Facing HPC Challenges with the PLUTO code

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Outline

I. The PLUTO code for astrophysical gasdynamics:
   - Overview
   - Available Physics
   - Parallelization and I/O

II. Challenges in Computational Astrophysics

III. Adaptive Mesh Refinement & Applications

IV. Particles Physics

I. THE PLUTO CODE

What is PLUTO ?

- PLUTO[1,2] is a modular parallel code providing a *multi-physics* as well as a *multi-algorithm* framework for the solution of mixed hyperbolic/parabolic conservation laws in astrophysics;

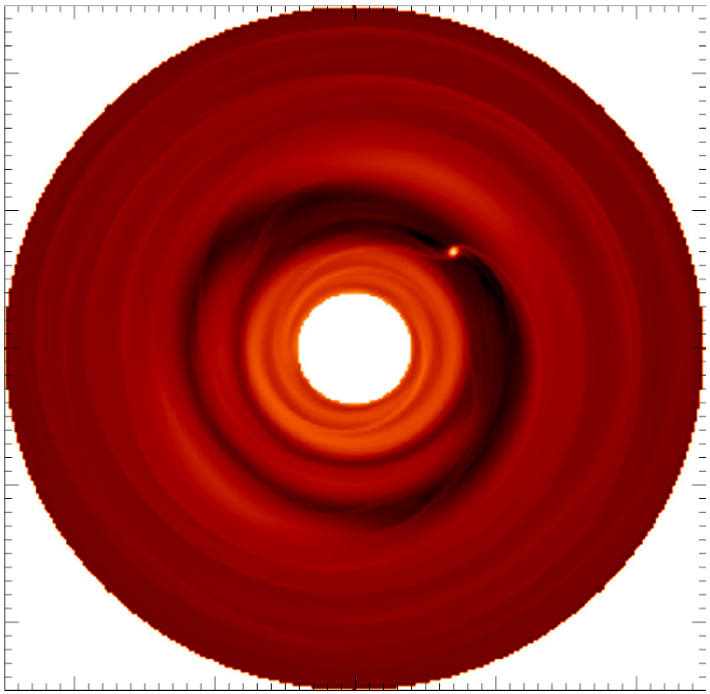
- ***Target***: multidimensional *compressible* flows with high Mach numbers:
  - Compressible Euler/Navier Stokes;
  - Newtonian (ideal/resistive) magnetohydrodynamics (MHD);
  - Special Relativistic hydro and MHD;
  - Heating/cooling processes, chemical network, …

- Freely distributed at http://plutocode.ph.unito.it (v. 4.2)

[1]Mignone et al. ApJS (2007), 170, 228-242; [2]Mignone et al, ApJS (2012), 198, 7

PLUTO Application Gallery

- Planet Formation
- Stellar Jets
- Radiative shocks
- Extragalactic Jets
- Jet Launching
- Magnetospheric accretion & star-disk Interaction
- Magneto-rotational instability (MRI) & accretion disks
- Relativistic Shock dynamics
- Fluid instabilities CD, KH, RT, etc…



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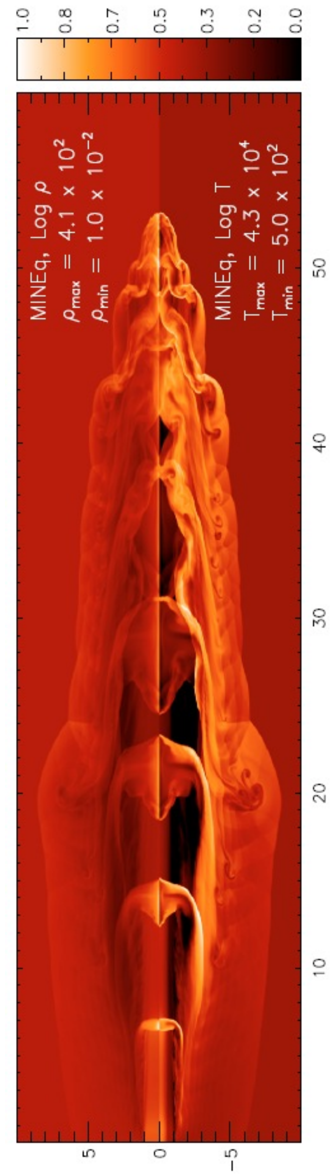

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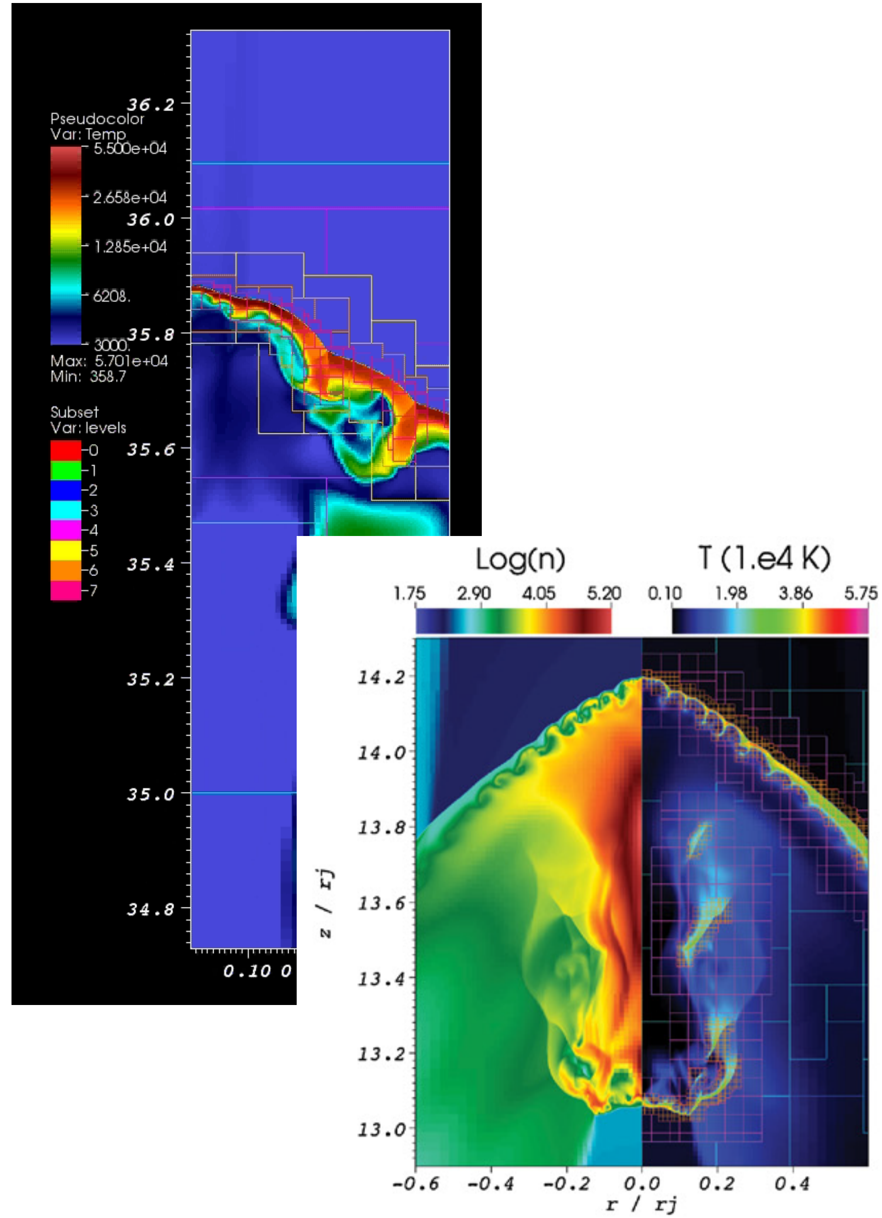

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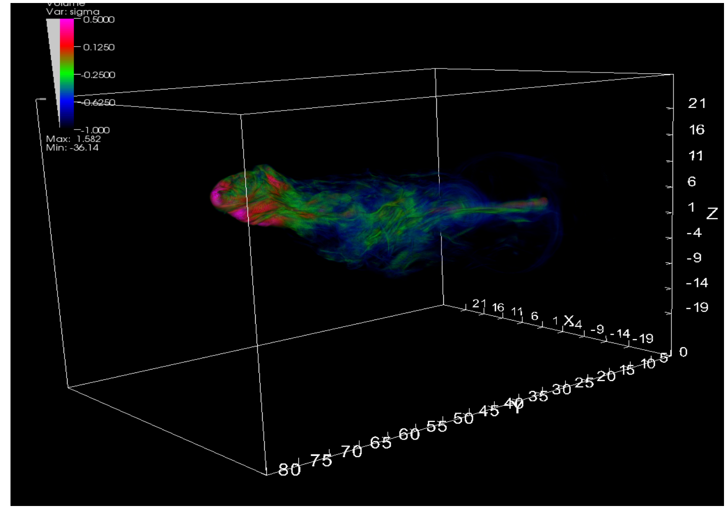
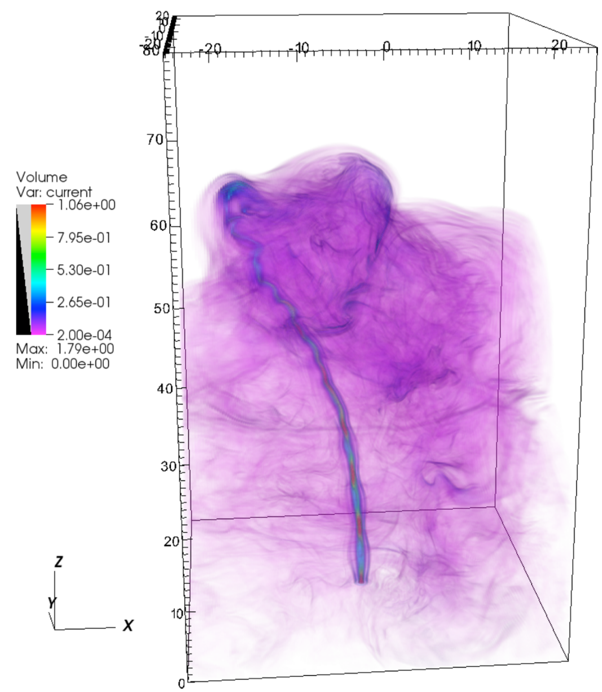


Case A3, t=89.48 (yrs)



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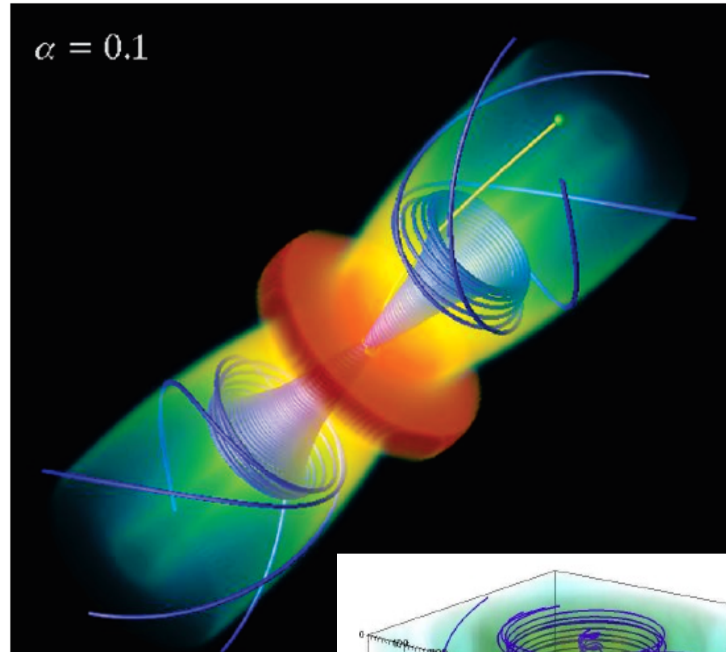

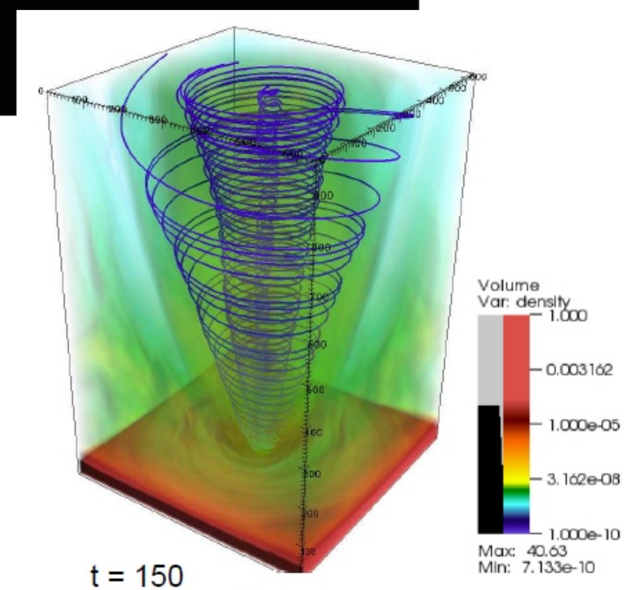

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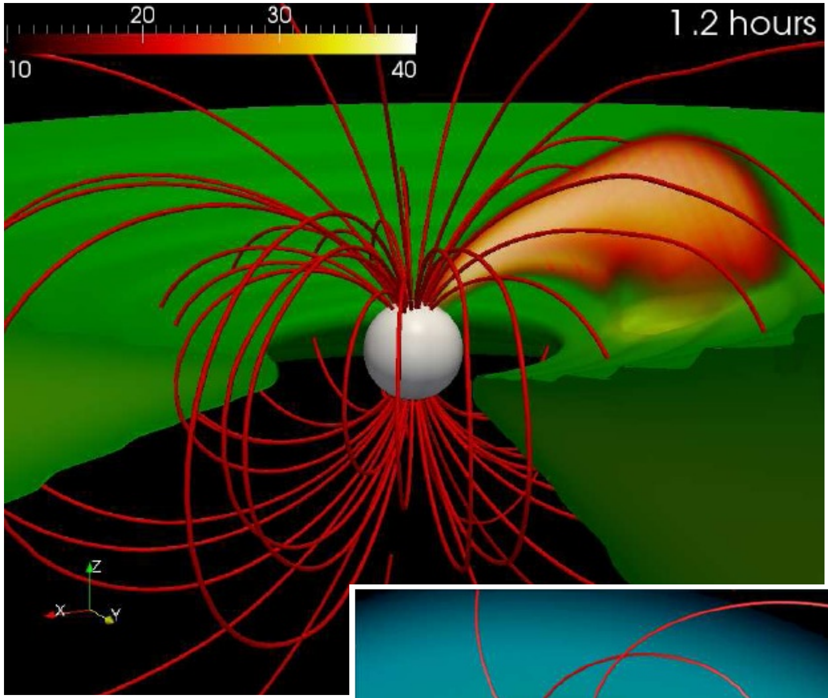

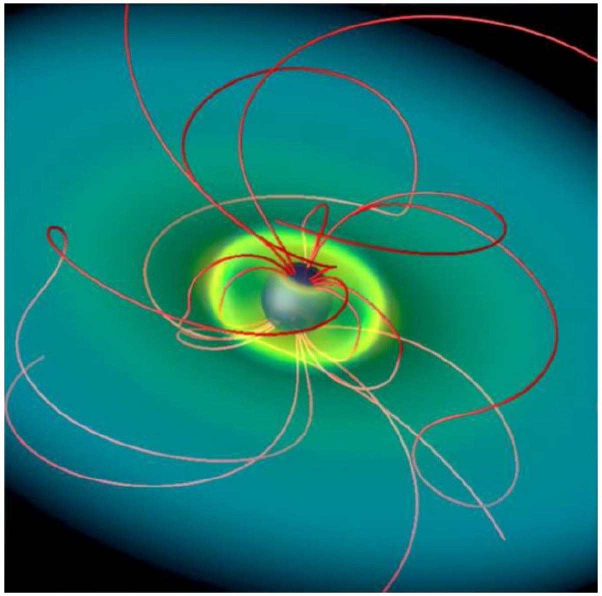

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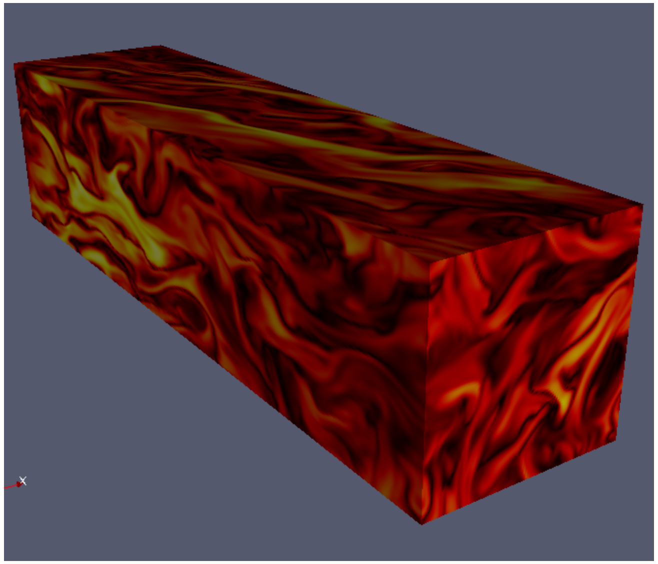

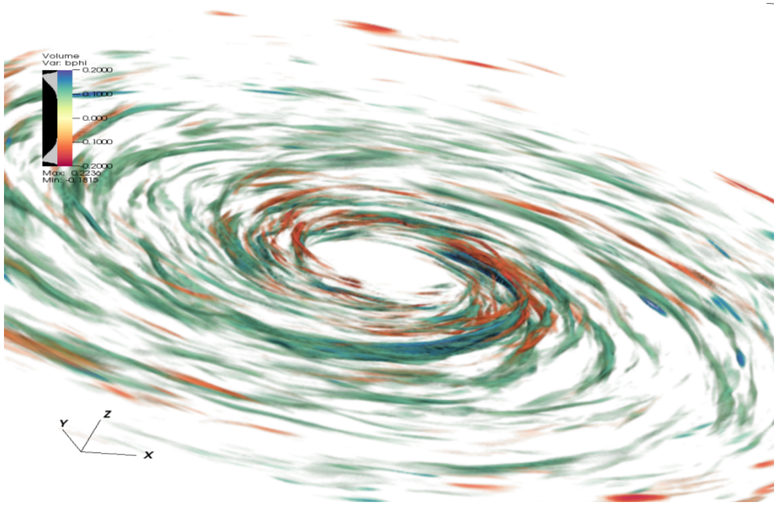

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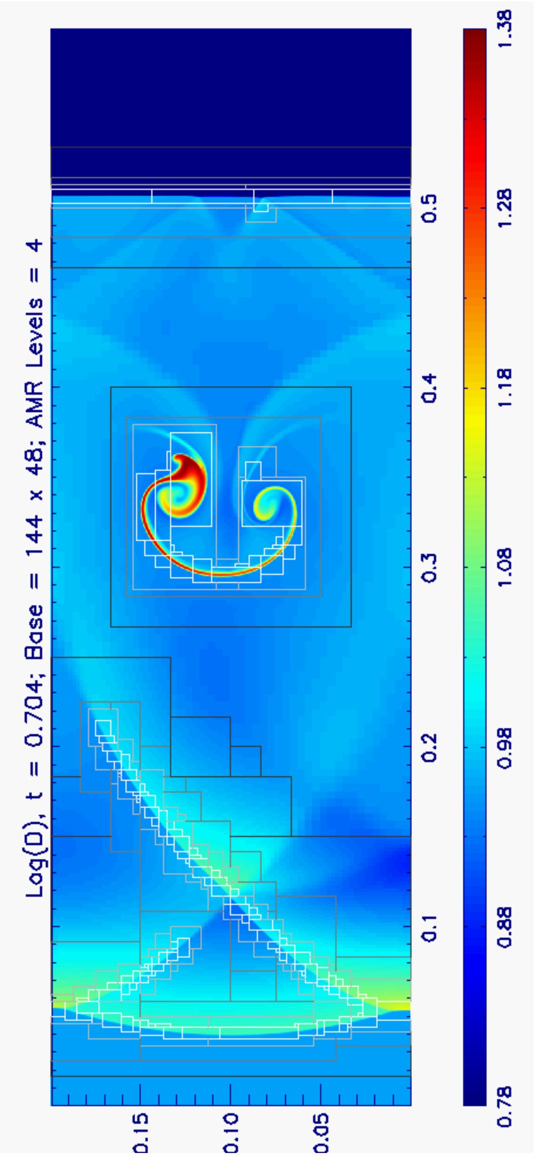

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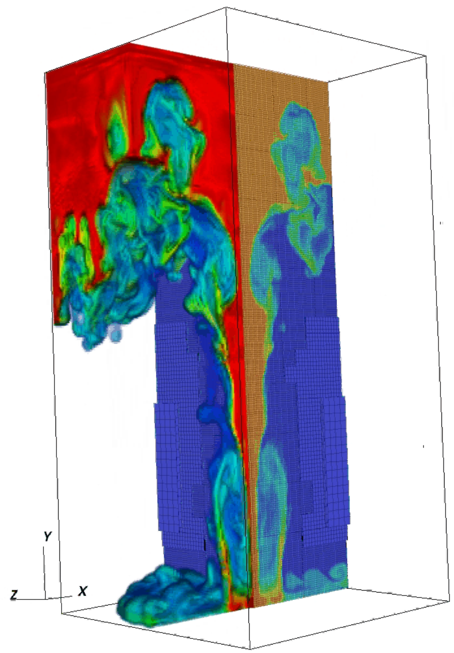
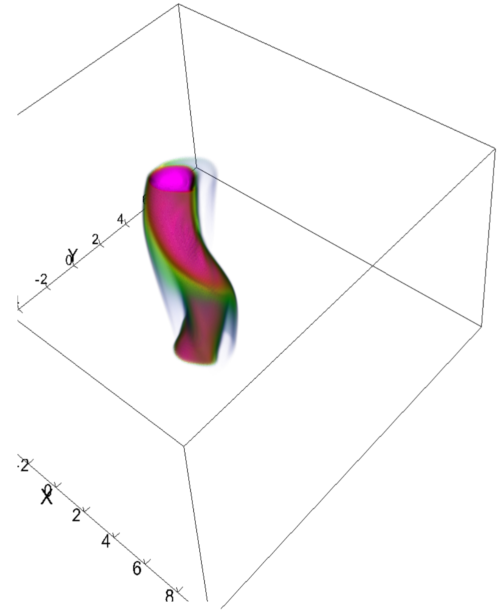
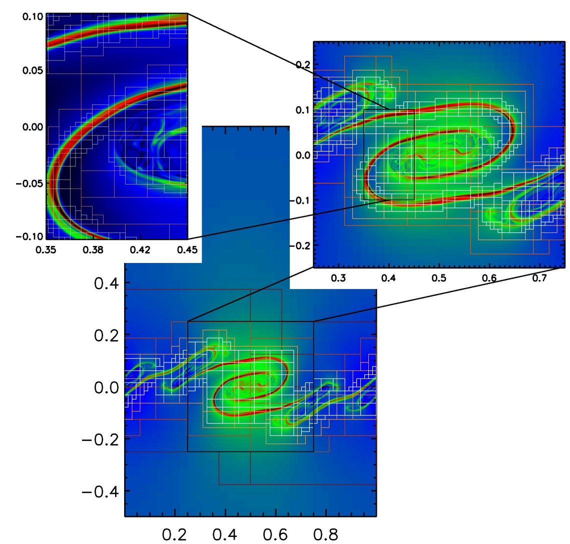
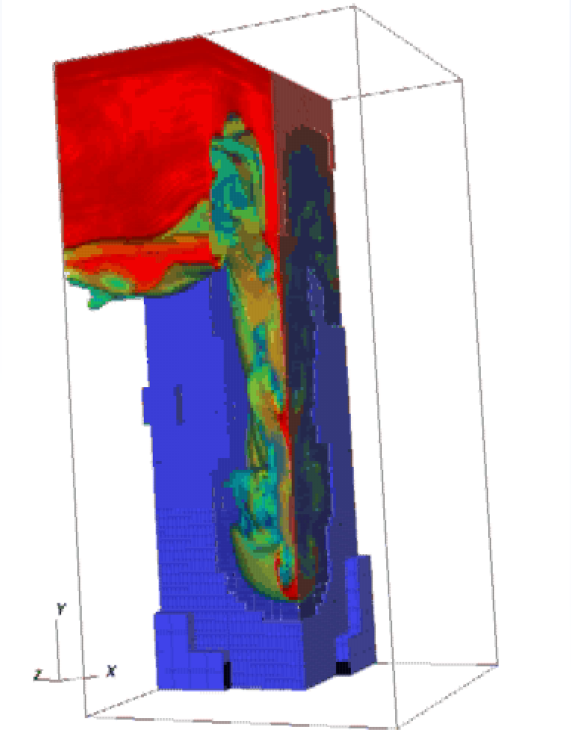






Introducing the PLUTO Code

- PLUTO is written in C (~80,000 lines) and C++ (12,000 lines);
- Support multi-dimensional parallel (MPI) computations from single processor to a large number of cores (tested up to 262,144);
- Tested on several platforms (Linux/Mac OS/SP6/ Blue Gene Q,P/Jugene/Fermi/Marconi);
- Computations may be performed on
  - Static grid : single fixed grid;
  - *Adaptive grid:* multiple refined, block-structured nested grids following and adapting to the solution



Available Physics Modules

Advection Physics (Hyperbolic PDE)

- Hydrodynamics (HD)
- Magnetohydrodynamics (MHD)
- Relativistic Hydrodynamics (RHD)
- Relativistic MHD (RMHD)

Thermodynamics

- Isothermal
- Ideal
- Non-constant gamma
- Synge Gas (relativistic)

Dissipation Physics (Parabolic PDE)

- Viscosity (Navier-Stokes)
- Thermal conduction (hydro and MHD)
- Magnetic resistivity
- Radiation Hydrodynamics (FLD[1], 2 temp)

Geometry

- Cartesian (1D, 2D, 3D)
- Cylindrical (1D, 2D, 3D)
- Spherical (1D, 2D, 3D)

Source Terms

- Gravity / Body forces
- Heating / optically thin cooling
- Chemical networks

Particle Physics

- Lagrangian particles (1D, 2D, 3D)
- Dust
- Cosmic Rays → MHD-PIC

[1]S. Kolb et al,A&A, *http://www.tat.physik.uni-tuebingen.de/~kolb/pluto_radiation*

Available Algorithms

- PLUTO supports 2nd order Finite-Volume as well as 5th order finite difference algorithms in multiple dimensions.

Time Stepping

- RK2, RK3
- MUSCL-Hancock
- Characteristic Tracing

Dimensionally split or fully unsplit methods.

Interpolation

- Piecewise Linear
- Piecewise Parabolic
- WENO 3rd – 5th order

Primitive or characteristic fields

Riemann Solver

- Two-shock
- AUSM
- Roe
- HLL / HLLC / HLLD
- TVDLF
- MUSTA

Parabolic Solver

- Explicit
- Super-Time-Stepping
- Runge-Kutta-Legendre

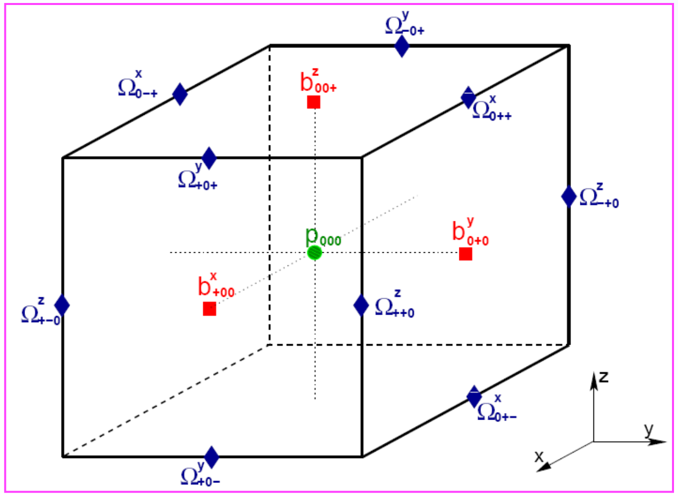
$\nabla\cdot B$ control

- 8-wave
- Constrained Transport
- Hyperbolic Divergence Cleaning

PLUTO & Magnetic Monopoles

- 8 wave: Cell centered approach, includes a source term $\propto \nabla\cdot B$
  - *Pros*: simple
  - *Cons*: $\nabla\cdot B=0$ to scheme accuracy, non conservative, error at shocks (Toth,2000)

- Constrained Transport: staggered approach, Stoke's theorem used for evolution
  - *Pros*: $\nabla\cdot B=0$ to machine accuracy, conservative, consistent formulation;
  - *Cons*: staggering requires solution of 2D R.P., extra care for AMR grids, high order and additional physics;



- Hyperbolic/Parabolic Div Cleaning[1]

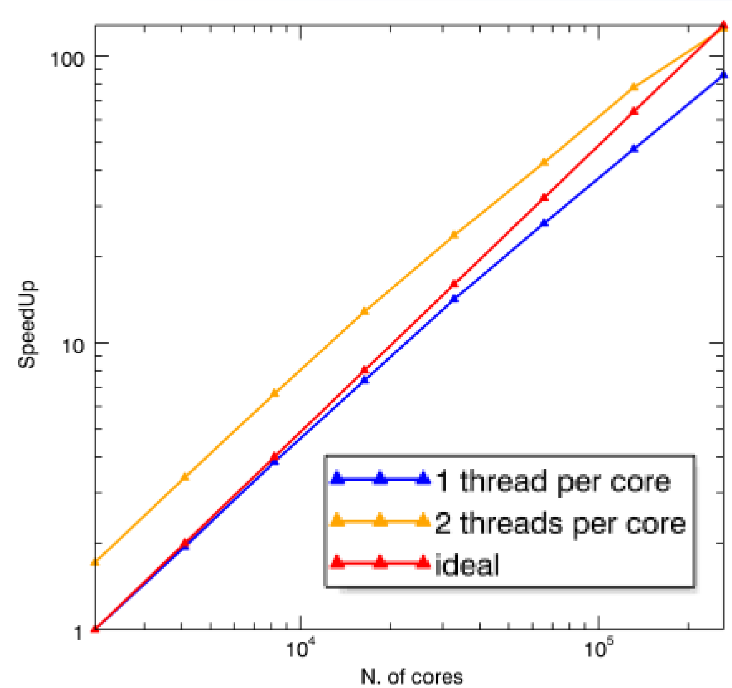
$$\begin{cases} \nabla\cdot\mathbf{B}=0, \\ \dfrac{\partial\mathbf{B}}{\partial t}=\nabla\times(\mathbf{v}\times\mathbf{B}), \end{cases} \Rightarrow \begin{cases} \mathcal{D}(\psi)+\nabla\cdot\mathbf{B}=0, \\ \dfrac{\partial\mathbf{B}}{\partial t}+\nabla\psi=\nabla\times(\mathbf{v}\times\mathbf{B}), \end{cases}$$

  - *Pros*: simple, conservative
  - *Cons*: $\nabla\cdot B=0$ to scheme accuracy, one additional scalar equation

[1]Dedner et al., JCP (2002)

Parallel Implementation

- Parallelization in PLUTO is achieved by standard domain decomposition;
- A built-in library (ArrayLib) provides an abstraction for distributed array objects and simple interfaces to the underlying MPI2 routines;
- Supports cell-centered and staggered meshes;
- Strong scaling tests up to 262,144 cores on both FERMI and the BG/Q MIRA at Argonne National Laboratories (USA)



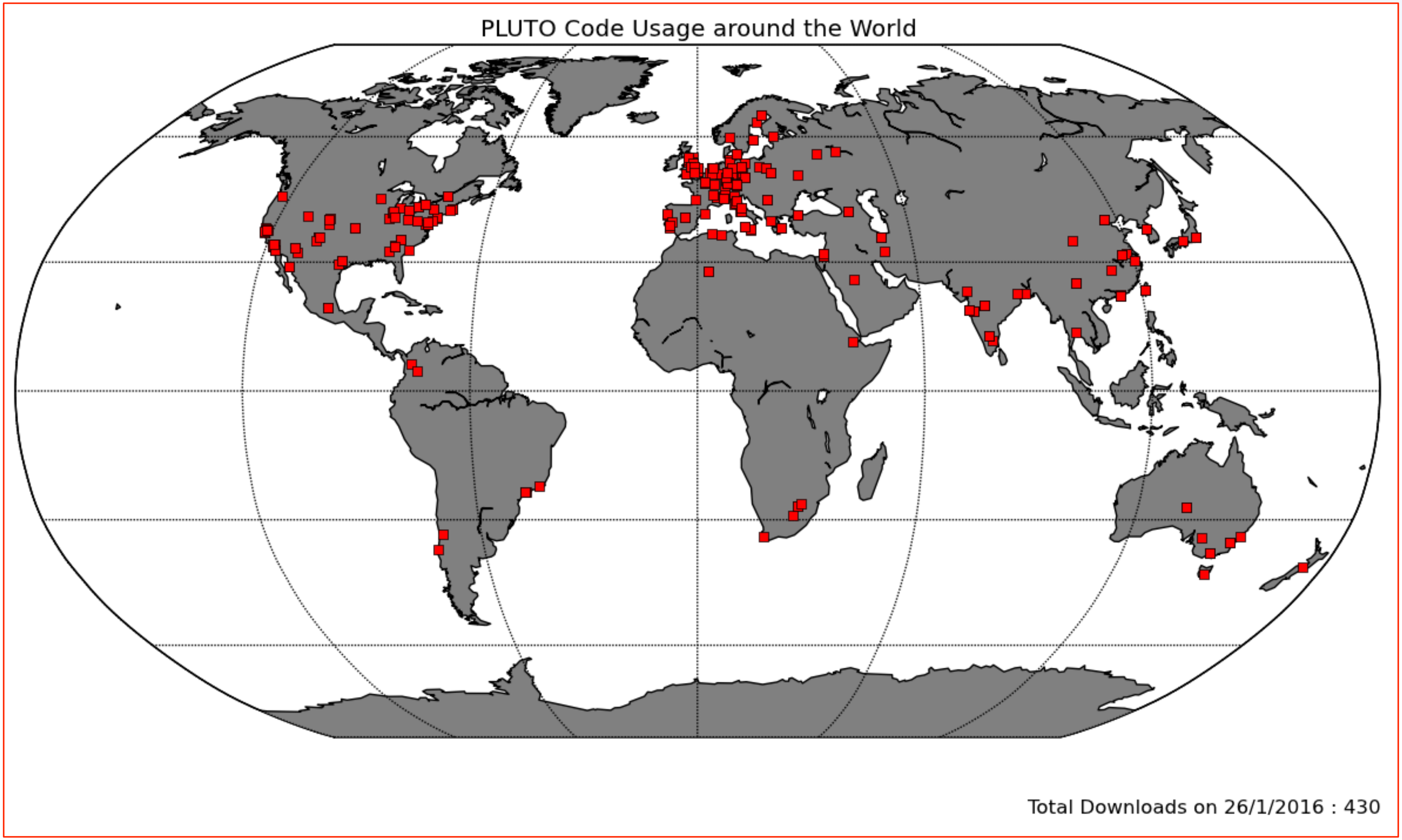
Parallel I/O

- PLUTO supports serial and fully parallel I/O (MPI2-standard);
- Several file formats:
  - Raw binary (single and double precision), [static grid]
  - Legacy VTK [static grid]
  - HDF5 [static grid, AMR]
  - ASCII [static grid]
- Parallel I/O improved to support both synchronous and asynchronous, 'split collective' calls (PRACE whitepaper[1]): this allows the transfer of data out/in the user's buffer to proceed concurrently with computation.

	$512 \times 1024 \times 512$			$512 \times 4096 \times 512$		
Nprocs	Synchronous time [sec]	Asynchronous time [sec]	Gain [%]	Synchronous time [sec]	Asynchronous time [sec]	Gain [%]
512	512	475	7.5	-	-	-
1024	295	277	6	-	-	-
2048	463	345	25	1368	1273	7
4096	246	193	21.5	863	697	19.2
8192	218	155	29	568	404	29

[1] http://www.hpc.cineca.it/content/io-optimizations-startegies-pluto-code

PLUTO Worldwide Distribution



II. ASTROPHYSICAL CHALLENGES

Astrophysical Plasma Conditions

- Astrophysical Plasmas are characterized by a wide disparity in spatial and temporal scales:

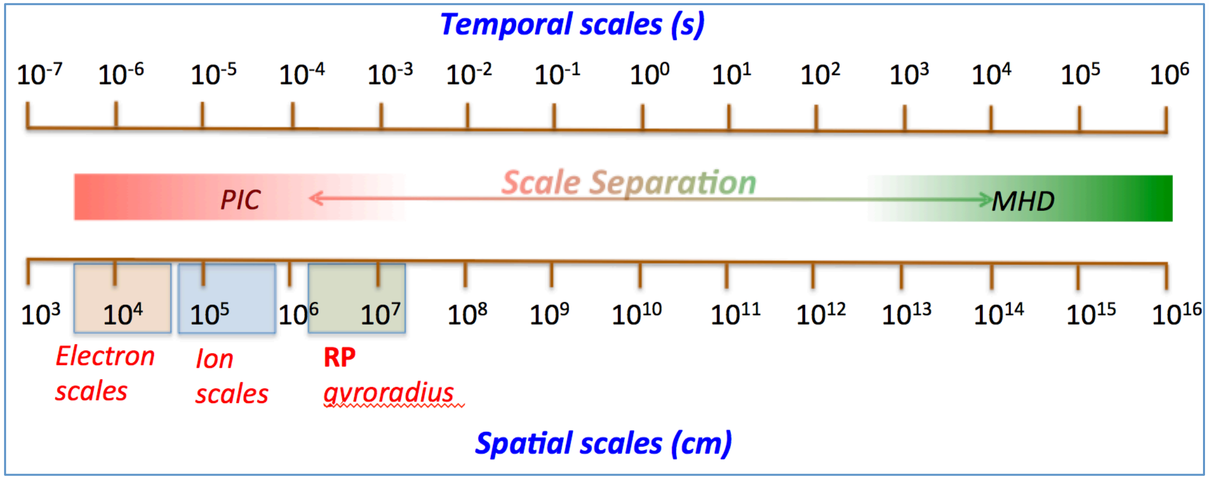
	L (cm)	n (cm^{-3})	T (K)	v(Km/s)	B (G)
Stellar interiors	$10^{10} \div 10^{12}$	10^{27}	$\geq 10^{7}$	$0 \div 500$	$1 \div 10^{4}$
Stellar winds	$10^{13} \div 10^{15}$	$10^{-2} \div 10^{3}$	$10^{2} \div 10^{3}$	$200 \div 4 \cdot 10^{3}$	$10^{-5} \div 10^{-3}$
Neutron star	10^{6}	10^{42}	$10^{6} \div 10^{9}$	-	10^{12}
Interstellar Medium	$10^{2} \div 10^{22}$	$10^{-1} \div 10$	10^{2}	$1 \div 30$	$\leq 10^{-5}$
Intergalactic Medium	$\geq 10^{24}$	$\leq 10^{-5}$	$10^{5} \div 10^{6}$	$10 \div 10^{3}$	$\leq 10^{-8}$
Jets from YSO	$10^{16} \div 10^{18}$	$10^{3} \div 10^{4}$	$10^{3} \div 10^{5}$	$100 \div 500$	$10^{-4} \div 10^{-3}$
Jets in AGN	$10^{21} \div 10^{24}$	$10^{-5} \div 10^{-3}$	-	$\sim c$	$\sim 10^{-3}$

- Flows are compressible, magnetized, supersonic, and possibly relativistic;
- Several physical effects: advection, dissipative (non-ideal effects), cooling/radiation, gravity, non-inertial effects, complex equations of state, stiff reaction networks, relativistic, etc…

Astrophysical Challenges: *Scale Separation*

- Astrophysical environments involve physical processes operating at *extremely different spatial* and *temporal scales*, and complex *interactions* between *plasmas* and *radiation*.

- Current computational *modeling* is still *largely fragmented* under the limited range of applicability of different models.



- A **large gap** stretches from theory to a clear interpretation of the observations of high-energy astrophysical sources.

Applications to Earth's Space Environment[1]

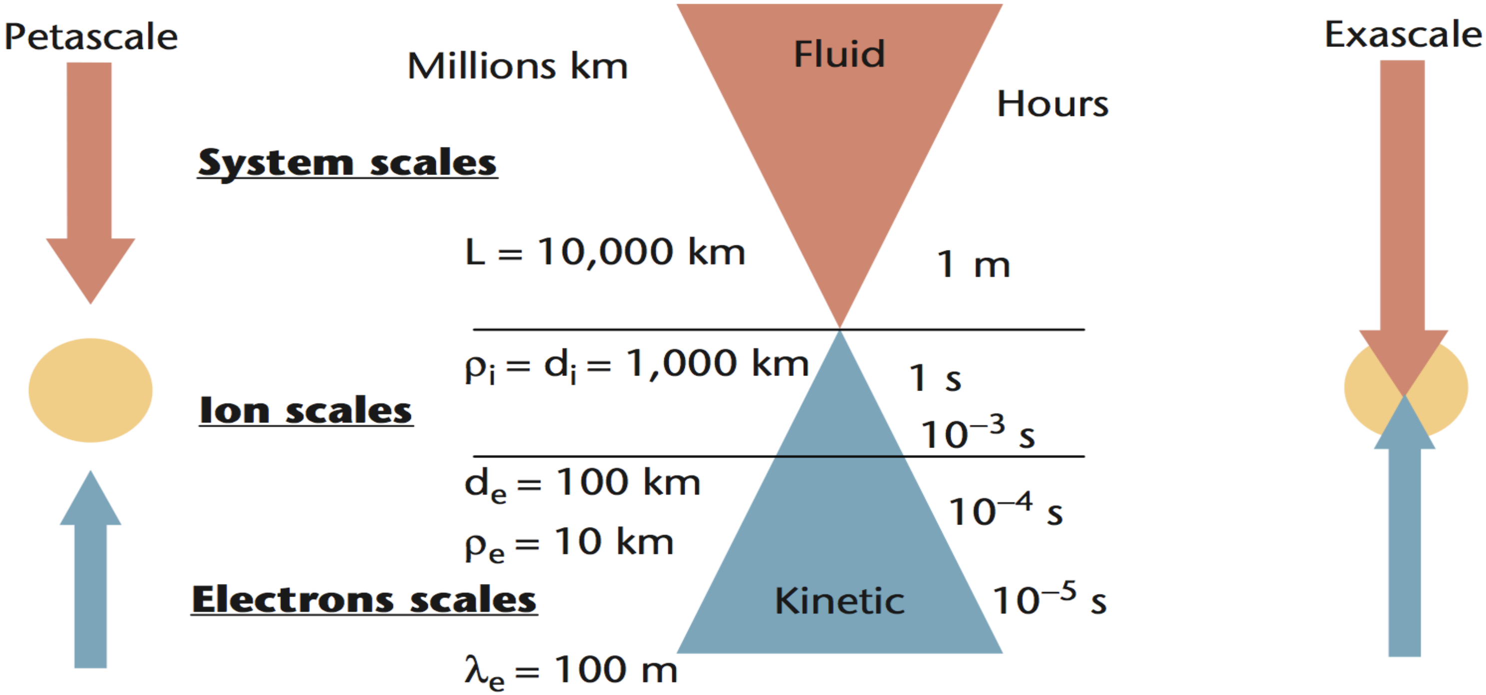


Figure 2. The physical scales of Earth's space environment. Typical scales observed during missions of exploration in Earth's space environment. The spatial scales are on the left and the temporal scales are on the right. Space plasmas are made of electrons and ions (mostly protons, the nuclei of hydrogen). Electrons are much lighter, and their scales are orders of magnitude smaller. A tremendous spread is present, requiring advanced modeling techniques and the largest computing resources conceivable.

[1]Lapenta JCP (2012), 231

III. ADAPTIVE MESH REFINEMENT

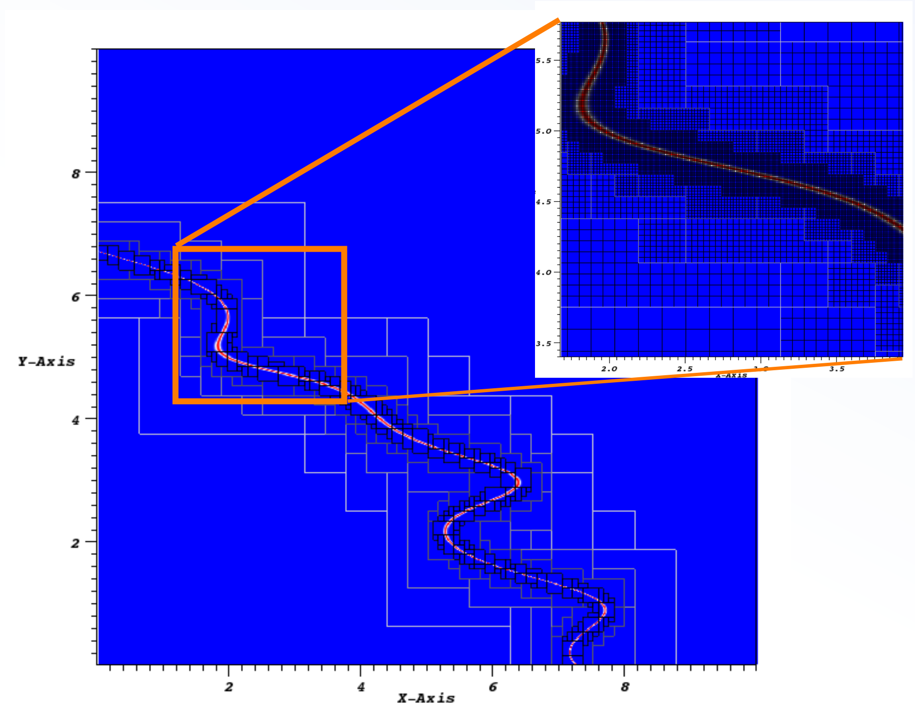
Grid Adaptive Computations

- Wide range of spatial and temporal scales

  → *<u>Adaptive Mesh Refinement</u>* (AMR)

- Goal of grid adaptivity:

  tracking features much smaller than overall scale of the problem providing adequate higher spatial and temporal resolution where needed.



- Dynamic grid vs. static grid approach:
  - Increased computational savings over a static grid approach.
  - Increased storage savings over a static grid approach.
  - Complete control of grid resolution, compared to the fixed resolution of a static grid approach.

Software for AMR Framework

Available frameworks for AMR:

- BoxLib (LBNL)
- Chombo (LBNL)
- AMRClaw (UW)
- SAMRAI (LLNL)
- ParaMesh (NASA)
- GRACE (Rutgers)

Parallelization Strategies:

- Individual grid distribution
- Separate distribution of each level
- Rigorous domain decomposition

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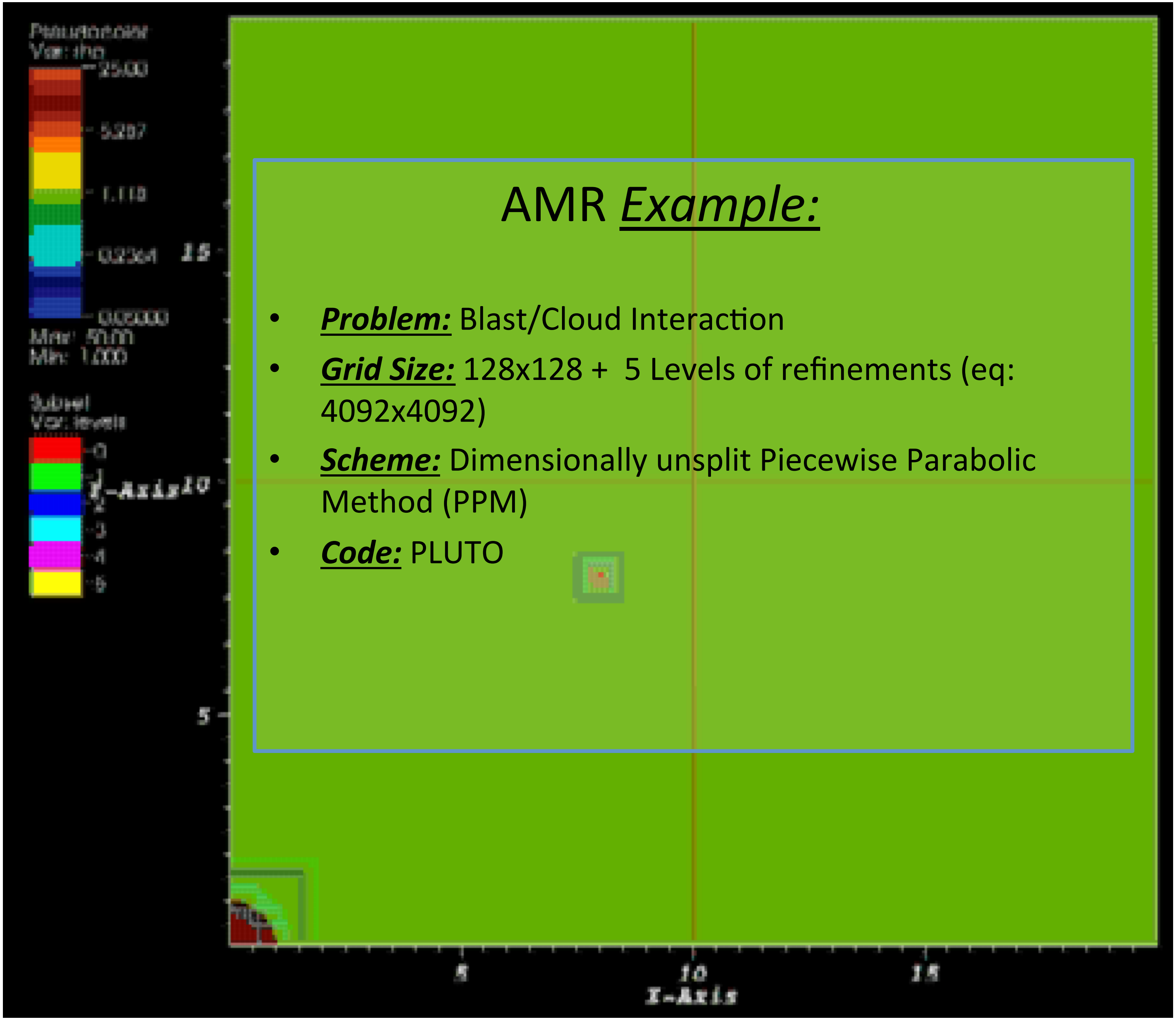
Parallelization Strategies:

- Individual grid distribution
- Separate distribution of each level
- Rigorous domain decomposition

- PLUTO takes advantage of the Chombo library: a distributed infrastructure for parallel computations over *block-structured* adaptively refined grids.

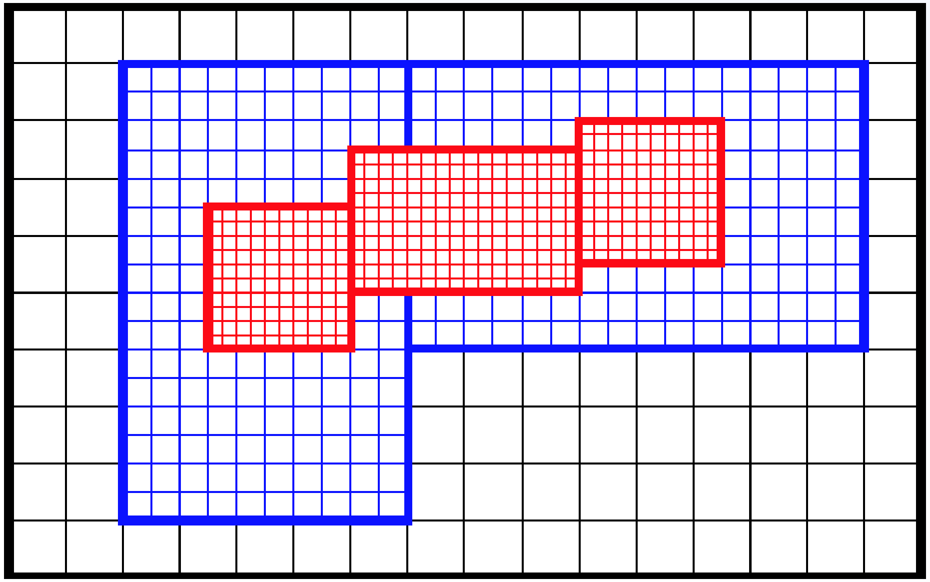
- The choice of block-structured AMR is justified by the need of exploiting the already implemented modular skeleton introducing the minimal amount of modification and, at the same time, maximizing code re-usability



AMR *Example:*

- ***Problem:*** Blast/Cloud Interaction
- ***Grid Size:*** 128x128 + 5 Levels of refinements (eq: 4092x4092)
- ***Scheme:*** Dimensionally unsplit Piecewise Parabolic Method (PPM)
- ***Code:*** PLUTO

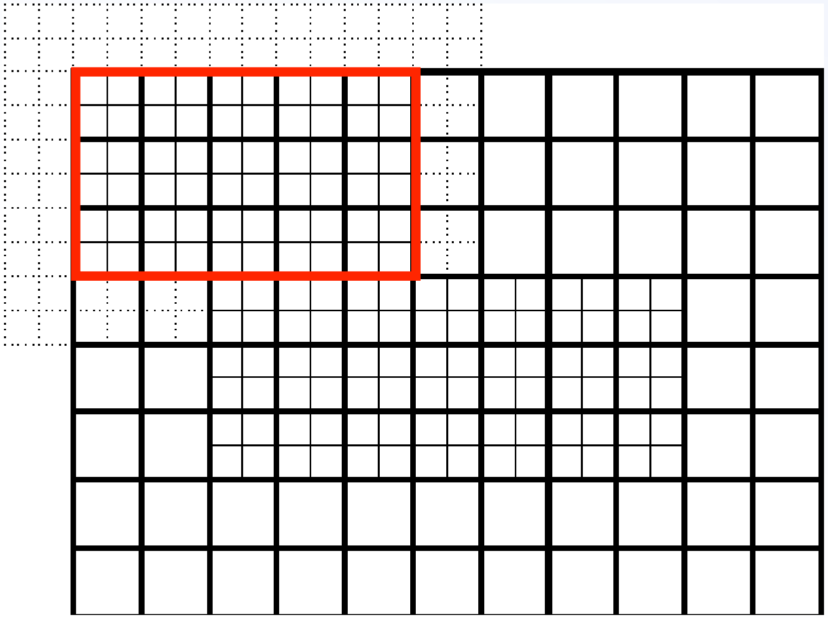
Block Structured AMR



- data blocks are created so that the same stencil can be used for all points and no special treatment is required.
- High level objects that encapsulate the functionality for AMR and its parallelization are independent of the details of the physics algorithms and the problem being solved.
- Simplifies the process of adding/replacing physics modules as long as they adhere to the interface requirements.

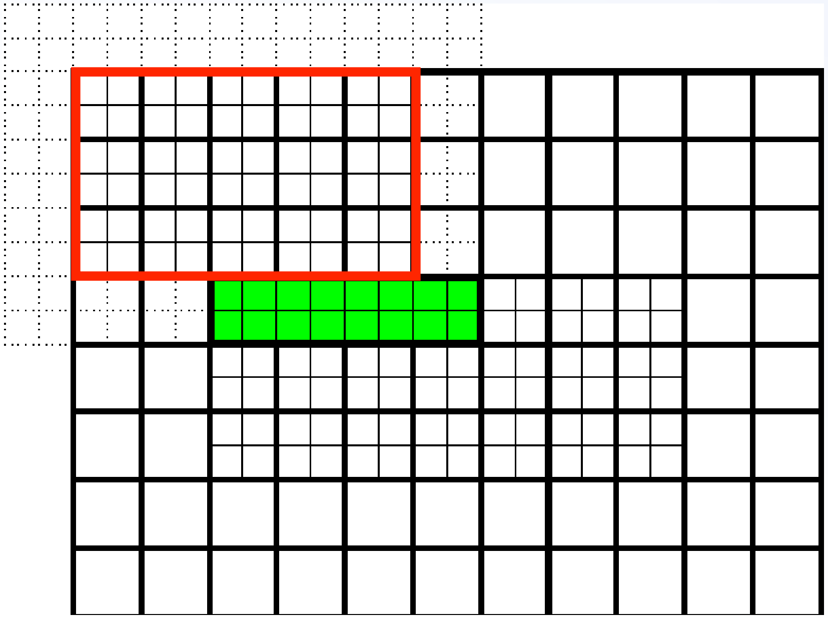
Single Level Integration

- ghost zones values need
  to be filled before integration;



Single Level Integration

- ghost zones values need to be filled before integration;
- Patches at the same level are synchronized.



Single Level Integration

- ghost zones values need
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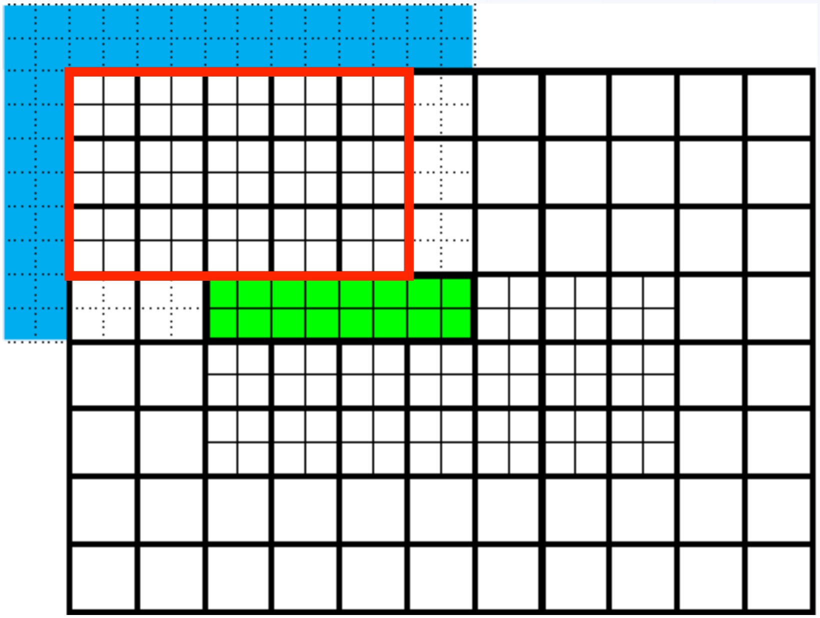
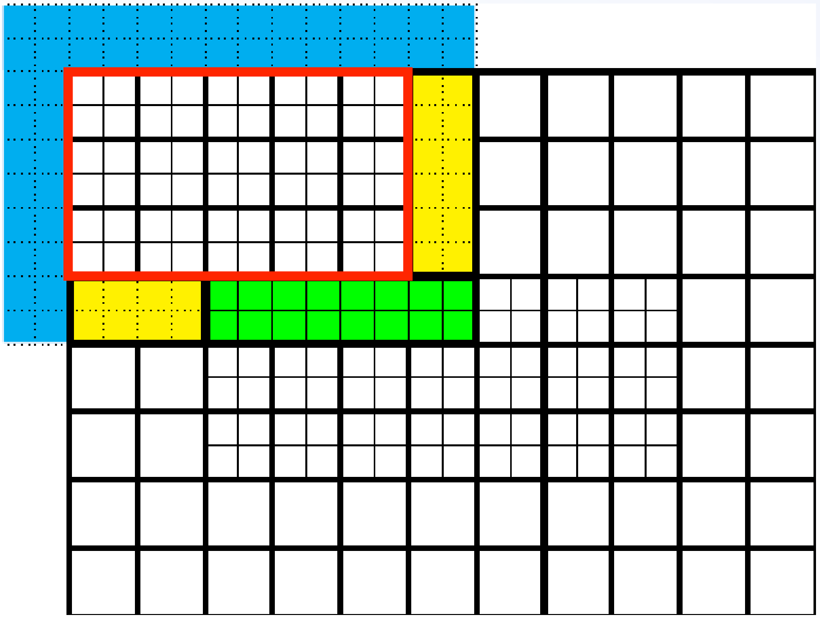
- Patches at the same level are synchronized;
- Physical boundaries are imposed externally;



Single Level Integration

- ghost zones values need to be filled before integration;
- patches at the same level are synchronized;
- Physical boundaries are imposed externally;
- Fine-Coarse and Coarse-Fine interface need interpolation / averaging



- Integration proceeds as for the single-grid case:

$$\mathbf{Q}_{jk}(t+\Delta t) = \mathbf{Q}_{jk}(t) - \frac{\Delta t}{\Delta x_1}\left(\mathbf{F}^1_{j+\frac{1}{2},k} - \mathbf{F}^1_{j-\frac{1}{2},k}\right) - \frac{\Delta t}{\Delta x_2}\left(\mathbf{F}^2_{j,k+\frac{1}{2}} - \mathbf{F}^2_{j,k-\frac{1}{2}}\right)$$

AMR PLUTO Implementation

- Time stepping based on the Corner Transport Upwind (CTU[1]) or Method of lines (RK2)
  - fully dimensionally unsplit inclusion of hyperbolic and parabolic terms;

$$\bar{\mathbf{U}}^{n+1} = \bar{\mathbf{U}}^{n} + \Delta t^{n} \sum_{d} \left(\mathcal{L}_{H,d}^{n+\frac{1}{2}} + \mathcal{L}_{P,d}^{n+\frac{1}{2}} \right)$$

  - CTU: one boundary call / step;

- PPM, WENO and linear reconstruction;

- Diffusion terms treated explicitly or via accelerated techniques (STS, RKL)

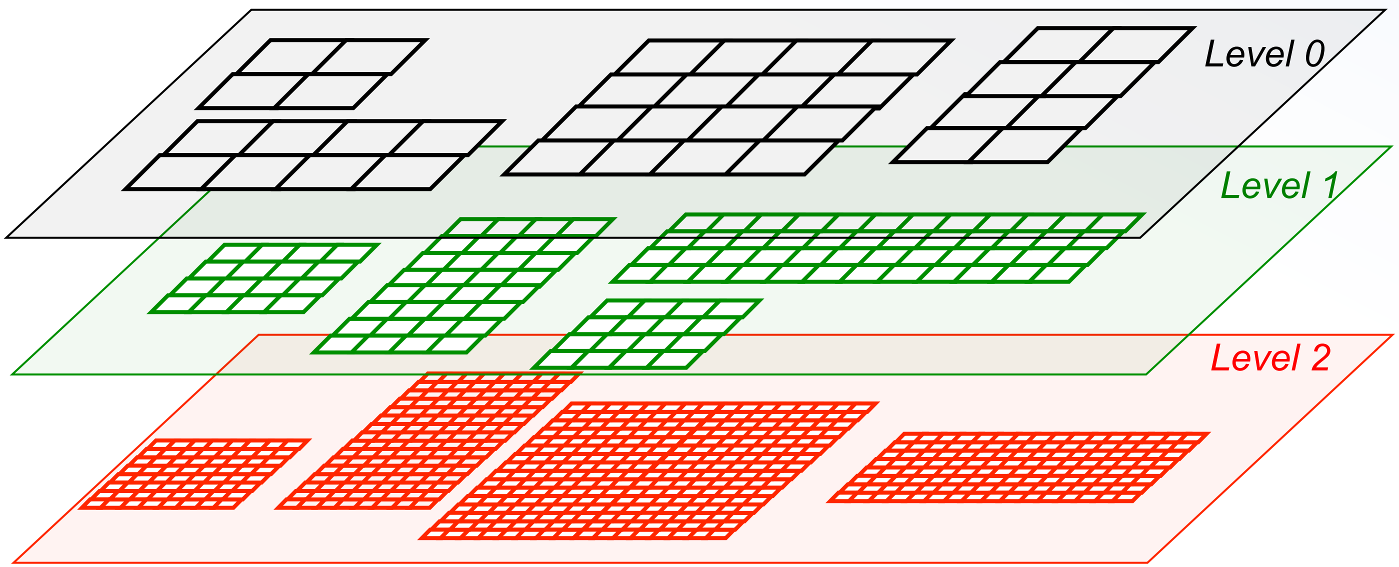
- Cell-centered GLM formulation of MHD equations

$$\begin{aligned} \frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) + \nabla \psi &= 0 \\ \frac{\partial \psi}{\partial t} + c_h^2 \nabla \cdot \mathbf{B} &= -\frac{c_h^2}{c_p^2} \psi \end{aligned}$$

[1]Colella JCP (1990); Saltzmann, JCP (1994)

Parallel Data Distribution

- For block-structured AMR, the solution at each level is defined on a collection of logically rectangular grid patches each containing a large number of points:



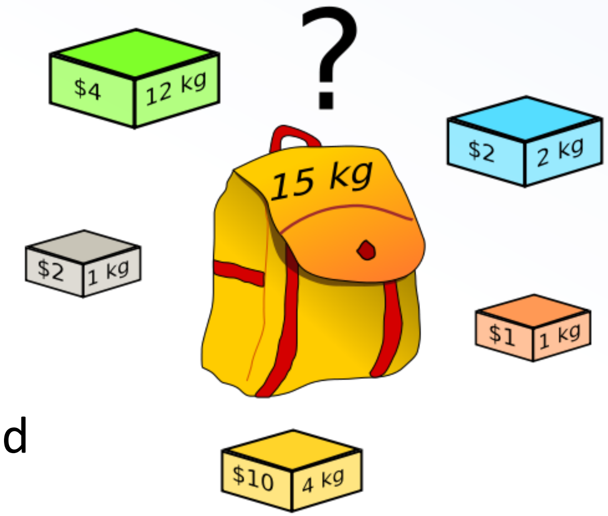
- This organization of data into large aggregate grid patches also provides a model for parallelization of the AMR methodology.

Parallel Data Distribution

- Data distributed among processor: different resolutions are distributed indipendently, separately load-balanced;

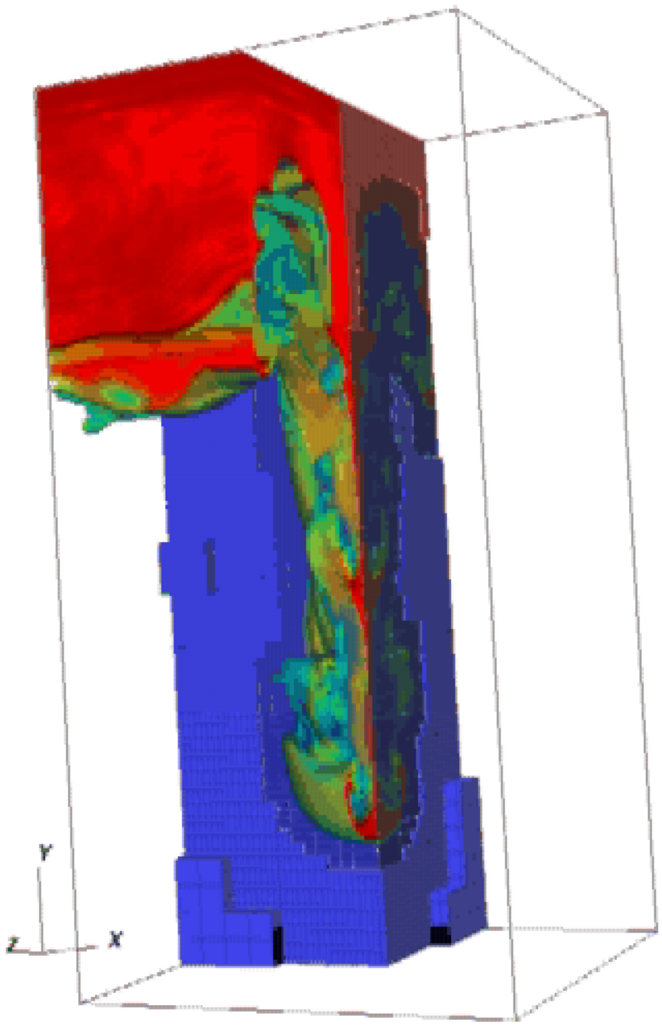
- Load-balancing based on the solution of the ***knapsack*** problem:
  - *Given a set of items, each with a weight and a value, determine the number of each item to include in a collection so that the total weight is less than a given limit and the total value is as large as possible*

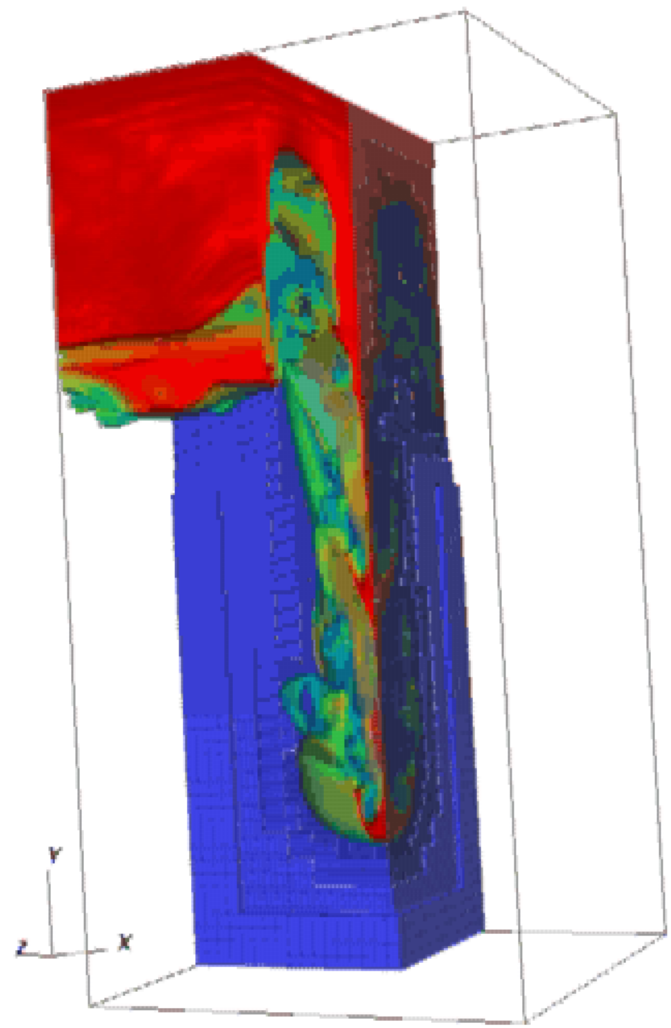
  → the computational work in the irregularly sized grids of the AMR data structures is equalized among the available processors.



- Knapsack algorithm provides good efficiency if the number of grids/processors > 3 (Crutchfield, 1993).

Parallel Performance, 3D Rayleigh-Taylor





<u>Base grid</u>: 16x32x16

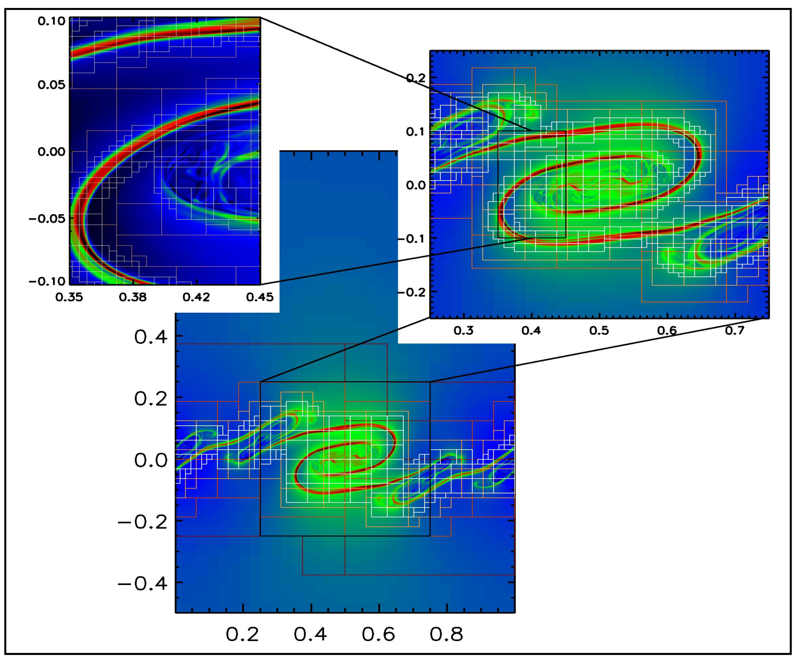
2 Levels, jump 4:4

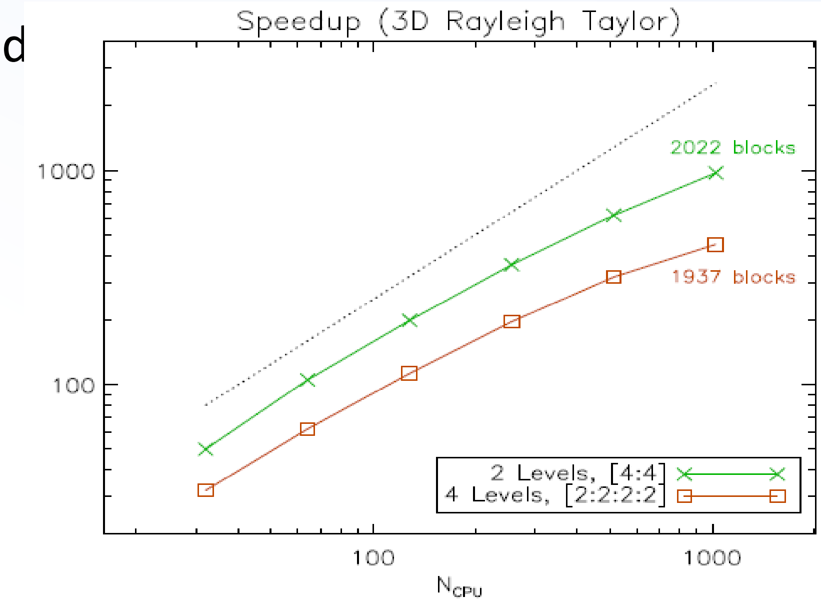
4 Levels, jump 2:2:2:2

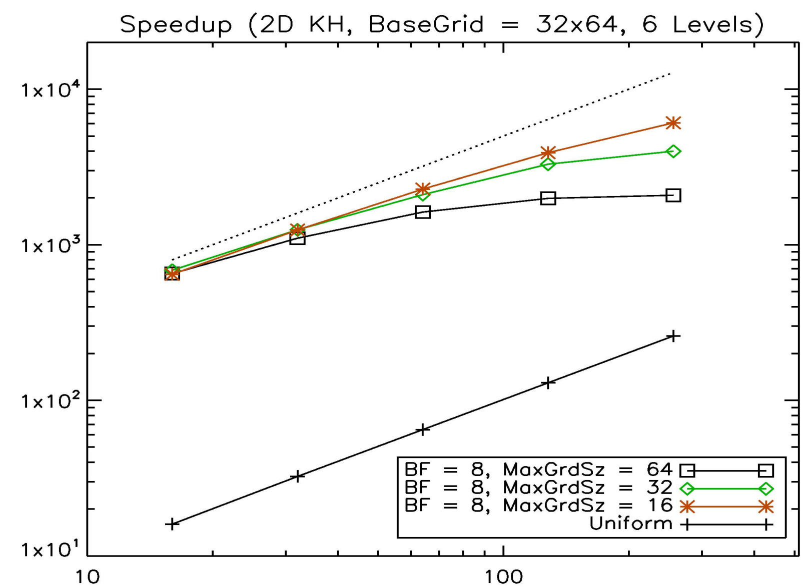
AMR PLUTO Parallel Performance

- 3D, RT: Efficiency > 0.8 for ≤ 512 CPUs and drops to 0.6 (2-lev) and 0.4 (4-lev) at 1024 CPUs;

- Smaller patches improve efficiency:
2D, Relativistic KH





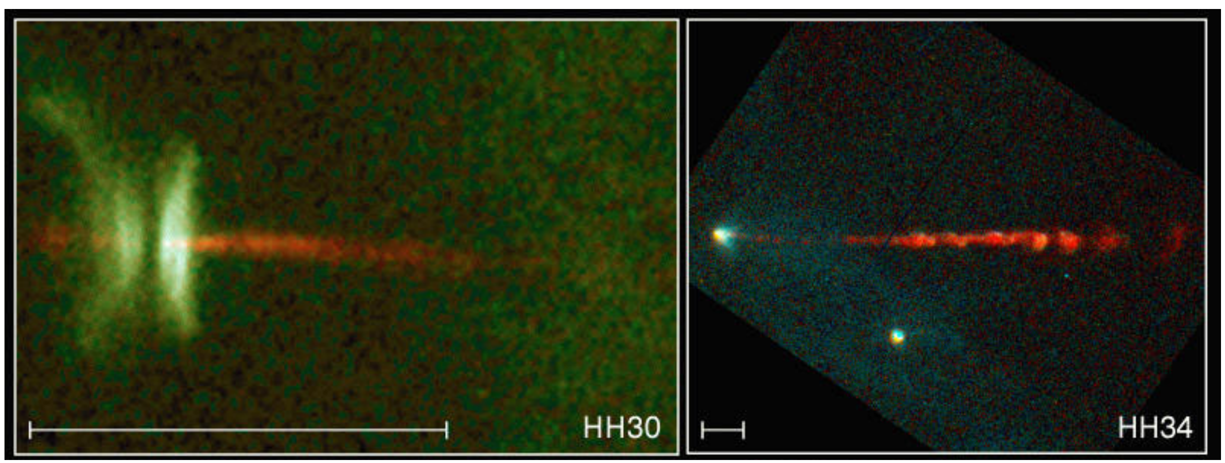


Application: Jets from young stellar objects

- Bibolar outflows from inner accretion disk in star formation regions;
- Strong shock waves that heat and ionize the gas;
- electrons and ions recombine → emission line spectrum characteristic of Herbig-Haro objects;
- Forbidden emission lines in the optical, IR emission
- Need to resolve different time and spatial scales:

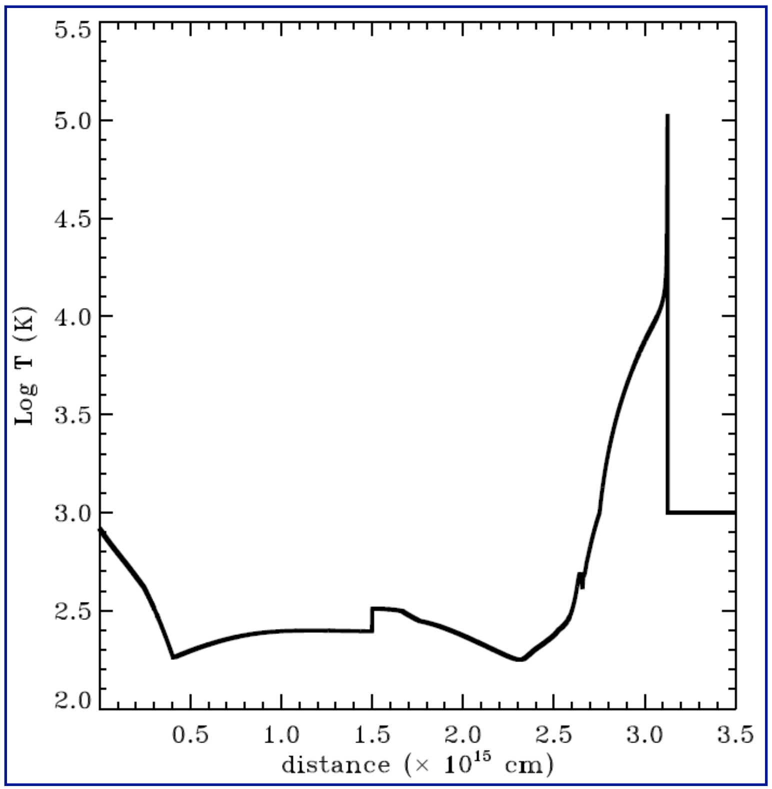
  Advection scales ~ 10 yrs/ ~10^{15} cm

  Cooling scales ~ week / ~10^{13}-10^{12}cm (! Stiff !)

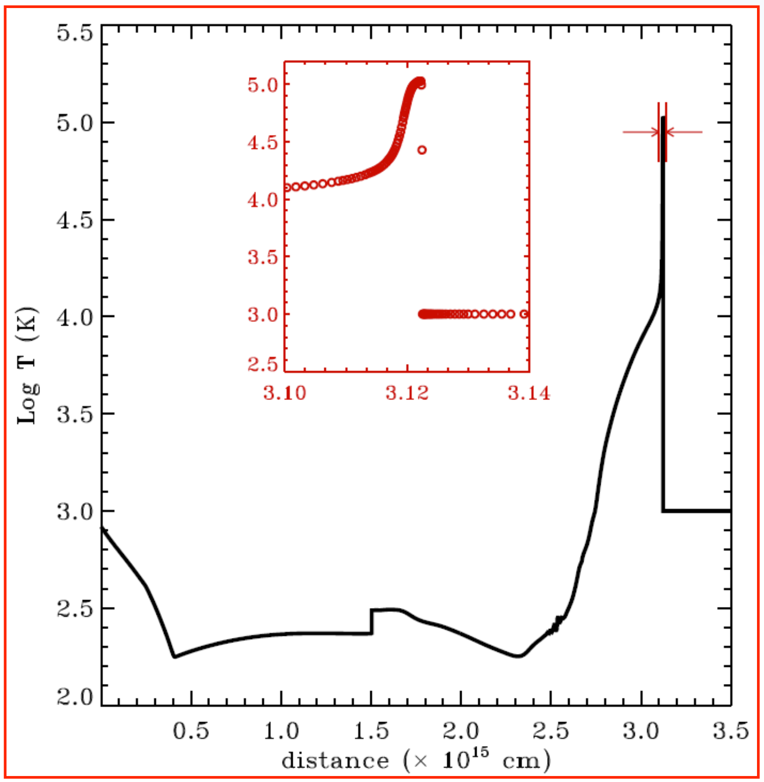


One-dimensional calculations

- Emission comes from very localized regions behind the shock
- Need for adaptive mesh refinement following the shock[1]:



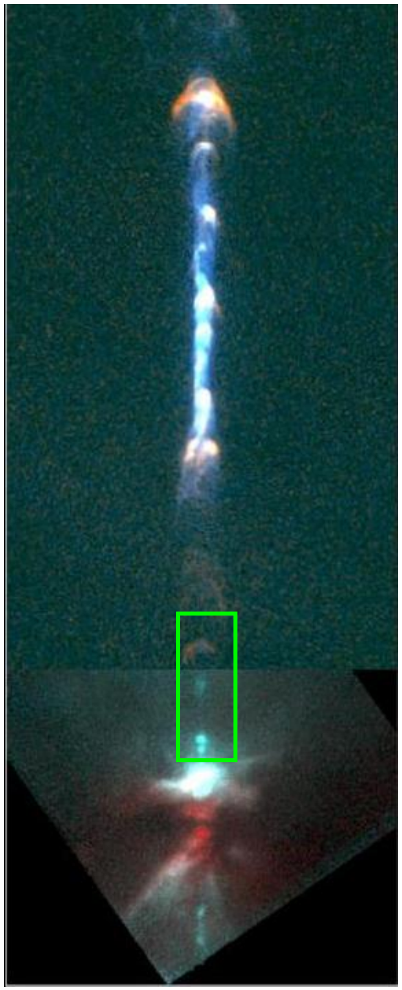
Static uniform grid (49152 zones), ~ 17 hrs

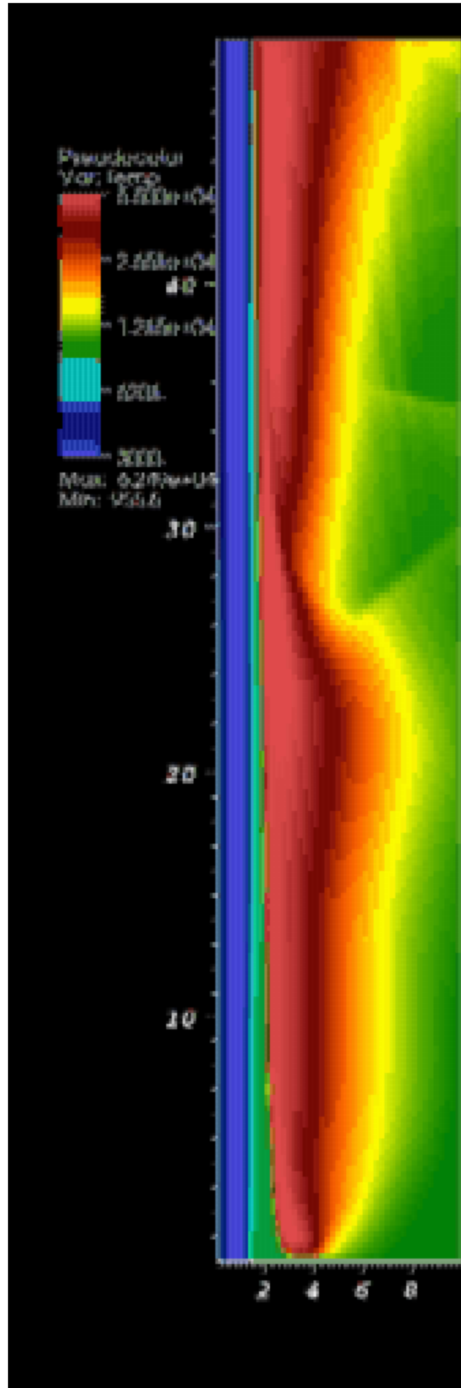


AMR (1536, 5 levels) ~ 4 min

[1]Tesileanu et al., ApJ (2012) 746:96

Axisymmetric Jet Model





Problem:

Radiative pulsed jet[1]

Base Grid:

128x640

Levels of Refinement:

7

(eq. Res = 16384 x 81920)

Method:

Unsplit PPM + Cooling

Code:

PLUTO + Chombo AMR

Description:

Jet perturbed at the inflow with a velocity variability (T = 50 yrs).

Parameters:

n_H = 500 cm^{-3},

v_j = 200 Km/s

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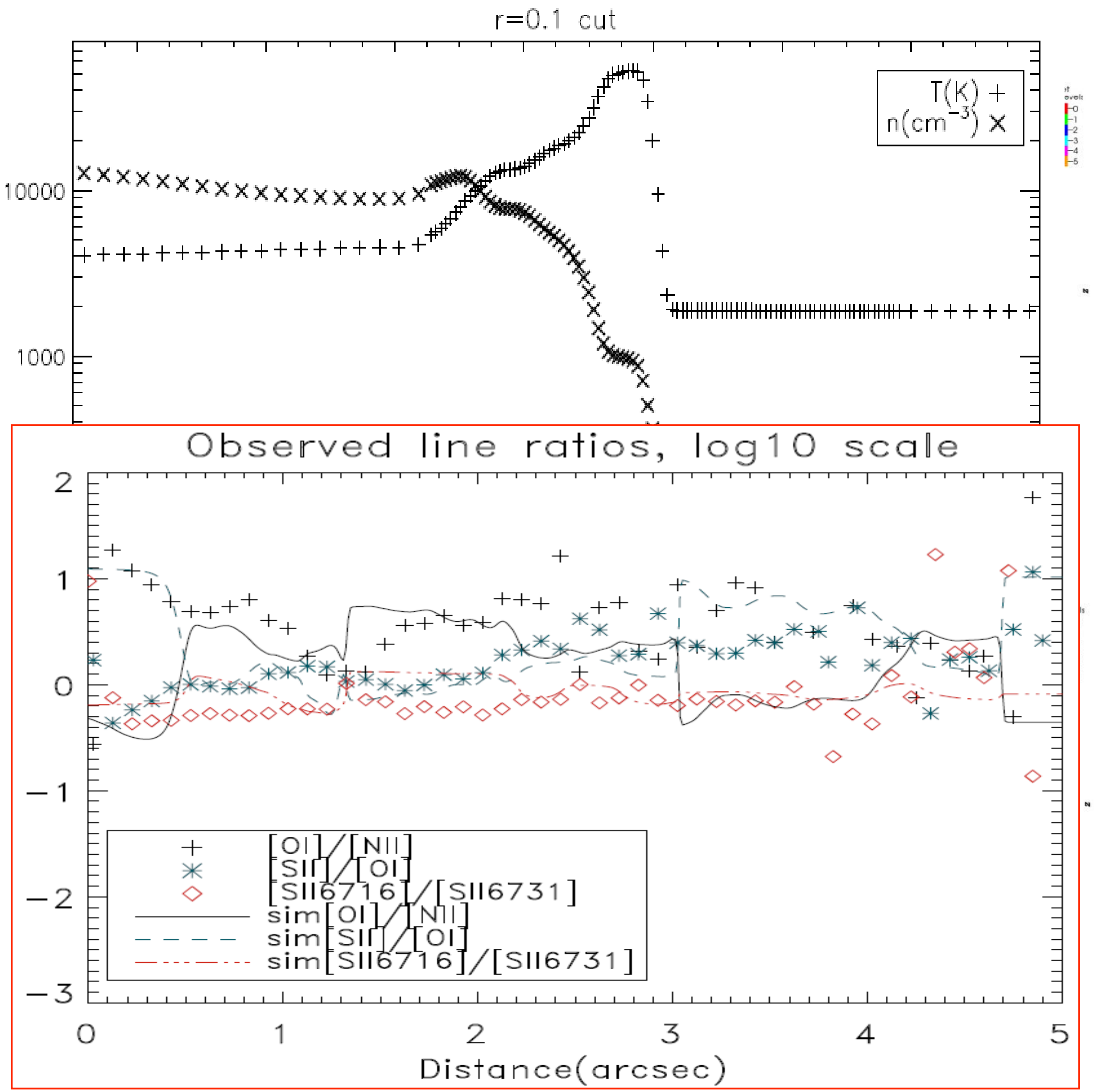
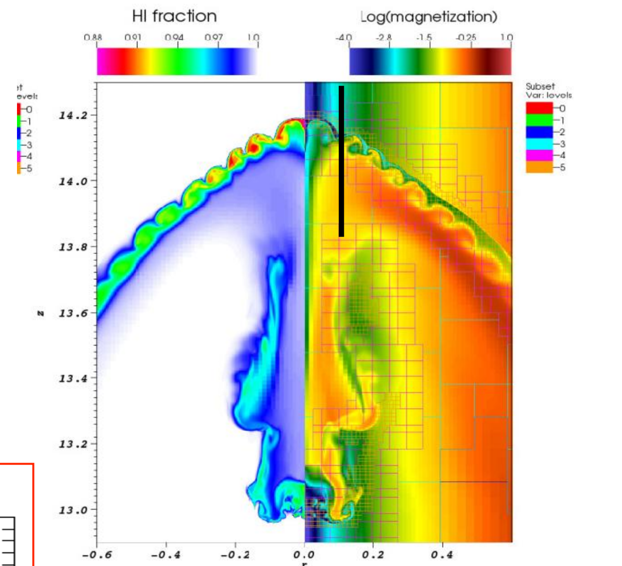
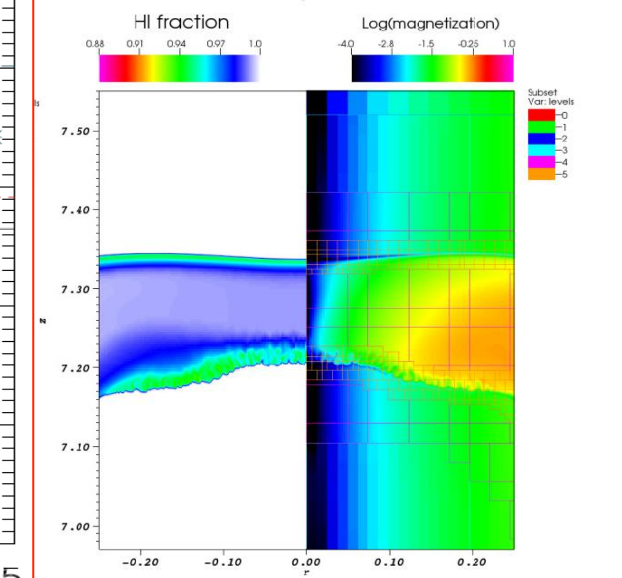
[1]Tesileanu et al., ApJ (2012) 746:96

Radiative Shock Structure







IV. PARTICLE PHYSICS

Particle Module in PLUTO

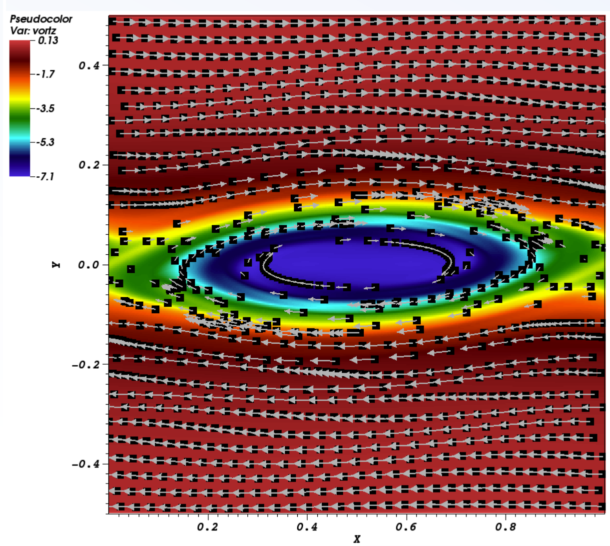
- *Sub-grid models*, *micro-scale physics* and/or *kinetic effects* can be (partially) restored by introducing particles.

- PLUTO offers type of particles may be used, depending on the application:

Particle type	Purpose	System Scale
Lagrangian (macro-particles)	Model non-thermal emission from AGN / PWN environments.	Largest
CR	Model CR streaming, turbulent field amplification and particle acceleration at shocks / reconnection layers.	Medium/Small
Dust	Models of proto-planetary disks.	Large
Superphotons	Monte-Carlo methods for radiation transport at arbitrary optical depth.	[Future]

Lagrangian Particles

- A Lagrangian macro-particle (MP) represents an ensemble of real particles (e.g., electrons) sufficiently close in physical space and associated with a *sub-grid physical modeling*.



- Each MP is characterized by a distribution function N(ε,t) representing the actual particle number density as a function of energy ε.

- The energy distribution changes in time according to several different physical processes (compression/expansion, synchrotron losses [Kardashev 1962])

- LPs are transported at the fluid speed, $dx/dt = v_g$;

Lagrangian Particles

- In energy space, the spectra is evolved by solving, for each particle, a Fokker-Planck equation

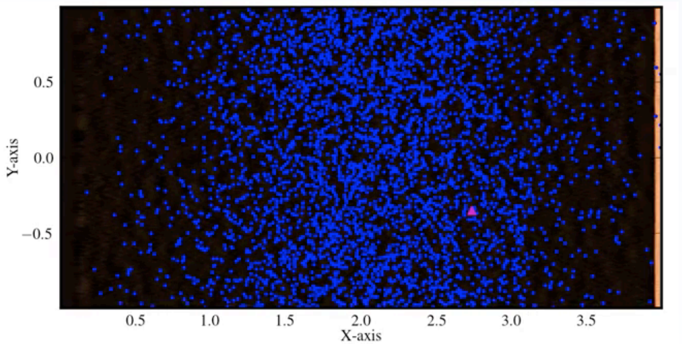
$$\boxed{\frac{\partial}{\partial t}\left[N(E,t)\right] = \frac{\partial^2}{\partial E^2}\left[D(E)N\right] - \frac{\partial}{\partial E}\left[\left(A(E) - \dot{E}_L\right)N\right] - \frac{N}{T_{esc}} + S(E,t)}$$

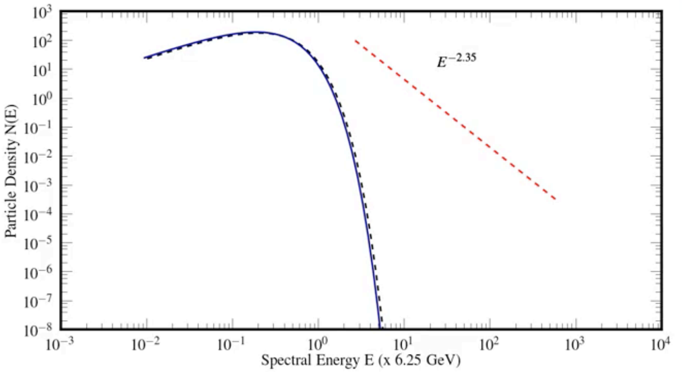
- Additional processes include sub-grid model for Fermi I acceleration (DSA) at shocks:

$$N(E,t)_+ = \lambda(\rho_+/\rho_-)N(E,t)_-$$

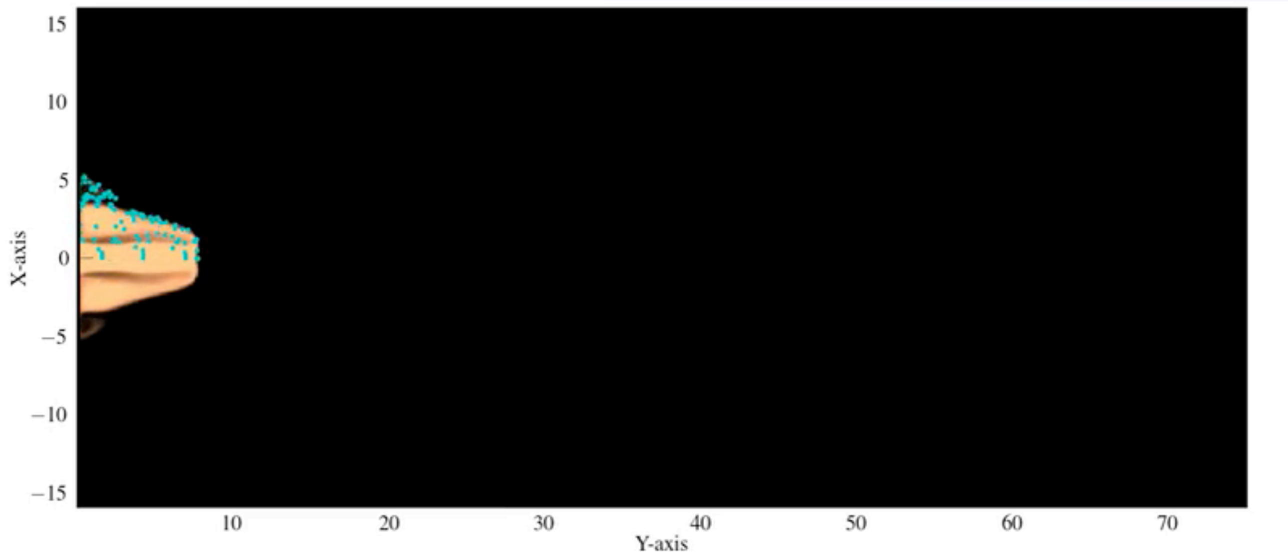
- Emissivity can be computed from particle distribution as

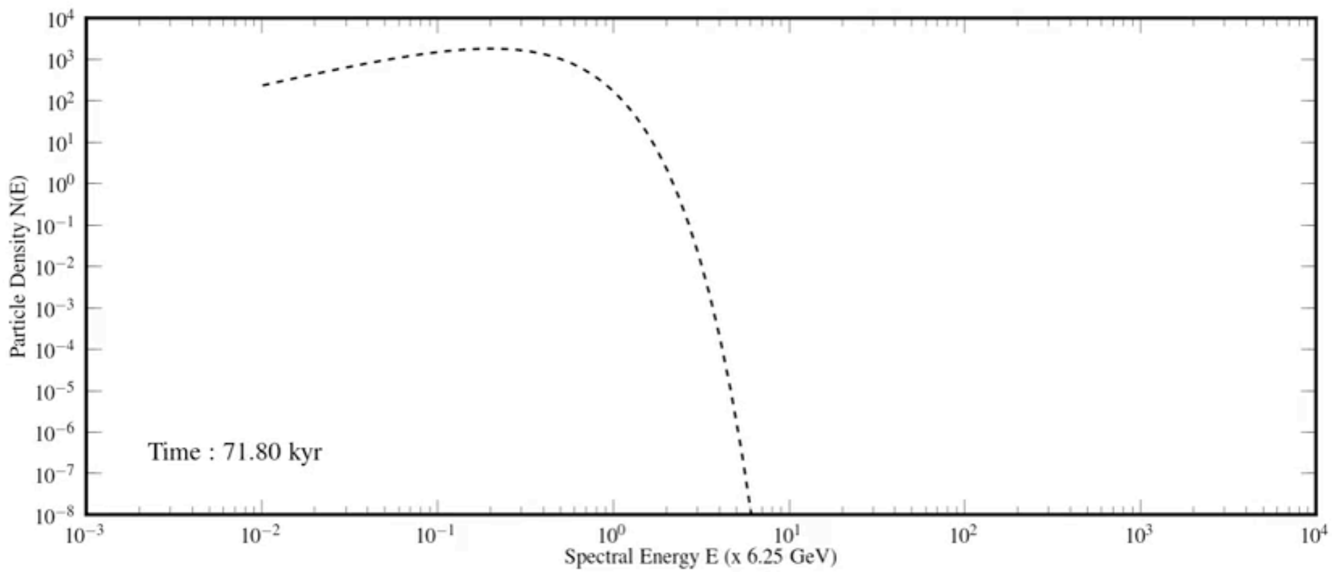
$$j_\nu \propto \int_0^\infty N(E',t)dE'$$





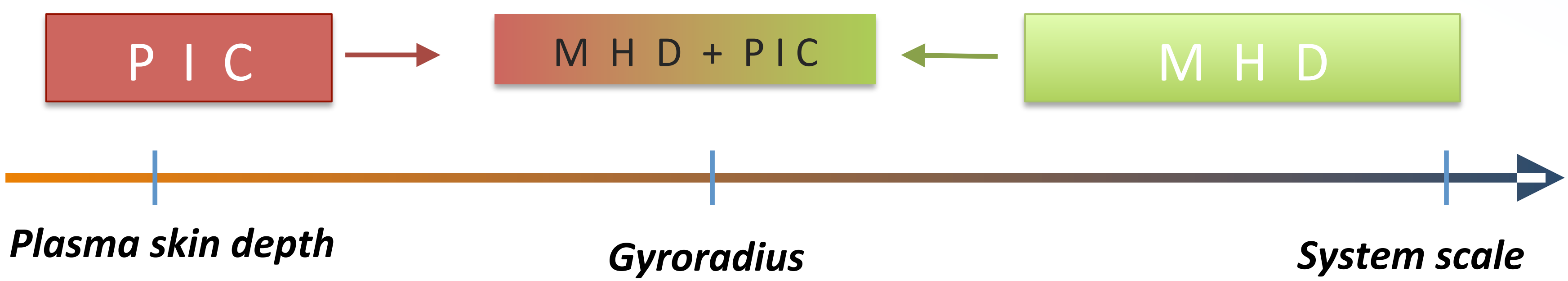
Application: Jet Propagation and Emission





Cosmic Rays: the MHD+PIC Model

- MHD+PIC hybrid model: Cosmic-Rays (CRs) particles treated with conventional PIC technique, while the rest of the thermal plasma (ions and electrons) is treated as MHD fluid[1].
- MHD+PIC properly describes the physics of the composite system on scales much larger than the ion inertial length, c/ω_{pi}.
- Avoid resolving microscopic scales, allowing simulations at much larger and even macroscopic scales at modest computational cost.
- Only gyration must be resolved.



$$\frac{c}{\omega_{pe}} \approx \frac{5.4 \times 10^5}{\sqrt{n}} \mathrm{cm}$$

$$\approx \frac{\gamma m c^2}{qB}$$

[1]Bai et al, ApJ (2015)

Hybrid MHD+PIC Equations

- MHD+PIC is a hybrid model using fluid (for the thermal plasma components) and particles (CRs, modeling the non-thermal component):

MHD Fluid ⟷ ***Particles***

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}_g) &= 0 \\
\frac{\partial (\rho \boldsymbol{v}_g)}{\partial t} + \nabla \cdot [\rho \boldsymbol{v}_g \boldsymbol{v}_g - \boldsymbol{B}\boldsymbol{B} + \mathsf{I} p_t] &= -\boldsymbol{F}_{\rm CR} \\
\frac{\partial \boldsymbol{B}}{\partial t} + c\nabla \times \boldsymbol{E} &= \boldsymbol{0} \\
\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \left[\left(\frac{1}{2}\rho \boldsymbol{v}_g^2 + \rho e + p\right)\boldsymbol{v}_g + \frac{c\boldsymbol{E} \times \boldsymbol{B}}{4\pi}\right] &= -\boldsymbol{v}_g \cdot \boldsymbol{F}_{\rm CR}
\end{aligned}
$$

Ohm’s law includes CR-induced Hall-term[1]:

$$
c\boldsymbol{E} = -\boldsymbol{v}_g \times \boldsymbol{B} - R(\boldsymbol{v}_{\rm CR} - \boldsymbol{v}_g) \times \boldsymbol{B}
$$

CRs are subject to the Lorentz force, and the force density they experience is:

$$
\boldsymbol{F}_{CR} = \left(\frac{q_{\rm CR}}{c}\right) c\boldsymbol{E} + \frac{1}{c}\boldsymbol{J}_{\rm CR} \times \boldsymbol{B}
$$

The equation of motion is

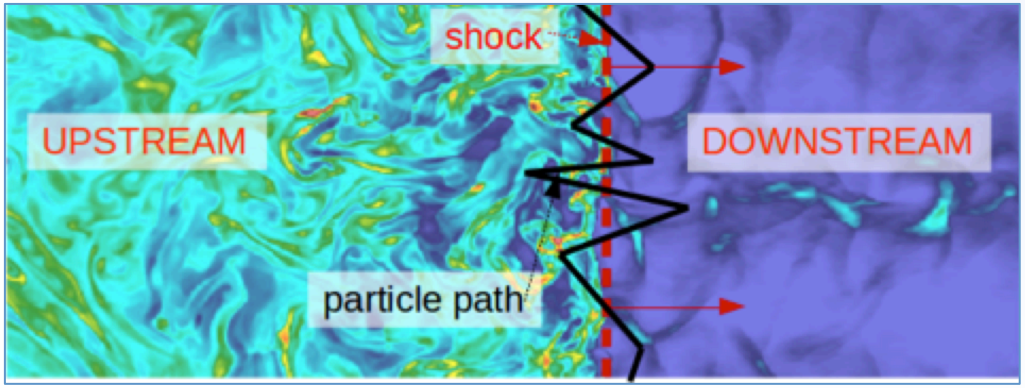
$$
\begin{aligned}
\frac{d\boldsymbol{x}_p}{dt} &= \boldsymbol{v}_p \\
\frac{d(\gamma \boldsymbol{v})_p}{dt} &= \left(\frac{e}{mc}\right)_p (c\boldsymbol{E} + \boldsymbol{v}_p \times \boldsymbol{B})
\end{aligned}
$$

[1] Bai et al, ApJ (2015) 809:55, Mignone et al. (2017) in preparation

Diffusive Shock Acceleration:

- DSA commonly invoked to explain production of high energy cosmic rays (CR) at shock waves.

- Acceleration of charged particles when being repeatedly scattered across a shock front:



- Important in many astrophysical models (e.g. shocks, solar flares and SNR).

- Scattering comes from magnetic field irregularities (acting as magnetic mirrors) / Alfven waves.

- → Requires substantial magnetic field amplification

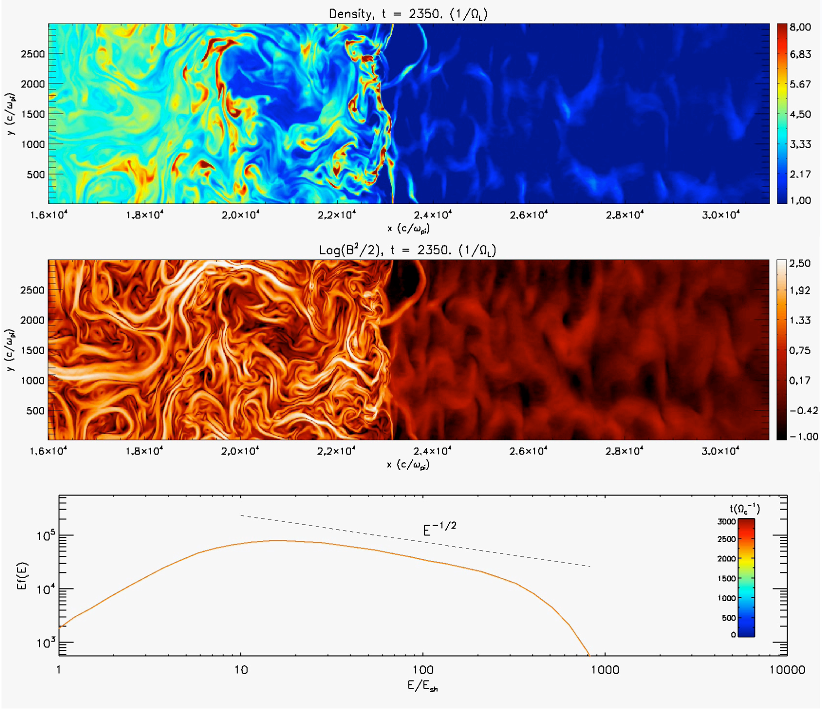
CR Acceleration at Shocks

- CR scattered by local turbulent magnetic field irregularities. Accelerated CRs drift with respect to the upstream fluid and the instability typically quickly enters its strongly nonlinear stage.

- Particles spectrum broadens in time, extending substantially to the high energy side.

- A high-energy power-law tail builds up, with spectral slope consistent with -3/2.

- The high-energy tail extends to higher energies with time, with a roughly exponential energy cutoff.



THE END