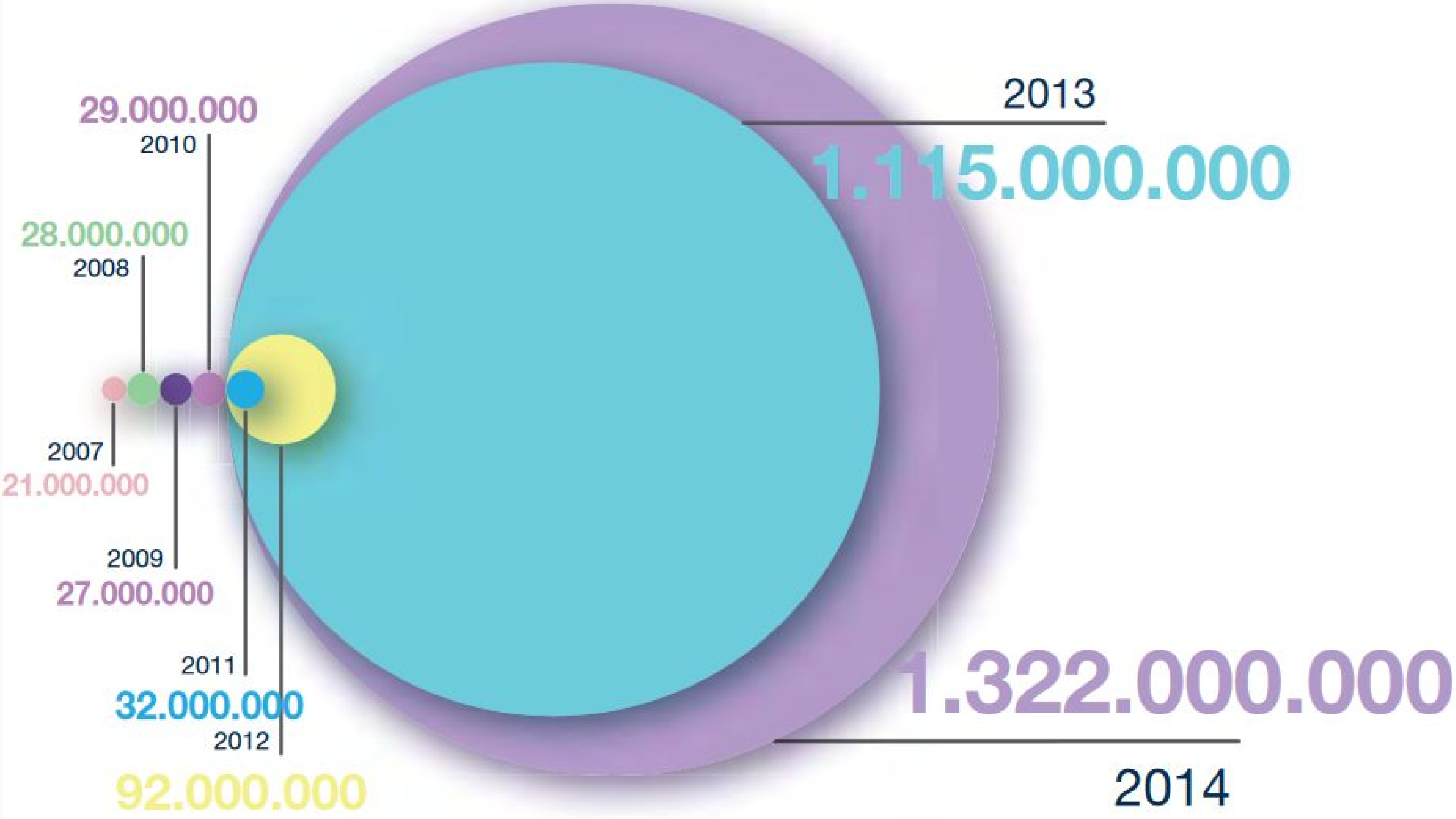
Aim of the workshop

- 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

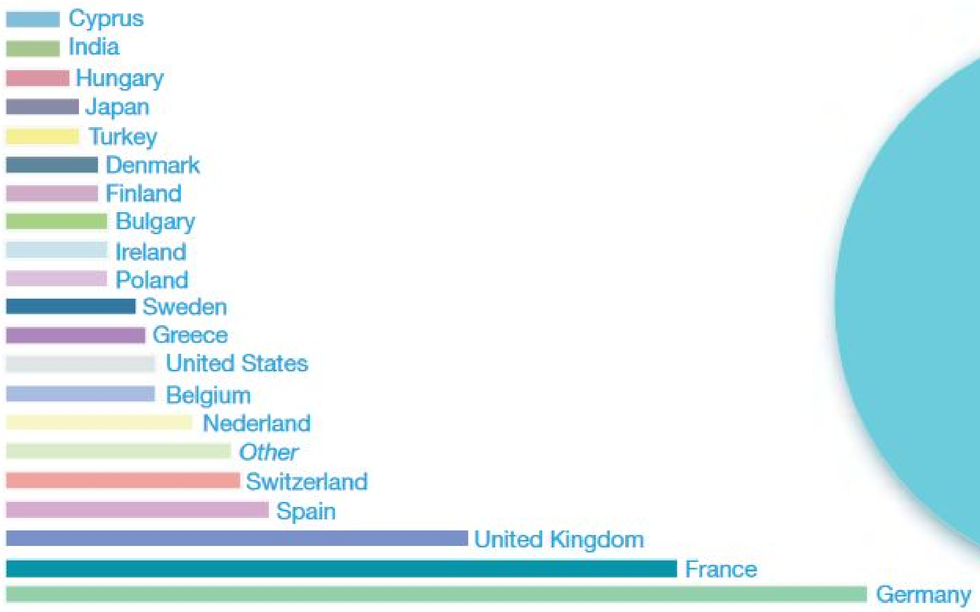
Disclaimer: It is NOT our intent to give a complete survey of the numerical methods used in HPC for the fields of CFD and Numerical Astrophysics. The present workshop shows some of the most used research/community codes granted for access to Tier-0 HPC european (and national) ecosystems in the recent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

HPC Usage by scientific Sector @ CINECA

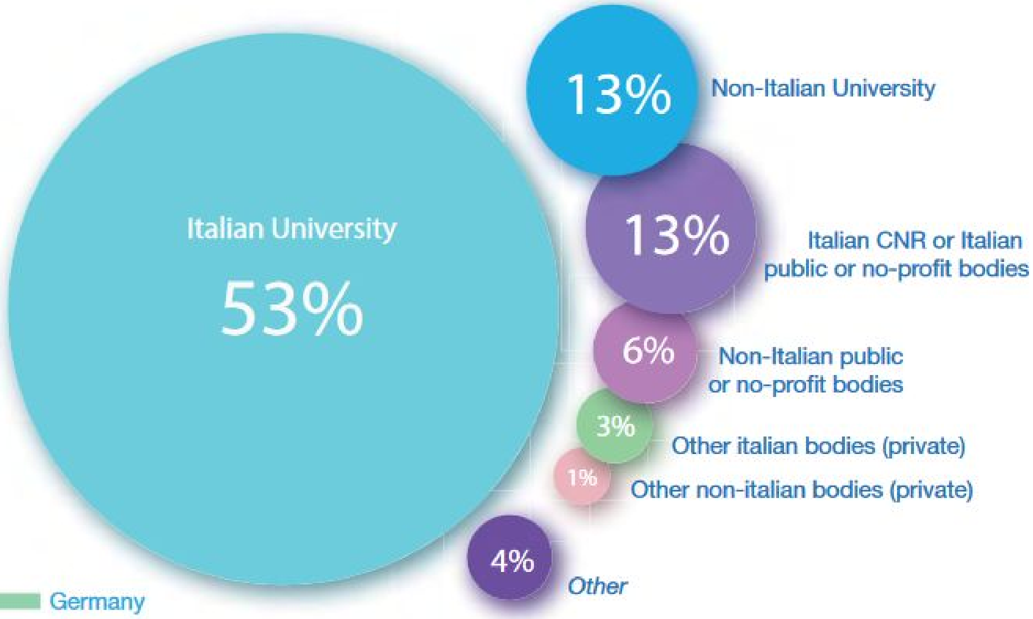
- Scientific computing core hours production



HPC Usage by scientific Sector @ CINECA

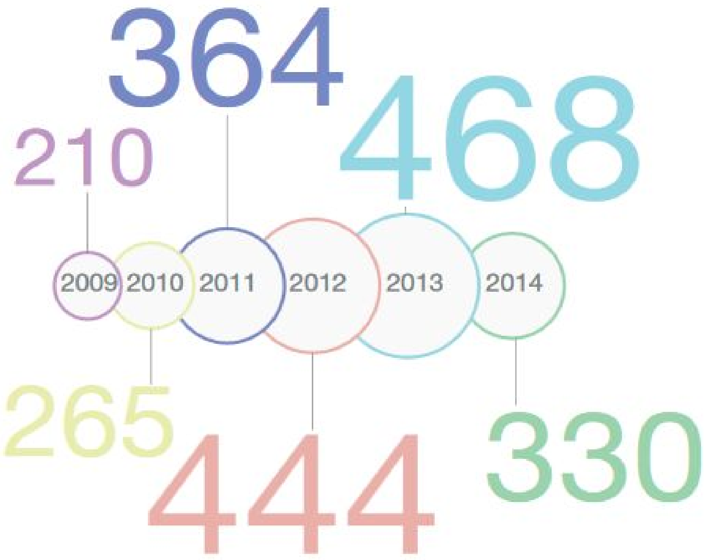


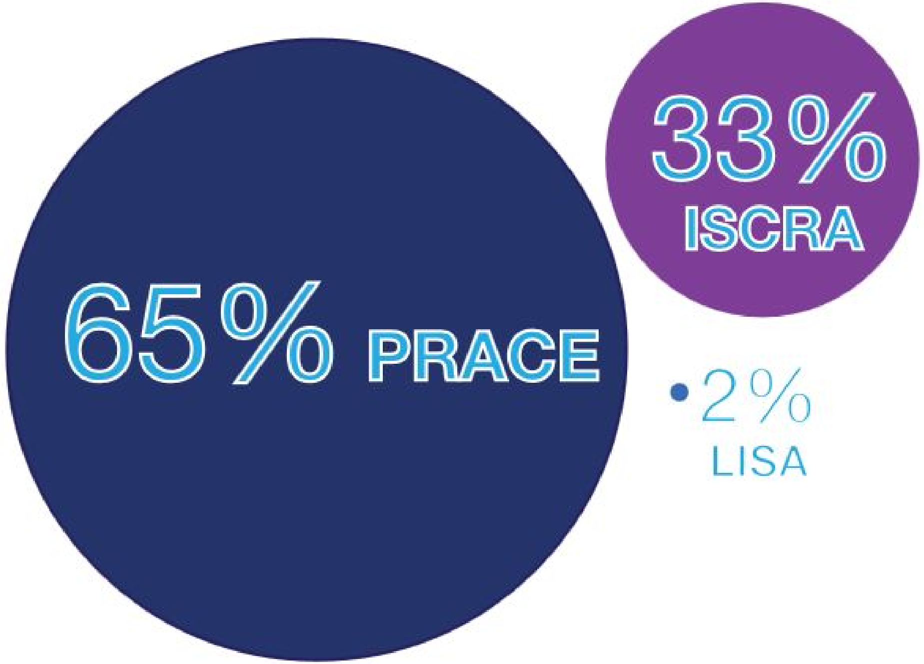
Cineca users with affiliation to foreign entities.



Classification User Institutes

HPC Usage by scientific Sector @ CINECA

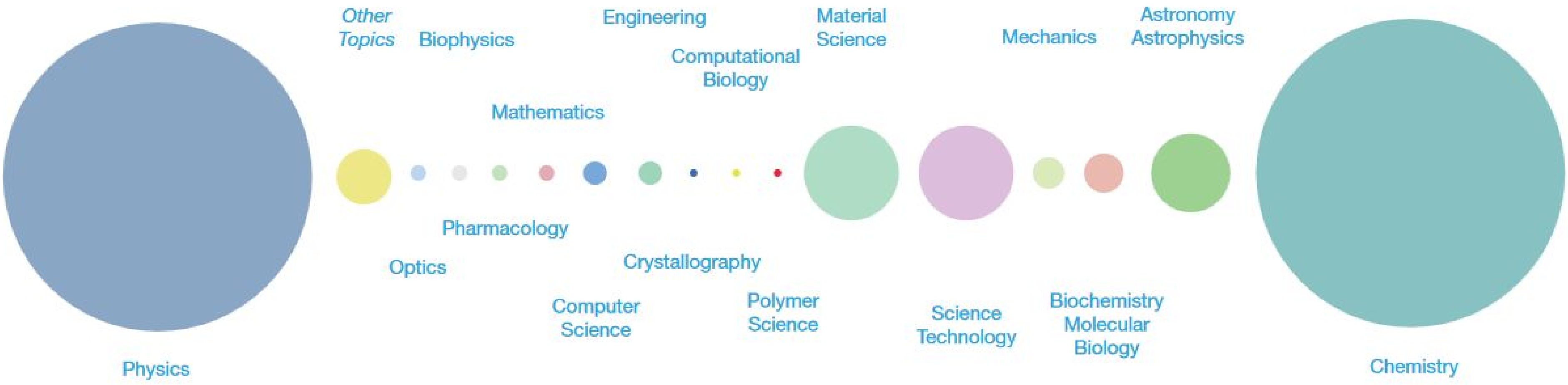




Total number of publications

Allocated resources

HPC Usage by scientific Sector @ CINECA

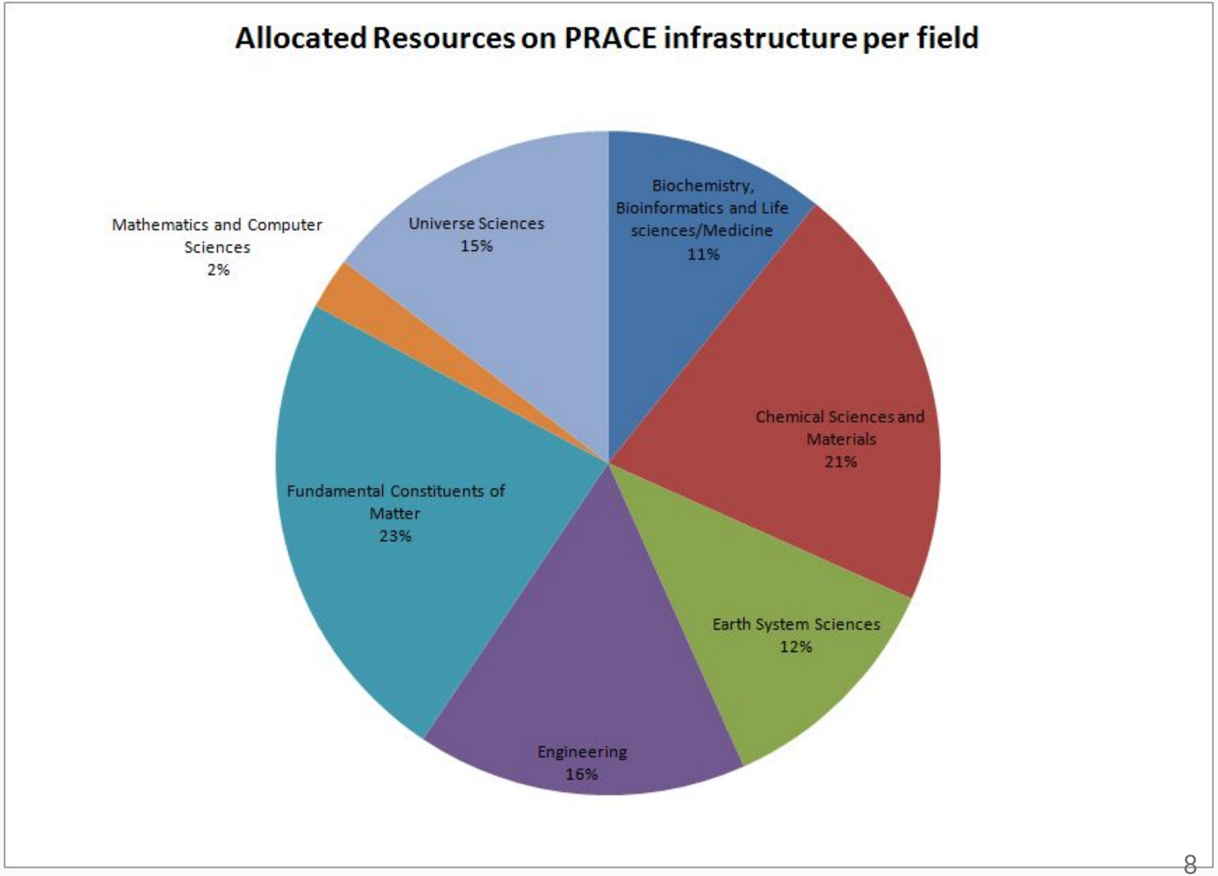


Research areas of the publications mentioning CINECA

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



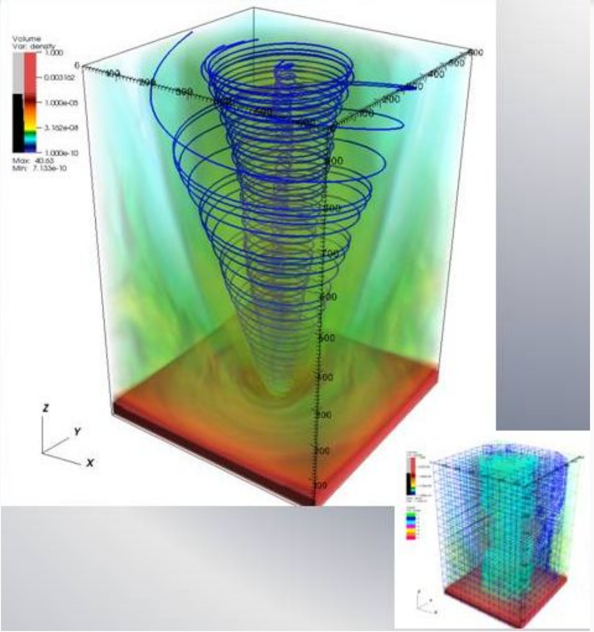
Overview of Numerical Methods and Algorithms

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

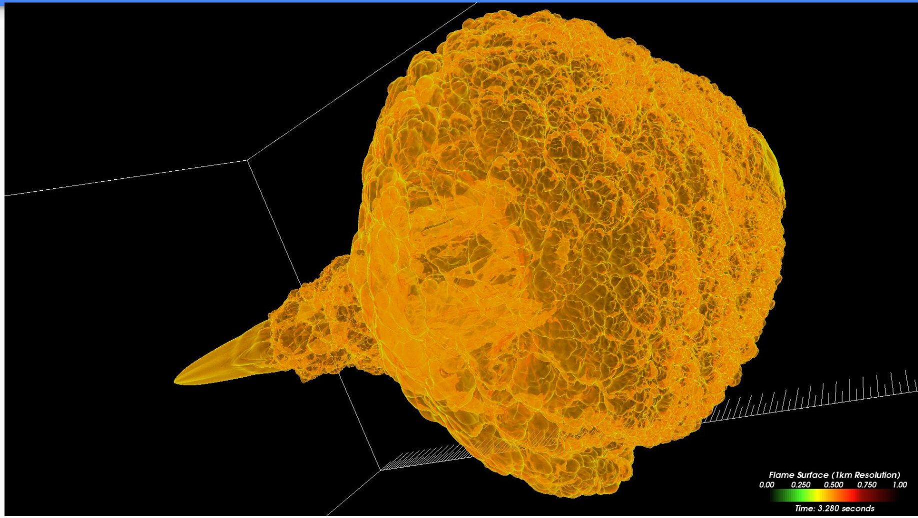
HPC Astrophysics Codes
A. Mignone: “Numerical method in computational fluid and Magnetohydrodynamics - Parallel implementation, static and adaptive grids”

- 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
S. Orlando: "Using the 3D MHD code FLASH to describe systems that span different scales in space and time"

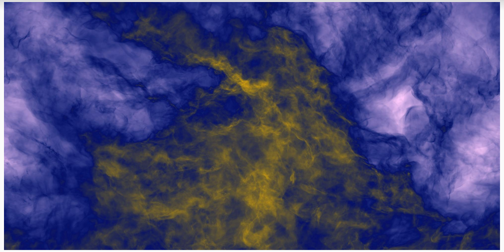
- Name of the code: Flash 4
- Authors: Several, mainly from Flash center for computational science
- Research Area: Astrophysics/Plasma Physics, CFD
- Governing Equations: HD, MHD, RHD, RMHD
- Numerical Method: multi-physics, multi-algorithm modular environment
- Implementation:
  - written in F90
  - parallelization MPI (+ OpenMP)
  - AMR by Paramesh or CHOMBO
  - HDF5
- Scalability: good weak and strong scaling up to 4k cores (with AMR)



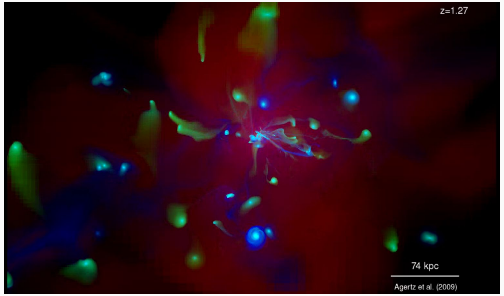
From http://flash.uchicago.edu

HPC Astrophysical Codes
C. Gheller: “ENZO and RAMSES codes for computational astrophysics”

- Name of the codes: ENZO and RAMSES
- Main Authors: Greg Bryan (ENZO), 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



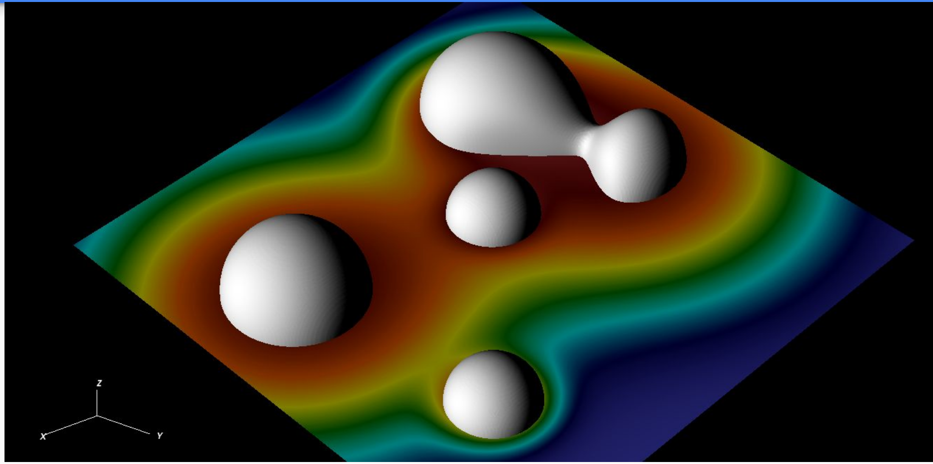
From http://enzo-project.org/



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

HPC Astrophysical Codes
R. De Pietri: “The Einstein Toolkit: an open framework for Numerical General Relativistic Astrophysics”

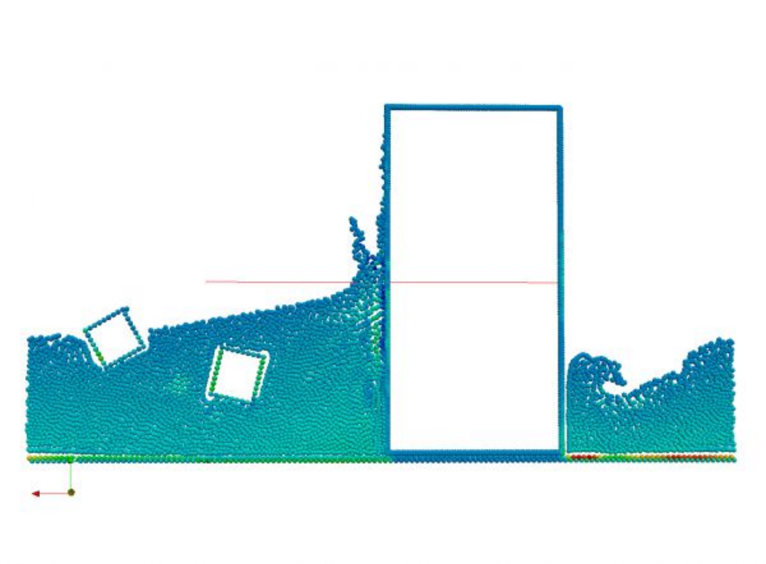
- Name of the code: Einstein Toolkit
- Authors: F. Löffler, J. Faber, E. Bentivegna, T. Bode, P. Diener, R. Haas, I. Hinder, B. C. Mundim, C. D. Ott, E. Schnetter, E. Allen, M. Campanelli, and P. Laguna.
- Research Area: Astrophysics, General relativity, Plasma physics
- Governing Equations: GRHD, GRMHD
- 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 Astrophysical Codes
G. Lodato: “SPH Methods”

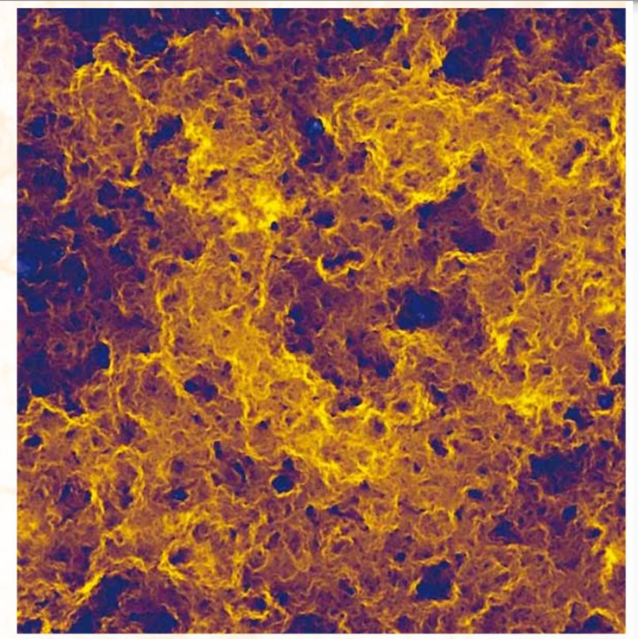
- Main Author: J. J. Monaghan
- Main Paper: Smoothed particle Hydrodynamics
- Research Area: Plasma Hysics, Astrophysics, cosmology, CFD
- Governing Equations: HD, RHD
- Numerical Method: SPH
- Various Implementations (e.g. Used in gadget code)
- Scalability: it depends by the code



From http://www.ged.rwth-aachen.de

HPC Astrophysical Codes
M. Baldi: “Numerical methods for standard and non-standard cosmological simulations”

- 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



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

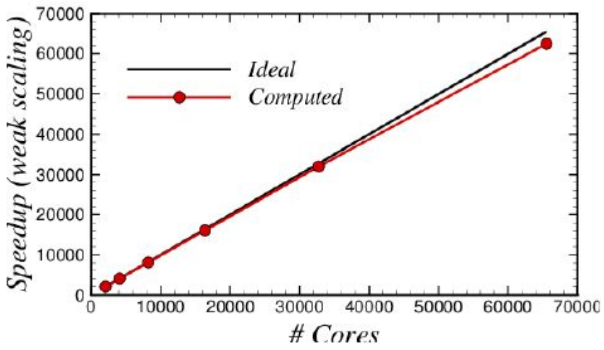


Figure 3: outcome of weak scalability tests

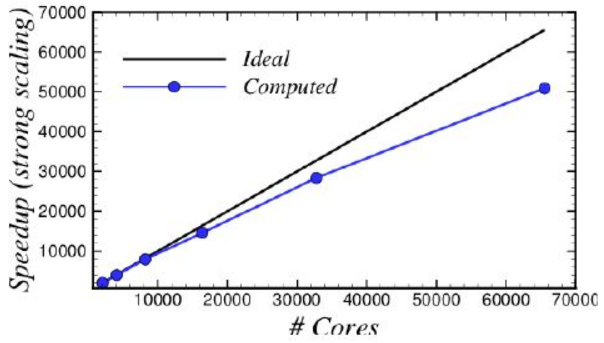
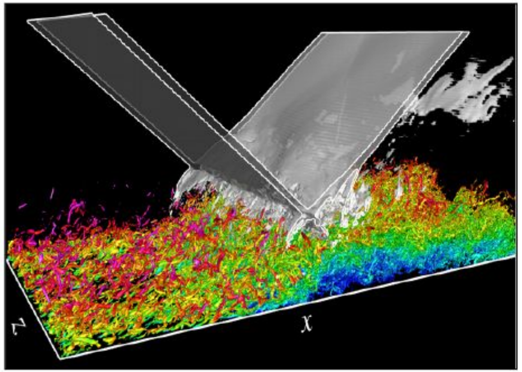
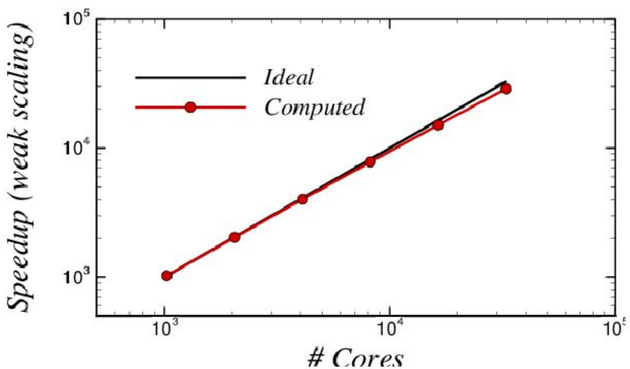


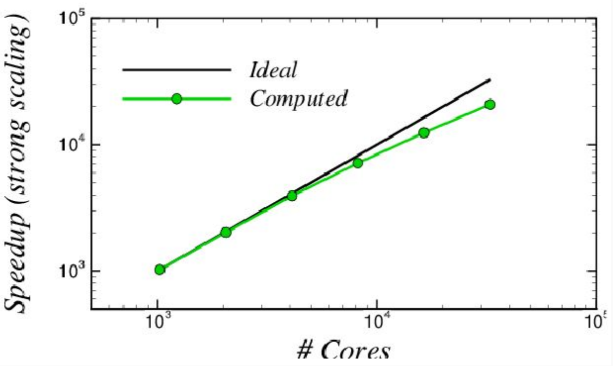
Figure 4: outcome of strong scalability tests.

HPC CFD Codes: S. Pirozzoli, Turbulence in wall-bounded flows

- Authors: S. Pirozzoli, M. Bernardini
- Research Area: DNS of turbulent flows, transonic and supersonic flows, Shock Boundary Layer Interaction (SBLI)
- Governing Equations: Full 3D compressible Navier-Stokes for perfect gas (DNS)
- Numerical Method: Method-of-lines, two-stage discretization.
  - Spatial discretization: hybrid conservative scheme, switch by the Ducros shock sensor
    - Explicit sixth-order central scheme
    - Fifth-order weighted-essentially non-oscillatory (WENO) scheme
    - Preservation of total kinetic energy at the discrete level (no spurious numerical dissipation) for convective term
  - Time advancement standard fourth-order explicit RK algorithm
- Implemented in F90, parallelization pure MPI by exploiting the Cartesian topological connectivity
- MPI I/O
- Scalability: excellent weak and strong scaling for channel flow simulations on FERMI

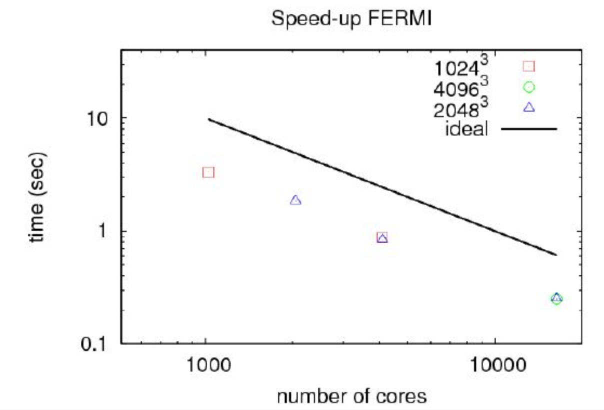






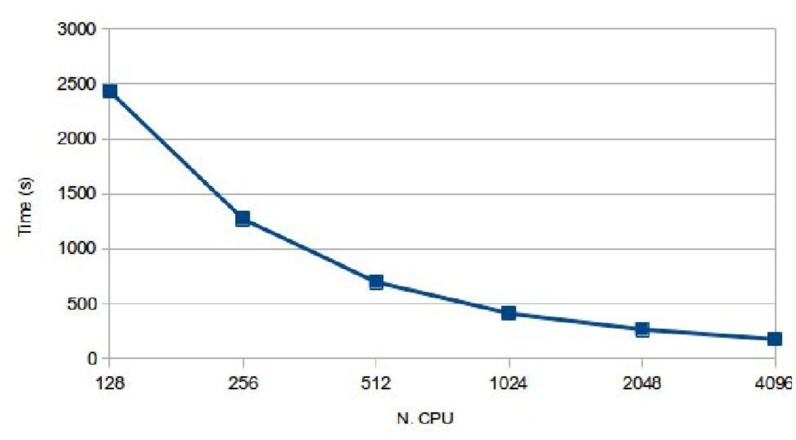
HPC CFD Codes: L. Biferale, Pseudo-spectral approach to high performance computing of MHD

- Authors: L. Biferale, F. Toschi, A. LaNotte, F. Bonaccorso (started 10 years ago)
- Research Area: turbulence, superfluid, intermittency, MHD
- Governing Equations: Navier-Stokes on a cubic regular, tri-periodic lattice
- Numerical Method:
    - Pseudo-spectral code integrates the evolution equation for the potential vector, whose curl is the velocity field. No explicit pressure term is calculated.
    - Time integration: second order Adams-Bashforth
- fully parallel with MPI. Lagrangian integration of particles seeding the flow is also parallelized with MPI.
    - Use of the pencil FFT, most of computational cost (P3DFFT with 1D FFT or ESSL libraries)
    - MPI I/O, HDF5
- Synergies with other European infrastructures (EuHIT, EUDAT) Projects
- Excellent scalability up to 32k cores on FERMI (PRACE call 4th, 9th,11th and 12th)



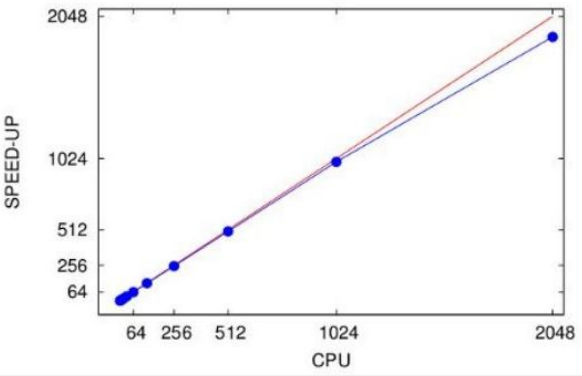
HPC CFD Codes: S. Frigio, Complex solutions of the 3D Navier-Stokes Equations in the Fourier Space: Numerical Evidence of Blow-Up

- Authors: S. Frigio
- Research Area: turbulence, singularities, blow-up mechanism
- Governing Equations: 3-D incompressible Navier-Stokes
- Numerical Method: Pseudo-spectral methods, integral equation in the Fourier space
  - integral equation is discretized by Nystrom method for the space variables and a marching scheme for time variable
  - discretization of the integral equation and the 2D-Pencil parallel decomposition of the 3-d computational domain
- Implemented in F90, parallelization pure MPI
- Use of the library 2Decomp&FFT
- Scalability: good strong scaling up to 5000 cores on FERMI BG/Q



HPC CFD Codes: F. Zonta, Physics and high performance computation of turbulent flows with interfaces

- Authors: F. Zonta, A. Soldati, M. Marchioli
- Research Area: multiphase flow, physics of turbulent flows with interfaces, droplets in turbulence
- Governing Equations: DNS of Cahn-Hilliard/Navier-Stokes system (Model H)
- Numerical Method: pseudo-spectral method
  - Fourier representations for the streamwise and spanwise directions and a Chebyshev representation for the wall-normal nonhomogeneous direction.
  - Time advancement of the solution via a two-level explicit Adams-Bashfort scheme for the nonlinear terms and an implicit Crank-Nicolson method for the viscous terms.
  - Implemented in F77, parallelization pure MPI
- Numerical Libraries
  - FISHPACK package for the solution of separable elliptic PDEs
  - FFTW3
- Scalability: good strong scaling up 4096 cores on FERMI BG/Q



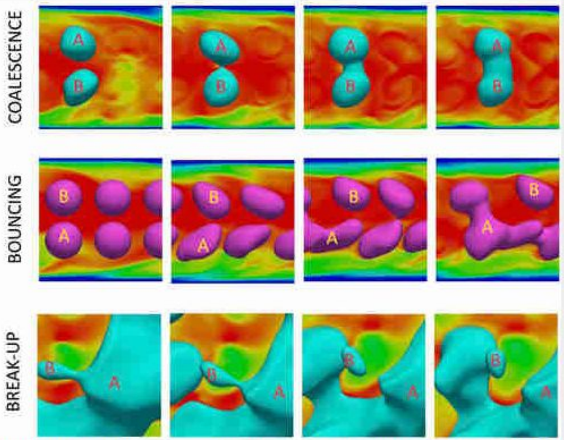
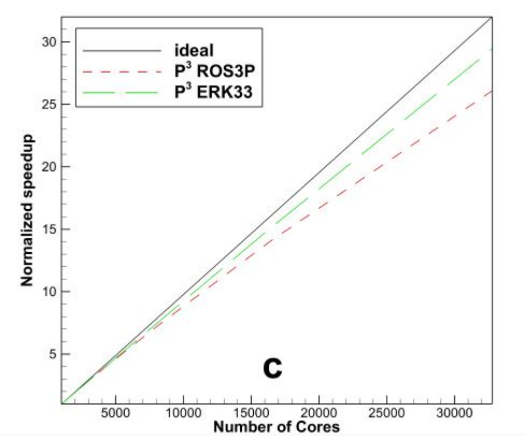


Figure1: Coalescence, Bouncing and Break-up of droplets in turbulence

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



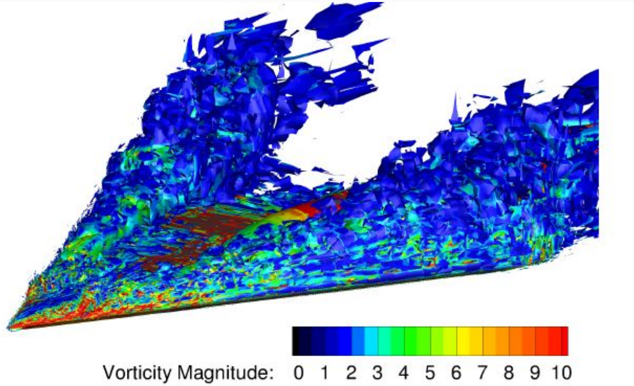


Figure 1: X-LES over the VFE-2 delta wing [1,2]

Missing Guest: OpenFOAM

- 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
- Work in progress inside the community
  - Modified version of OpenFOAM available scaling up to 50/100 k cores
  - Implementation of Adios MPI I/O library on-going

Thank You

Overview of Numerical Methods and Algorithms, CFD Codes

Speaker	Area of research	Governing Equations	Numerical Method	Parallelization	Scalability	Total of CPU hours granted (Millons)
L. Biferale	DNS/LES/Particle	MHD				
S. Pirozzoli	Turbulents flows	Navier-Stokes	DNS Compressible, high-order explicit FD schemes. Incompressible	MPI + (Accelerators)	Up to 32/64 k cores (BGQ)	200 / 300
S. Frigio			Spectral Methods			
P. Orlandi			Immersed Boundary			
Francesco Zonta			Multiphase flow			
A. Colombo			Discontinuous Galerkin			

Overview of Numerical Methods and Algorithms ???

- Present numerical methods and algorithms for Astrophysics and CFD:
  - Eulerian (ASTRO, CFD);
  - Lagrangian (ASTRO, CFD);
  - Implicit methods (ASTRO, CFD);
  - Explicit methods (ASTRO, CFD);
  - Regular grids (ASTRO, CFD), AMR (ASTRO, CFD) , unstructured meshes (CFD), Immersed Boundary (CFD)
  - HD (ASTRO, CFD), MHD (ASTRO, CFD), RHD (ASTRO), RMHD (ASTRO);
  - Multi-Physics modules (ASTRO, CFD);
  - Parallel implementation (ASTRO, CFD);
- State of the art HPC architectures;
- State of the art and community codes.

HPC CFD Codes: L. Biferale, Pseudo-spectral approach to high performance computing of MHD

- Authors: L. Biferale, K. Jansen, R. Tripiccione
- Research Area: turbulence, micro-fluids, particles physics, lattice QCD
- Governing Equations: Hybrid Monte Carlo (HMC)
- Numerical Method: Fourier space for the velocity field, time integration backward time discretization
- Implemented in C/C++, parallelization pure MPI with Fourier acceleration
    - Use of FFTW3, statistical software R, random number generator ranlux
- MPI I/O
- Scalability: tested up to 4000 cores on FERMI BG/Q
- Reference: 13th Call PRACE, BurgersHMC - Instantons and Intermittency in Hydrodynamic Turbulence: A Lattice Monte Carlo Approach