MHD in AthenaK

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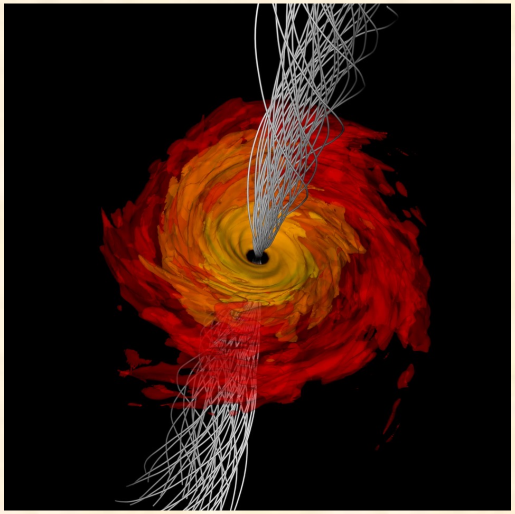
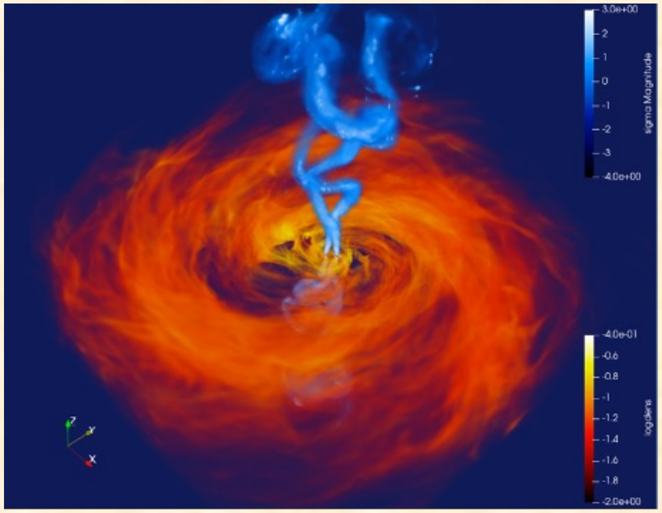
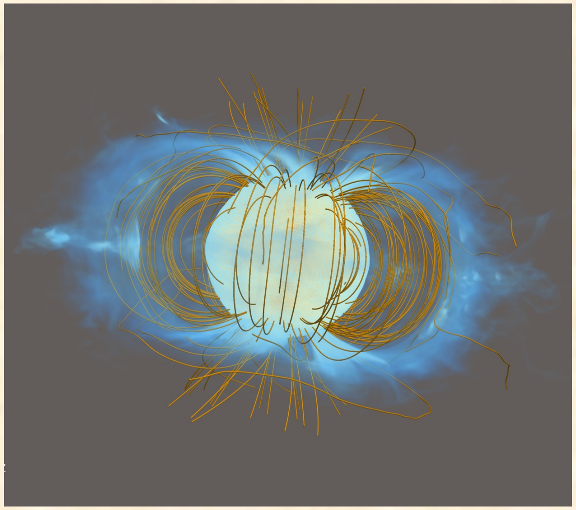






Three lectures on AthenaK

1. Introduction to AthenaK
2. MHD Algorithms
3. Black hole accretion disks

Lecture 2: MHD Algorithms

1. Introduction to MHD
2. Numerical Methods: Finite Volumes
3. Test Problems
4. Adding explicit diffusion
5. Running MHD with AthenaK

Start with the equations of compressible viscous and resistive non-relativistic MHD:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot [\rho \mathbf{v}] = 0$$

$$\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot [\rho \mathbf{v}\mathbf{v} - \mathbf{B}\mathbf{B} + \mathsf{P}^* + \Pi] = 0$$

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + P^*)\mathbf{v} - \mathbf{B}\,(\mathbf{B}\cdot\mathbf{v}) + \Pi \cdot \mathbf{v} + \eta \mathbf{J} \times \mathbf{B}] = 0$$

$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B}) - \eta \mathbf{J} = 0$$

$$P^* = P + \frac{\mathbf{B}\cdot\mathbf{B}}{2}$$

$$E = P/(\gamma - 1) + \frac{\rho(\mathbf{v}\cdot\mathbf{v})}{2} + \frac{\mathbf{B}\cdot\mathbf{B}}{2}$$

$$\Pi_{ij} = \rho\nu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_j} - \frac{2}{3}\delta_{ij} \nabla \cdot \mathbf{v} \right)$$

Also need an equation of state P = P(ρ,T). Usually adopt the ideal gas law $\boxed{P=nkT}$ or $\boxed{P = (\gamma\text{-}1)e}$ where for monoatomic gas (H), $\gamma=5/3$

Equations in SR/GR have similar form: $\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = 0,$

Linear Waves

The MHD equations are a set of hyperbolic conservation laws.

An important characteristic of hyperbolic PDEs is they admit wave-like solutions of the form:

$$a = a_0 + \delta a = a_0 + a_1 \exp(i\mathbf{k} \cdot \mathbf{x} - i\omega t)$$

Where a_0 = constant and $a_1/a_0 << 1$. That is, small amplitude perturbations propagate as waves.

To see this:

- Substitute this form of solution into MHD equations
- Drop terms quadratic in δa

Write resulting system of linear equations for perturbations $\mathbf{W} = \delta a_i$ as

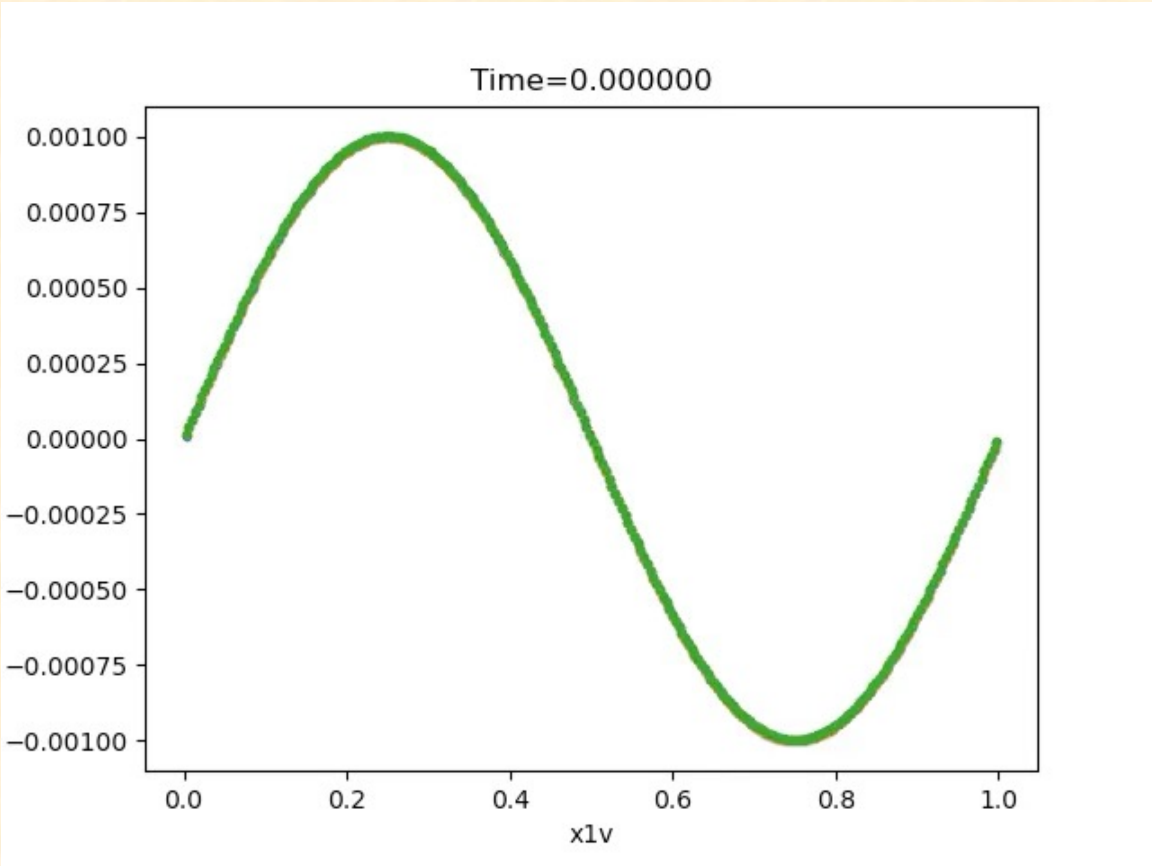
$$\frac{\partial \mathbf{W_1}}{\partial t} + \mathsf{A}(\mathbf{W_0}) \frac{\partial \mathbf{W_1}}{\partial x} = 0$$

Each of the eigenvalues and eigenvectors of A correspond to different wave modes in the system, with the eigenvalues given by the characteristic equation (dispersion relation) equal to the phase velocity.

Pure hydrodynamics (no magnetic field) modes are:

- sound waves propagating at (v_0 +/- C_s)
- entropy mode propagating at v_0

ρ, P, v in propagating sound wave



(numerical solution computed AthenaK)

Dispersion relation for MHD waves.

Dispersion relation for ideal MHD waves is much more complicated:

$$[\omega^2 - (\mathbf{k}\cdot\mathbf{v}_A)^2][\omega^4 - \omega^2 k^2 (v_A^2 + C^2) + k^2 C^2 (\mathbf{k}\cdot\mathbf{v}_A)^2] = 0$$

Where $\mathbf{v}_A = \frac{\mathbf{B}}{\sqrt{4\pi\rho}}$ is the Alfven speed

$C^2 = \gamma P_0/\rho_0$ is the sound speed

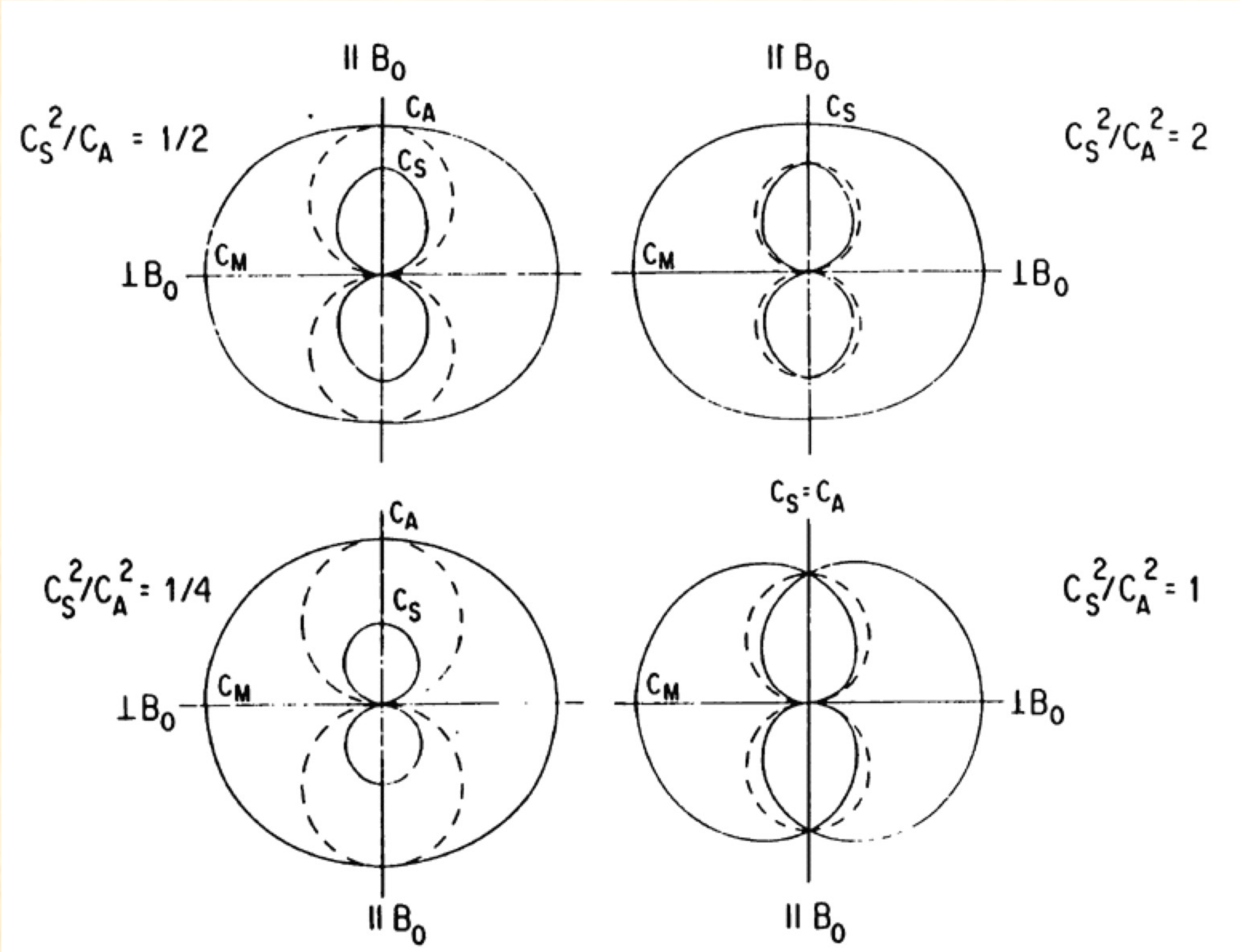
In MHD there are three wave families (in addition to the entropy mode). Note there is only one in hydrodynamics!:

1) Alfven wave propagates at V_A

2) and 3) Fast and slow magnetosonic waves propagating at $C_{f,s}$

$$C_{f,s}^2 = \frac{1}{2}\left([C^2 + v_A^2] \pm \sqrt{[C^2 + v_A^2]^2 - 4C^2 v_{Ax}^2}\right)$$

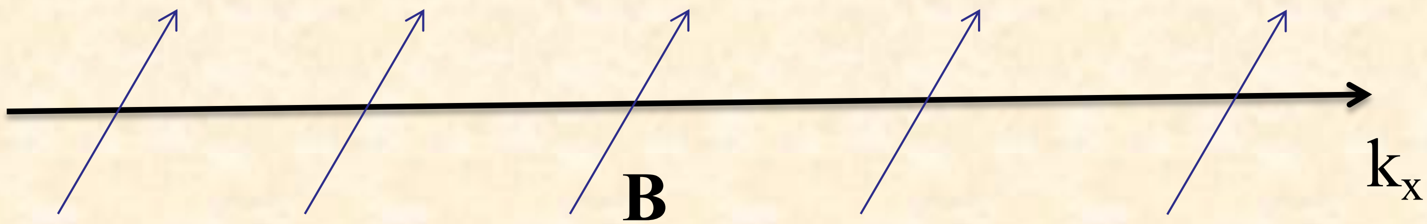
Phase velocities of MHD waves: Friedrichs diagrams.



Note for in some cases, modes are degenerate. Eigenvalues of linearized MHD equations are not always linearly independent. MHD equations are not *strictly hyperbolic*.

Examples of MHD waves

Consider a 1D domain with $\rho = 1$, $P = 1/\gamma$, $B_x = 1$, $B_\perp = 1.5$



Then $C^2 = \gamma P/\rho = 1$

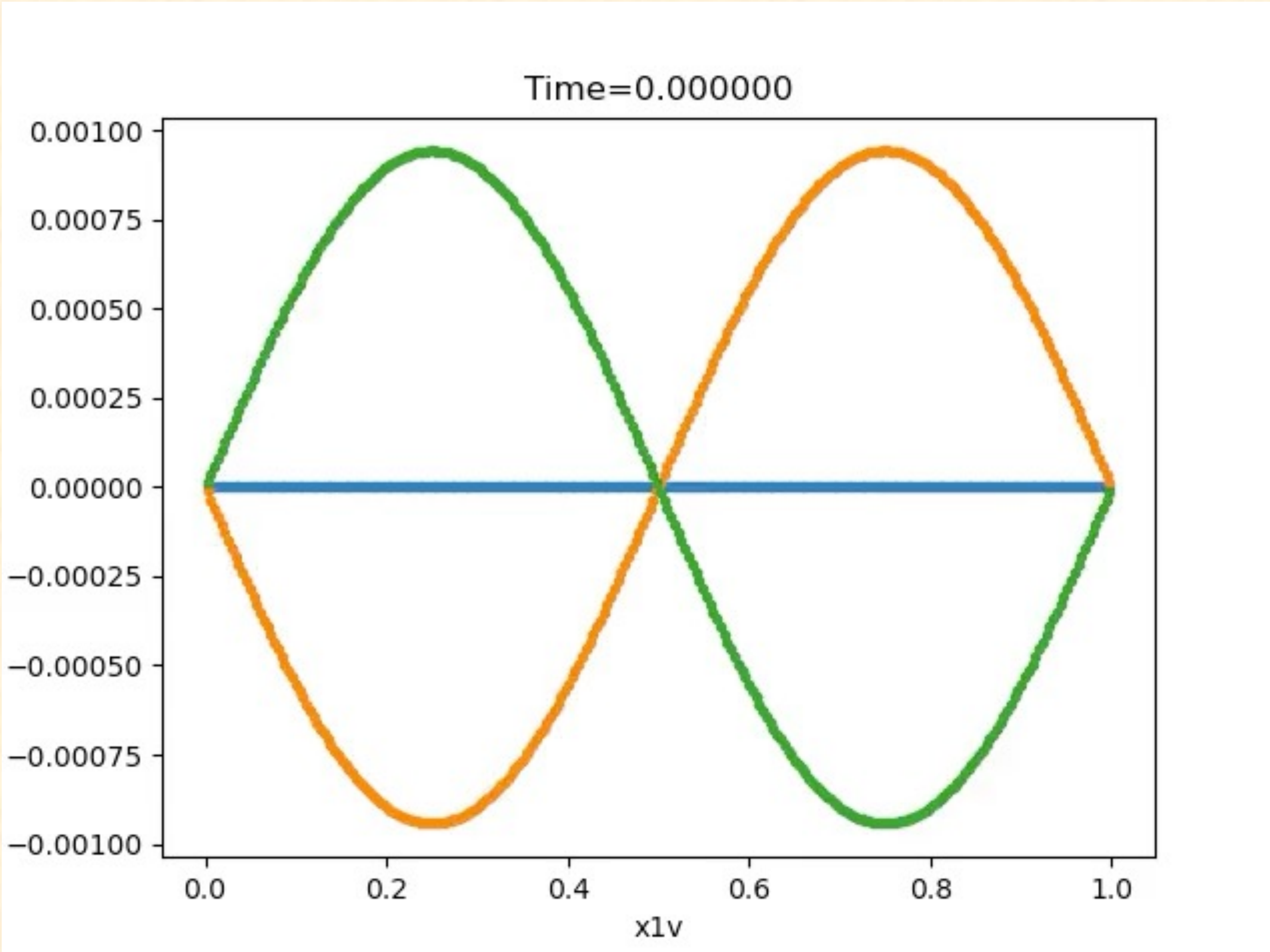
$V_{A,x}{}^2 = B^2/\rho = 1$

$C_f{}^2 = 2$

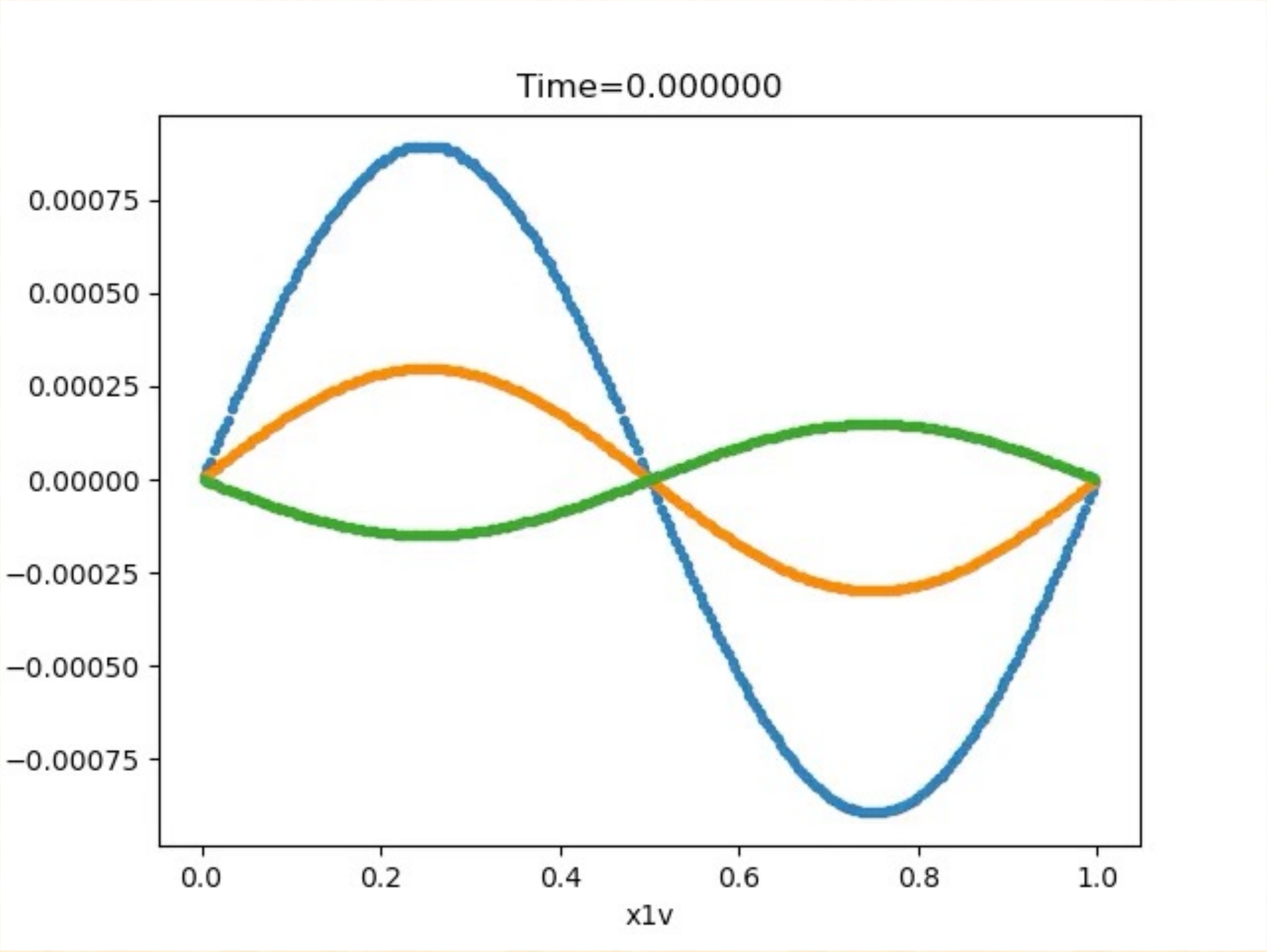
$C_s{}^2 = 1/2$

$\tan(\theta) = 3/2$, $\theta = 56^o$

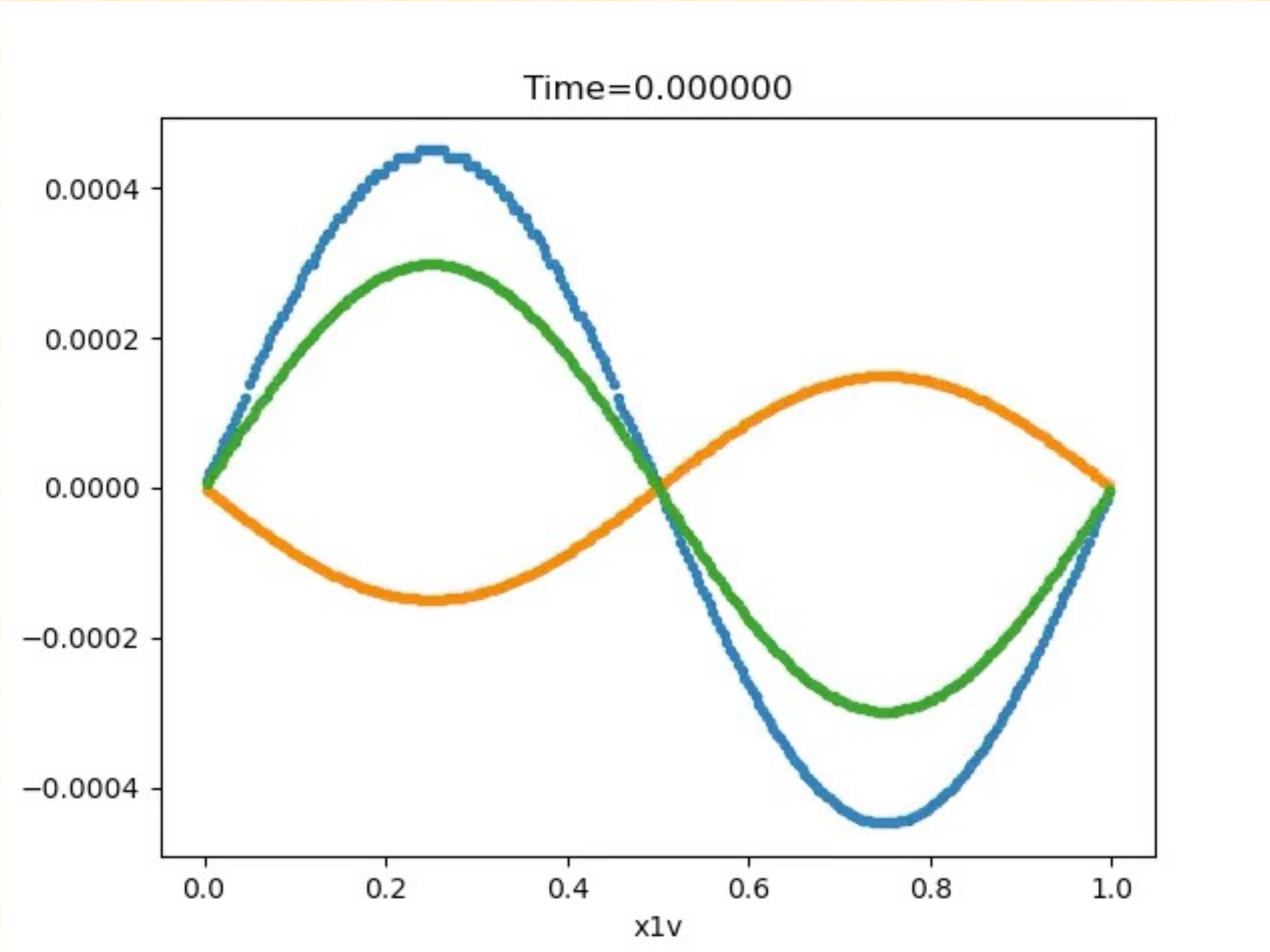
ρ (blue), $B_\perp$(green), $v_\perp$(orange) in propagating Alfven wave



ρ (blue), $B_\perp$(green), $v_\perp$(orange) in propagating slow magnetosonic wave



ρ (blue), $B_{\perp}$(green), $v_{\perp}$(orange) in propagating fast magnetosonic wave



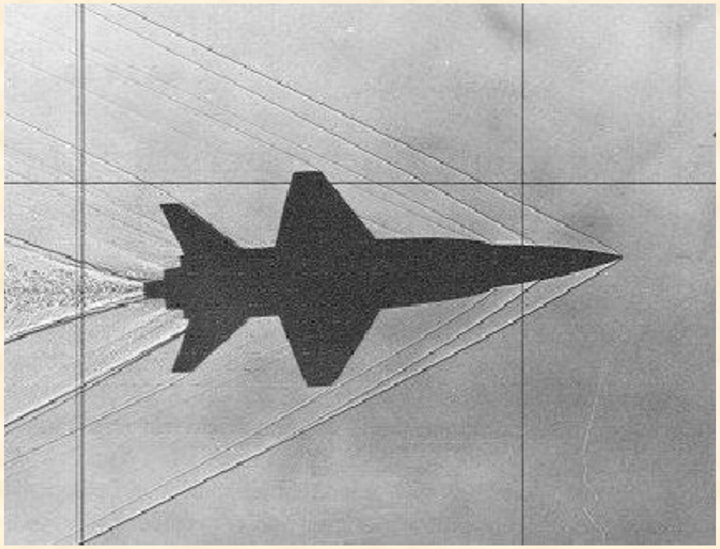
Shocks

Remarkably, hyperbolic PDEs admit discontinuous solutions.

Example: ***contact discontinuity***:
discontinuous change in density (with constant P) advected at constant v.

Shocks: discontinuous changes in all variables

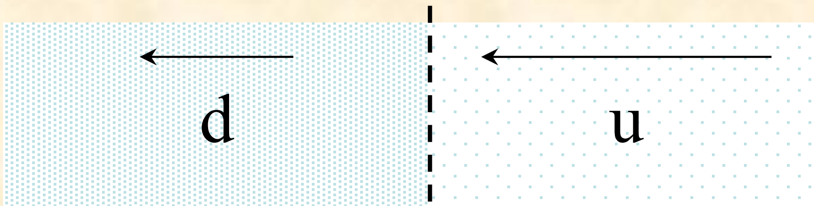
Shocks result from nonlinear steepening of smooth waves, or from disturbances that propagate faster then the compressive wave speeds



HST image of Tycho SNR

Hydrodynamic shocks

In the frame of reference of the shock, there is a steady fluid flow toward the shock from the upstream direction, and away from the shock in the downstream direction.



v_u = shock speed

Mass, momentum and energy must all be conserved in this frame

$$\rho_d v_d = \rho_u v_u$$

$$\rho_d v_d^2 + P_d = \rho_u v_u^2 + P_u$$

$$\frac{1}{2}\rho_d v_d^3 + (e_d + P_d)v_d = \frac{1}{2}\rho_u v_u^3 + (e_u + P_u)v_u$$

Can solve these equations for the ***Rankine-Hugoniot jump conditions*** (ratios of downstream to upstream quantities). For example:

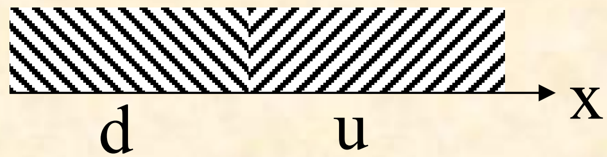
$$\frac{\rho_d}{\rho_u} = \frac{(\gamma+1)\mathcal{M}^2}{(\gamma-1)\mathcal{M}^2+2}$$

$M = v_u/C_u$ = shock Mach number

MHD shocks

Alfven "shocks" (rotational discontinuity).

$V_{x,u} = V_{x,d}$ (no compression), but transverse components of V and B change discontunusously (field undergoes discontinuous rotation)



Slow shock

Field "decompresses" through shock, $C_s < V_x < C_f$. Field direction deflected towards normal.

Fast shock

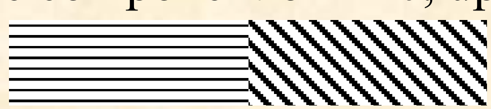
Field compresses through shock. $V_x > C_f$. Field direction deflected away from normal.

Switch-on shock

Upstream transverse component of B=0, downstream non-zero

Switch-off shock

Downstream transverse component of B=0, upstream non-zero



Finite Volume Methods

Challenge for numerical methods is to capture both linear and nonlinear waves and shocks accurately and stably.

Finite volume (FV) methods have emerged as accurate and robust methods for shock capturing, and they are ideally suited for modern HPC systems.

They are implemented in many public codes.

Athena, Athena++, AthenaK
AthenaPK, Pheobus
Enzo, Enzo-E
Einstein Toolkit
FLASH
HARM, HARM3D, H-AMR
PLUTO
RAMSES
VAC, BHAC

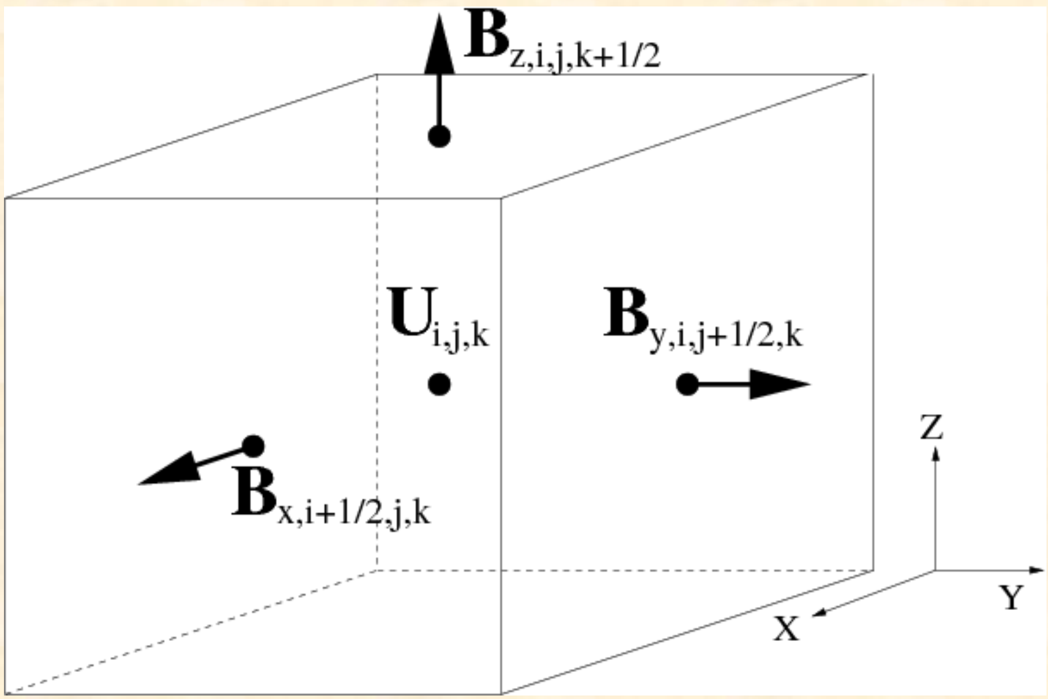
Discretization with FV Methods.

Uses cell-centered mass, momentum, energy and face-centered fields where cell-centered values are averaged over the volume:

$$\mathbf{U}^n_{i,j,k} = \frac{1}{\delta x \delta y \delta z} \int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} \mathbf{U}(x, y, z, t^n)\ \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z$$

and face centered values are averaged over areas, e.g.;

$$B^n_{x,i-1/2,j,k} = \frac{1}{\delta y \delta z} \int_{z_{k-1/2}}^{z_{k+1/2}} \int_{y_{j-1/2}}^{y_{j+1/2}} B_x(x_{i-1/2}, y, z, t^n)\ \mathrm{d}y\ \mathrm{d}z$$



Finite Volume Discretization

Integrate conservation laws over the volume of a grid cell, and over a timestep dt, apply the divergence theorem to give:

$$
\begin{aligned}
\mathbf{U}^{n+1}_{i,j,k} = \mathbf{U}^{n}_{i,j,k} \quad &- \quad \frac{\delta t}{\delta x}\left(\mathbf{F}^{n+1/2}_{i+1/2,j,k} - \mathbf{F}^{n+1/2}_{i-1/2,j,k}\right) \\
&- \quad \frac{\delta t}{\delta y}\left(\mathbf{G}^{n+1/2}_{i,j+1/2,k} - \mathbf{G}^{n+1/2}_{i,j-1/2,k}\right) \\
&- \quad \frac{\delta t}{\delta z}\left(\mathbf{H}^{n+1/2}_{i,j,k+1/2} - \mathbf{H}^{n+1/2}_{i,j,k-1/2}\right)
\end{aligned}
$$

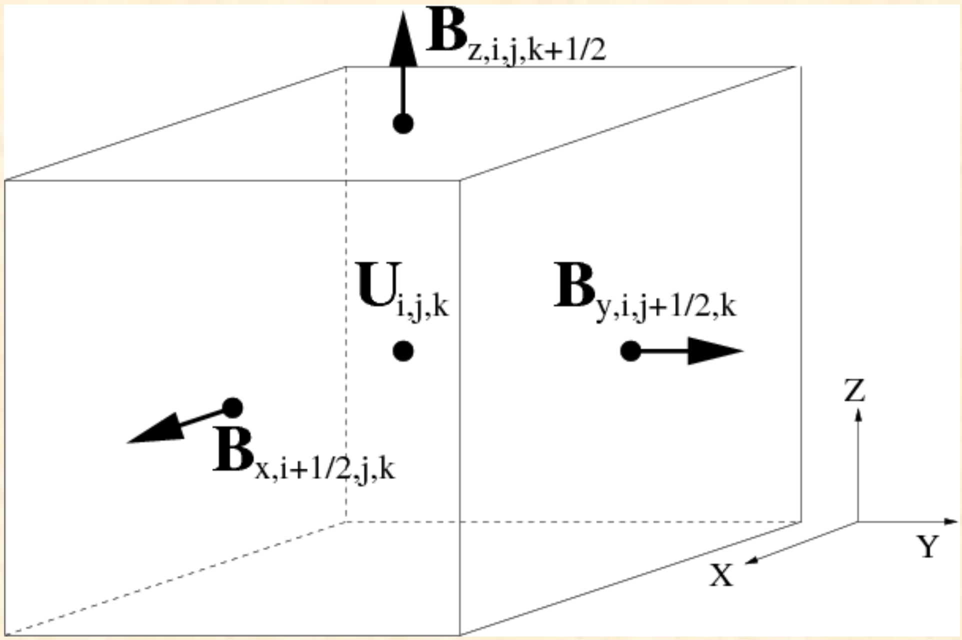
Integrate the induction equation over area of each cell face and dt, apply Stokes Law to give **Constrained Transport** method:

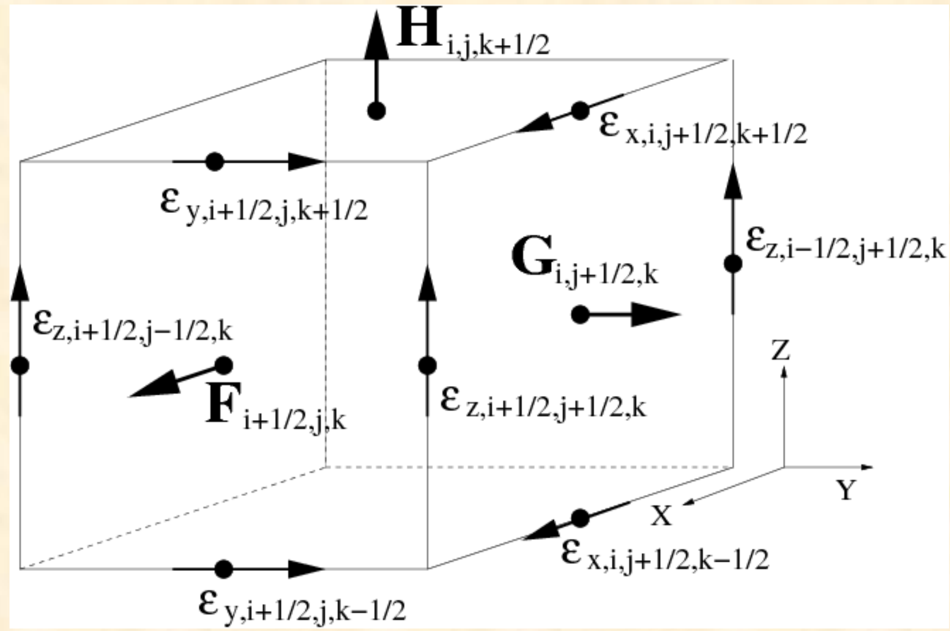
$$
\begin{aligned}
B^{n+1}_{x,i-1/2,j,k} = B^{n}_{x,i-1/2,j,k} \quad &- \quad \frac{\delta t}{\delta y}(\mathcal{E}^{n+1/2}_{z,i-1/2,j+1/2,k} - \mathcal{E}^{n+1/2}_{z,i-1/2,j-1/2,} \\
&+ \quad \frac{\delta t}{\delta z}(\mathcal{E}^{n+1/2}_{y,i-1/2,j,k+1/2} - \mathcal{E}^{n+1/2}_{y,i-1/2,j,k-1/}
\end{aligned}
$$

These equations are exact -- no approximations have been made!

Discretization with FV Methods.

Cell-centered mass, momentum, energy; face-centered magnetic field; face-centered fluxes; edge-centered electric fields





Importantly, FV discretization preserves volume-integrated values of **U** and magnetic flux (and therefore div(B)) to machine precision.

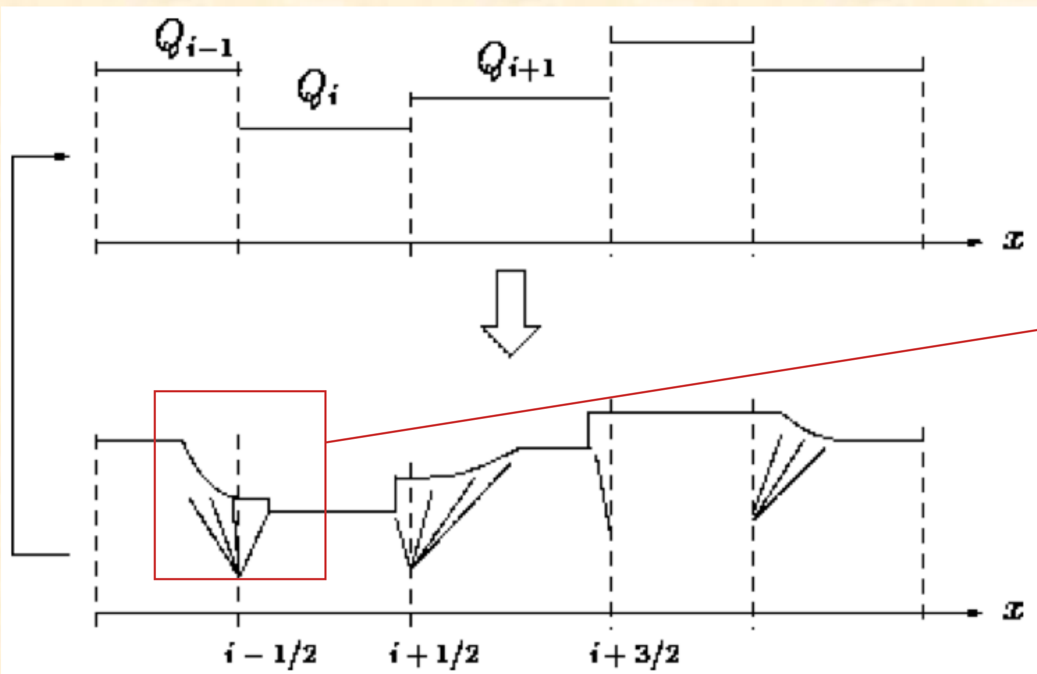
The key is how to compute these fluxes and EMFs all at once!

Godunov's orginal (first-order) method

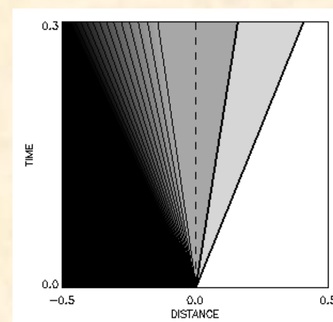
• Difference in cell-averaged values at each grid interface define set of Riemann problems (evolution of initially discontinuous states).

• Solution of Riemann problems averaged over cell give time-evolution of cell-averaged values, until waves from one interface crosses the grid and interacts with the other, that is for $\Delta t \leq \Delta x/(v+C)$

• Due to conservation, don't actually need to solve Riemann problem exactly. Just need to compute state *at location of interface* to compute fluxes.



Flux given by solution along x=0



Then, solution evolved according to

$$\frac{\mathbf{U}_j^{n+1} - \mathbf{U}_j^n}{\Delta t} = -\frac{\mathbf{F}_{j+1/2}^{n+1/2} - \mathbf{F}_{j-1/2}^{n+1/2}}{\Delta x}$$

Riemann solvers

For pure hydrodynamics of ideal gases, exact/efficient nonlinear Riemann solvers are possible.

In MHD, nonlinear Riemann solvers are complex because:

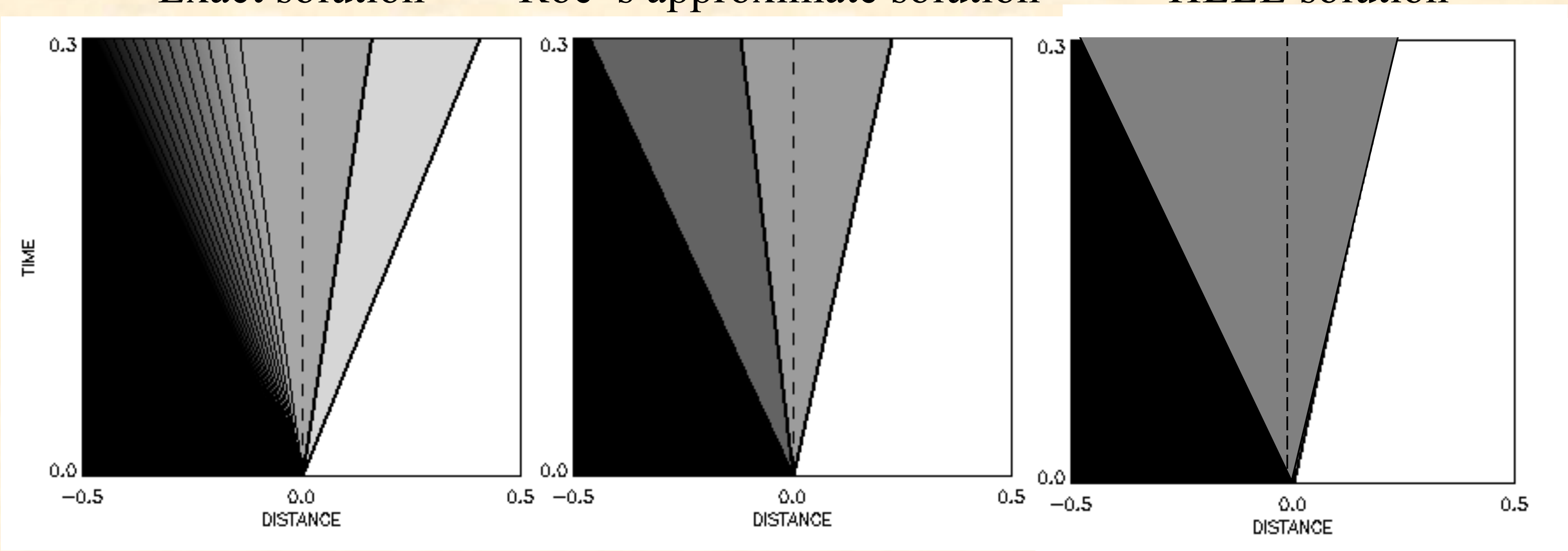
1. There are 3 wave families in MHD – 7 characteristics
2. In some circumstances, 2 of the 3 waves can be degenerate (e.g. $V_{Alfven} = V_{slow}$)

Equations of MHD are not *strictly hyperbolic*
(Brio & Wu, Zachary & Colella)

Thus, in practice, MHD Godunov schemes use approximate and/or linearized Riemann solvers.

Effect of various approximations on the solution to the Riemann problem in hydrodynamics

Exact solution — Roe’s approximate solution — HLLE solution



So which approximation is “best”? Must explore the use of each.

Use of a Riemann solvers is a benefit, not a weakness, of a Godunov method: makes shock capturing more accurate.

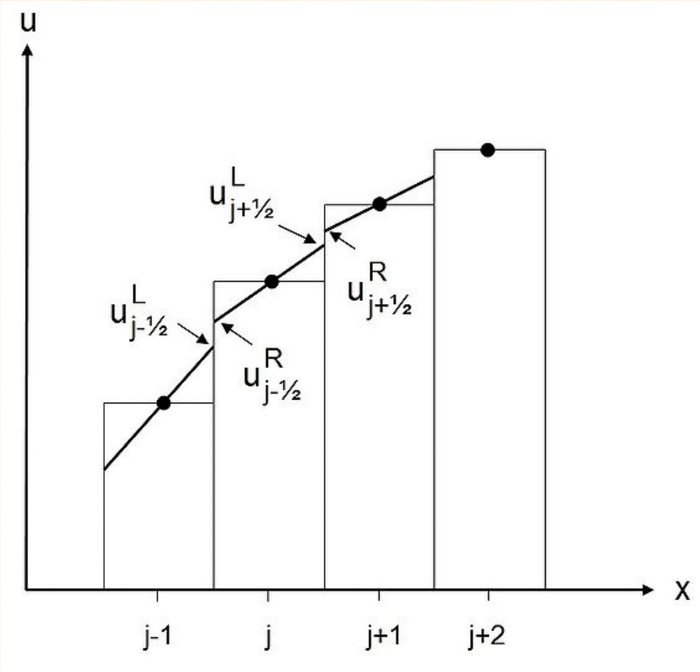
Ingredients of FV methods

Riemann Solvers:

- Equations of MHD admit three wave families; not *strictly hyperbolic*
- In practice, requires approximate and/or linearized solvers (LLF, HLLE, HLLD, Roe's method)

Spatially higher-order

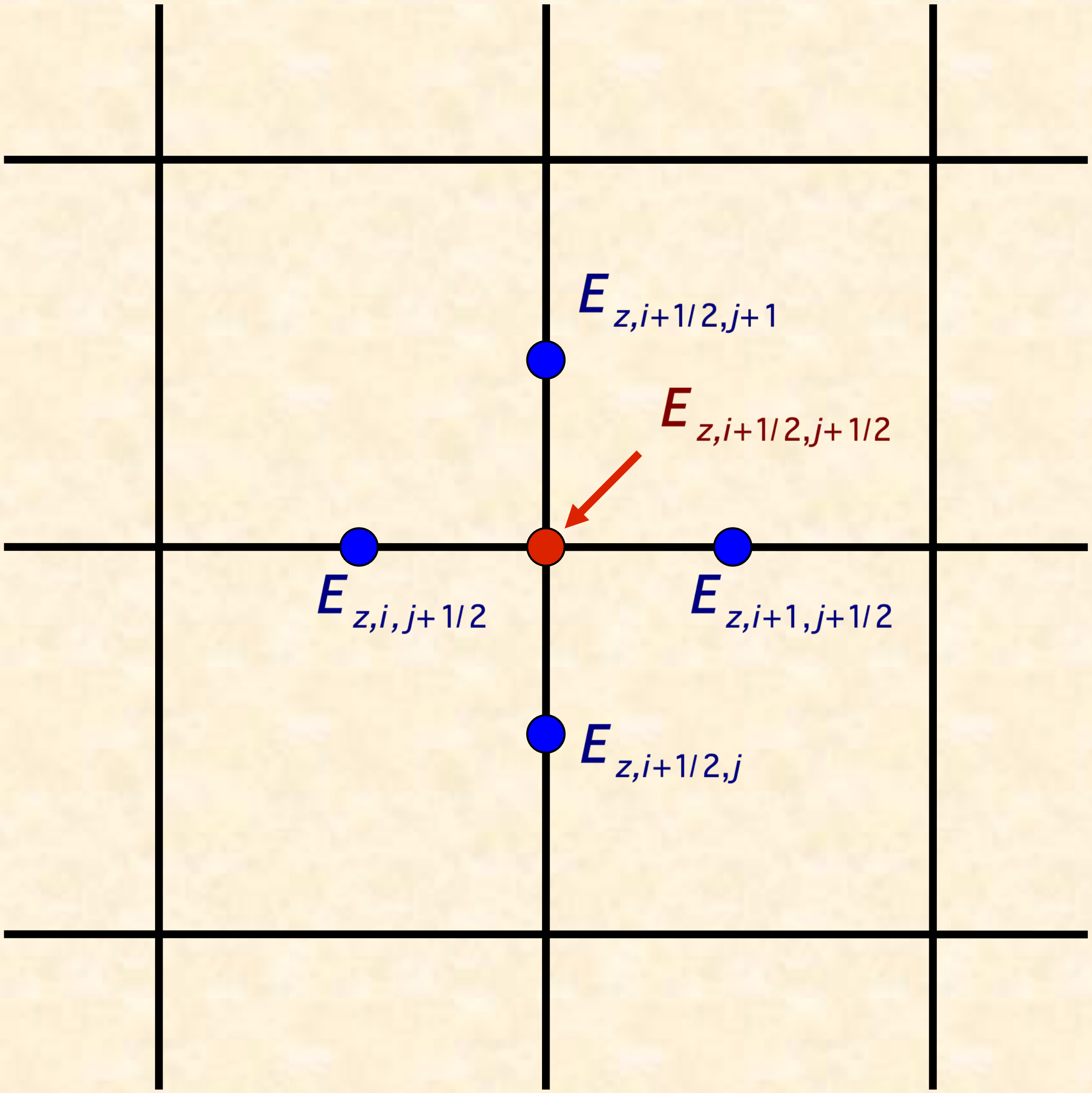
- Higher-order polynomial reconstruction with total-variation diminishing (TVD) and extremum-preserving reconstruction methods.



Temporally higher-order

- multistep strong-stability-preserving (SSP) Runge-Kutta integrators can be used, e.g. RK2, RK3, RK4 (Suresh & Huynh).
- Fourth-order in space, third-order in time seem to be most effective (for shocks and discontinuities, all methods are first-order)

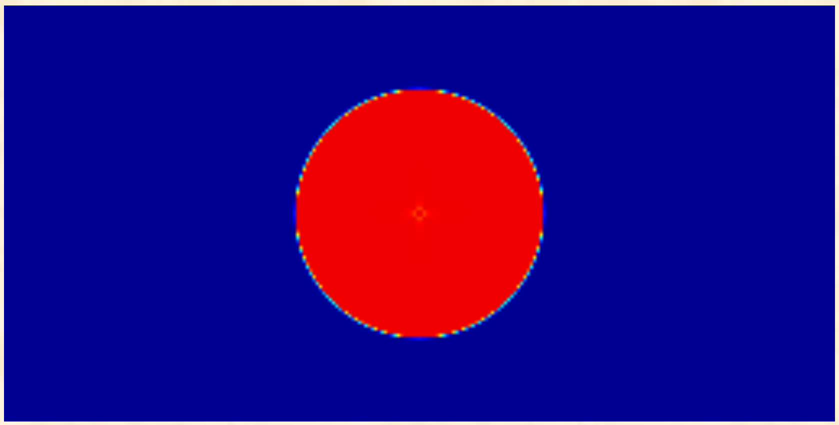
Constrained Transport in multidimensions



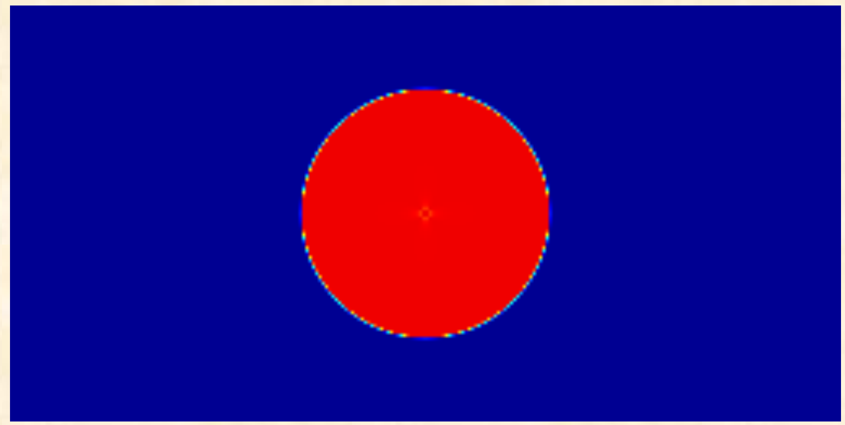
- Finite Volume / Godunov algorithm gives E-field at face centers.
- "CT Algorithm" needs E-field at grid cell corners.
- Arithmetic averaging: 2D plane-parallel flow does not reduce to equivalent 1D problem
- Algorithms which reconstruct E-field at corner are superior Gardiner & Stone 2005
- Some codes use a 2D Riemann solver to compute upwind EMF (e.g. PLUTO, RAMSES)

Advection of a field loop (2N x N grid)

Field Loop Advection ($\beta = 10^6$): MUSCL - Hancock integrator
Movies of B^2



Arithmetic average
(Balsara & Spicer 1999)



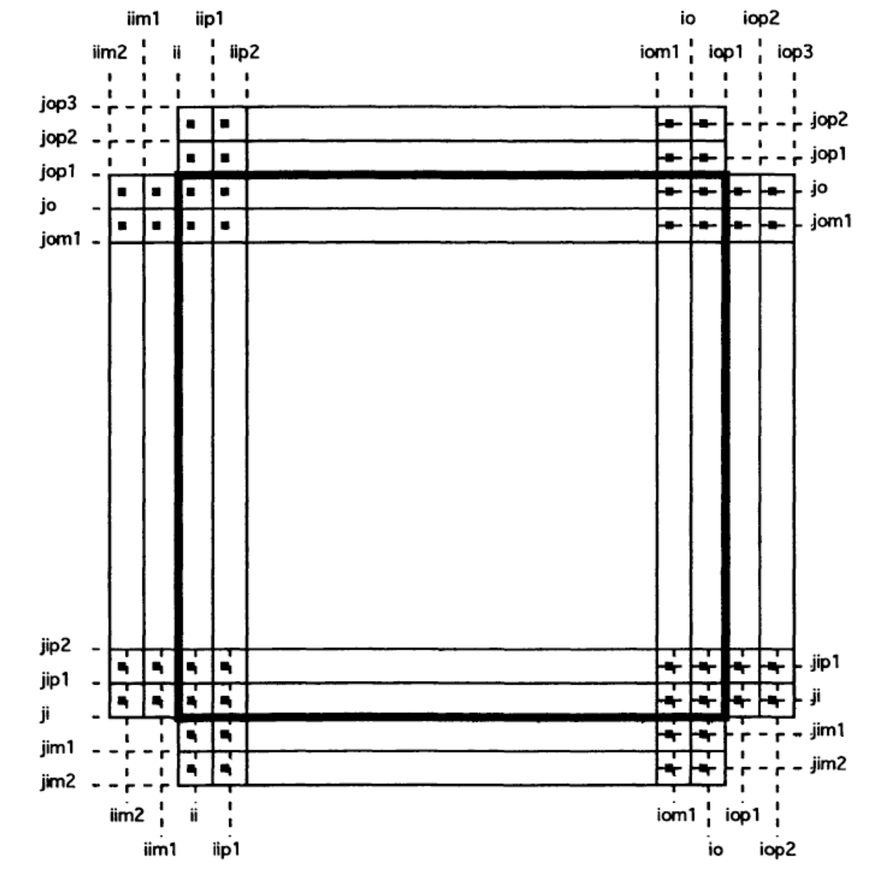
Gardiner & Stone 2005

Good test of proper upwinding of electric fields in CT.

Good test of whether codes preserves div(B) on appropriate stencil:
Run in 3D with non-zero V_z. Does method keep B_z zero?

Boundary conditions

Most grid codes apply boundary conditions by specifying solution in extra rows of cells ("ghost" or "guard" zones) at boundary of grid. This algorithm requires 2 or 3 rows (for 2nd or 4th order upwind reconstruction respectively)



There are different ways of specifying solution in ghost zones for different BCs, e.g.

1. Reflecting
2. Inflow
3. Outflow
4. Periodic

BCs must be applied after every stage in multi-stage integrators.

Practical time step control

For stability, the integration time step is limited by the Courant-Freidrichs-Lewy (CFL) condition:

$$\Delta t \leq \Delta x / (v + C)$$

Must take minimum timestep over whole grid.

Can be thought of as limiting distance fastest wave travels in one time step is less than cell size everywhere on mesh.

Also can be derived more rigorously from formal von Neumann stability analysis.

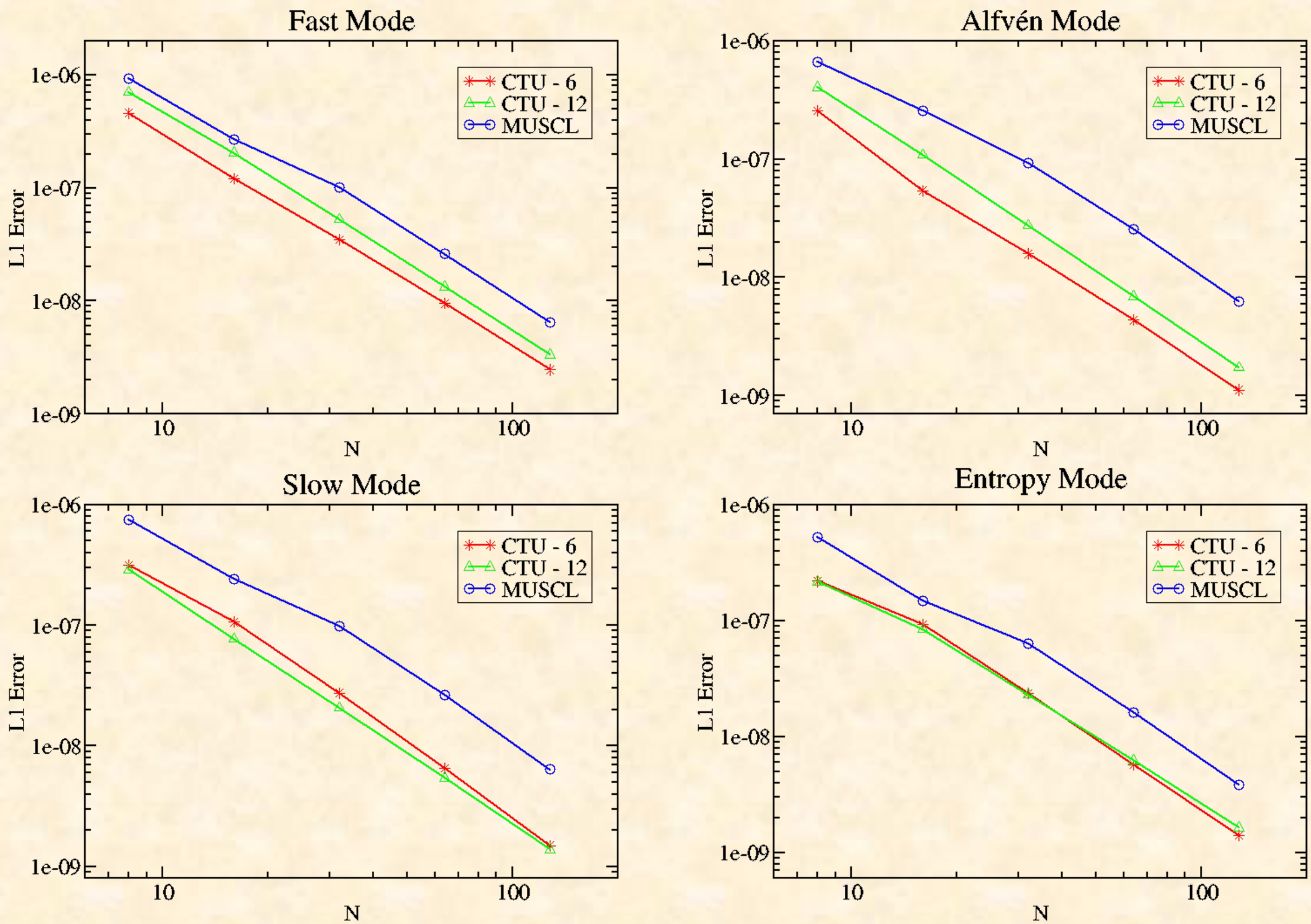
Define Courant number: $C = \dfrac{\Delta t}{\Delta x / (v + C)}$

For stability C < 1

In multi-dimensions, $C < 1/N_{dim}$ for most RK integrators.

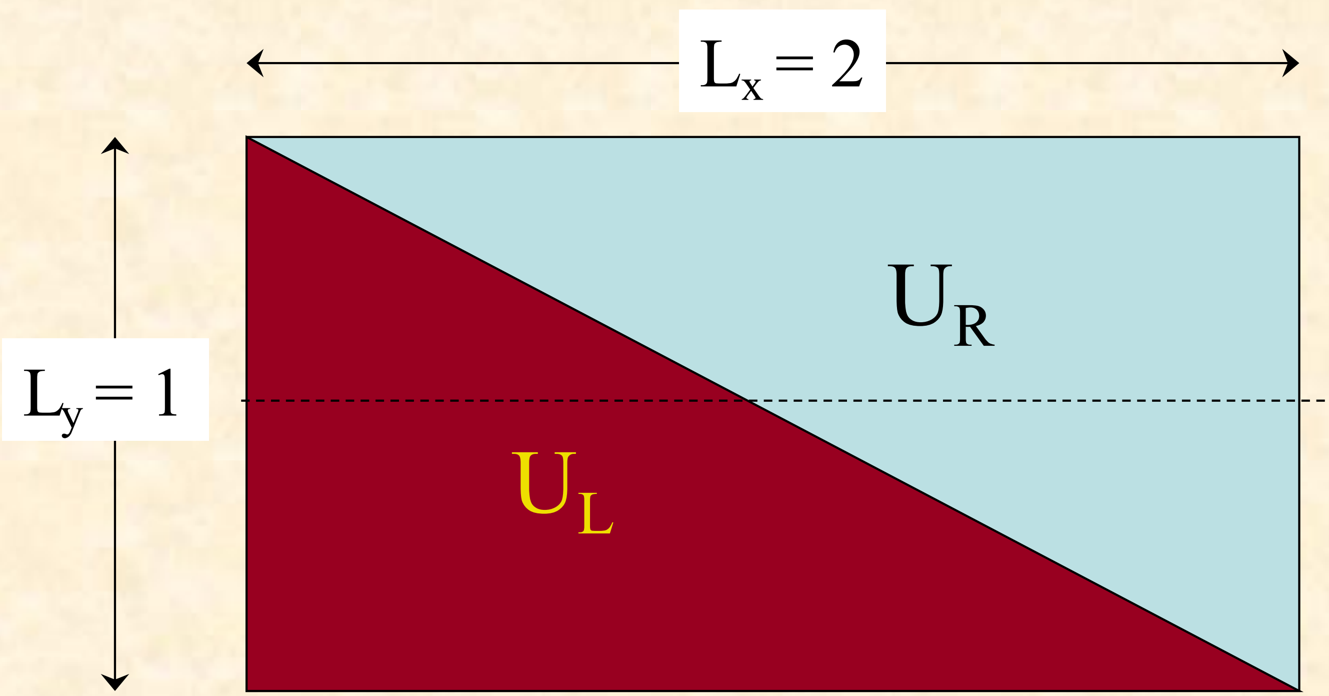
Tests: Linear Wave Convergence

Initialize pure eigenmode for each wave family
Measure RMS error in U after propagating one wavelength
quantitative test of accuracy of scheme



Tests: Shock Tubes (RJ2a)

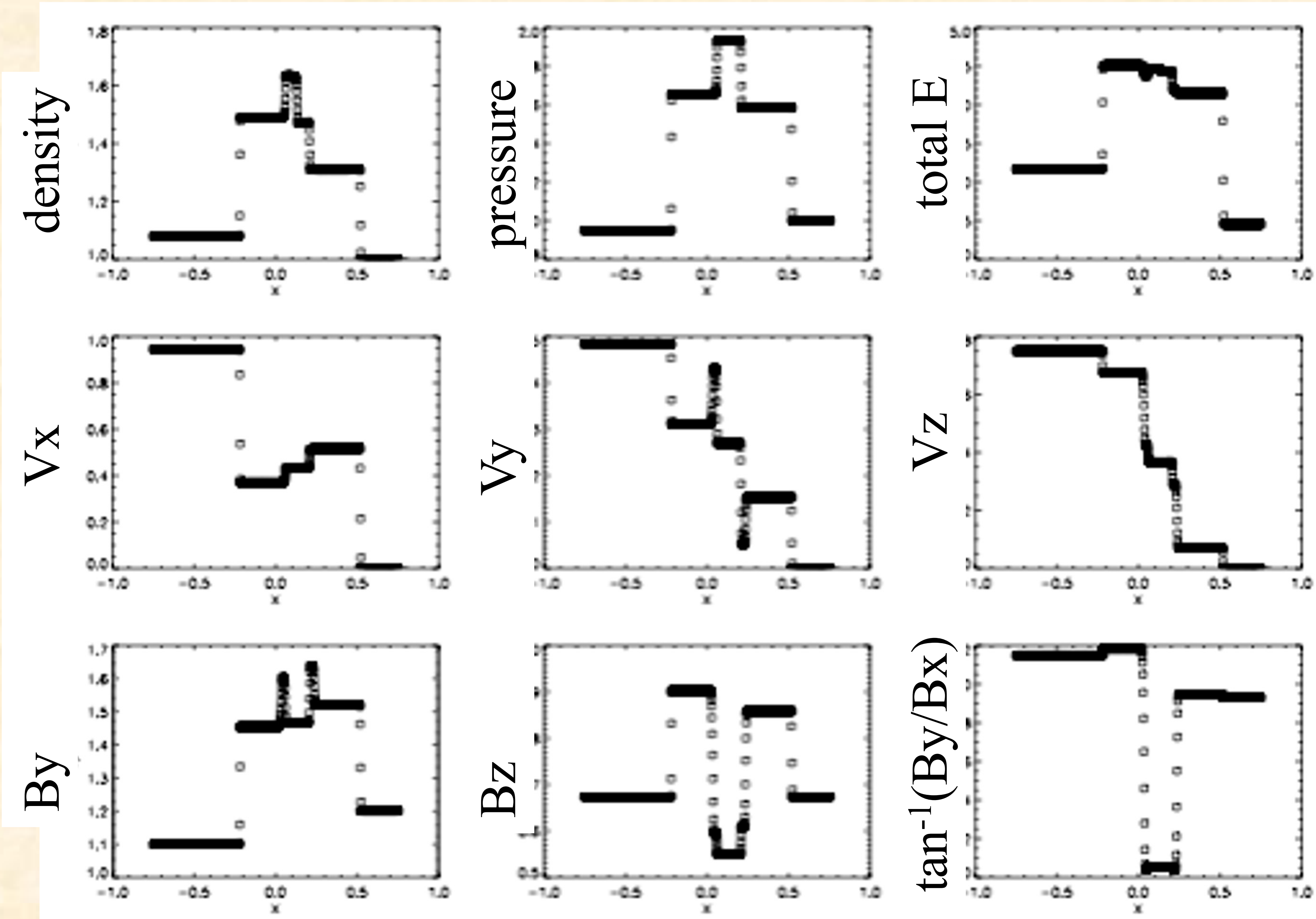
Initial discontinuity inclined to grid at $\tan^{-1}\theta = 1/2$
Magnetic field initialized from vector potential to ensure div(B)=0
$\Delta x = \Delta y$, 512 x 256 grid



Problem is Fig. 2a from Ryu & Jones 1995

Final result plotted along horizontal line at center of grid

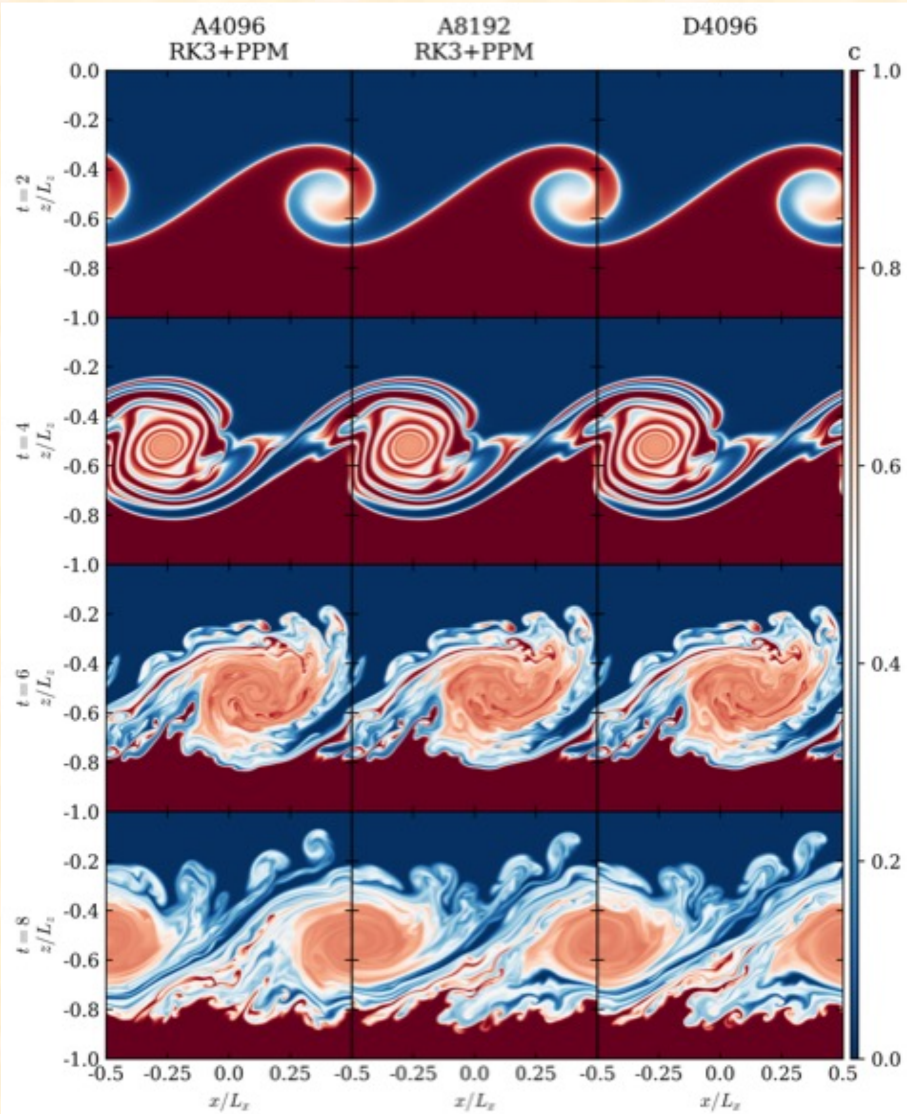
RJ2a shocktube in 2D (2N x N grid)

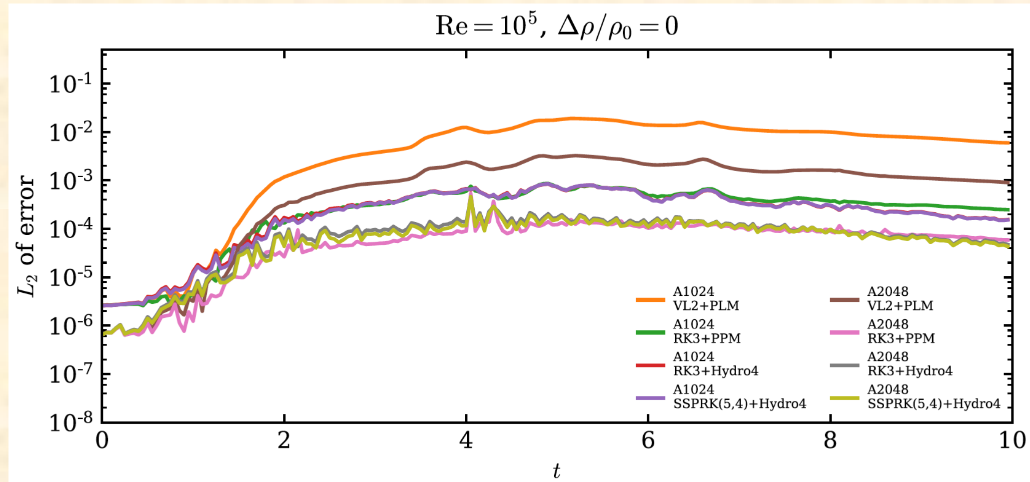


HLLD solver, all 7 MHD waves captured well.

Validation: Nonlinear regime of KH instability

- Resolved shear layer with tanh profile. Single more perturbation.
- Explicit viscosity and heat conduction: ***resolved reference solution***
- Good agreement between Athena and Dedalus (spectral code)





L_1 errors versus time at different resolutions

FV methods reproduce spectral code results at comparable cost.

Lecoanet+ 2016

Adding explicit diffusion: Viscosity and thermal conduction

Momentum equation: $\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \mathbf{F}_{\rho \mathbf{v}} = \nabla \cdot (\nu \nabla \mathbf{v})$

Energy equation: $\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{F}_E = \nabla \cdot (\kappa \nabla \mathbf{T}) + \nabla \cdot (\mathbf{v} \cdot (\nu \nabla \mathbf{v}))$

Both cases can be differenced using FTCS: $\frac{q_j^{n+1} - q_j^n}{\Delta t} = D \left(\frac{q_{j+1}^n - 2q_j^n + q_{j-1}^n}{\Delta t} \right)$

But stability constraint on FTCS for parabolic equations is very restrictive $\Delta t_D \leq (\Delta x)^2 / 4D$ (in 2D)

Solution: (1) sub-stepping: take many steps at Δt_D for every MHD Δt.

(2) super-timestepping; size of sub-time steps varied.

(3) implicit differencing: $\frac{q_j^{n+1} - q_j^n}{\Delta t} = D \left(\frac{q_{j+1}^{n+1} - 2q_j^{n+1} + q_{j-1}^{n+1}}{\Delta t} \right)$

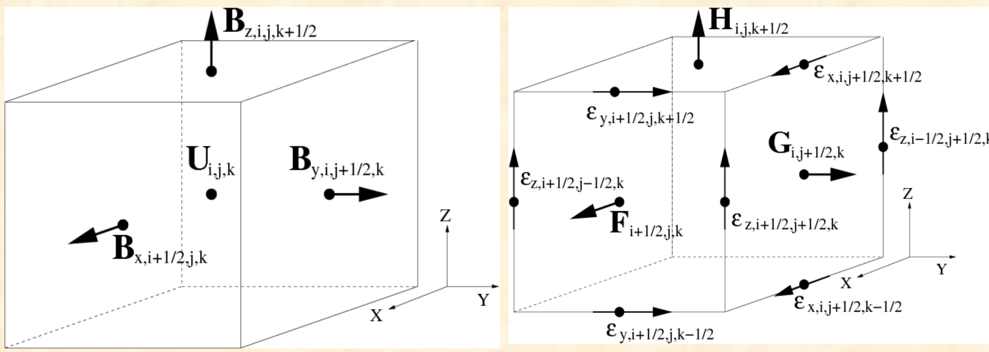
Latter leads to large sparse-banded matrices in 2D and 3D, which must be solved using, e.g. multigrid.

Explicit Diffusion: Ohmic resistivity

Induction equation becomes: $\dfrac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{v} \times \mathbf{B} - \eta \mathbf{J}) = 0$

$\mathbf{J}$ = current density

Over-riding concern is to keep div(B)=0. This suggests a CT differencing is required, using an "effective" EMF **E**=η**J** located at cell corners



Once again, time step constraint very restrictive: $\Delta t_\eta \leq (\Delta x)^2 / 4\eta$

Can use (1) sub-stepping, or (2) super-timestepping. Implicit CT differencing is complex.

Can be extended to ambipolar-diffusion and Hall regimes by appropriate definition of AD or Hall EMF.

Running Hydro and MHD problems with AthenaK

Either (1) write your own problem generator, or (2) use one of the default (built-in) pgens.

Build and compile code.

In the input file:

- Choose the mesh, using parameters in `<mesh>` and `<meshblock>`
- Add SMR or AMR using `<mesh_refinement>` and `<refined_regionN>` and/or `<amr_criterionN>`

Running Hydro and MHD problems with AthenaK

- For SR/GR problems, set flag in a `<coord>` block, e.g. `special_rel = true`
- For hydro problem, set parameters in a `<hydro>` block

- `eos` (**mandatory**): equation of state, `ideal` or `isothermal` (isothermal is Newtonian only).
- `gamma` (**mandatory if** `eos = ideal`): ratio of specific heats γ.
- `iso_sound_speed` (**mandatory if** `eos = isothermal`): isothermal sound speed.
- `reconstruct` (default `plm`): spatial reconstruction. Options: `dc` (donor cell), `plm` (piecewise linear), `ppm4` and `ppmx` (piecewise parabolic), `wenoz` (WENO-Z). The higher-order methods require more ghost zones (set `<mesh>/nghost` to at least 3, or 4 when combined with `fofc`).
- `rsolver` (**mandatory**): approximate Riemann solver. Valid choices depend on the regime:
  - Newtonian: `llf`, `hlle`, `hllc` (ideal only), `roe`
  - special/general relativistic: `llf`, `hlle`, `hllc` (SR only)
  - kinematic evolution (`<time>/evolution = kinematic`): `advect`
- `nscalars` (default `0`): number of passively advected scalars carried by the fluid.
- `fofc` (default `false`): enable first-order flux correction, which locally falls back to a diffusive first-order update in troubled cells to preserve positivity.

Running Hydro and MHD problems with AthenaK

- For MHD problem, set parameters in a `<mhd>` block

The `<mhd>` block shares most of its parameters with `<hydro>`:

- `eos` (**mandatory**): `ideal` or `isothermal`.
- `gamma` / `iso_sound_speed`: as for hydro (one is mandatory depending on `eos`).
- `reconstruct` (default `plm`): `dc`, `plm`, `ppm4`, `ppmx`, or `wenoz` (the higher-order options require more ghost zones).
- `rsolver` (**mandatory**): approximate Riemann solver. Valid choices:
  - Newtonian MHD: `llf`, `hlle`, `hlld`
  - special/general relativistic MHD: `llf`, `hlle`
  - kinematic evolution: `advect`
- `nscalars` (default `0`): number of passive scalars.
- `fofc` (default `false`): first-order flux correction.
- floors/ceilings: `dfloor`, `pfloor`, `tfloor`, `sfloor`, `gamma_max` (SR/GR).

- Choose run time, etc. in <time> block
- Add some outputs specified by `<outputN>` blocks
- Run the code, analyze results!

Physics Solvers

Wide variety of physics solvers implemented in AthenaK is one of its strengths:

- NR/SR/GR Hydro and MHD
- Diffusion processes: conduction, viscosity, resistivity
- Ambipolar diffusion
- Ion-neutral fluids
- Self-gravity (Velasco)
- Numerical Relativity (Zhu)
- GRMHD in dynamical spacetimes (Fields)
- Relativistic radiation transport (Zhang)
- Particles (Wong)

Plus, much more being implemented…