# A versatile, adaptive toolkit for Solar and Astrophysical Applications

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# Philosophy

- targets **any set of equations of generic type**

$$\partial_t \mathbf{U} + \nabla \cdot \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U}, \partial_i \mathbf{U}, \partial_i \partial_j \mathbf{U}, \mathbf{x}, t)$$

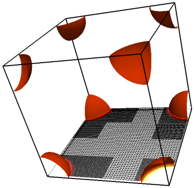
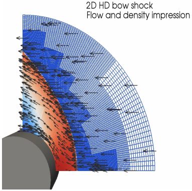
  - $\Rightarrow$ conserved variables **U**, fluxes **F**, sources **S**
  - $\Rightarrow$ (near-) conservation laws: hyperbolic PDEs
- emphasis on shock-governed dynamics
  - $\Rightarrow$ shock-capturing schemes
- **any-dimensionality**: `Perl` preprocessor to `Fortran 90`
  - $\Rightarrow$ can handle Cartesian, cylindrical, spherical geometries
- **several physics modules pre-implemented**

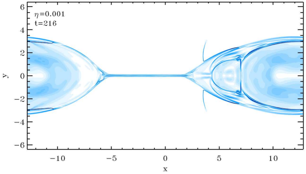
- **User defines initial conditions, can select predefined or add personal boundary conditions**, may add source terms, and possibly I/O additions
  - ⇒ many example setups provided in repository version
  - ⇒ code obtained via `gitlab` through

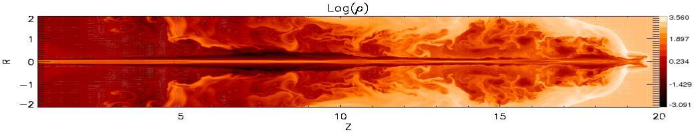
```
git clone https://gitlab.com/mpi-amrvac/amrvac.git
```

- (some) `HTML` documentation info at `http://homes.esat.kuleuven.be/~keppens`
  - ⇒ develop **Porth**, **Xia**, Hendrix, Meliani, van Marle, RK, ...
  - ⇒ AMR described in **Keppens et al, 2012, JCP 231, 741**

- **open source software MPI-AMRVAC**
  - ⇒ any-D, explicit **grid adaptive framework**
  - ⇒ **full MPI octree AMR, cartesian/cylindrical/spherical**
- physics: **advection**, **HD**, **MHD**, **relativistic HD-MHD**

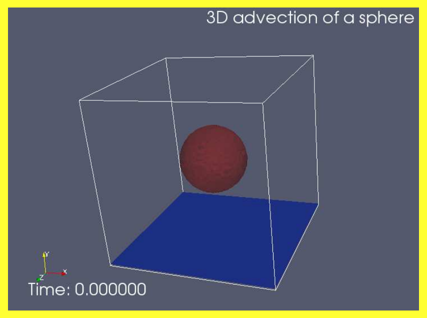








- **Porth et al, 2014, ApJS, 214, 4**
  - ⇒ addition of gas+dust modules, Hall-MHD extensions
  - ⇒ generic **slice & collapse** procedures for 3D block AMR
- **active-passive** grids as exploited in Porth et al 2013,2014

- **Test module: pure advection**
  - ⇒ with $\mathbf{U} = \rho$, $\mathbf{F} = \rho \mathbf{v}$ with $\mathbf{v}$ uniform velocity
  - ⇒ testing novel functionality in discretization or adaptivity
  - ⇒ demonstrating convergence, order of accuracy, . . .
- Discontinuity dominated 2D profile: `VAC` logo
  - ⇒ **advected diagonally on unit square**
- 3D advection test: constant $\rho$ in sphere, different $\rho$ out
  - ⇒ **movie shows isosurface, slice plane**



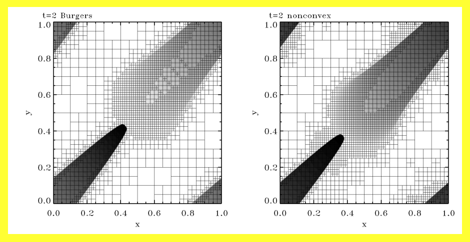
- **Nonlinear Scalar equation**: `nonlinear/amrvacphys.t`
  - ⇒ `eqpar(fluxtype_)` switch for different flux expressions
  - ⇒ inviscid Burgers (case 1), nonconvex equation (case 2)

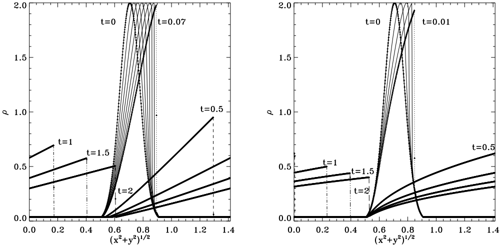
$$\rho_t + \nabla \cdot \left( \frac{1}{2} \rho^2 \mathbf{e} \right) = 0$$

$$\rho_t + \nabla \cdot \left( \rho^3 \mathbf{e} \right) = 0$$

  - ⇒ in any dimensionality as $\mathbf{e} \equiv \sum_{i=1}^{D} \hat{\mathbf{e}}_i$

- evolution of Gaussian, **compare Burgers to nonconvex case**

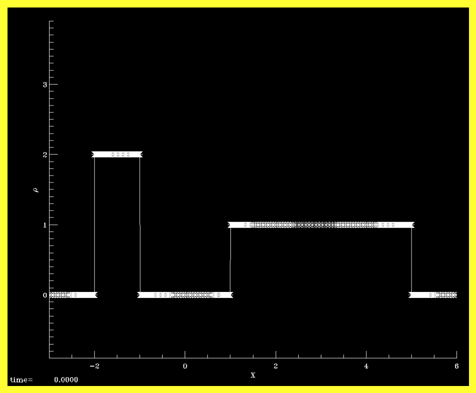



⇒ smooth initial condition steepens, shock formation

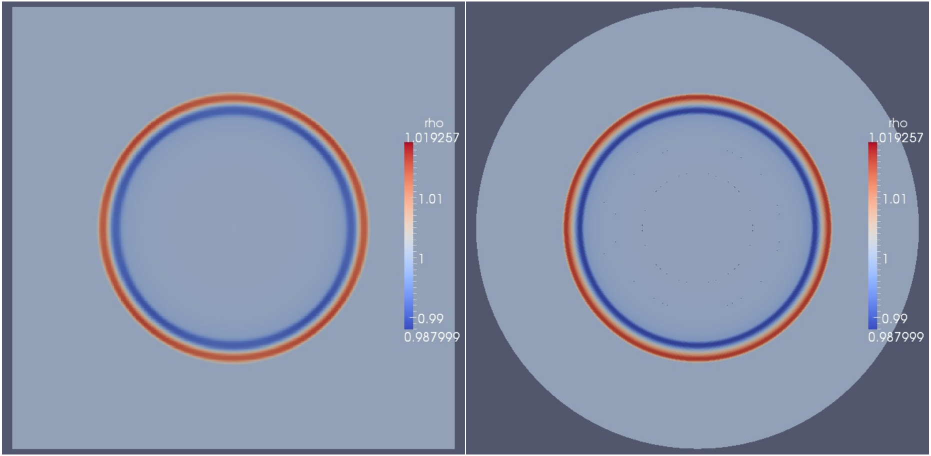
⇒ **Rankine-Hugoniot relations** explain different speeds

- **adiabatic HD** set, $\mathbf{U} = (\rho, \rho\mathbf{v})$ and $\mathbf{F} = (\rho\mathbf{v}, \rho\mathbf{v}\mathbf{v} + c_{ad}\rho^{\gamma})$
  - ⇒ parameters $c_{ad}$, $\gamma$ for **isothermal or polytropic** scenarios
- can do **dust dynamics where pressure vanishes** ($c_{ad} = 0$)
  - ⇒ ultimate challenge for grid adaptivity: $\delta$ **waves!**

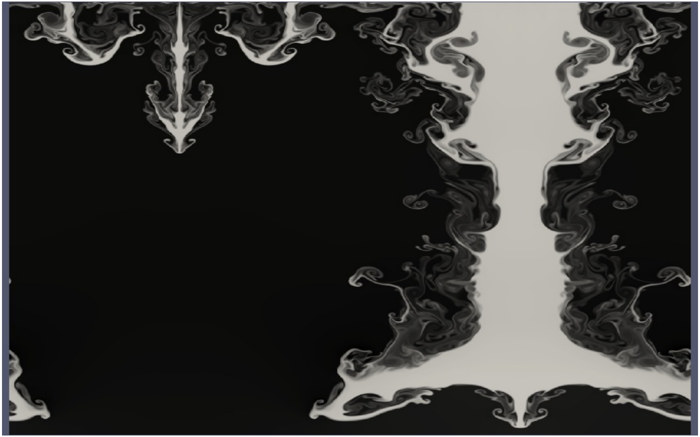



⇒ reproduces analytic result from Leveque (2004)

- adiabatic hydro encompasses 'shallow water' equations
  - $\Rightarrow$ interpret $\rho = h$ as water height, $\gamma = 2$ and gravity $g = 2\, c_{\mathrm{ad}}$
  - $\Rightarrow$ follow water waves in a square or **round pool**

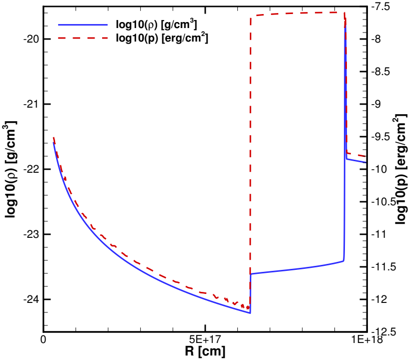


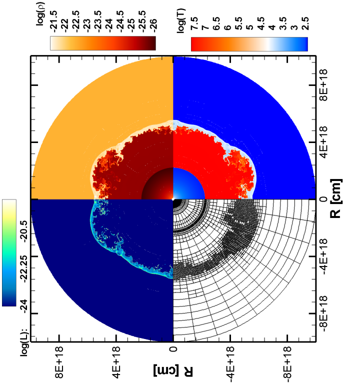
- **Euler equations**, with or without sources
  - $\Rightarrow$ external gravity (planar or point)
  - $\Rightarrow$ optically thin radiative losses (various cooling curves)
- Example with uniform gravity: **Rayleigh-Taylor evolution**



- 2D HD example useful for symmetry-preservation test
  - ⇒ **Liska test: 2D ‘shock tube’ in closed box**
- 2D HD example with spatio-temporal BC
  - ⇒ **Woodward & Collela shock reflection**
  - ⇒ (old) movie compares patch-based with hybrid block AMR

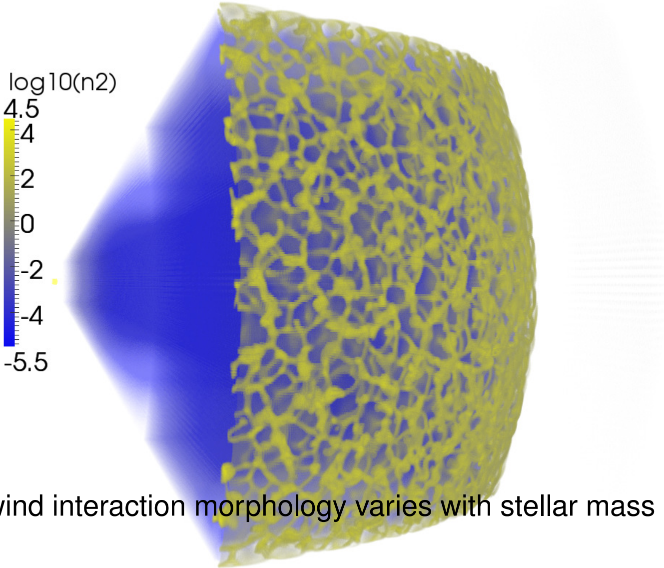
- modern applications: circumstellar environments **(van Marle et al.)**: Euler with optically thin radiative losses: 1D to 3D




- **3D hydro+radiative losses** for massive star environments
  ⇒ mass loss & wind speed change from LBV to WR stage
  ⇒ adiabatic compression at WR wind termination shock, radiative at swept up LBV matter

- thin shell instabilities shape the 3D environment: density view




⇒ wind-wind interaction morphology varies with stellar mass loss history

# Need for dust inclusion

- wind-blown bubbles: infrared observations show dust concentrations, assume stellar dust mass loss fixed fraction (promille) of gas outflow
  - $\Rightarrow$ dust distribution inversely proportional to grainsize

$$n(a) \propto a^{-3.5}$$

- Star movement through ISM creates bow shock
  - $\Rightarrow$ in free-streaming wind: dust species flowing along
  - $\Rightarrow$ between reverse shock-contact discontinuity
  - $\Rightarrow$ small grains 'trapped' [ **ApJ Letters**, 734, L26 (2011)]
  - $\Rightarrow$ **dust (small grains) versus gas evolution**
- **need equations governing gas-dust interactions!**

- discretize dust in grainsize bins $a_d \in [0.005, 0.25]\mu\mathrm{m}$
  $\Rightarrow$ solve **coupled gas-dust equations**

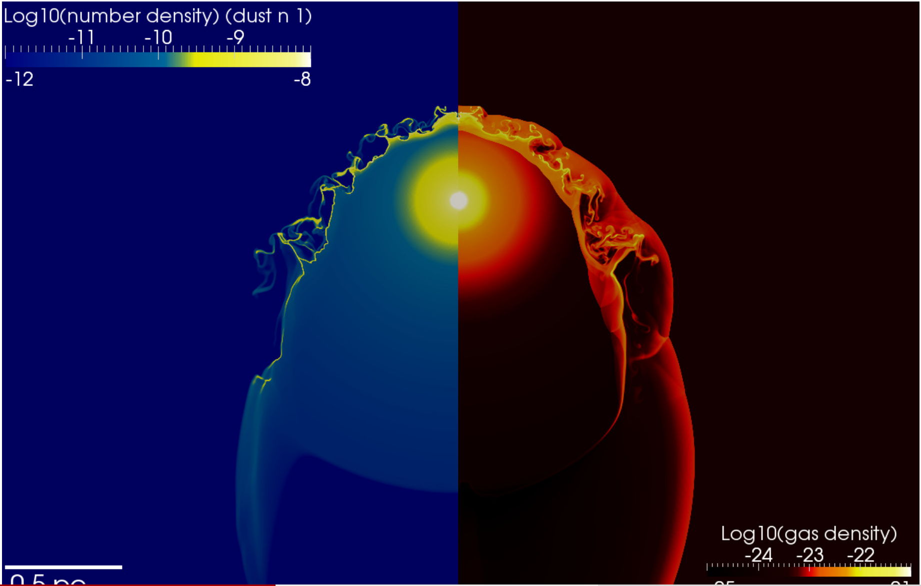
$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) &= -\nabla p + \sum_{d=1}^{n} \mathbf{f}_{\mathrm{d}} \\
\frac{\partial e}{\partial t} + \nabla \cdot \left[ (p+e)\mathbf{v} \right] &= \sum_{d=1}^{n} \mathbf{v} \cdot \mathbf{f}_{\mathrm{d}} - \frac{\rho^2}{m_{\mathrm{h}}^2} \Lambda(T)
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial \rho_{\mathrm{d}}}{\partial t} + \nabla \cdot (\rho_{\mathrm{d}} \mathbf{v}_{\mathrm{d}}) &= 0 \\
\frac{\partial (\rho_{\mathrm{d}} \mathbf{v}_{\mathrm{d}})}{\partial t} + \nabla \cdot (\rho_{\mathrm{d}} \mathbf{v}_{\mathrm{d}} \mathbf{v}_{\mathrm{d}}) &= -\mathbf{f}_{\mathrm{d}}
\end{aligned}
$$

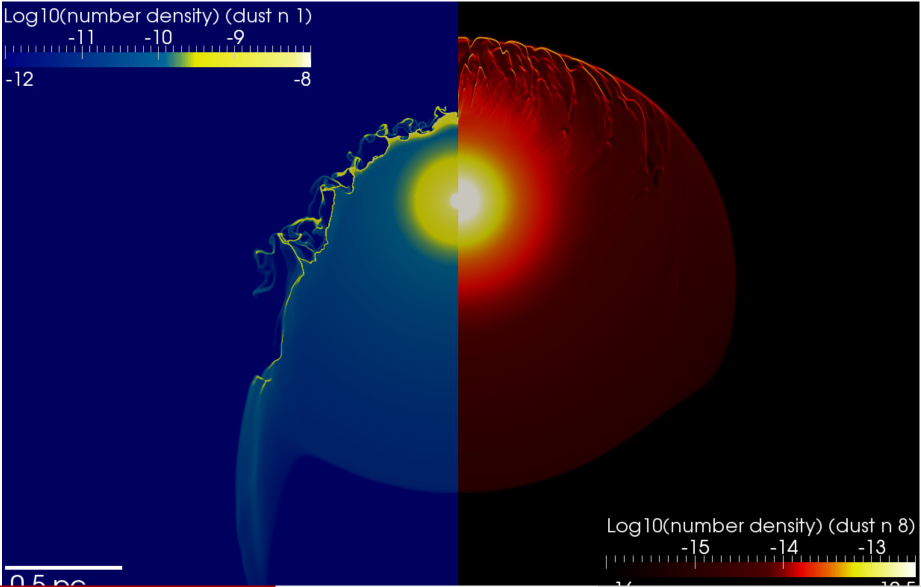
  $\Rightarrow$ **drag combines Epstein/Stokes** (sub/supersonic) regime

$$
\mathbf{f}_{\mathrm{d}} = -(1-\alpha)\pi n_{\mathrm{d}} \rho a_{\mathrm{d}}^2 (\mathbf{v} - \mathbf{v}_{\mathrm{d}}) \sqrt{(\mathbf{v} - \mathbf{v}_{\mathrm{d}})^2 + v_{\mathrm{t}}^2}
$$

- when simulating up to 10 dust species (note: **34 PDEs in 2D**)
  - ⇒ small grains pile up at wind-ISM transition (CD)



- largest dust grains: can move ahead of forward shock!
  - ⇒ less influence from hydrodynamic instabilities



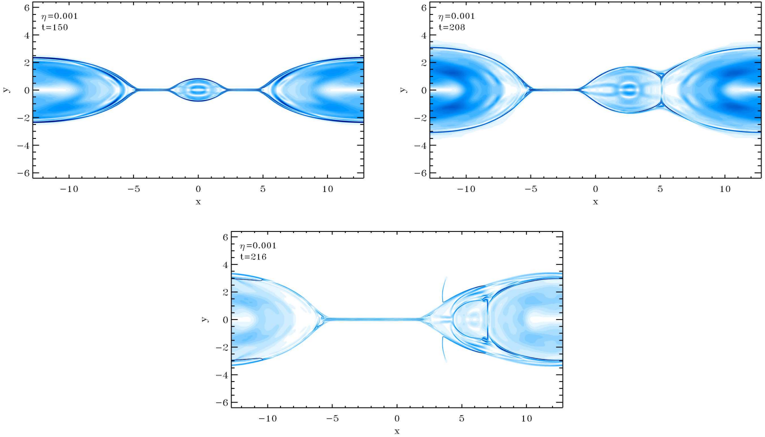
- **Ideal and resistive MHD**, with or without sources
  - $\Rightarrow$ external gravity; optically thin radiative losses
- ideal MHD and conservation laws for density $\rho$, momentum density $\mathbf{m} = \rho\mathbf{v}$, $\mathcal{H}$ and $\mathbf{B}$ ($+$ sink/source terms)

$$\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v}\rho) &= S_\rho \\
\frac{\partial \mathbf{m}}{\partial t} + \nabla \cdot (\mathbf{v}\rho\mathbf{v} - \mathbf{B}\mathbf{B}) + \nabla p_{tot} &= \mathbf{S}_{\rho v} \\
\frac{\partial \mathcal{H}}{\partial t} + \nabla \cdot (\mathbf{v}\mathcal{H} + \mathbf{v}p_{tot} - \mathbf{B}\mathbf{B}\cdot\mathbf{v}) &= S_e \\
\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v}) &= \mathbf{S}_B
\end{aligned}$$

- $p_{tot} \equiv$ thermal pressure + magnetic pressure
- total energy density $\mathcal{H}$ has 3 contributions

$$\mathcal{H} = \underbrace{\frac{p}{\gamma - 1}}_{\text{internal}} + \underbrace{\frac{\rho v^2}{2}}_{\text{kinetic}} + \underbrace{\frac{1}{2}B^2}_{\text{magnetic}}$$

- many standard (shock-governed) tests, different strategies for $\nabla \cdot \mathbf{B} = 0$, splitting off strong background fields, ...




$\Rightarrow$ 2D resistive MHD, GEM Challenge, $\eta = 0.001$ case

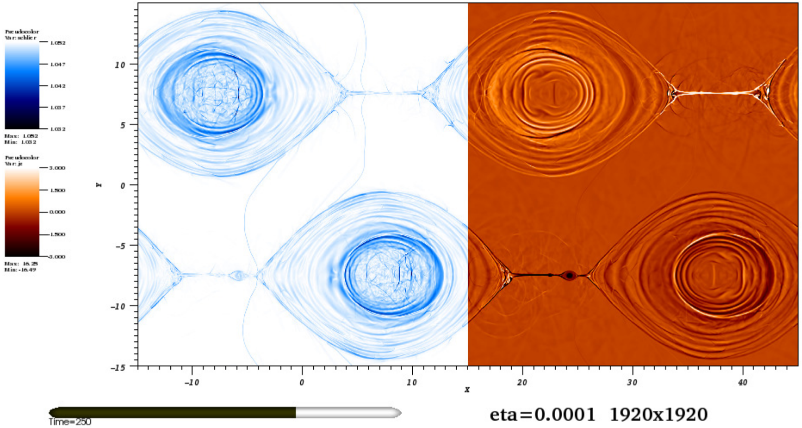
# Reconnection benchmark test

- resistive MHD code comparison on 2D GEM variant
  - ⇒ **Keppens et al, PoP 20, 092109 (2013)**
  - ⇒ double periodic setup on square $[-15, 15]^2$
  - ⇒ lower/upper current layer

$$B_x(y) = B_0 \left[-1 + \tanh\left(y - y_{\mathrm{low}}\right) + \tanh\left(y_{\mathrm{up}} - y\right)\right]$$

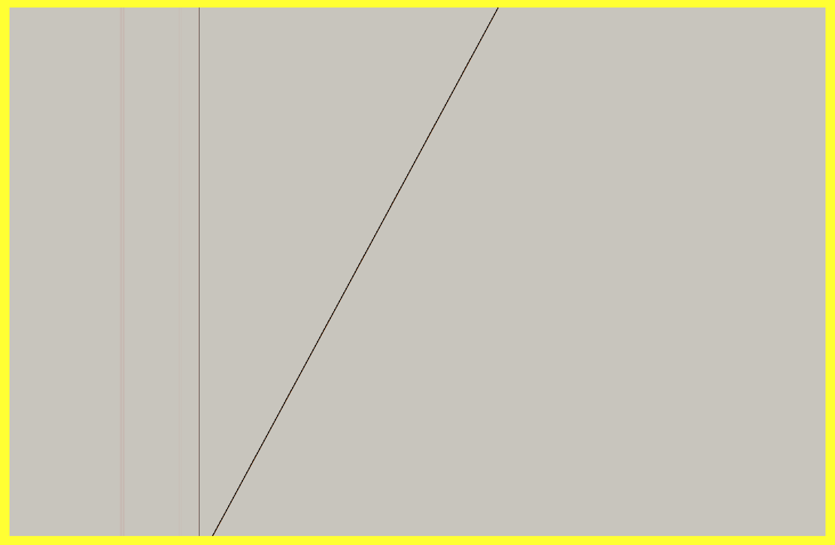
  - ⇒ deterministic perturbation, 10% amplitude (non-linear!)
  - ⇒ compared finite volume, difference and PIC-type (visco-)resistive MHD evolutions
- **resolving long-term, chaotic dynamics** for lower $\eta$

- magnetic↔internal through compressive interactions
  - $\Rightarrow$ **evolution for $\eta = 0.0001$**

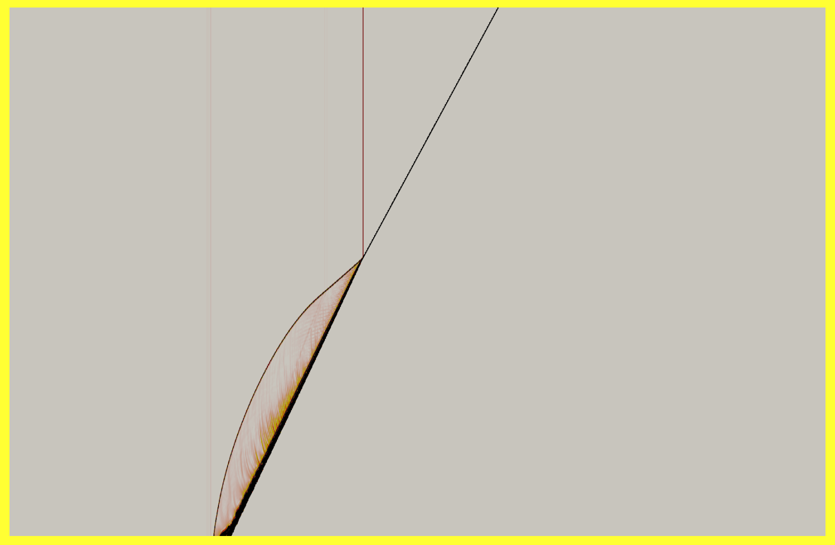


- **Special relativistic HD and MHD**
- extreme contrasts, positive $p, \rho, \tau$, $v < 1$, $\Gamma \geq 1$, solenoidal **B**
  - $\Rightarrow$ stringent demands on numerics and accuracy: **AMR vital**
  - $\Rightarrow$ **different EOS implemented for relativistic modules**
- Relativistic hydro refraction
  - $\Rightarrow$ 7 levels, effective $1536 \times 7680$ in day(s) on local desktop!

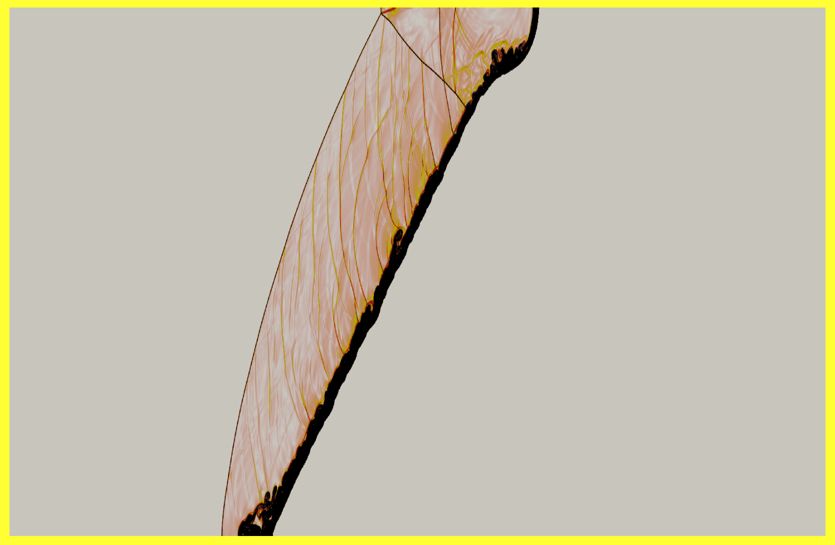
# Relativistic hydro refraction $t = 0.5$



# Relativistic hydro refraction $t = 1$



# Relativistic hydro refraction $t = 2$

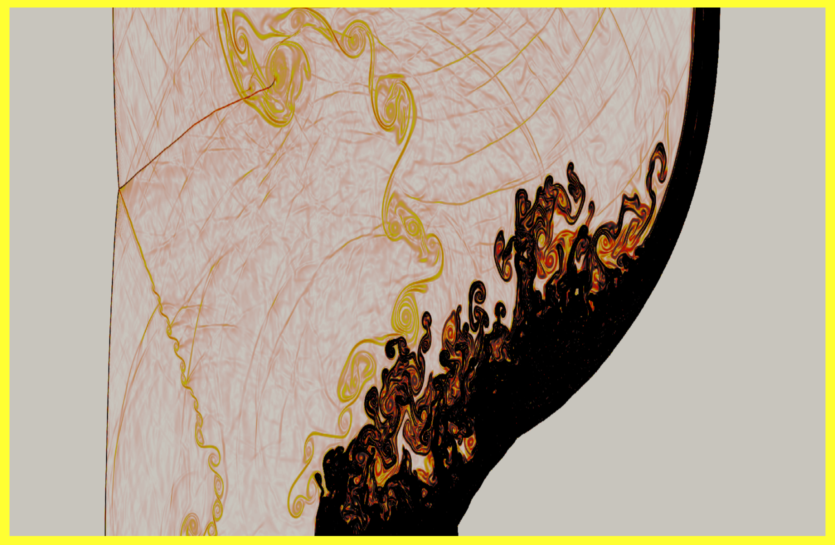


# Relativistic hydro refraction $t = 3$

# Relativistic hydro refraction $t = 4$

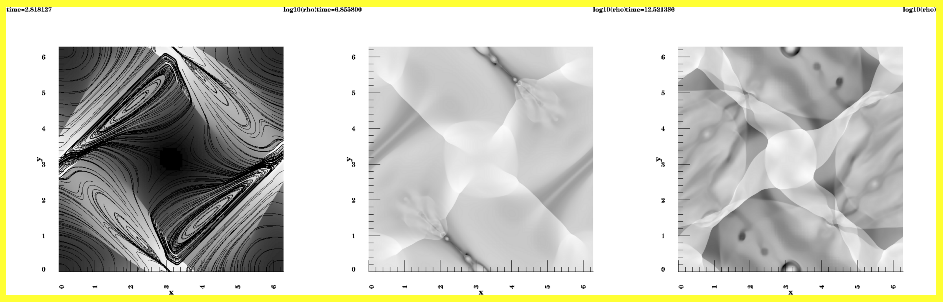
# Relativistic hydro refraction $t = 5$

# Relativistic hydro refraction $t = 6$



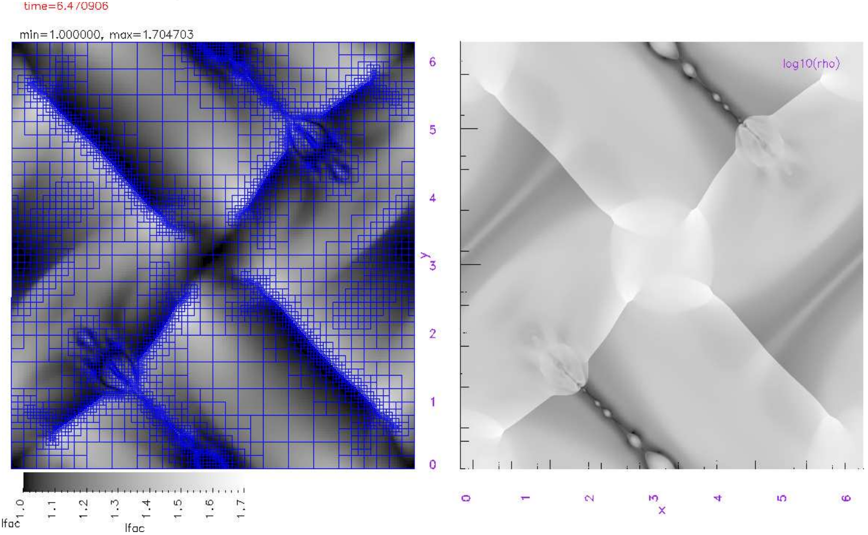
# RMHD Orszag-Tang test

- relativistic analogue of 2D MHD Orszag-Tang test
  - ⇒ double periodic, supersonic relativistic vortex rotation
  - ⇒ initial field configuration: double island structure

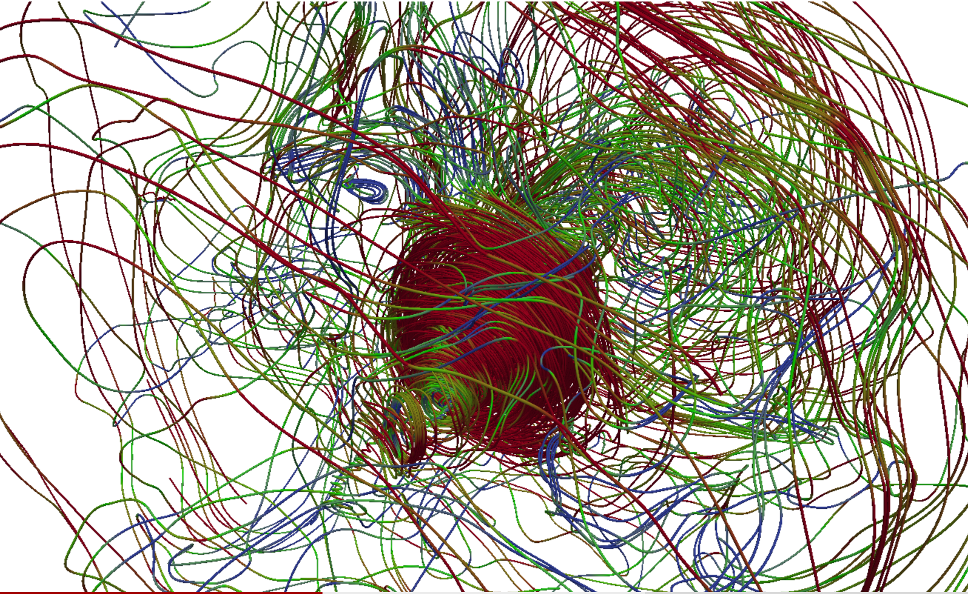



⇒ **current sheets form, shock interactions, reconnections**

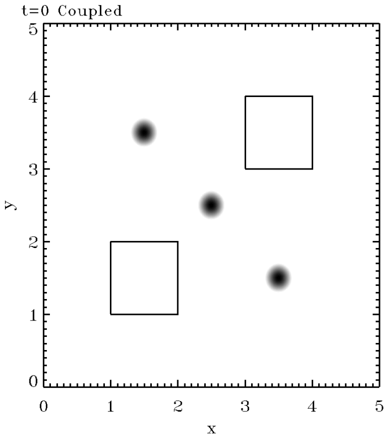
- AMR captures small-scale reconnection effects



# 3D (special) relativistic MHD simulations of Crab nebula (Porth et al 2013, 2014) [active-passive grids!]

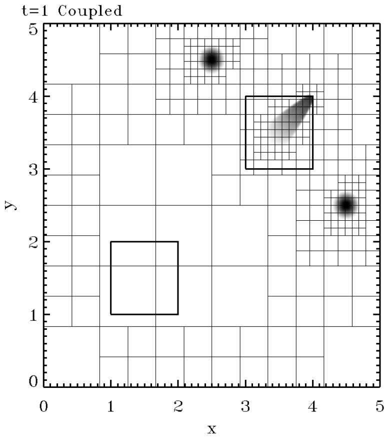


- **Force-free electrodynamics**: Maxwell's equations with Ohm's law: tomorrow's talk by Oliver Porth (and hands-on session 4)
- **coupled physics: nonlinear+rho**: 2D advection on square, with embedded Burgers (UR) and nonconvex region (LL)



# Boundary coupling:multi-D

- 2D advection on square, with embedded Burgers (UR) and nonconvex region (LL)



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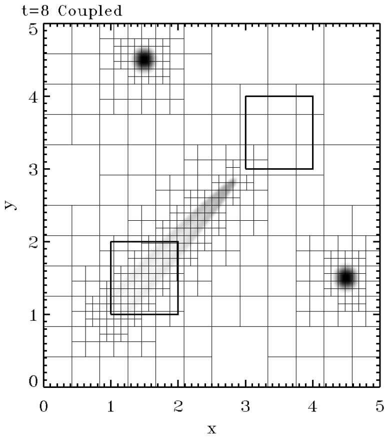

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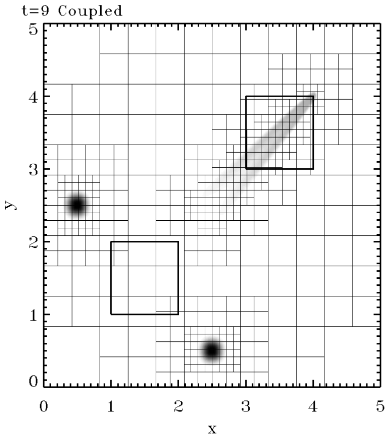
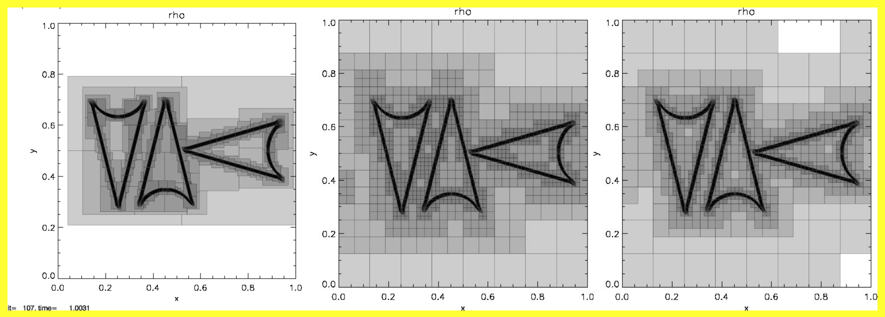


# Patch, block, hybrid block AMR

- 3 approaches to nested grids




⇒ **patch (left)**, **quadtree**, **hybrid block-based (right)**

⇒ **233 sec**; **196 sec**; **159 sec**

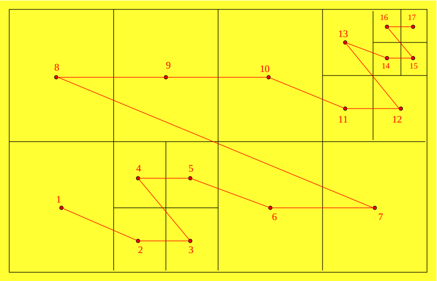
⇒ van der Holst & Keppens, JCP 2007, **226**, 925

- Current `MPI-AMRVAC` only pure block-based (quadtree/octree)

⇒ easier parallelization: Keppens et al., JCP 2012, **231**, 718

# Quadtree-Octree AMR

- example 2D domain covered by $8 = 4 \times 2$ base level grid blocks
  - $\Rightarrow$ **hierarchically nested** AMR levels, **proper nesting**
  - $\Rightarrow$ fixed **factor** 2 **refinement**




- **Space-filling Morton** ($Z$-order) **curve**
  - $\Rightarrow$ for $N_{block} = 17$ grid blocks
  - $\Rightarrow$ load-balancing: $N_p$ CPUs each $N_{block}/N_p$ 'adjacent' blocks
  - $\Rightarrow$ **every $k$-th timestep: full grid-tree re-evaluated**

# Quadtree-Octree AMR

- Octree (3D) or Quadtree (2D) AMR
  - $\Rightarrow$ use **blocks of user-set size (at compile) divide domain**
  - $\Rightarrow$ use **same CFL-limited $\Delta t$ for all grids**
- parallelization using MPI
  - $\Rightarrow$ 1 AMR level = Domain Decomposition strategy

# Generic AMR code skeleton

```
timeloop : do
  exit time loop by user-defined criteria
  compute timestep constraint for all grids
  conditionally save data
  advance all grids for one time step dt
      distinguish source and flux addition strategies
          select numerical scheme, geometric sources, ...
          collect fluxes at fine-coarse boundaries
      after every parallel update of grids on all processors
          fill all ghost cells for all grid blocks
      at final temporal update, fix for conservation
  regrid
      Quantify the error estimator on all grids
      Create new grid structure, ensure proper nesting
      Load balance the new grid structure
  update time counters
end do timeloop
```

# AMR criteria

- automated block-based regridding procedure: 3 steps
  - ⇒ consider all blocks at level $1 < l < l_{\mathrm{max}}$
  - ⇒ quantify **local error $\mathcal{E}_i$ at each gridpoint $\mathbf{x}_i$** in a grid block
  - ⇒ if **ANY point has $\mathcal{E}_i > \mathrm{Tol}^l$ refine** block (ensure nesting)
  - ⇒ if **ALL points have $\mathcal{E}_i \leq f^l_{\mathrm{Tol}}\mathrm{Tol}^l$ coarsen** block
- involves (user) parameters:
  - ⇒ **coarsen fraction $f^l_{\mathrm{Tol}}$ per level**
  - ⇒ **error tolerance per level $\mathrm{Tol}^l$** [for Löhner $\mathcal{O}(0.1)$, smaller for Richardson/Local]

# Error estimation

- choice between **3 different local error $\mathcal{E}_i$ estimators**

  $\Rightarrow$ **Richardson-based**: quantify error at $t^{n+1}$, use $w^{n-1}$, $w^n$

  $\Rightarrow$ **local comparison** between $w^{n-1}$, $w^n$

  $\Rightarrow$ **Löhner (& FLASH3) estimator**: use $w^n$, normalized 2nd derivatives [used typically for all our applications]
- all use user-selection of (conserved or auxiliary) variables

$$\mathcal{E}_i = \sum_{\mathrm{iw}} \sigma_{\mathrm{iw}} \mathcal{E}_{iw}^{\mathrm{Rel}}$$

  $\Rightarrow$ local relative variable errors $\mathcal{E}_{iw}^{\mathrm{Rel}}$

  $\Rightarrow$ weights obey $\sum_{\mathrm{iw}} \sigma_{\mathrm{iw}} = 1$
- all estimators augmented with **user-coded (de)refinement**

# Löhner estimator I

- Löhner (1987) as adjusted in PARAMESH & FLASH3
  - $\Rightarrow$ instantaneous $w^n$
  - $\Rightarrow$ **quantifies normalized 2nd derivatives**
  - $\Rightarrow$ local relative variable errors $\mathcal{E}_{iw}^{\mathrm{Rel}}$ from

$$\mathcal{E}_{iw}^{\mathrm{Rel}} = \sqrt{\frac{N_{\mathrm{iw}}}{\max\left(D_{\mathrm{iw}}, \epsilon\right)}}$$

$\Rightarrow$ numerator $N_{\mathrm{iw}} = \sum_{i_1} \sum_{i_2} \left[\Delta_{i_1}(\Delta_{i_2} w_{\mathrm{iw}})\right]^2$, denominator

$$D_{\mathrm{iw}} = \sum_{i_1} \sum_{i_2} \left[ \mid L_{i_1} w_{\mathrm{iw}} \mid + \mid R_{i_1} w_{\mathrm{iw}} \mid + f^I S_{i_2} (S_{i_1} \mid w_{\mathrm{iw}} \mid) \right]^2$$

$\Rightarrow$ discrete **central, left and right shifts $\Delta_i$, $L_i$, $R_i$, sum** operator $S_i$ for direction $i$

# Löhner estimator II

- estimator quantifies weighted 2nd derivative in **grid point** $i$ as in

$$\left\{ \frac{\sum_{i_1} \sum_{i_2} \left( \Delta x_{i_1} \Delta x_{i_2} \frac{\partial^2 w}{\partial x_{i_1} \partial x_{i_2}}\Big|_{\mathbf{i}} \right)^2}{\sum_{i_1} \sum_{i_2} \left[ \left| \Delta x_{i_1} \frac{\partial w}{\partial x_{i_1}}\Big|_{\mathbf{i-1}} \right| + \left| \Delta x_{i_1} \frac{\partial w}{\partial x_{i_1}}\Big|_{\mathbf{i+1}} \right| + \mathbf{f^l} \left| \mathbf{w^m} \right| \right]^2} \right\}^{\frac{1}{2}}$$

- (level dependent) **‘wavefilter’ parameter** $f^l$, order $10^{-2}$
  $\Rightarrow$ can also use logarithm for (positive) variables

# Parallel I/O

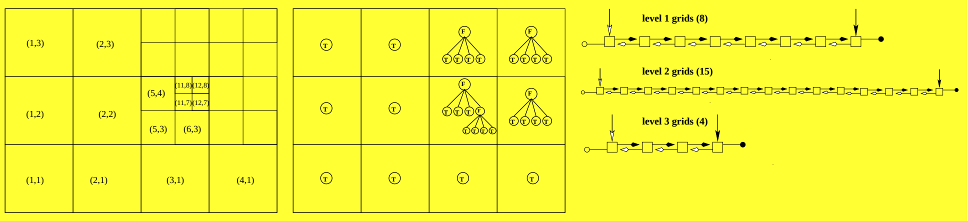
- using full MPI-2 functionality

  ⇒ all **processors write simultaneously to single file**, with MPI_FILE_IWRITE_AT constructions, and offset from Morton-ordered space filling curve
- pure master-slave data file dump option as well
- Files in *.dat format used for restarts

  ⇒ can increase AMR levels, change HPC platform/desktop
- postprocess or on-the-fly **conversions to unstructured** VTK **format, for use with** Paraview **or** Visit**, or data formats native to** Idl**,** Tecplot **or** OpenDX

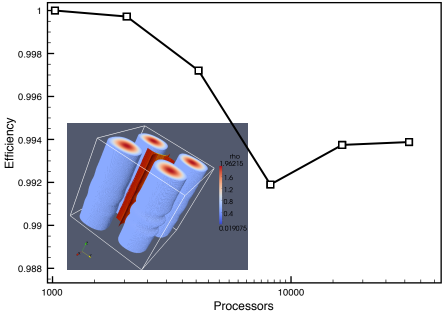
# Data structures

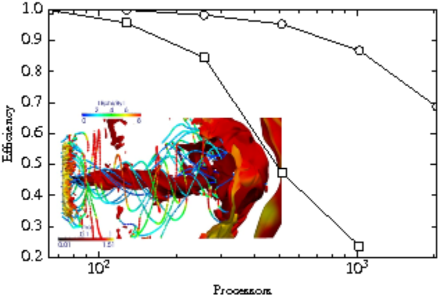
- grid blocks indexed in variety of ways
  - ⇒ **global grid indices**, identifying block location
  - ⇒ **boolean tree**, identifying block presence/absence
  - ⇒ **linked list**, with pointers to same grid level blocks




  - ⇒ Morton ordered space curve index

- weak/strong scaling, with(out) AMR, several 1000-10000 CPUs
  ⇒ see **Porth et al, 2014, ApJS, 214, 4**



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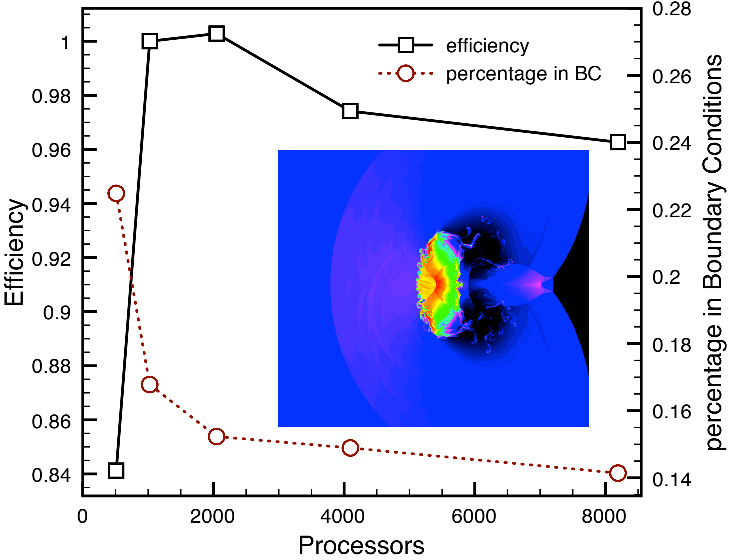
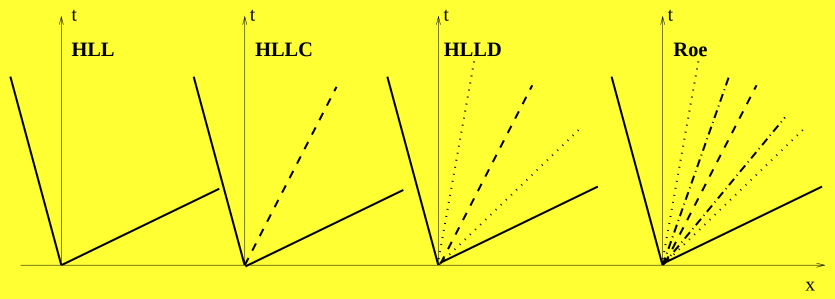


# Discretizations

- emphasis **shock-capturing schemes, finite volume approach**

  $\Rightarrow$ from TVDLF (readily used for any system) to successively more advanced schemes, incorporating better approximations to the local Riemann fans at cell interfaces

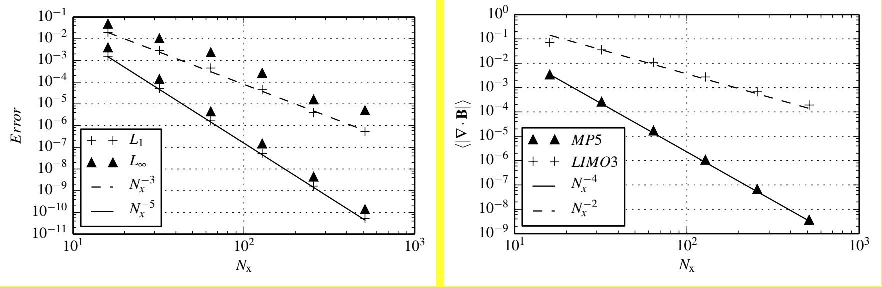



- limited linear reconstruction (2nd to 3d order); PPM (parabolic)

  $\Rightarrow$ **different discretization possible per grid level!**

- Convergence for **3D MHD circularly polarized Alfvén wave**

  ⇒ high order **conservative Finite Differences** (Porth et al ApJS 2014) & **Strong Stability Preserving Runge-Kutta** steppers (CFL $> 1$!)




⇒ RK3 + 3d order limiter: third order, SSPRK with MP5 limiter: even 5th order! [right: 2nd & 4th on $\nabla \cdot \mathbf{B} = 0$]

# Boundary conditions

- (stencil-dependent number of) **ghost cell** layers

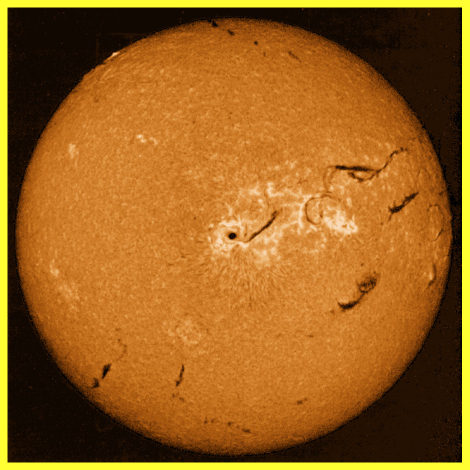
  $\Rightarrow$ physical domain boundaries: user set or preselect

  - (a)symmetry for reflective walls;
  - continuous extrapolation for open boundaries;
  - limited inflow conditions, allowing turbulent flow structures to cross boundaries unhampered;
  - periodic boundaries;
  - $\pi$-periodicity at 'poles' (cylindrical/spherical)

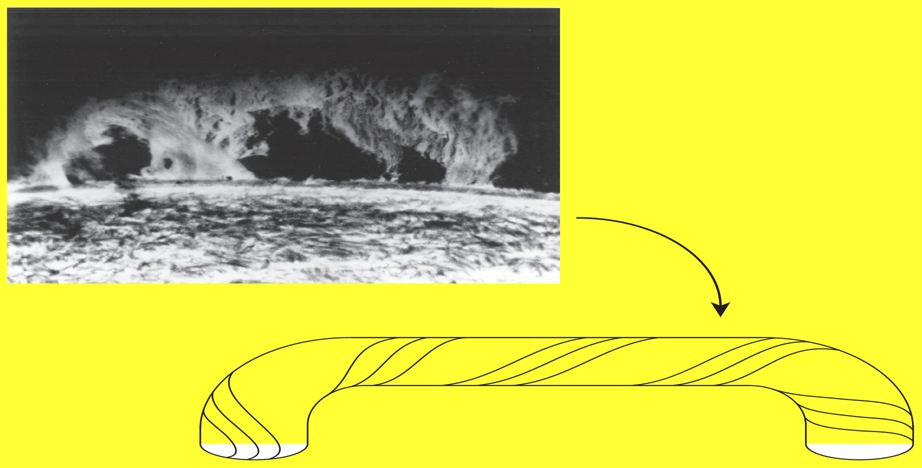
- user can **set spatio-temporally varying combinations of primitive/conservative variables in boundary regions**

# Solar filaments

- solar atmosphere: $T$ from several 1000 to million K corona
- View sun in selected spectral lines: sample different heights
- **H$\alpha$ image at 6563 Å:**
  - solar chromosphere
  - bright active regions
  - dark filaments (on disk) $\equiv$ prominences (at limb)



- Prominences **suspended magnetically against gravity**
  - up in corona, 100 denser, cooler than surroundings
  - 200 Mm long, 50 Mm high, 6 Mm wide
  - ‘quiescent prominences’ live months: **stable equilibria!**



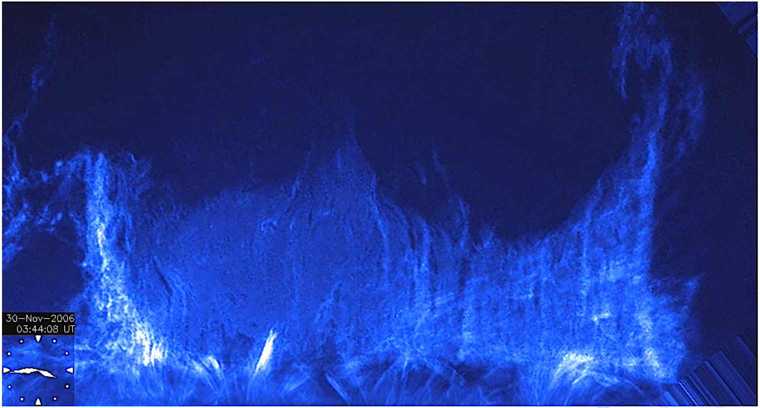
# Hinode prominence views

- contemporary high resolution observations (Hinode)

  http://solarb.msfc.nasa.gov

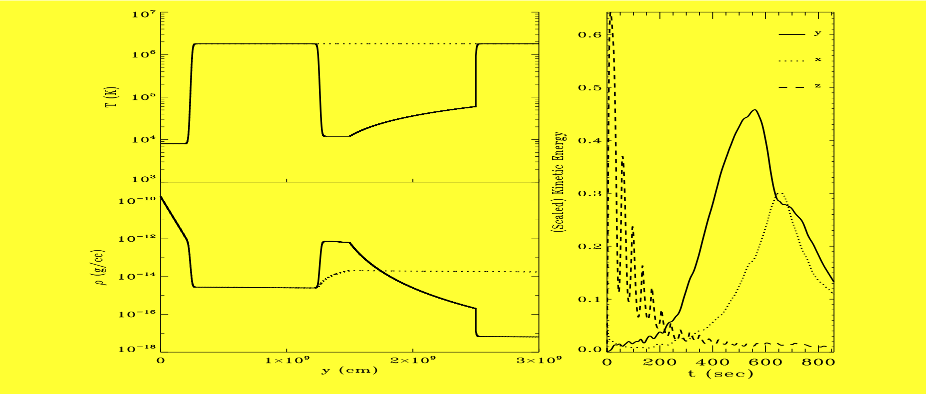
  ⇒ **lots of turbulent upflows**

  ⇒ from Berger et al., ApJ 2010, 716, 1288



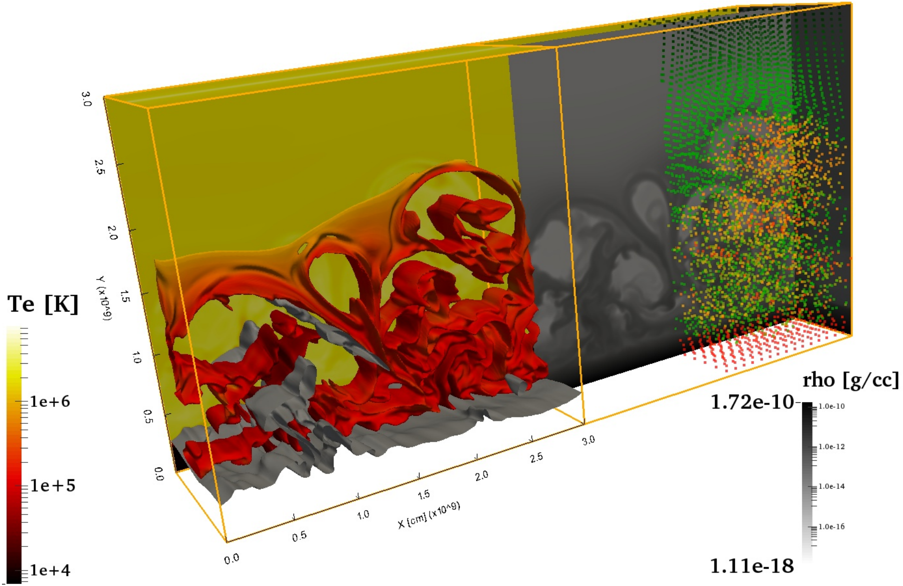
# Rayleigh-Taylor in prominences

- Keppens et al. 2015: 3D MHD in chromosphere-to-corona
  - $\Rightarrow$ initial $T - \rho$ variation [left], kinetic energy evolution [right]

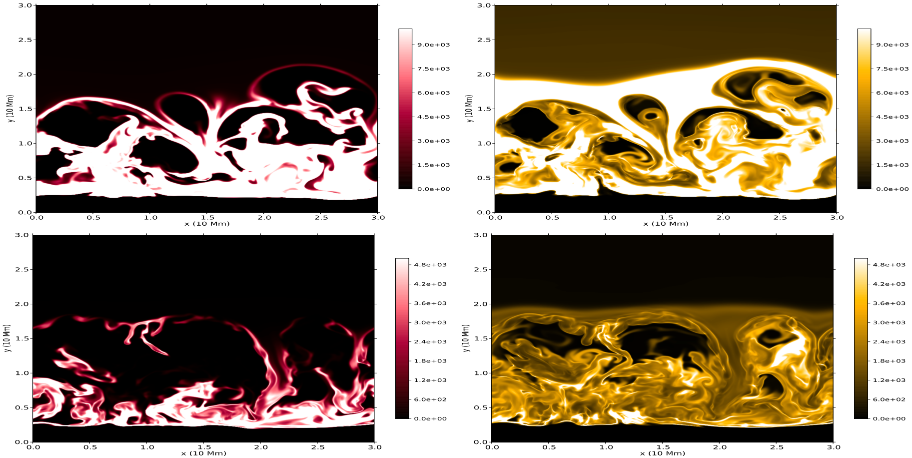



$\Rightarrow$ vertical force-balanced prominence in $30 \times 30 \times 14\,\mathrm{Mm}^3$, with AMR up to $600 \times 600 \times 280$ resolution, follow for $\pm 15$ minutes

# Rayleigh-Taylor dynamics in quiescent prominences



- **7 min virtual SDO/AIA view**




- 20 Gauss (top) to 8 Gauss (bottom), at 304 (left) to 171 (right)
  $\Rightarrow$ complex multi-temperature up-down motions, KH effects

# Summary

- MPI-AMRVAC open-source effort
  - ⇒ extended with particle treatments in MHD fields [Porth]
- MHD description for solar prominence configurations
  - ⇒ formation of prominences from first principles [Xia et al.]
- simulations of further nonlinear dynamics
  - ⇒ modern **High Performance Computing** challenges

# Summary

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# CSAM 2015 and MPI-AMRVAC

- developer **Chun Xia**: modern solar physics applications

  $\Rightarrow$ emphasis on (Newtonian) MHD with thermal conduction, optically thin radiative losses, parametrized heating, applications to solar filaments/prominences
- **Stefaan Poedts**: space weather type simulations (Coronal Mass Ejections, initiation and interplanetary propagation)
- developer **Oliver Porth**: applications with particle treatments [e.g. accelerations in electromagnetic field evolutions]

- Hands-on sessions: `$AMRVAC_DIR/tests/CSAM2015`

  ⇒ **test suite for hydro to MHD** [jet-cloud interactions, dusty Richtmyer-Meshkov, circumstellar wind bubbles, Orszag-Tang, double GEM]

  ⇒ **Rayleigh-Taylor in prominences** [ideal MHD setup]

  ⇒ using **MPI-AMRVAC for magnetic field extrapolations** [LFFF, PFSS] from local to global magnetograms

  ⇒ example **applications with particle treatments** [tilt-kink evolutions, electrodynamics]

- `when used for follow-up research, please contact (and acknowledge) us!!! [rony.keppens@wis.kuleuven.be]`