

Divergence Cleaning for MHD

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Overview

1. A (really) brief review on MHD and the project
2. How cleaning works
3. 1D Riemann solver for MHD & Test Problems
4. 2D Riemann solver & revision
5. MPI Parallelization

Task Required

- Implement a divergence cleaning method for MHD - done!(in some sense)
- Compare the divergence errors with and without this correction - done!
- No need to adopt the constraint transport technique - done!
- Apply to a MHD test problem (e.g., MHD Riemann problems) - done!
- Measure the performance scaling - done!

Ideal MHD Equations

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot \left[\rho \mathbf{u} \mathbf{u}^T + \left(p + \frac{1}{2} |\mathbf{B}|^2 \right) \mathcal{I} - \mathbf{B} \mathbf{B}^T \right] = 0$$

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) = 0$$

$$\partial_t e + \nabla \cdot \left[\left(e + p + \frac{1}{2} |\mathbf{B}|^2 \right) \mathbf{u} - \mathbf{B} (\mathbf{u} \cdot \mathbf{B}) \right] = 0$$

With the additional constraint on \mathbf{B} (also our favorite one)

$$\nabla \cdot \mathbf{B} = 0$$

combine the divergence free constraint and the third equation,

$$\partial_t \mathbf{B} + \nabla \times (\mathbf{B} \times \mathbf{u}) = 0$$

and we have $\nabla \cdot (\nabla \times \cdot) \equiv 0$.

$$\frac{\partial}{\partial t} \mathbf{U} + \nabla \cdot \mathbf{F} = \mathbf{S}$$

Divergence error

However!! For divergence to be discretized $\nabla \cdot \mathbf{B} \neq 0$

$\nabla \cdot \mathbf{B}$ errors arise $\frac{\partial}{\partial t} (\nabla \cdot \mathbf{B}) = 0 + O(\Delta x^m, \Delta t^n)$
magnetic flux, momentum, and energy are not conserved

Effect:

- Unphysical force

- The magnetic topology is distorted

Divergence Cleaning Method - GLM

Generalized Lagrange Multiplier - Boris(1971), Munz *et al*(2000)

Introducing a Lagrange multiplier to couple the divergence constraints

Operator-splitting procedure:

First step: Equations are solved numerically;

Second step: Divergence constraint is enforced by solving an Poisson equation

Divergence errors are transported to the boundary

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) + \nabla \psi = 0$$

$$\mathcal{D}(\psi) + \nabla \cdot \mathbf{B} = 0$$

Motivated by C.-D. Munz 1999

Advantage

Straightforward way

Efficient

Highly flexible

```
# GLM_hyperbolic
def hyperbolic_secondstep(flux, L, R):
    flux_hyp = flux.copy()
    b_xm = L[5] + 0.5*( R[5] - L[5]) - ( R[8] - L[8] ) / ( 2*ch )
    psi_m = L[8] + 0.5*( R[8] - L[8]) - 0.5*ch*( R[5] - L[5] )
    flux_hyp[8] = flux[8] + psi_m
    flux_hyp[5] = flux[5] + ch**2*b_xm

    return flux_hyp
```

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot \left[\rho \mathbf{u} \mathbf{u}^T + \left(p + \frac{1}{2} |\mathbf{B}|^2 \right) \mathcal{I} - \mathbf{B} \mathbf{B}^T \right] = 0$$

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) + \nabla \psi = 0$$

$$\partial_t e + \nabla \cdot \left[\left(e + p + \frac{1}{2} |\mathbf{B}|^2 \right) \mathbf{u} - \mathbf{B} (\mathbf{u} \cdot \mathbf{B}) \right] = 0$$

$$\mathcal{D}(\psi) + \nabla \cdot \mathbf{B} = 0$$

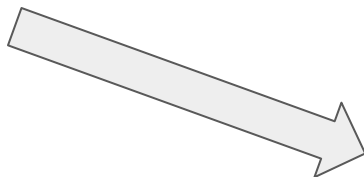
$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) + \nabla \psi = 0$$

$$\mathcal{D}(\psi) + \nabla \cdot \mathbf{B} = 0$$



$$\partial_t (\nabla \cdot \mathbf{B}) + \Delta \psi = 0,$$

$$\partial_t \mathcal{D}(\psi) + \partial_t (\nabla \cdot \mathbf{B}) = 0,$$



$$\partial_t \mathcal{D}(\psi) - \Delta \psi = 0$$

Correction Methods - A Dedner *et al*(2002)

Proposed three different choices for the linear operator D .

$$\mathcal{D}(\psi) := 0$$

$$\Delta \psi = 0$$

$$\mathcal{D}(\psi) := \frac{1}{c_p^2} \psi \quad \text{with } c_p \in (0, \infty)$$

$$\partial_t \psi - c_p^2 \Delta \psi = 0$$

$$\mathcal{D}(\psi) := \frac{1}{c_h^2} \partial_t \psi \quad \text{with } c_h \in (0, \infty)$$

$$\partial_{tt}^2 \psi - c_h^2 \Delta \psi = 0$$

$$\mathcal{D}(\psi) := \frac{1}{c_h^2} \partial_t \psi + \frac{1}{c_p^2} \psi$$

$$\partial_{tt}^2 \psi + \frac{c_h^2}{c_p^2} \partial_t \psi - c_h^2 \Delta \psi = 0$$

$$\partial_t \mathcal{D}(\psi) - \Delta \psi = 0$$

Elliptic $\mathcal{D}(\psi) := 0$

then ψ is just a Lagrange multiplier

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) + \nabla \psi = 0,$$

$$\partial_t (\nabla \cdot \mathbf{B}) + \Delta \psi = 0.$$

- First step: solve the hyperbolic system (Resulting in \mathbf{B}_n)
- 1.5 step : Solve the poisson equation (Resulting in ψ)

$$-\Delta \psi^{n*} = \frac{1}{\Delta t_n} (\nabla \cdot \mathbf{B}^{n*} - \nabla \cdot \mathbf{B}^n) = \frac{1}{\Delta t_n} \nabla \cdot \mathbf{B}^{n*}.$$

- Second step: update the magnetic field with ψ

$$\mathbf{B}^{n+1} = \mathbf{B}^{n*} - \Delta t_n \nabla \psi^{n*}.$$

Elliptic $\mathcal{D}(\psi) := 0$,

Projection method

- Possesses elliptical character
- B_{n+1} is simply the projection of B_n^* into the space of divergence-free vector fields.

Parabolic

$$\mathcal{D}(\psi) := \frac{1}{c_p^2} \psi \quad \text{with } c_p \in (0, \infty),$$

$$\partial_t \psi - c_p^2 \Delta \psi = 0$$

Heat Equation

- Coupled with a strength
- Local divergence errors are dissipated and smoothed out

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) = c_p^2 \nabla (\nabla \cdot \mathbf{B})$$

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) + \nabla \psi = 0$$

$$\mathcal{D}(\psi) + \nabla \cdot \mathbf{B} = 0$$

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot \left[\rho \mathbf{u} \mathbf{u}^T + \left(p + \frac{1}{2} |\mathbf{B}|^2 \right) \mathcal{I} - \mathbf{B} \mathbf{B}^T \right] = 0$$

$$\partial_t \mathbf{B} + \nabla \cdot (\mathbf{u} \mathbf{B}^T - \mathbf{B} \mathbf{u}^T) + \nabla \psi = 0$$

$$\partial_t e + \nabla \cdot \left[\left(e + p + \frac{1}{2} |\mathbf{B}|^2 \right) \mathbf{u} - \mathbf{B} (\mathbf{u} \cdot \mathbf{B}) \right] = 0$$

$$\mathcal{D}(\psi) + \nabla \cdot \mathbf{B} = 0$$

Hyperbolic $\mathcal{D}(\psi) := \frac{1}{c_h^2} \partial_t \psi$ with $c_h \in (0, \infty)$

$$\partial_{tt}^2 \psi - c_h^2 \Delta \psi = 0 \quad \Delta t_n = c_{cf} l \min_{1 \leq j \leq N} \min_{1 \leq l \leq 3} \frac{h_{jl}}{c_h}.$$

wave equation

- local divergence error are propagated to the boundary with finite speed $c_h > 0$

Hyperbolic

$$\begin{aligned}\partial_t \rho + \partial_x(\rho u_x) &= 0, \\ \partial_t(\rho u_x) + \partial_x \left(\rho u_x^2 + p + \frac{1}{2}(B_y^2 + B_z^2 - B_x^2) \right) &= 0, \\ \partial_t(\rho u_y) + \partial_x(\rho u_x u_y - B_x B_y) &= 0, \\ \partial_t(\rho u_z) + \partial_x(\rho u_x u_z - B_x B_z) &= 0, \\ \partial_t B_x + \partial_x \psi &= 0, \\ \partial_t B_y + \partial_x(B_y u_x - B_x u_y) &= 0, \\ \partial_t B_z + \partial_x(B_z u_x - B_x u_z) &= 0, \\ \partial_t e + \partial_x \left[u_x \left(e + p + \frac{1}{2} \mathbf{B}^2 \right) - B_x(u_x B_x + u_y B_y + u_z B_z) \right] &= 0, \\ \partial_t \psi + c_h^2 \partial_x B_x &= 0,\end{aligned} \quad \frac{\partial}{\partial t} \mathbf{U} + \frac{\partial}{\partial x} \mathbf{F} + \frac{\partial}{\partial y} \mathbf{G} + \frac{\partial}{\partial z} \mathbf{H} = 0$$

$$\partial_t \psi + c_h^2 \partial_x B_x = 0,$$

$$\partial_t \begin{pmatrix} B_x \\ \psi \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ c_h^2 & 0 \end{pmatrix} \partial_x \begin{pmatrix} B_x \\ \psi \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Decoupled from the other seven equations

It's actually a **Riemann problem**

$$\begin{pmatrix} B_{x,m} \\ \psi_m \end{pmatrix} = \begin{pmatrix} B_{x,l} \\ \psi_l \end{pmatrix} + \begin{pmatrix} \frac{1}{2}(B_{x,r} - B_{x,l}) - \frac{1}{2c_h}(\psi_r - \psi_l) \\ \frac{1}{2}(\psi_r - \psi_l) - \frac{c_h}{2}(B_{x,r} - B_{x,l}) \end{pmatrix}$$

we obtain $(\psi_m, c_h^2 B_{x,m})^T$ as numerical flux.

$$\mathbf{G}(\mathcal{R}(\mathbf{n}_{jl})\mathbf{U}_j^n, \mathcal{R}(\mathbf{n}_{jl})\mathbf{U}_{jl}^n)$$

$$:= \mathbf{G}_{mhd}(\mathcal{R}(\mathbf{n}_{jl})\mathbf{U}_j^n, \mathcal{R}(\mathbf{n}_{jl})\mathbf{U}_{jl}^n; B_{jl}^n) + (0, 0, 0, 0, \psi_{jl}^n, 0, 0, 0, c_h^2 B_{jl}^n)^T.$$

Mixed

$$\mathcal{D}(\psi) := \frac{1}{c_h^2} \partial_t \psi + \frac{1}{c_p^2} \psi.$$

- Offers both dissipation and propagation of divergence errors

The “divergence constraint” takes the form $\partial_t \psi + c_h^2 \nabla \cdot \mathbf{B} = -\frac{c_h^2}{c_p^2} \psi.$

Initial value problem

First step : Solve the homogenous system

1.5step : solve the initial value problem, with $\psi_j(0) = \psi_j^{n*}$

$$\partial_t \psi_j = -\frac{c_h^2}{c_p^2} \psi_j \quad \Longrightarrow \quad \psi_j^{n+1} := e^{-\Delta t_n c_h^2 / c_p^2} \psi_j^{n*}.$$

Second step: $\mathbf{B}^{n+1} = \mathbf{B}^{n*} - \Delta t_n \nabla \psi^{n*}.$

c_p is still a free parameter

We can set it as a function of c_h .

1. $c_d := e^{-\Delta t_n c_h^2 / c_p^2}$ fix a constant $c_d \in (0, 1)$

$$c_p(c_d, c_h, \Delta t_n) = \sqrt{-\Delta t_n \frac{c_h^2}{\ln(c_d)}}.$$

2. $c_r := c_p^2 / c_h \in (0, \infty)$

Mirrors the ratio between hyperbolic and parabolic effects

MHD Riemann Solver in 1D

Riemann Solvers

On our way to make a Riemann solver for MHD, we've tried the following solvers.

1. **Roe Solver**
2. **HLL - Einfeldt, et al (1991)**
3. **HLLC - Toro, et al (1994)**

These three solvers have been successfully implemented for 1D hydro problems.

For MHD, we choose to use the HLL solver.

Riemann Solvers

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ B_y \\ B_z \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} \rho u \\ \rho u^2 + p_T - B_x^2 \\ \rho v u - B_x B_y \\ \rho w u - B_x B_z \\ B_y u - B_x v \\ B_z u - B_x w \end{pmatrix}$$

HLL Solver

Advantages

- No need to deal with the Roe matrix.
- The entropy condition is satisfied.
- **Easier to code.**
- Because that's also what Athena did.
(but HLLD is a bit too hard, so we just stayed with HLL)

Choice	Comment	Physics	Reference
force	Toro's FORCE flux	Hydro and MHD	Toro section 7.4.2
two-shock	Two-shock approximation	Hydro	Toro section 9.4.2
exact	exact solver	Hydro	Toro chapter 4
hllc	Harten-Lax-van Leer with contact	Hydro	Toro section 10.4
hll	Harten-Lax-van Leer with Einfeldt fix	Hydro and MHD	Toro section 10.3
hll	Harten-Lax-van Leer with contact and Alfven mode	MHD	Miyoshi & Kusano, JCP, 208, 305
Roe	Roe's linearized solver	Hydro and MHD	Toro chapter 11

For **hydrodynamics**, use of the **Roe or HLLC solver** is strongly recommended.

For **MHD**, use of the **Roe or HLLD solver** is strongly recommended.

Taken from the Athena documentation

(Really) Basic Ideas of HLL Solver

Roe : solve the exact solutions to the approximated equations.

HLL- : solve the approximated solutions to the original equations.

- HLL : Using **one intermediate state** to approximate the solutions.
- HLLC : Using **two intermediate states** to approximate the solutions.
- HLLD : Using **four intermediate states** to approximate the solutions.

We just stayed with the one state approximate.

$$\mathbf{U}(x, 0) = \begin{cases} \mathbf{U}_l, & \text{if } x < 0 \\ \mathbf{U}_r, & \text{if } x > 0 \end{cases} \quad \mathbf{U}_{\text{HLL}} = \begin{cases} \mathbf{U}_l, & \text{if } S_L > 0, \\ \mathbf{U}^*, & \text{if } S_L \leq 0 \leq S_R \\ \mathbf{U}_r, & \text{if } S_R < 0, \end{cases}$$

where S_L and S_R are numerical approximations for the largest and smallest physical signal-velocities - B Einfeldt.(1991)

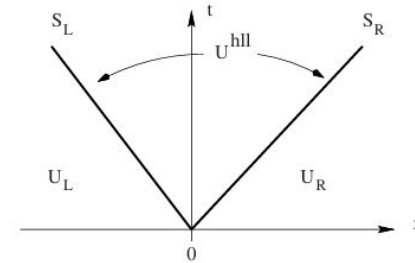


Fig. 10.3. Approximate HLL Riemann solver. Solution in the *Star Region* consists of a single state \mathbf{U}^{hll} separated from data states by two waves of speeds S_L and S_R .

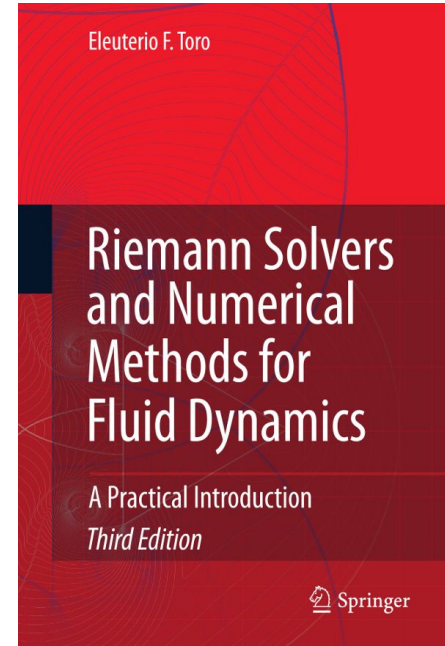
(Really) Basic Ideas of HLL Solver

After some mathematics, physics, assumptions and approximations, we have the following formulas.
Check out **E.F. Toro. (1999)** for more details.

$$\mathbf{U}^* = \frac{S_R \mathbf{U}_r - S_L \mathbf{U}_l - (F_r - F_l)}{S_R - S_L} \quad \mathbf{U}_{\text{HLL}} = \begin{cases} \mathbf{U}_l, & \text{if } S_L > 0, \\ \mathbf{U}^*, & \text{if } S_L \leq 0 \leq S_R \\ \mathbf{U}_r, & \text{if } S_R < 0, \end{cases}$$

Or in terms of fluxes, L and R denote the states or fluxes of the left and right side.

$$\mathbf{F}_{i+\frac{1}{2}}^{hll} = \begin{cases} \mathbf{F}_L & \text{if } 0 \leq S_L, \\ \frac{S_R \mathbf{F}_L - S_L \mathbf{F}_R + S_L S_R (\mathbf{U}_R - \mathbf{U}_L)}{S_R - S_L}, & \text{if } S_L \leq 0 \leq S_R \\ \mathbf{F}_R & \text{if } 0 \geq S_R. \end{cases}$$



On the Estimation of SL and SR

Final step is to find **SL** and **SR**. Several methods for estimating SL and SR exist, we adapt the one proposed by B Einfeldt, et al.(1991).

$$S_L = \min\{b_L, 0\} \quad b_L = \min\{\lambda_i, u_L - c_L\}$$

$$S_R = \max\{b_R, 0\} \quad b_R = \max\{\lambda_i, u_R + c_R\}$$

where the lambdas are the eigenvalues of **the Roe matrix**. CL and CR are the sound speed in the left and right state in hydro, but for MHD, we uses the “fast wave speed”.

$$\lambda_{f\pm} = u \pm c_f, \quad \lambda_{s\pm} = u \pm c_s, \quad \lambda_{a\pm} = u \pm c_a, \quad c_a = |b_x|,$$

$$c_f = \sqrt{\frac{1}{2}(a^2 + b^2 + \sqrt{(a^2 + b^2)^2 - 4a^2b_x^2})},$$

$$c_s = \sqrt{\frac{1}{2}(a^2 + b^2 - \sqrt{(a^2 + b^2)^2 - 4a^2b_x^2})}$$

$$b_x := \sqrt{\frac{B_x^2}{\rho}}, \quad b^2 := \frac{|\mathbf{B}|^2}{\rho}, \quad a := \sqrt{\frac{\gamma p}{\rho}}$$

The Roe Matrix (The Fun Stuff)

The 7 eigenvalues correspond to 7 waves.

- Two fast magnetosonic waves - Cs
- Two fast magnetosonic waves - Cf
- One Alfvén wave - Ca

$$\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ \delta_{21} & \delta_{22} & \delta_{23} & \delta_{24} & \delta_{25} & \delta_{26} & \delta_{27} \\ -\bar{u}\bar{v} & \bar{v} & \bar{u} & 0 & -B_x & 0 & 0 \\ -\bar{u}\bar{w} & \bar{w} & 0 & \bar{u} & 0 & -B_x & 0 \\ \frac{-B_y}{\rho}\bar{u} + \frac{B_x}{\rho}\bar{v} & \frac{B_y}{\rho} & \frac{-B_x}{\rho} & 0 & \bar{u} & 0 & 0 \\ \frac{-B_z}{\rho}\bar{u} + \frac{B_x}{\rho}\bar{w} & \frac{B_z}{\rho} & 0 & \frac{-B_x}{\rho} & 0 & \bar{u} & 0 \\ \delta_{71} & \delta_{72} & \delta_{73} & \delta_{74} & \delta_{75} & \delta_{76} & \delta_{77} \end{bmatrix}$$

$$\delta_{21} = -\bar{u}^2 + (2 - \gamma)X + \frac{\gamma - 1}{2}\bar{V}^2, \delta_{22} = 2\bar{u} - (\gamma - 1)\bar{u}$$

$$\delta_{23} = -(\gamma - 1)\bar{v}, \delta_{24} = -(\gamma - 1)\bar{w}$$

$$\delta_{25} = (2 - \gamma)\underline{B}_y, \delta_{26} = (2 - \gamma)\underline{B}_z, \delta_{27} = \gamma - 1$$

$$\delta_{71} = -\bar{u}\bar{H}^* + \bar{u}(\delta_{21} + \bar{u}^2) + \frac{B_x}{\rho}(\bar{V} \cdot \underline{B})$$

$$\delta_{72} = \bar{H}^* + \bar{u}(\delta_{22} - 2\bar{u}) - \frac{B_x^2}{\rho}, \delta_{73} = \bar{u}\delta_{23} - \frac{B_x}{\rho}\underline{B}_y,$$

$$\delta_{74} = \bar{u}\delta_{24} - \frac{B_x}{\rho}\underline{B}_z$$

$$\delta_{75} = \bar{u}\delta_{25} - B_x\bar{v}, \delta_{76} = \bar{u}\delta_{26} - B_x\bar{w}, \delta_{77} = \bar{u} + \bar{u}\delta_{27}$$

Roe-averaged Values

The wave speeds are calculated using Roe-averaged values. \mathbf{B} and \mathbf{u} are **vectors**.

$$\bar{u} = \frac{\sqrt{\rho_L}u_L + \sqrt{\rho_R}u_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

$$\bar{H} = \frac{\sqrt{\rho_L}H_L + \sqrt{\rho_R}H_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

$$\bar{B} = \frac{\sqrt{\rho_L}B_L + \sqrt{\rho_R}B_R}{\sqrt{\rho_L} + \sqrt{\rho_R}}$$

$$\bar{\rho} = \sqrt{\rho_L}\sqrt{\rho_R}$$

Recall that:

$$\lambda_{f\pm} = u \pm c_f, \quad \lambda_{s\pm} = u \pm c_s, \quad \lambda_{a\pm} = u \pm c_a,$$

$$c_a = |b_x|,$$

$$c_f = \sqrt{\frac{1}{2}(a^2 + b^2 + \sqrt{(a^2 + b^2)^2 - 4a^2b_x^2})},$$

$$c_s = \sqrt{\frac{1}{2}(a^2 + b^2 - \sqrt{(a^2 + b^2)^2 - 4a^2b_x^2})}$$

$$b_x := \sqrt{\frac{B_x^2}{\rho}}, \quad b^2 := \frac{|\mathbf{B}|^2}{\rho}, \quad a := \sqrt{\frac{\gamma p}{\rho}}$$

Python Code for HLL

See the function “**HLL**” in our code for details. I’ll just go through the process here.

- Given the left and right state and compute the Roe-averaged values.
- Use the Roe-averaged values to compute the eigenvalues.
- Estimate S_L and S_R .
- Determine which state to use using S_L and S_R .
- Compute the HLL-estimated flux.
- Return flux and update.(we use MUSCL-Hancock, van-leer limiter and PLM)

$$\mathbf{U}_{\text{HLL}} = \begin{cases} \mathbf{U}_L, & \text{if } S_L > 0, \\ \mathbf{U}^*, & \text{if } S_L \leq 0 \leq S_R \\ \mathbf{U}_R, & \text{if } S_R < 0, \end{cases} \quad \mathbf{F}_{i+\frac{1}{2}}^{\text{hll}} = \begin{cases} \mathbf{F}_L & \text{if } 0 \leq S_L, \\ \frac{S_R \mathbf{F}_L - S_L \mathbf{F}_R + S_L S_R (\mathbf{U}_R - \mathbf{U}_L)}{S_R - S_L}, & \text{if } S_L \leq 0 \leq S_R \\ \mathbf{F}_R & \text{if } 0 \geq S_R. \end{cases}$$

Test Problems for Our Solver

Test Problems

To verify if our solver yields correct result, we use several test problems, including hydro and MHD problems.

- **Hydro: Sod's Shock Tube**
- **Hydro: Strong Shock Problem**
- **MHD: Brio-Wu Shock Tube**

We also verify the conserved quantities (Brio-Wu Shock Tube).

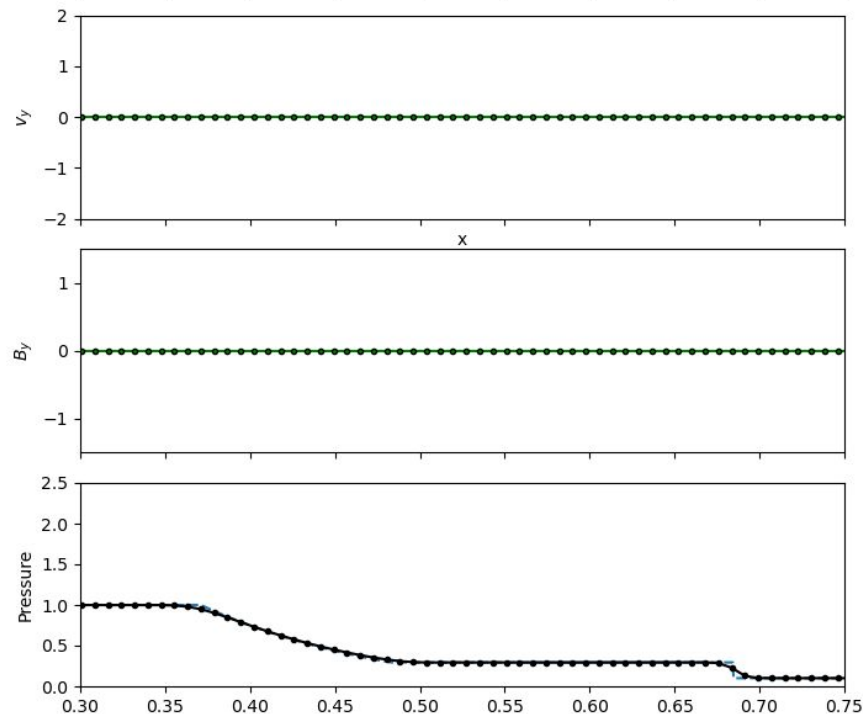
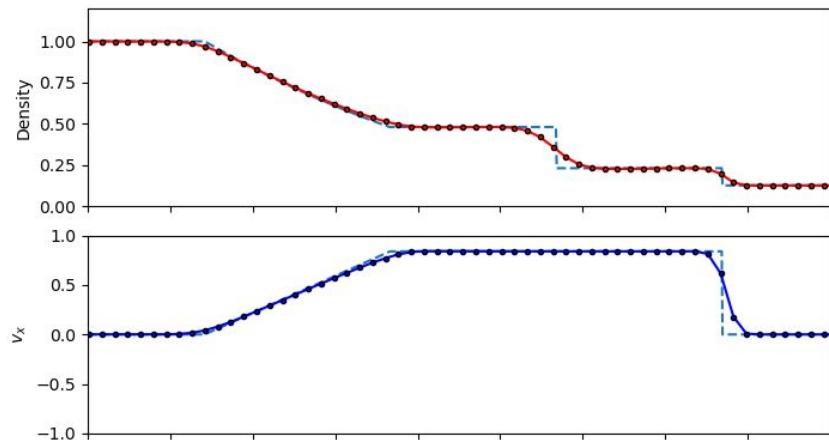
- **Mass conservation**
- **Energy conservation**

Lastly, we will show the performance scaling (with some unsolved mysteries).

Sod's Shock Tube

Hydro test problem. (BC: Outflow)

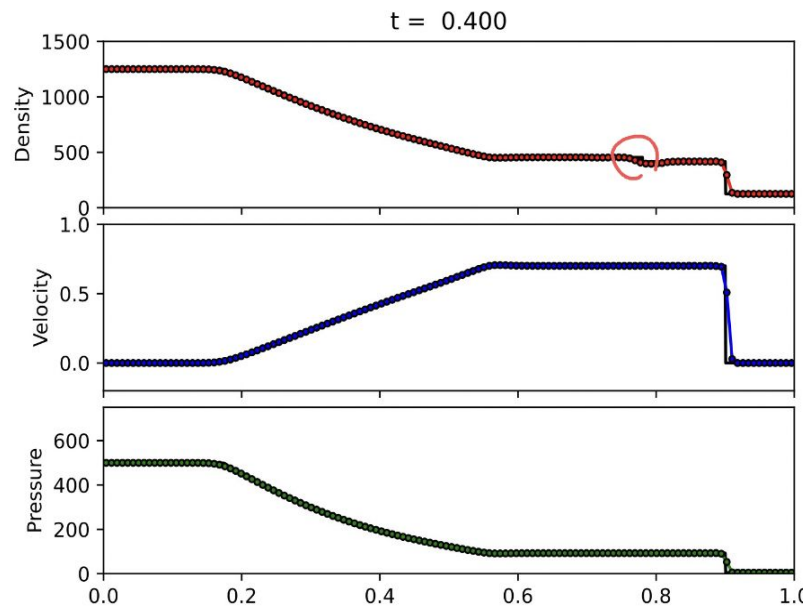
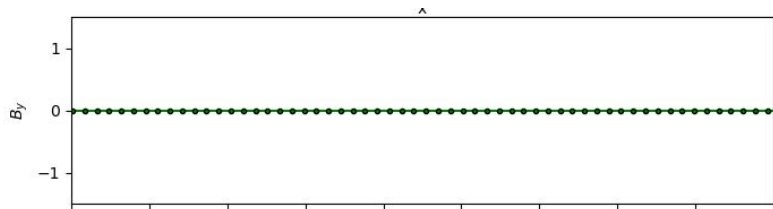
- Left state: $\rho = 1.0$, $\mathbf{u} = 0.0$, $\mathbf{B} = 0.0$, $P = 1.0$
- Right state: $\rho = 0.125$, $\mathbf{u} = 0.0$, $\mathbf{B} = 0.0$, $P = 0.1$
- End time = 0.1, cfl = 0.475, 128 cells were used



Strong Shock Tube

Hydro test problem. (BC: Outflow)

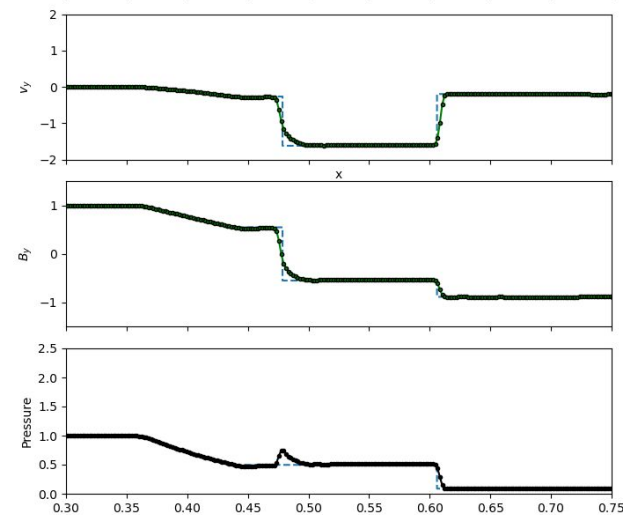
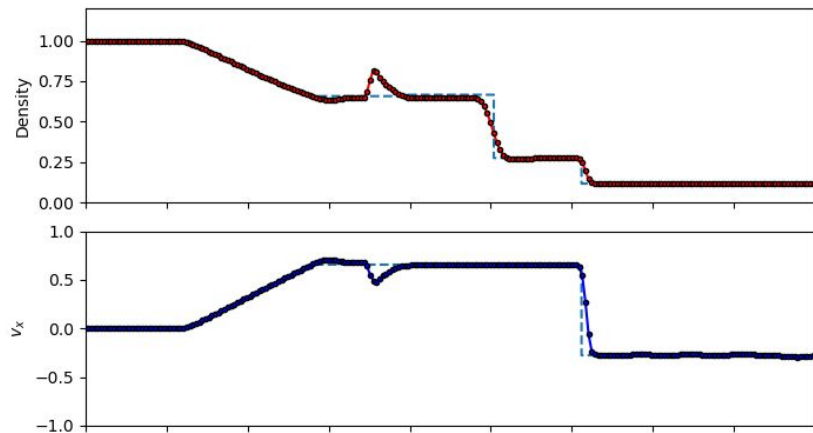
- Left state: $\rho = 1.25\text{e}+3$, $\mathbf{u} = 0.0$, $\mathbf{B} = 0.0$, $P = 5.0\text{e}+2$
- Right state: $\rho = 1.25\text{e}+2$, $\mathbf{u} = 0.0$, $\mathbf{B} = 0.0$, $P = 5.0$
- End time = 0.4, cfl = 0.475, 128 cells were used.



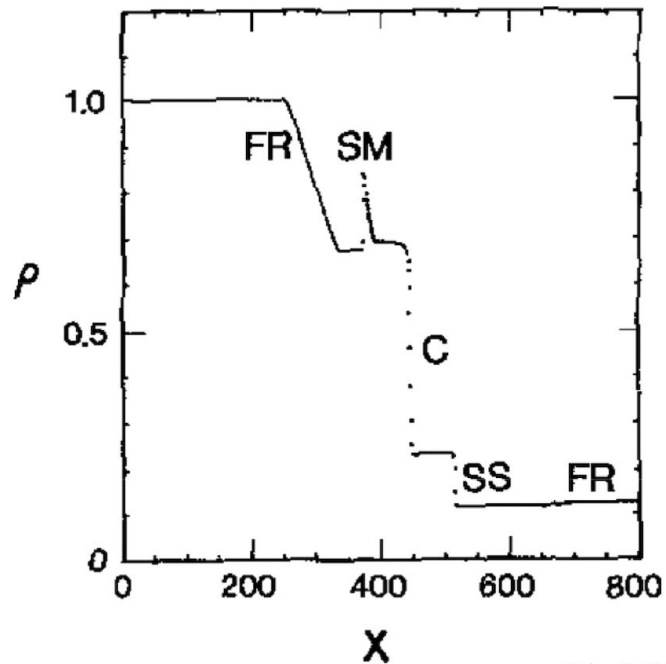
Brio-Wu shock tube

MHD test problem. (BC: Dirichlet)

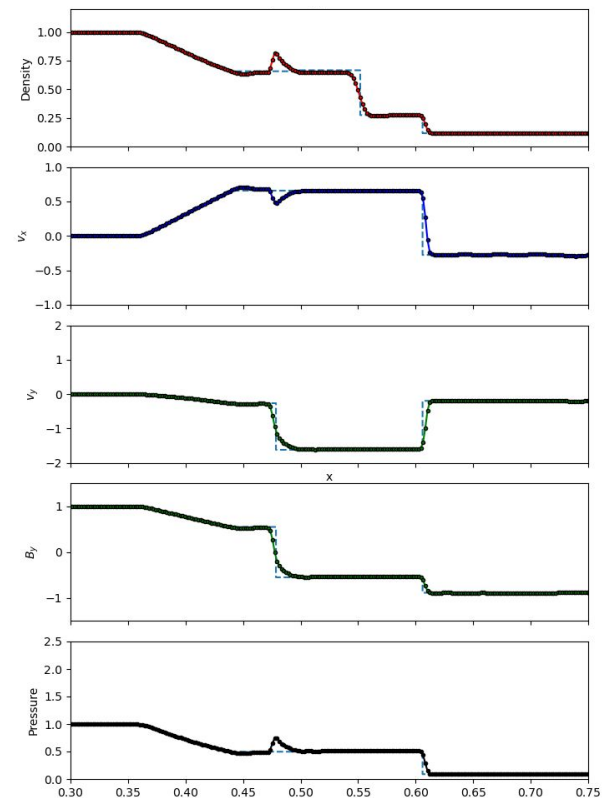
- Left state: $\rho = 1.0$, $\mathbf{u} = 0.0$, $\mathbf{B} = (0.75, 1.0, 0.0)$, $P = 1.0$
- Right state: $\rho = 0.125$, $\mathbf{u} = 0.0$, $\mathbf{B} = (0.75, -1.0, 0.0)$, $P = 0.1$
- End time = 0.08, cfl = 0.475, 512 cells were used.



Brio-Wu shock tube



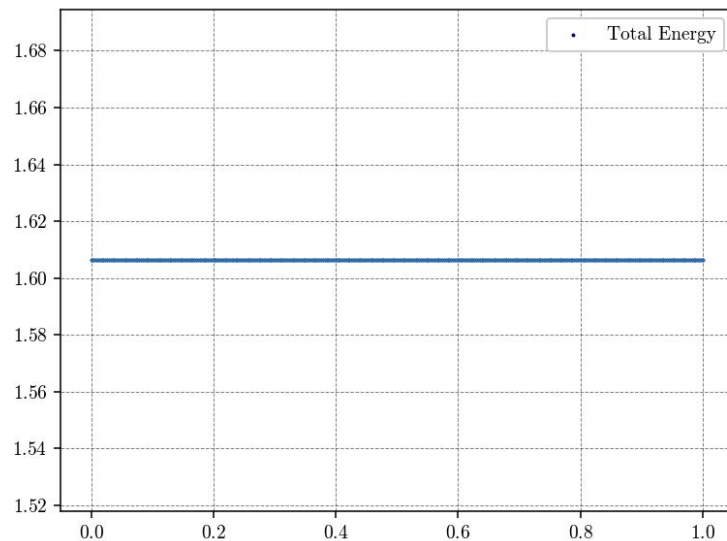
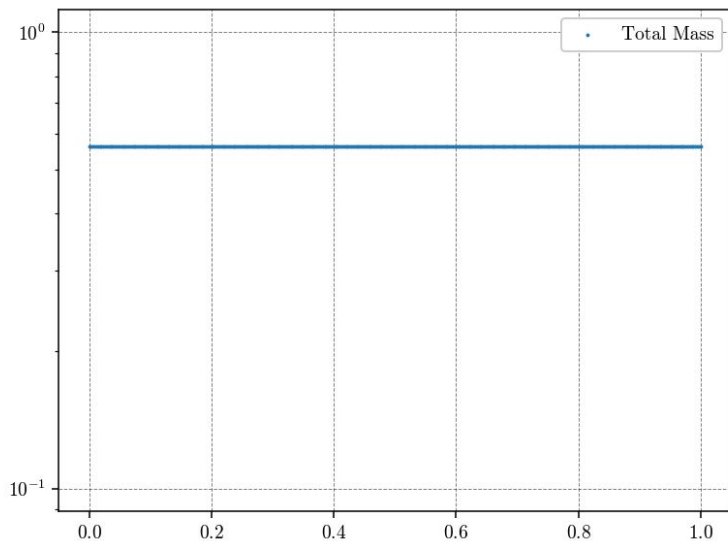
Brio & Wu 1988



Conserved Quantities

Using the Brio-Wu tube as an example. The result seems a bit too good.

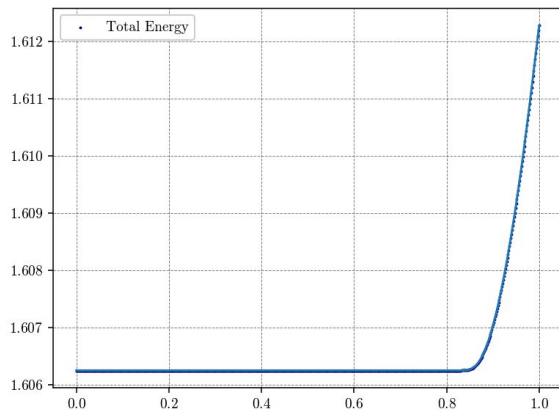
The energy error has an order of magnitude of -16 (double precision).



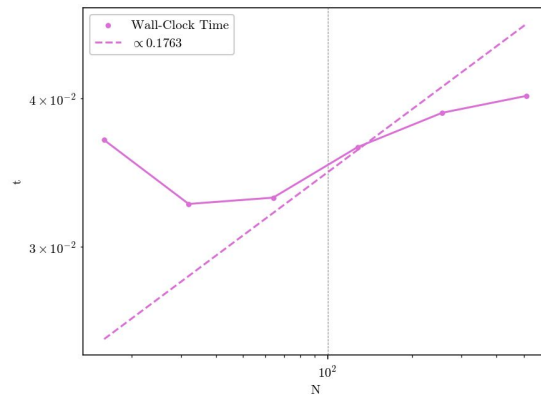
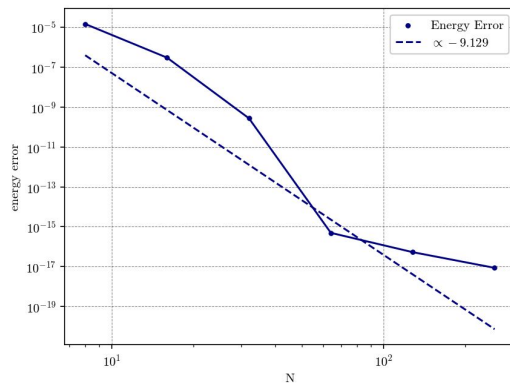
Performance Scaling

Using the Brio-Wu tube as an example. Endtime = 0.16.

- In theory, MUSCL-Hancock should give us a **second-order accuracy**.
- The error decrease with the number of computing cells(**ninth-order**?).
- The wall-clock is roughly the same, despite the increasing number of cells.
- The error starts increasing after $t=0.8$. (due to Dirichlet boundary conditions).



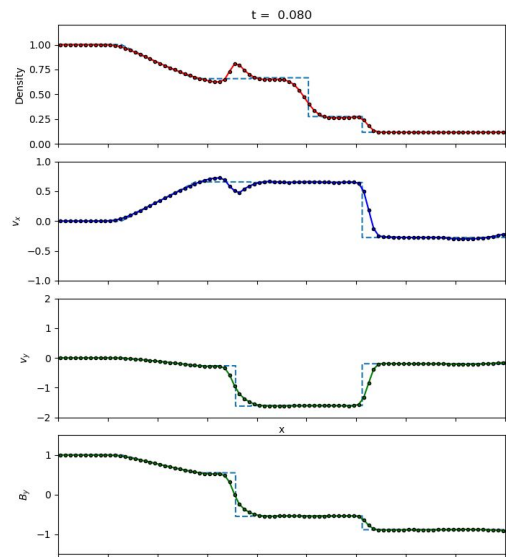
$$Error = \left| \frac{E - E_0}{\bar{E}_0} \right|$$



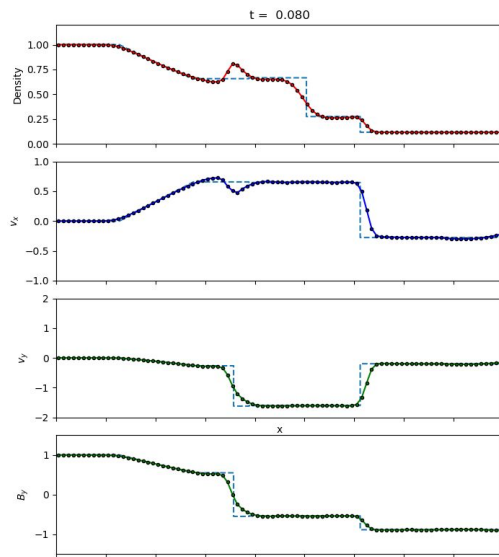
Compare the Divergence Errors

But there's no error. With or without the cleaning, we all obtained the same result.

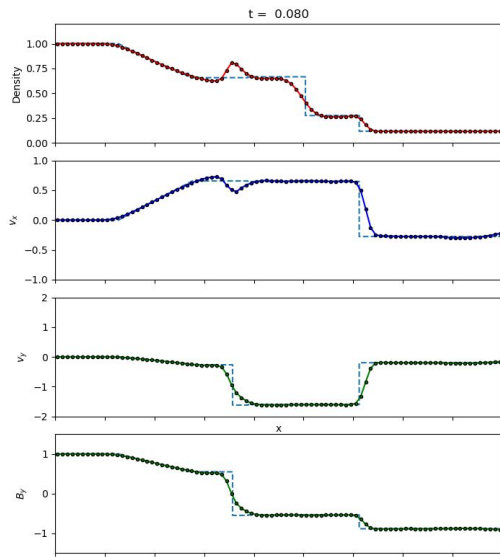
Since the divergence free condition **is trivially satisfied in 1D** (We have more on this later.)



No correction



Hyperbolic correction



Mixed correction

2D MHD ?

$$U_t + G(U)_y = 0$$

$$U = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{Bmatrix}; G(U) = \begin{Bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(E + p) \end{Bmatrix}$$

$$U_B = \bar{U}_n$$

$$U_T = \bar{U}_s$$

$$G_B = G(\bar{U}_n)$$

$$G_T = G(\bar{U}_s)$$

$$s_B = \min(v_B - a_B, v_T - a_T)$$

$$s_T = \min(v_B + a_B, v_T + a_T)$$

$$G = \begin{cases} G_B & \text{if } 0 \leq s_B \\ \frac{s_T G_B - s_B G_T + s_B s_T (U_T - U_B)}{s_T - s_B} & \text{if } s_B \leq 0 \leq s_T \\ G_T & \text{if } 0 \geq s_T \end{cases}$$

$$U_t + F(U)_x = 0$$

$$U = \begin{Bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{Bmatrix}; F(U) = \begin{Bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(E + p) \end{Bmatrix}$$

$$U_L = \bar{U}_e$$

$$U_R = \bar{U}_w$$

$$F_L = F(\bar{U}_e)$$

$$F_R = F(\bar{U}_w)$$

$$s_L = \min(u_L - a_L, u_R - a_R)$$

$$s_R = \min(u_L + a_L, u_R + a_R)$$

$$F = \begin{cases} F_L & \text{if } 0 \leq s_L \\ \frac{s_R F_L - s_L F_R + s_L s_R (U_R - U_L)}{s_R - s_L} & \text{if } s_L \leq 0 \leq s_R \\ F_R & \text{if } 0 \geq s_R \end{cases}$$

2D MHD ?

HLL in 2D - DS Balsara(2011)

$$\partial_t \mathbf{U} + \partial_x \mathbf{F} + \partial_y \mathbf{G} = 0$$

$$\begin{aligned} \mathbf{F}^* = & 2 \mathbf{U}^* S_R - \frac{S_U}{S_U - S_D} \mathbf{F}_U^{\text{HLL}} + \frac{S_D}{S_U - S_D} \mathbf{F}_D^{\text{HLL}} \\ & + 2 \frac{\mathbf{F}_{RU} S_U - \mathbf{F}_{RD} S_D + (\mathbf{G}_{RU} - \mathbf{G}_{RD}) S_R - (\mathbf{U}_{RU} S_U - \mathbf{U}_{RD} S_D) S_R}{S_U - S_D} \\ & + \frac{(\mathbf{F}_{RD} - \mathbf{F}_R^*) S_D^R - (\mathbf{F}_{RU} - \mathbf{F}_R^*) S_U^R - (\mathbf{G}_{RU} - \mathbf{G}_U^*) S_R^{U+} + (\mathbf{G}_{LU} - \mathbf{G}_U^*) S_L^{U+} + (\mathbf{G}_{RD} - \mathbf{G}_D^*) S_R^{D+} - (\mathbf{G}_{LD} - \mathbf{G}_D^*) S_L^{D+}}{S_U - S_D} \end{aligned}$$

$$\begin{aligned} S_R^U &= \max(\lambda_x^N(\mathbf{U}_{RU}), \bar{\lambda}_x^N(\mathbf{U}_{LU}, \mathbf{U}_{RU})) \quad ; \quad S_L^U = \min(\lambda_x^1(\mathbf{U}_{LU}), \bar{\lambda}_x^1(\mathbf{U}_{LU}, \mathbf{U}_{RU})) \quad S_U^R = \max(\lambda_y^N(\mathbf{U}_{RU}), \bar{\lambda}_y^N(\mathbf{U}_{RD}, \mathbf{U}_{RU})) \quad ; \quad S_D^R = \min(\lambda_y^1(\mathbf{U}_{RD}), \bar{\lambda}_y^1(\mathbf{U}_{RD}, \mathbf{U}_{RU})) \\ S_R^D &= \max(\lambda_x^N(\mathbf{U}_{RD}), \bar{\lambda}_x^N(\mathbf{U}_{LD}, \mathbf{U}_{RD})) \quad ; \quad S_L^D = \min(\lambda_x^1(\mathbf{U}_{LD}), \bar{\lambda}_x^1(\mathbf{U}_{LD}, \mathbf{U}_{RD})) \quad S_U^L = \max(\lambda_y^N(\mathbf{U}_{LU}), \bar{\lambda}_y^N(\mathbf{U}_{LD}, \mathbf{U}_{LU})) \quad ; \quad S_D^L = \min(\lambda_y^1(\mathbf{U}_{LD}), \bar{\lambda}_y^1(\mathbf{U}_{LD}, \mathbf{U}_{LU})) \\ S_R &= \max(S_R^U, S_R^D) \quad ; \quad S_L = \min(S_L^U, S_L^D) \quad S_U = \max(S_U^R, S_U^L) \quad ; \quad S_D = \min(S_D^R, S_D^L) \end{aligned}$$

Orszag-Tang Vortex

2D test problem. (BC: Periodic)

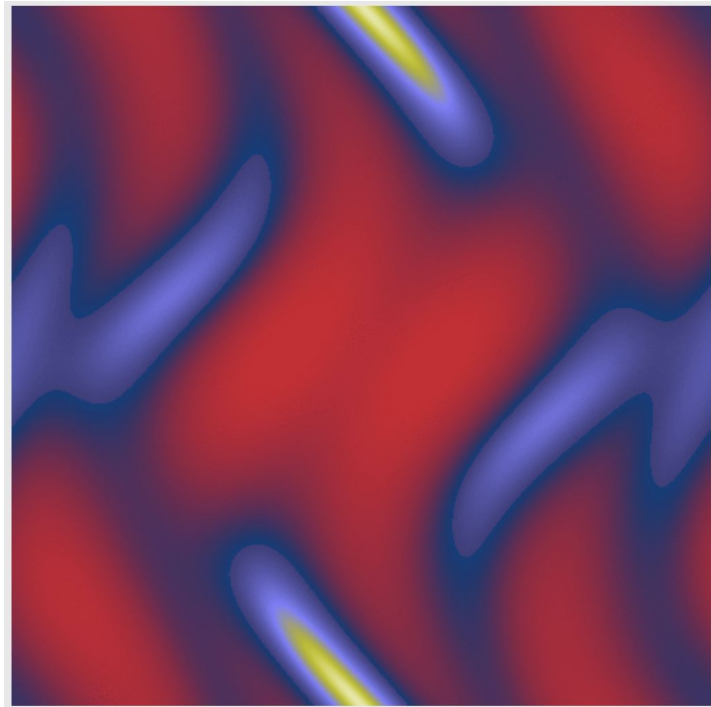
$$\rho(\mathbf{r}, 0) = \frac{\gamma^2}{4\pi},$$

$$p(\mathbf{r}, 0) = \frac{\gamma}{4\pi},$$

$$\mathbf{v}(\mathbf{r}, 0) = (-\sin(2\pi y), \sin(2\pi x)),$$

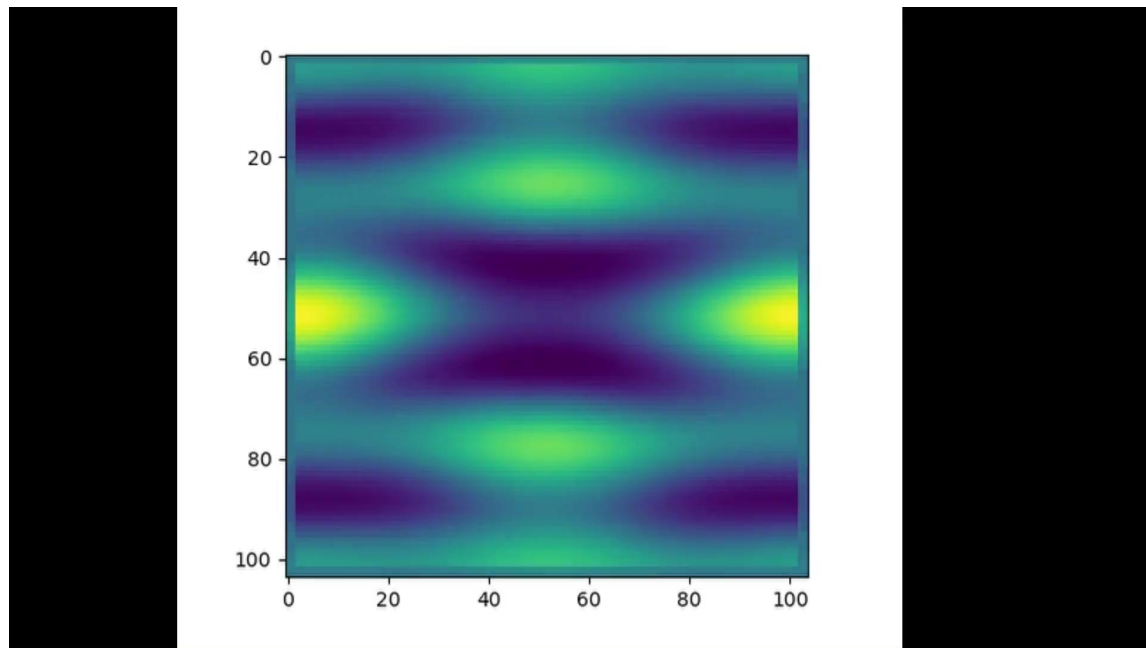
$$\mathbf{B}(\mathbf{r}, 0) = \frac{1}{2\pi\sqrt{4\pi}} \nabla_{\perp} \left(\frac{\cos(4\pi x)}{2} + \cos(2\pi y) \right)$$

Negative pressure ?!



openMHD

Current Progress

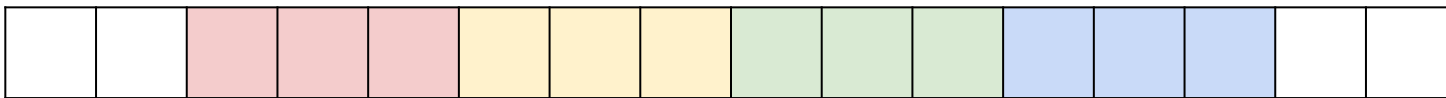


MPI Parallelization

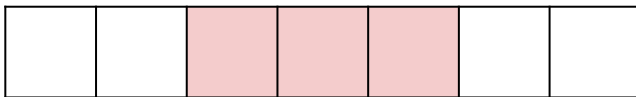
Syntax

- `comm = MPI.COMM_WORLD`
- `rank = comm.Get_rank()`
- `nrank = comm.Get_size()`
- `comm.Send()`
- `comm.Recv()`
- `comm.gather()`
- `comm.bcast()`

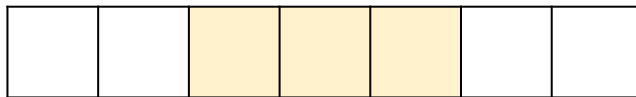
Split cells - 1D



Rank = 0



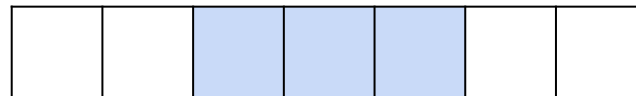
Rank = 1



Rank = 2

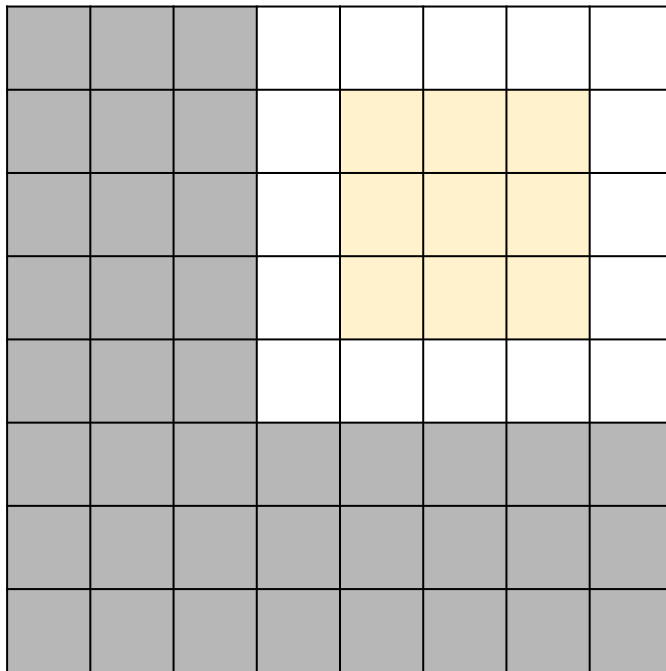


Rank = 3



	Red	Red	Red	Yellow	Yellow	Yellow	
	Red	Red	Red	Yellow	Yellow	Yellow	
	Red	Red	Red	Yellow	Yellow	Yellow	
	Green	Green	Green	Blue	Blue	Blue	
	Green	Green	Green	Blue	Blue	Blue	
	Green	Green	Green	Blue	Blue	Blue	

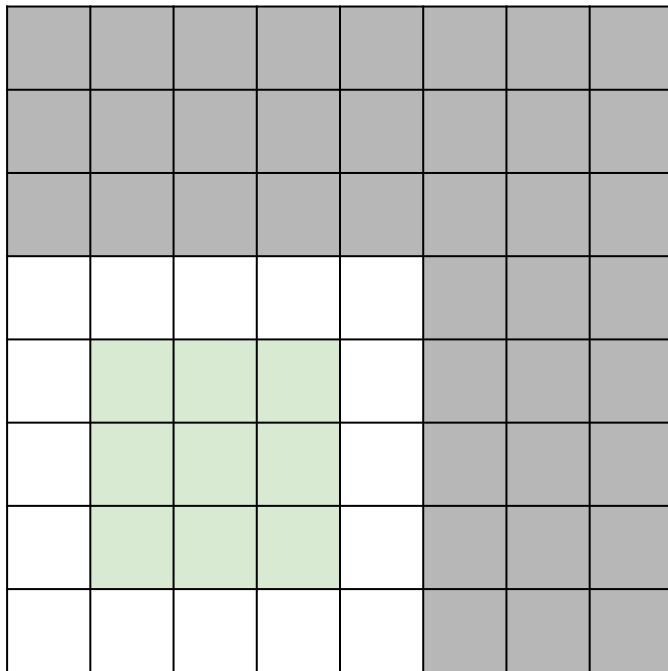
Split cells - 2D



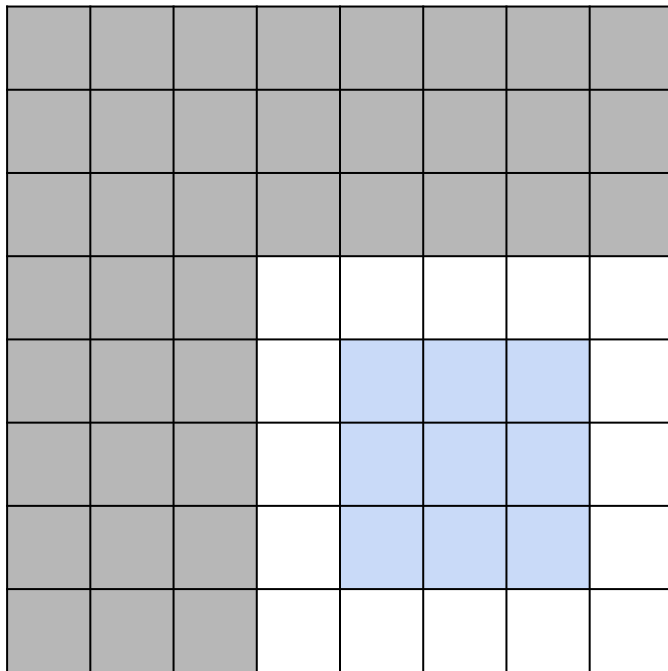
Rank = 1

Split cells - 2D

Rank = 2

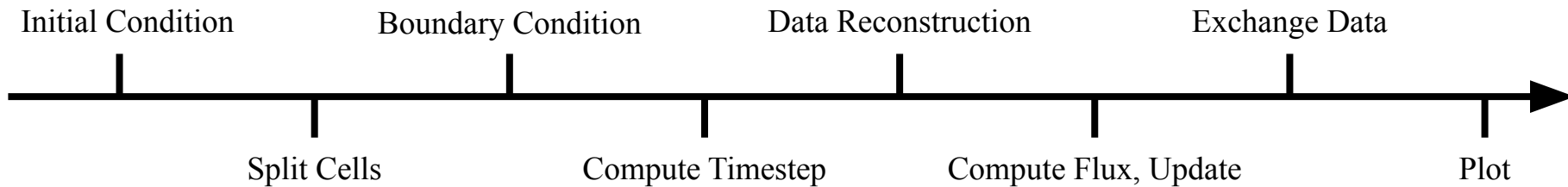


Split cells - 2D

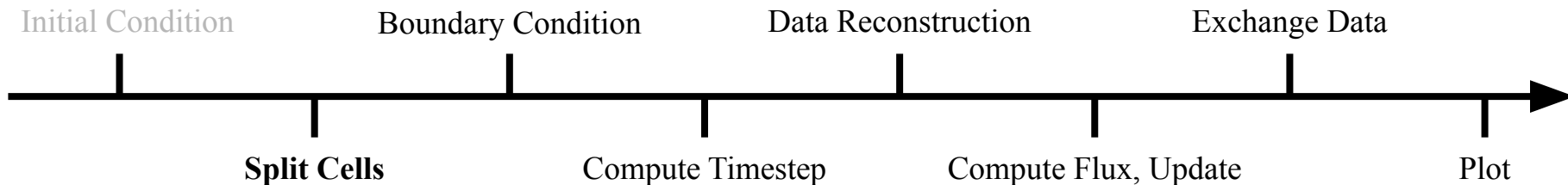


Rank = 3

Modifications



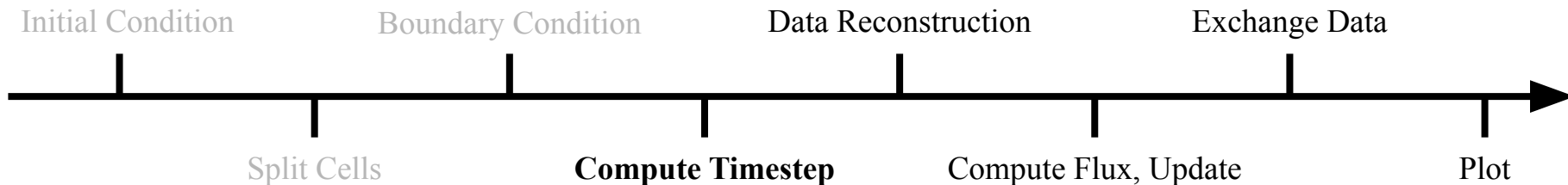
Modifications



```
u = np.empty((n,9))
U[0:nghost] = U[nghost]
U[N-nghost:N] = U[N-nghost-1]
u = U[rank*n_In:(rank+1)*n_In+4]
```

```
u = np.empty((n,n,9))
if rank == 0:
    u = U[:n,:n]
elif rank == 1:
    u = U[:n,-n:]
elif rank == 2:
    u = U[-n,:n]
elif rank == 3:
    u = U[-n,-n:]
```

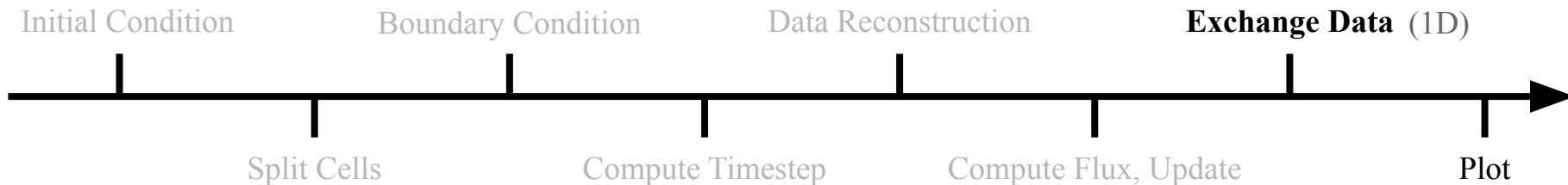
Modifications



```
max_info_speed = np.amax( u + cf )
dt_cfl         = cfl*dx/max_info_speed
dt_end         = end_time - t

dt_l = comm.gather(dt_cfl, root = 0)
DT = comm.bcast(dt_l, root = 0)
DT.append(dt_end)
dt = min(DT)
```

Modifications



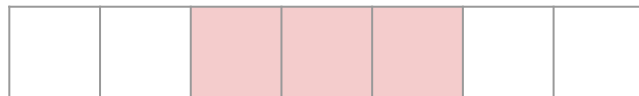
```
recv_l = np.empty((nghost,9))
recv_r = np.empty((nghost,9))
send_l = u[nghost:nghost+nghost]
send_r = u[n-nghost-nghost:n-nghost]

if rank%2 == 0:
    comm.Send(send_r, rank+1, tag = it+rank)
    comm.Recv(recv_r, rank+1, tag = it+rank+1)
    bd_r = recv_r
else:
    comm.Recv(recv_l, rank-1, tag = it+rank-1)
    comm.Send(send_l, rank-1, tag = it+rank)
    bd_l = recv_l
```

```
if rank != 0 and rank != nrank-1:
    if rank%2 == 0:
        comm.Send(send_l, rank-1, tag = it+rank)
        comm.Recv(recv_l, rank-1, tag = it+rank-1)
        bd_l = recv_l
    else:
        comm.Recv(recv_r, rank+1, tag = it+rank+1)
        comm.Send(send_r, rank+1, tag = it+rank)
        bd_r = recv_r
elif rank == 0:
    bd_l = u[0:nghost]
elif rank == nrank-1:
    bd_r = u[n-nghost:n]
```

Sending & Receiving data

Rank = 0



Rank = 1



Rank = 2

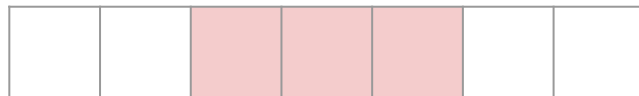


Rank = 3

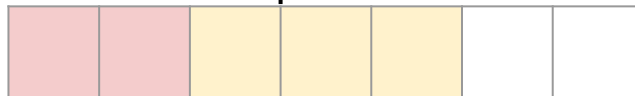


Sending & Receiving data

Rank = 0



Rank = 1



Rank = 2

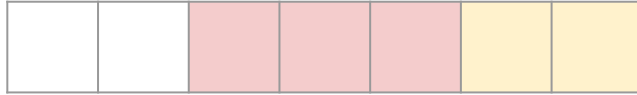


Rank = 3

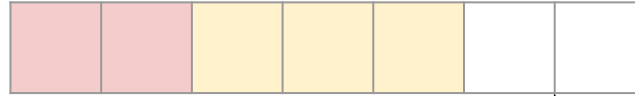


Sending & Receiving data

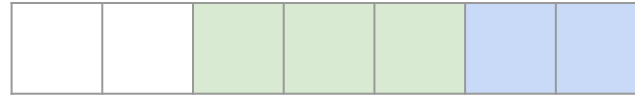
Rank = 0



Rank = 1



Rank = 2

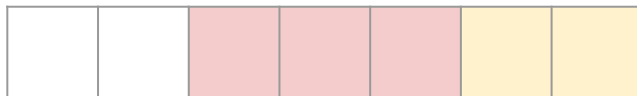


Rank = 3

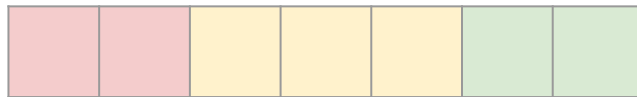


Sending & Receiving data

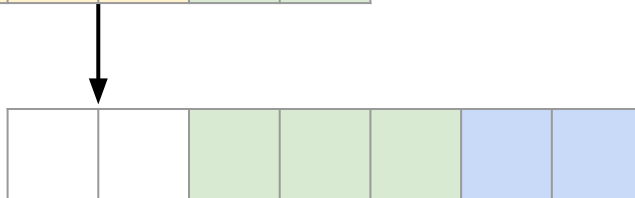
Rank = 0



Rank = 1



Rank = 2

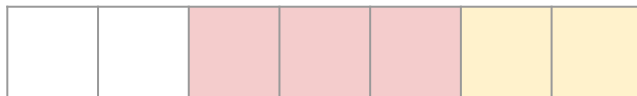


Rank = 3



Done!

Rank = 0



Rank = 1



Rank = 2



Rank = 3



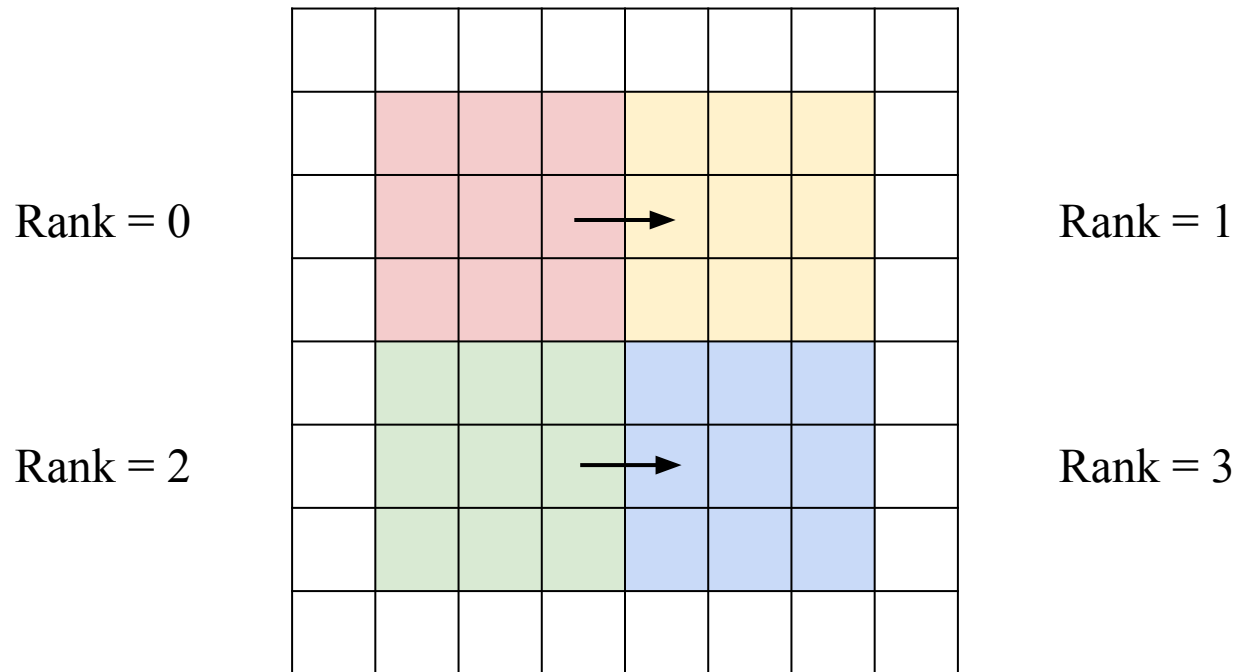
Modifications



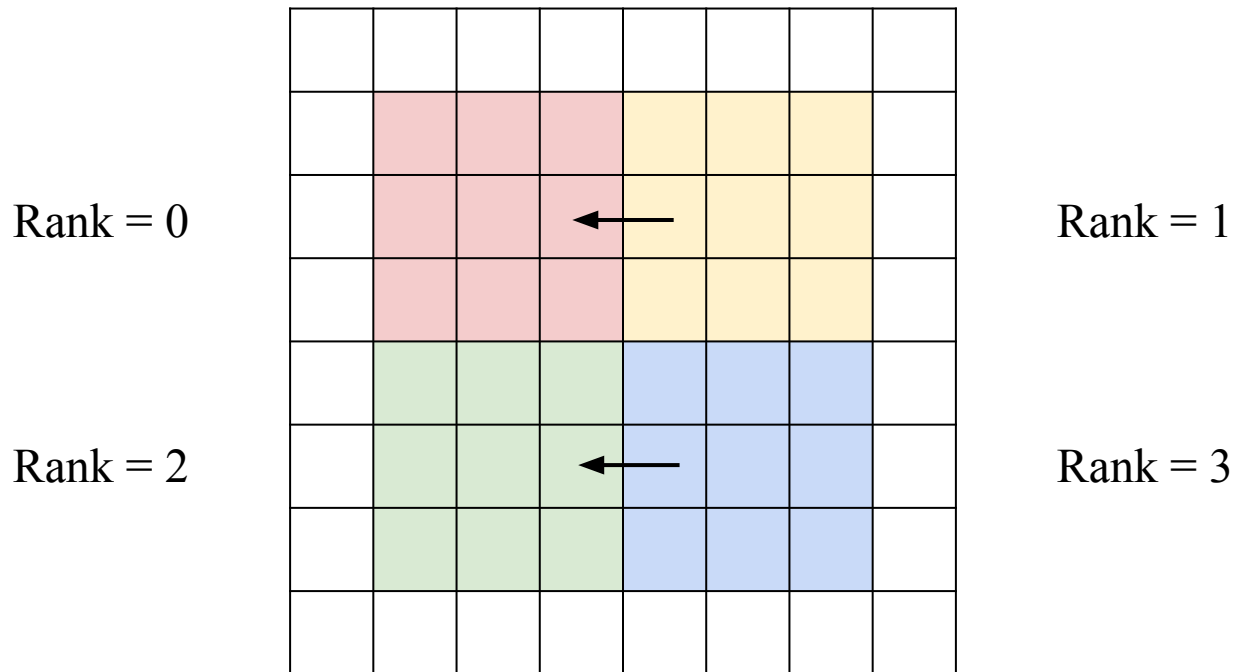
```
recv_u = np.empty((nghost*n,9))
recv_d = np.empty((nghost*n,9))
recv_r = np.empty((n*nghost,9))
recv_l = np.empty((n*nghost,9))
send_u = u[nghost:nghost+nghost].reshape(nghost*n,9)
send_d = u[n-nghost-nghost:n-nghost].reshape(nghost*n,9)
send_l = u[:, nghost:nghost+nghost].reshape(n*nghost,9)
send_r = u[:, n-nghost-nghost:n-nghost].reshape(n*nghost,9)
```

```
if rank%2 == 0:
    comm.Send(send_r, rank+1, tag = it+rank)
    comm.Recv(recv_r, rank+1, tag = it+rank+1)
    bd_r = recv_r.reshape(n,nghost,9)
    bd_l = u[:, :nghost]
else:
    comm.Recv(recv_l, rank-1, tag = it+rank-1)
    comm.Send(send_l, rank-1, tag = it+rank)
    bd_l = recv_l.reshape(n,nghost,9)
    bd_r = u[:, -nghost:]
if int(rank/2) == 0:
    comm.Send(send_d, rank+2, tag = it+rank+10)
    comm.Recv(recv_d, rank+2, tag = it+rank+12)
    bd_d = recv_d.reshape(nghost,n,9)
    bd_u = u[:,nghost, :]
else:
    comm.Recv(recv_u, rank-2, tag = it+rank+8)
    comm.Send(send_u, rank-2, tag = it+rank+10)
    bd_u = recv_u.reshape(nghost,n,9)
    bd_d = u[-nghost:, :]
```

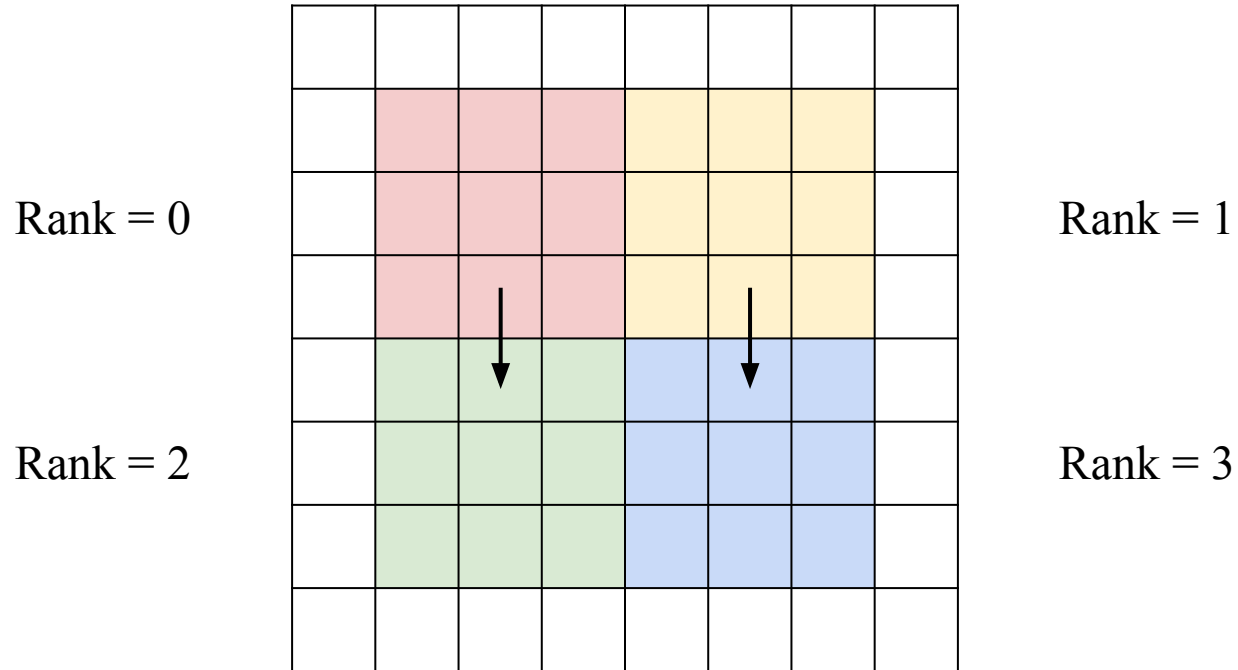
Sending & Receiving data



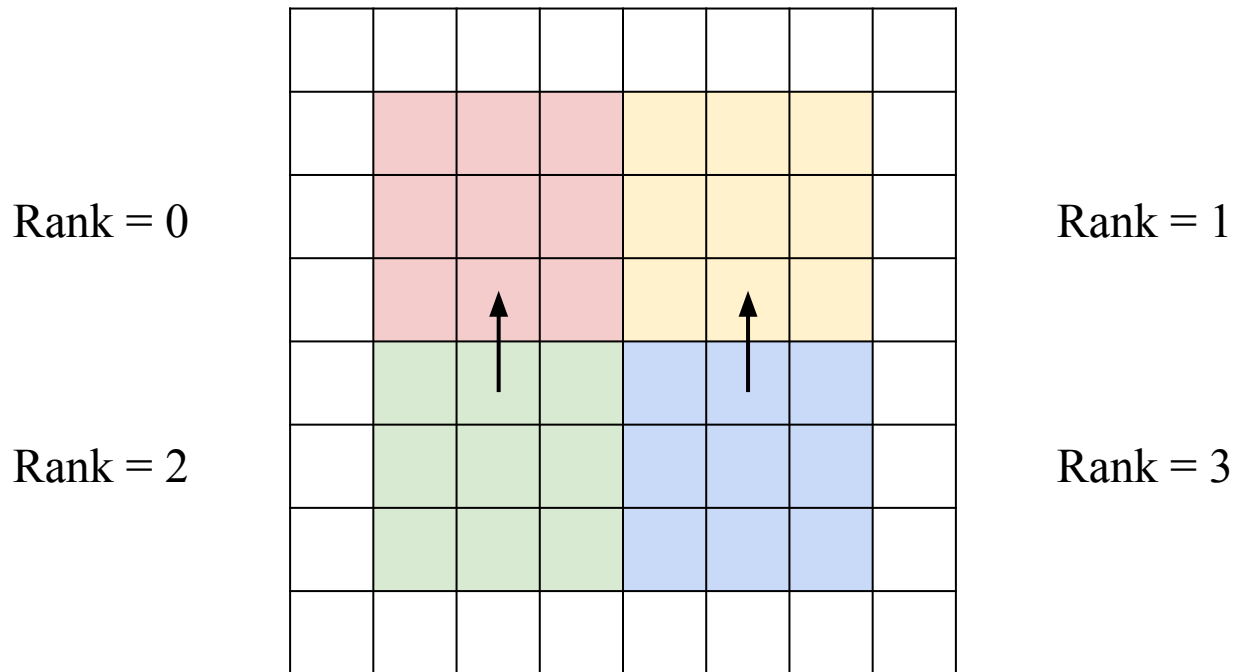
Sending & Receiving data



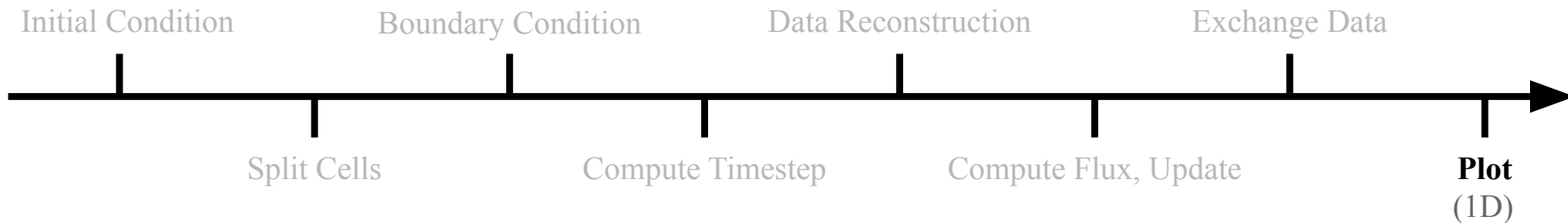
Sending & Receiving data



Sending & Receiving data

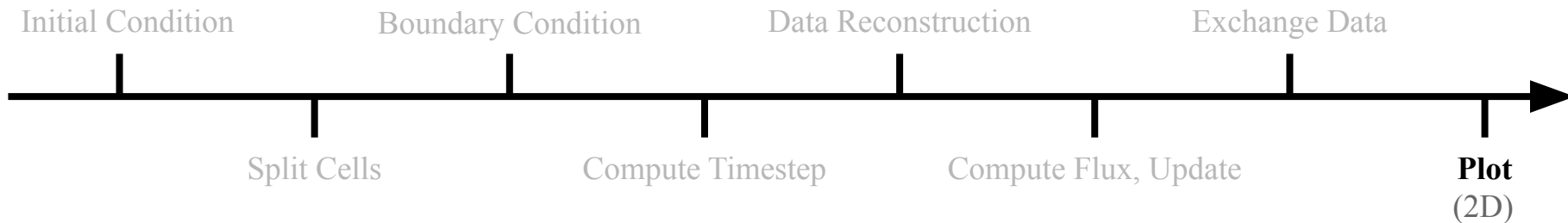


Modifications



```
Send = list(u[nghost:n-ghost])
Recv = comm.gather(Send, root = 0)
Bcast = comm.bcast(Recv, root = 0)
Cells = np.array( np.concatenate( np.array(Bcast), axis = None ) ).reshape((N_In,9))
U[nghost:N-ghost] = Cells
```

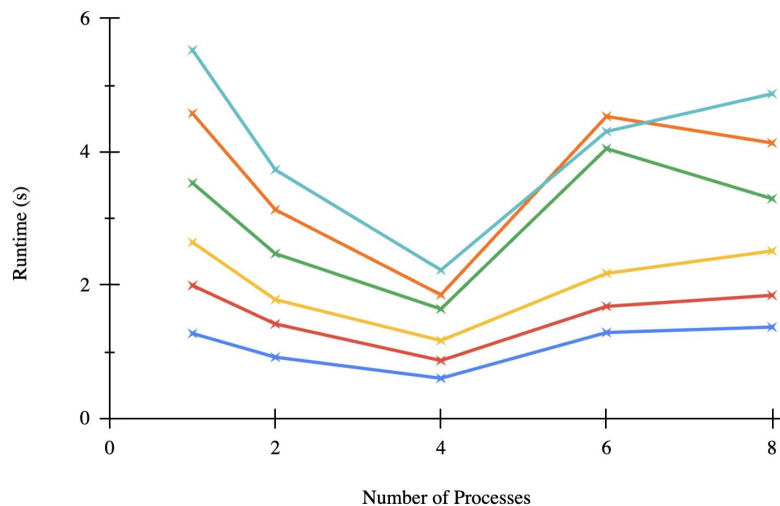
Modifications



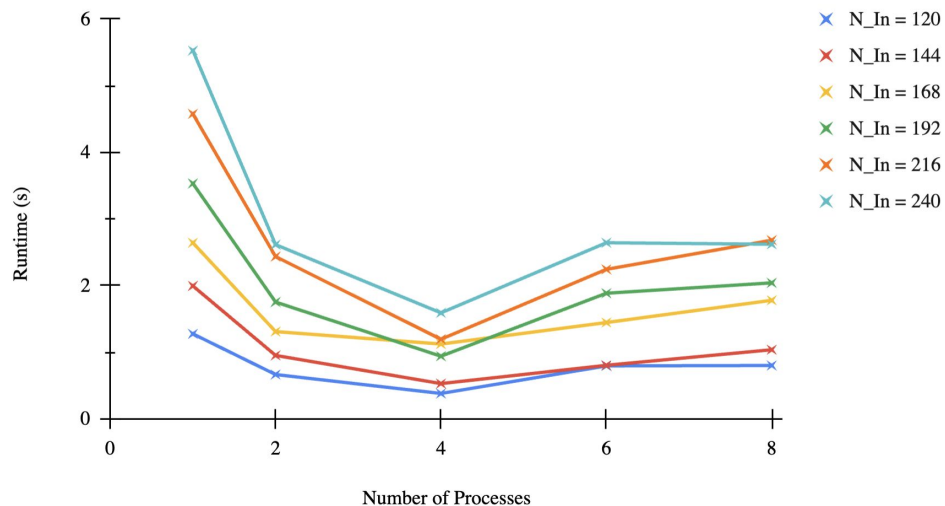
```
Send = list(u[nghost:n-nghost,nghost:n-nghost])
Bcast0 = comm.bcast(Send, root = 0)
Bcast1 = comm.bcast(Send, root = 1)
Bcast2 = comm.bcast(Send, root = 2)
Bcast3 = comm.bcast(Send, root = 3)
Cell0 = np.array( np.concatenate( np.array(Bcast0), axis = None ) ).reshape((n_In,n_In,9))
Cell1 = np.array( np.concatenate( np.array(Bcast1), axis = None ) ).reshape((n_In,n_In,9))
Cell2 = np.array( np.concatenate( np.array(Bcast2), axis = None ) ).reshape((n_In,n_In,9))
Cell3 = np.array( np.concatenate( np.array(Bcast3), axis = None ) ).reshape((n_In,n_In,9))
U[nghost:int(N/2),nghost:int(N/2)] = Cell0
U[nghost:int(N/2),int(N/2):N-nghost] = Cell1
U[int(N/2):N-nghost,nghost:int(N/2)] = Cell2
U[int(N/2):N-nghost,int(N/2):N-nghost] = Cell3
```

Performance

With gather() and bcast() in HLL

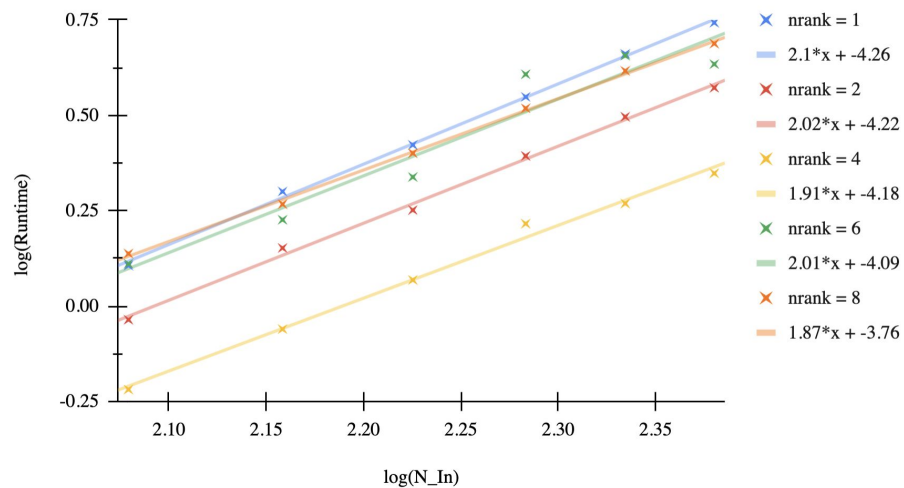


Without gather() and bcast() in HLL

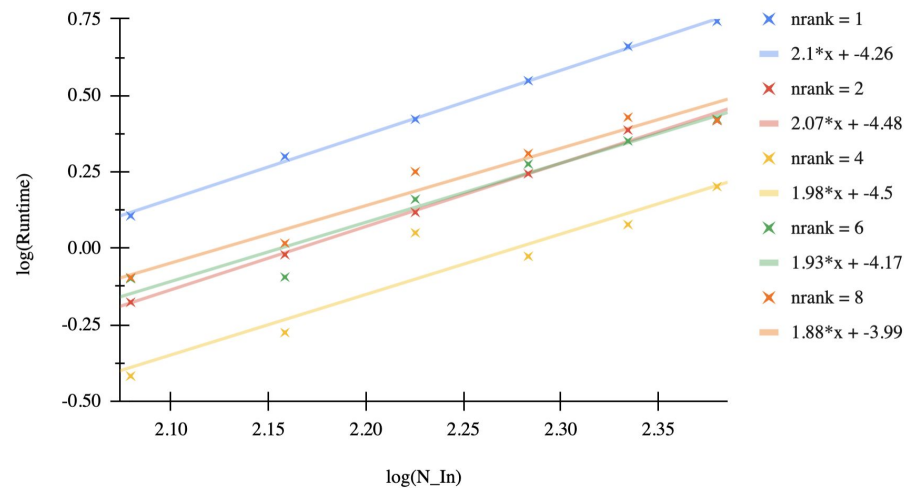


Performance

With gather() and bcast() in HLL



Without gather() and bcast() in HLL



Discussion

Most time consuming step: gather and bcast

Turns out that the gather and bcast was unnecessary inside **def HLL**, because the signs of SL and SR stayed the same

gather and bcast are still necessary in **ComputeTimestep**, and when nrank went from 4 to 6, the average time it takes to compute went up a whopping 30 times.

The scaling of runtime with N is as expected for other steps

Sending and receiving data took less time than expected

(Possible) Far Future Works

- HLL in 2D - DS Balsara(2011) - WIP ('bout to RIP)
- Compare different correction methods.
- Compare with CT method.
- HLLC, HLLD, Roe.....
- GPU parallel
- Update our Github pages.
- Lots of thing to do, but not lots of time.....
- Have some good sleeps finally.....

Reference

- [1] Brio, M. ; Wu, C. C. An Upwind Differencing Scheme for the Equations of Ideal Magnetohydrodynamics. Journal of Computational Physics, Volume 75, Issue 2, p. 400-422.
- [2] Li, Shengtai. An HLLC Riemann solver for magneto-hydrodynamics. Journal of Computational Physics, Volume 203, Issue 1, p. 344-357.
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Contribution Table

Divergence Cleaning: 賴伯熏

1D MHD Riemann Solver: 黃品睿

2D MHD: 吳冠霖

MPI Parallelization: 曾映舫

Github Page

We didn't really have time to sort out our Github pages. Most of the code is still in our personal branches, but they are public. You may take a look if wanted, and sorry for the inconvenience.

- pipimei: Hydro Riemann solver and MHD Riemann solver (single process)
- grid: MPI parallelization, supporting 1D hydro and MHD (both 1D and 2D). Cleaning included for 1D MHD.
- JW: 2D MHD and CT test code

Project-V: Divergence Cleaning for MHD

1. Implement a divergence cleaning method for MHD
 - a. Compare the **divergence errors** with and without this correction
 - b. No need to adopt the constraint transport technique
 - c. Apply to a **MHD test problem** (e.g., MHD Riemann problems)
 - d. Measure the **performance scaling** (i.e., wall-clock time vs. number of cells)
2. Bonus points
 - a. You get **bonus points automatically** since this topic is not covered by our lecture
 - b. Incorporate with a **high-resolution shock capturing scheme**
3. Reference
 - a. Hyperbolic Divergence Cleaning for the MHD Equations:
<https://www.sciencedirect.com/science/article/pii/S002199910196961X>

1D —> Grade : F

Thank you !

And wish you all a great summer.