

Removal of pseudo-convergence in near-coplanar  
Riemann problems of ideal  
magnetohydrodynamics  
and  
parallel fluid simulations on shared memory  
processors

Andrew Kercher

George Mason University

29 September 2014

# Outline

## Introduction

Shocks in space plasma

Overview

Riemann problems of ideal MHD

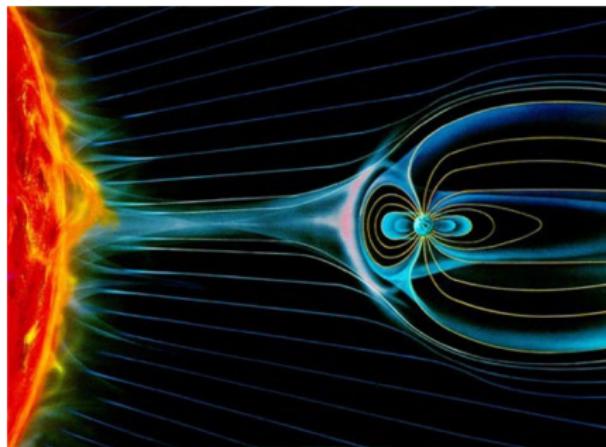
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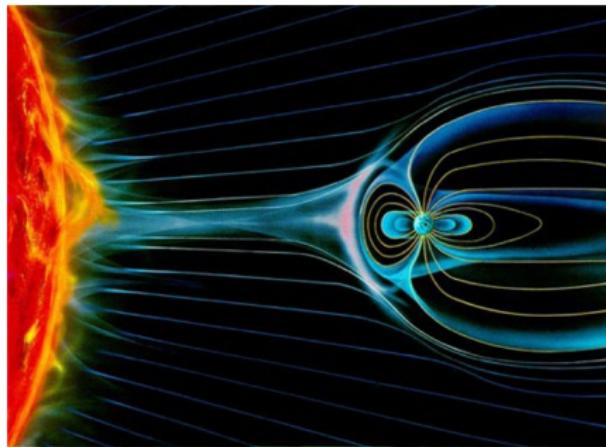
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Source [10]

- Sun-earth interaction:
  - ▶ Super-sonic plasma originating at sun travels toward earth.

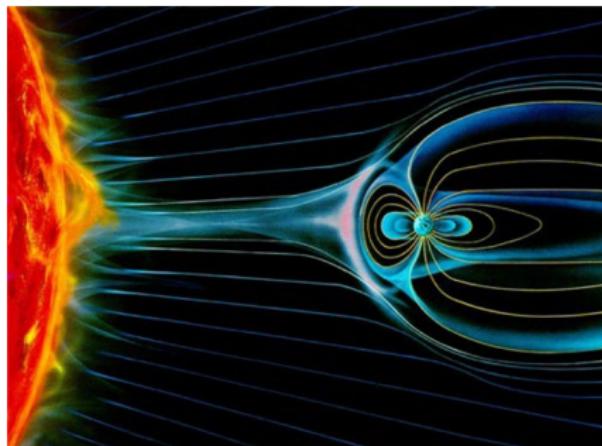
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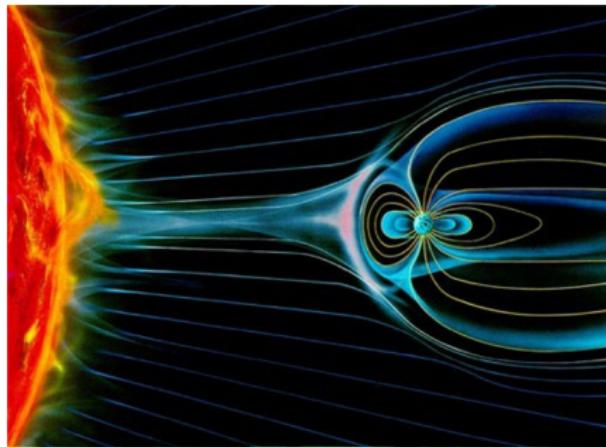
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- Sun-earth interaction:
  - ▶ Super-sonic plasma originating at sun travels toward earth.
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  - ▶ Plasma flow becomes subsonic forming a bow shock.

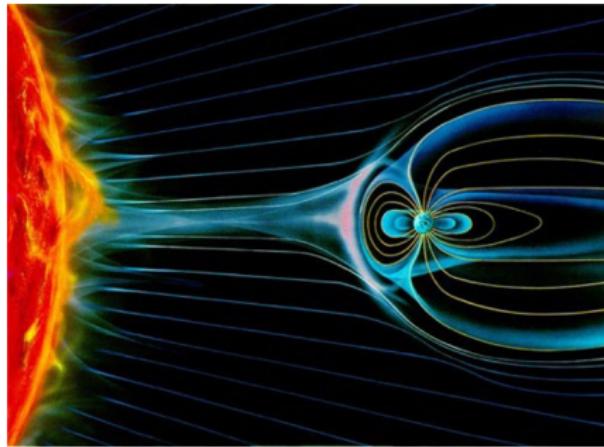
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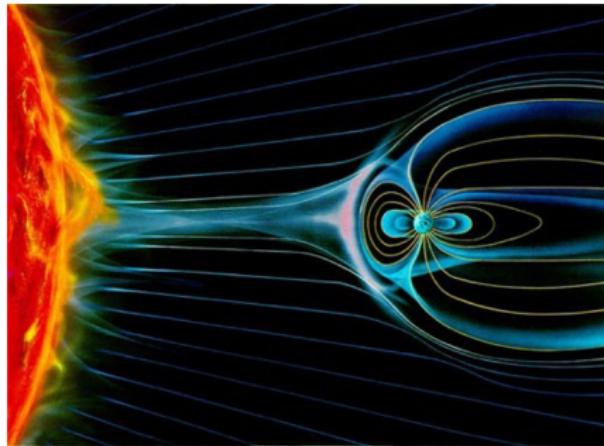
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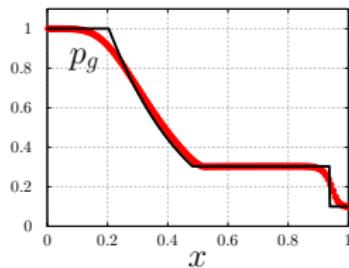
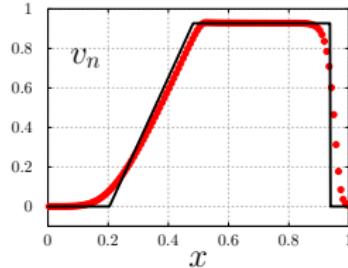
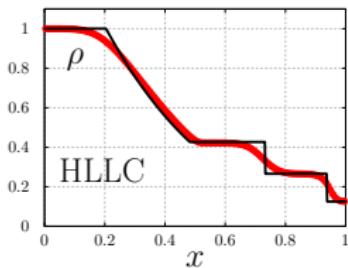
- Compound wave formation in MHD bow shock simulations.
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- Slow convergence with finite volume schemes.
- Compound wave modification (CWM).
  - ▶ Modification to the HLLD approximate Riemann solver of Athena [11].
  - ▶ Removes compound wave, correctly computes rotational discontinuity.
  - ▶ Converges at all grid resolutions.
  - ▶ FAST! HLLD intermediate states are already calculated.

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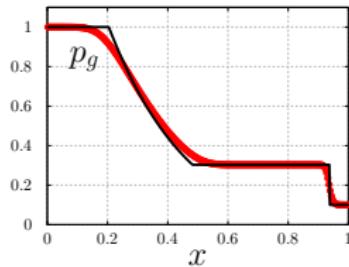
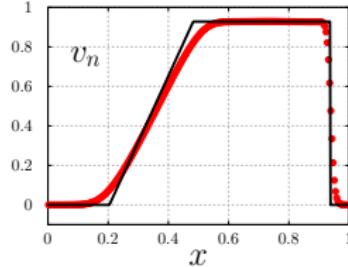
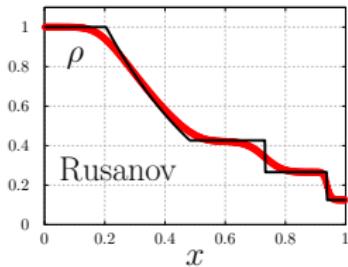
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- Description multi-dimensional fluid solver capable of shared memory parallelism.
  - ▶ Hydrodynamics and ideal MHD.
  - ▶ Algorithms implemented for unstructured grids.

# Limiting numerical diffusion

- **Total variation diminishing (TVD): Limit slope [5].**



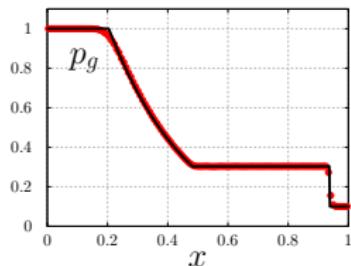
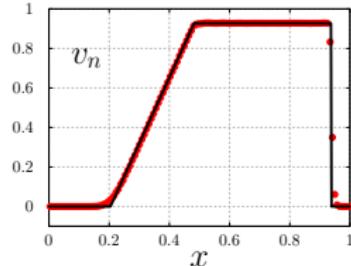
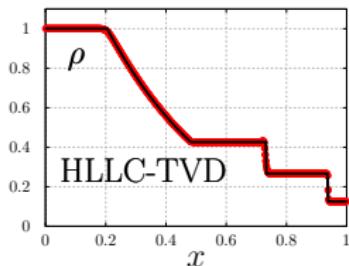
- **Flux corrected transport (FCT): Limit flux [1].**



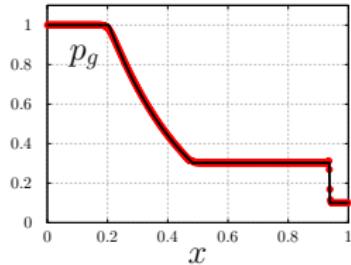
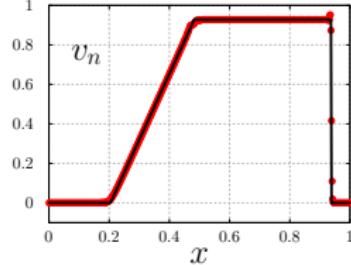
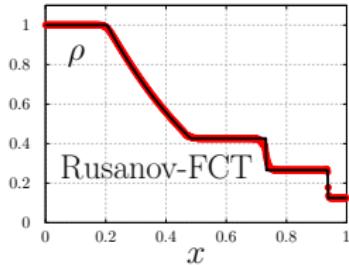
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## Ideal magnetohydrodynamics

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 ,$$

$$\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \otimes \mathbf{v} + \left( p_g + \frac{B^2}{2} \right) \mathbf{I} - \mathbf{B} \otimes \mathbf{B} \right] = 0 ,$$

$$\frac{\partial E}{\partial t} + \nabla \cdot \left[ \left( E + p_g + \frac{B^2}{2} \right) \mathbf{v} - \mathbf{v} \cdot \mathbf{B} \otimes \mathbf{B} \right] = 0 , \text{ and}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot [\mathbf{v} \otimes \mathbf{B} - \mathbf{B} \otimes \mathbf{v}] = 0 ,$$

where the energy density is defined as

$$E = \frac{p_g}{\gamma - 1} + \frac{\rho v^2}{2} + \frac{B^2}{2} ,$$

# Ideal magnetohydrodynamics

**Non-strictly** hyperbolic.

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = 0.$$

Real, but **not** necessarily distinct eigenvalues:

$\nu_n$  : contact or tangential discontinuity (entropy),

$\nu_n \pm c_s$  : slow rarefaction or shock,

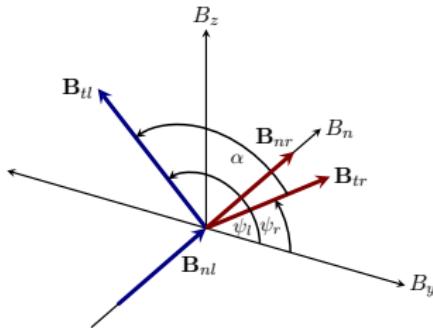
$\nu_n \pm c_a$  : rotational discontinuity (Alfvén), and

$\nu_n \pm c_f$  : fast rarefaction or shock,

$$c_{f,s}^2 = \frac{1}{2} \left[ a^2 + c_a^2 + c_t^2 \pm \sqrt{(a^2 + c_a^2 + c_t^2)^2 - 4a^2 c_a^2} \right],$$

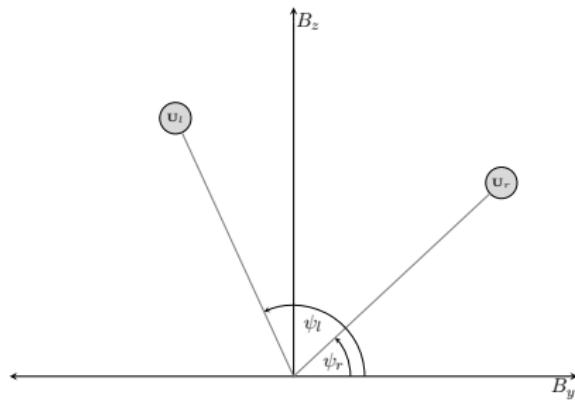
$$c_a^2 = \frac{B_n^2}{\rho}, \text{ and } c_t^2 = \frac{B_t^2}{\rho}.$$

# Riemann problems of ideal MHD



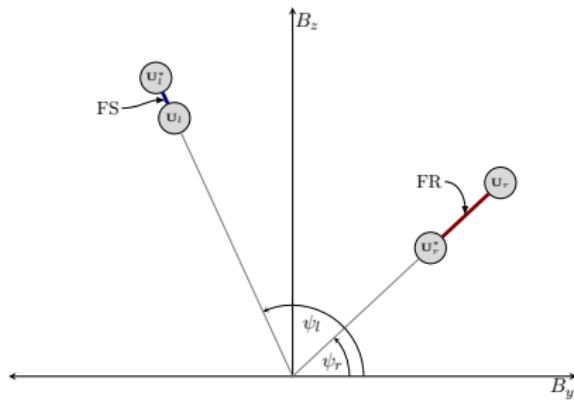
- Initial discontinuity separates two states.
- Rotation angle:  $\psi = \arctan(B_z/B_y)$ .
- Twist angle:  $\alpha = \psi_r - \psi_l$ .
- Solution: waves separating distinct states.

# Riemann problems of ideal MHD



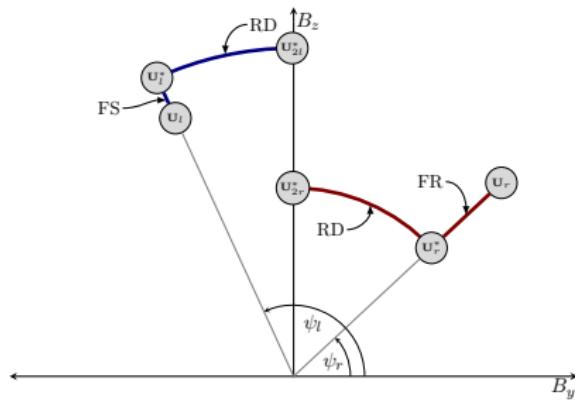
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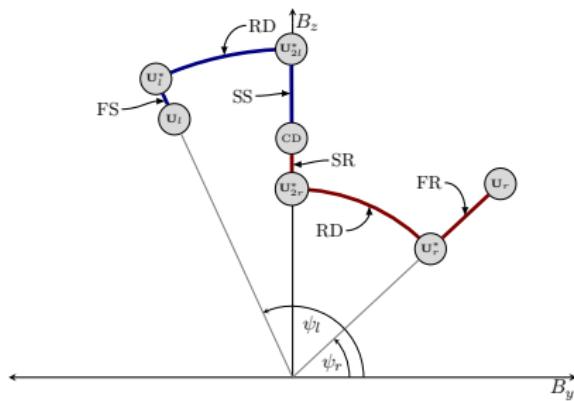
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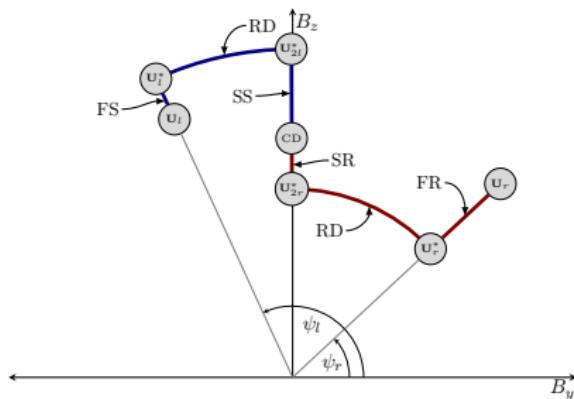
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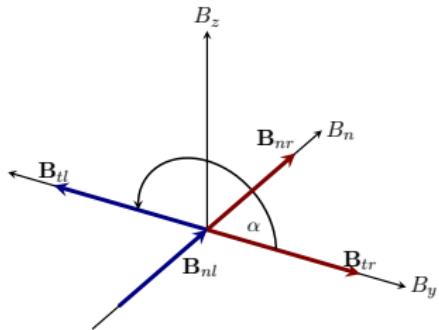
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- Slow shock:  $B_t \downarrow$ , slow rarefaction:  $B_t \uparrow$ .
- Contact discontinuity: no change.

# Riemann problems of ideal MHD



- Coplanar magnetic field

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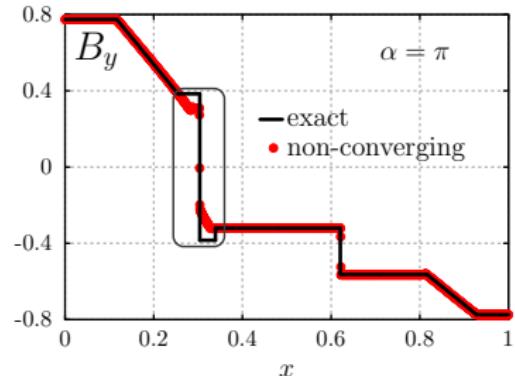
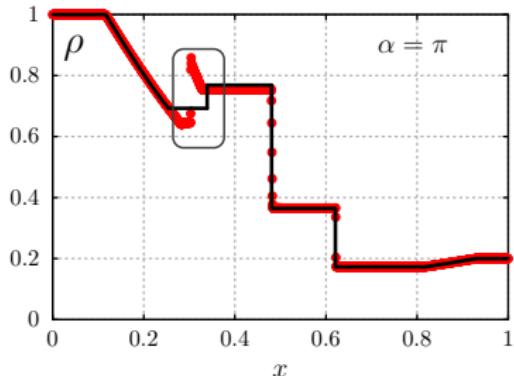
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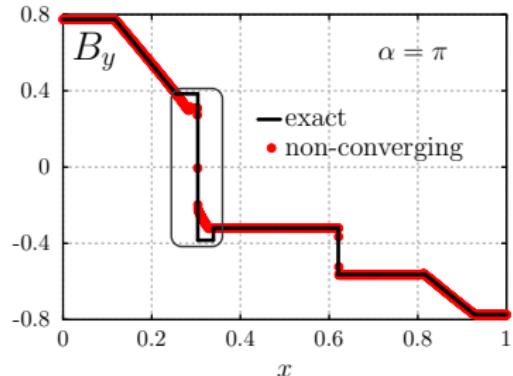
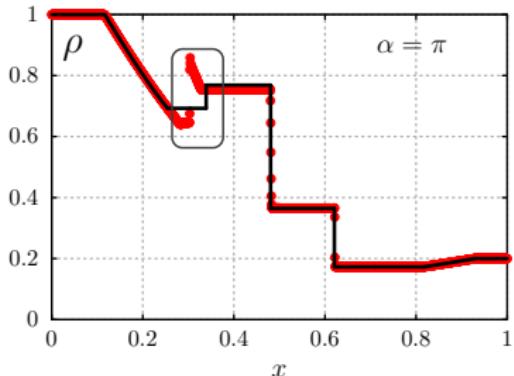
Shared memory parallelism

# Non-unique solutions



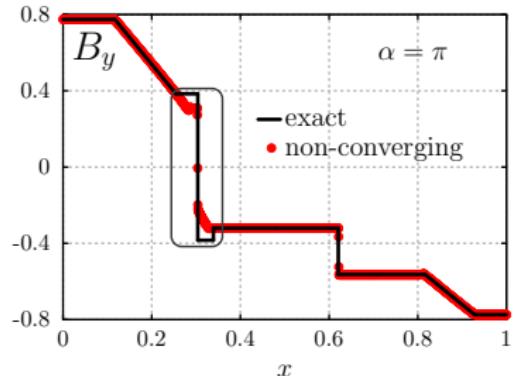
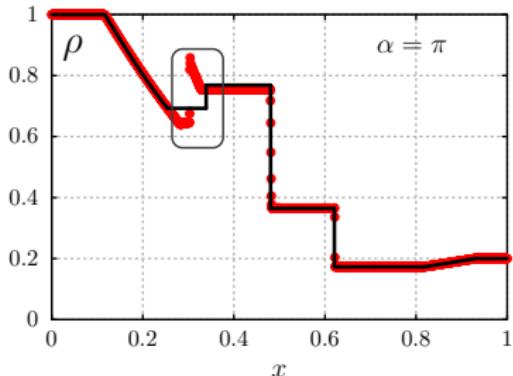
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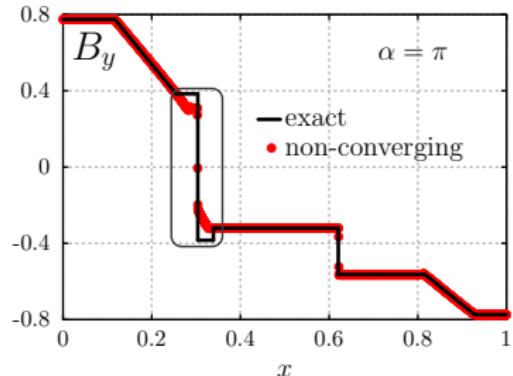
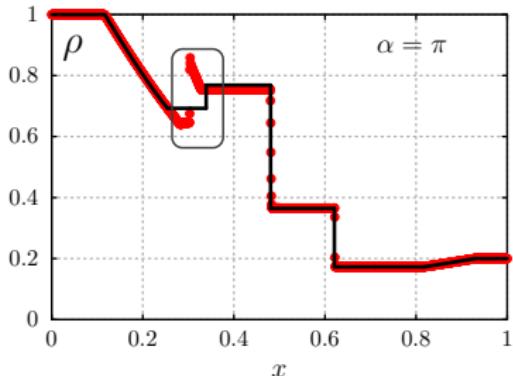
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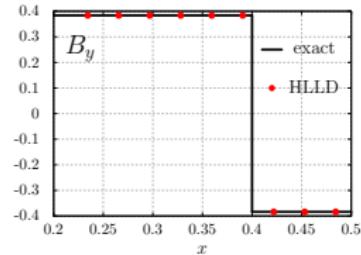
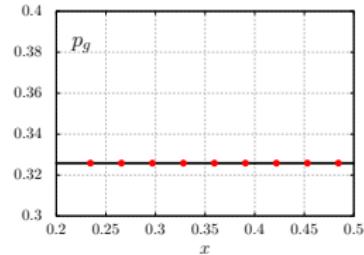
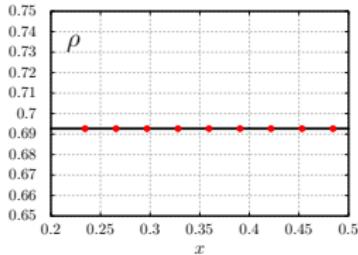
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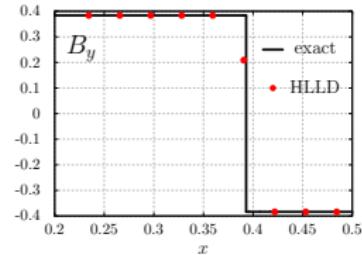
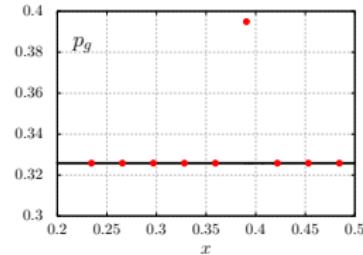
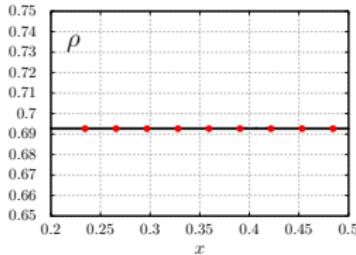
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  - ▶ Unstable for under small perturbations [7].
  - ▶ Satisfy jump conditions (coplanar case).

# Compound wave formation



- Compound waves are a product of numerical diffusion.

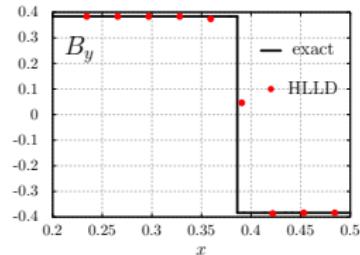
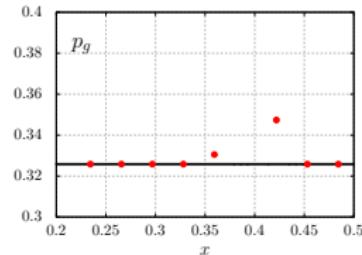
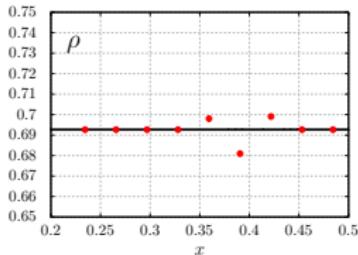
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$$p_g = (\gamma - 1) \left( E - \frac{\rho v^2}{2} - \frac{B^2}{2} \right)$$

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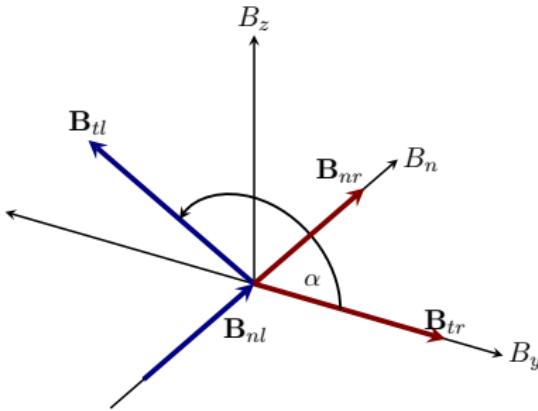


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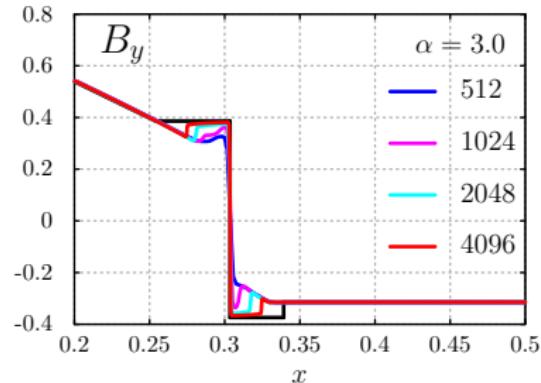
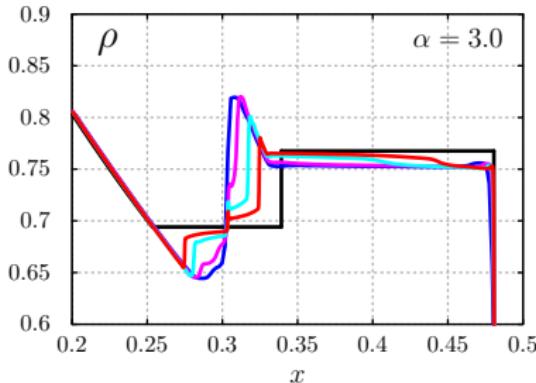
- Increase  $p_g \rightarrow$  compound wave.

# Pseudo-convergence



- $\alpha < \pi$ , compound waves at lower resolutions.

# Pseudo-convergence



- $\alpha < \pi$ , compound waves at lower resolutions.
- Pseudo-convergence: rotational discontinuity at higher resolutions [13].
- Transition between 1024 and 2048 grid points.
- $\alpha \rightarrow \pi$ , grid resolution increases.
- $\pi = \alpha$ , compound wave at all resolutions.

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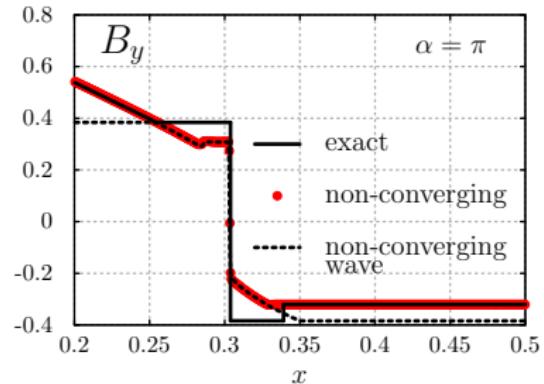
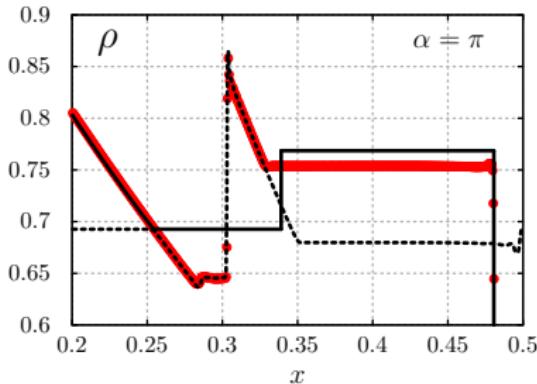
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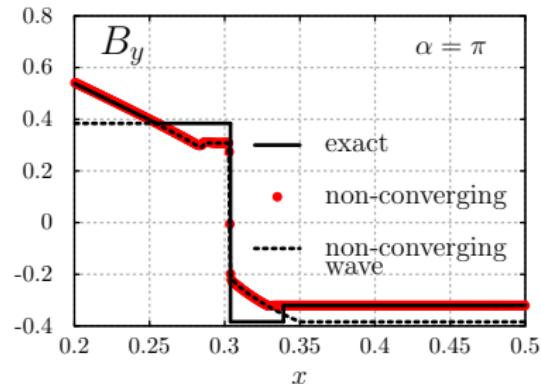
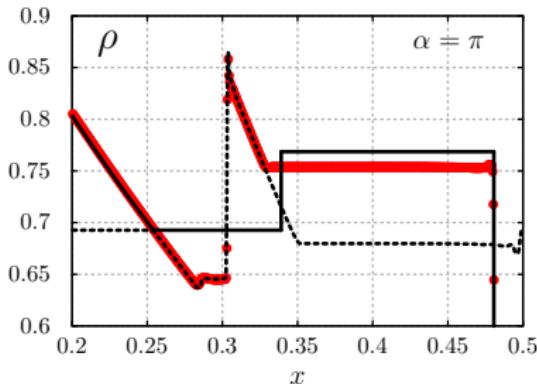
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# Compound wave modification



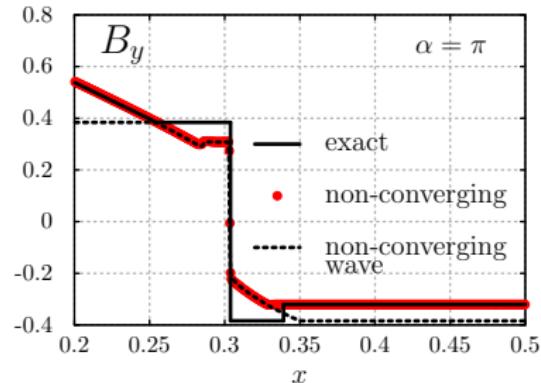
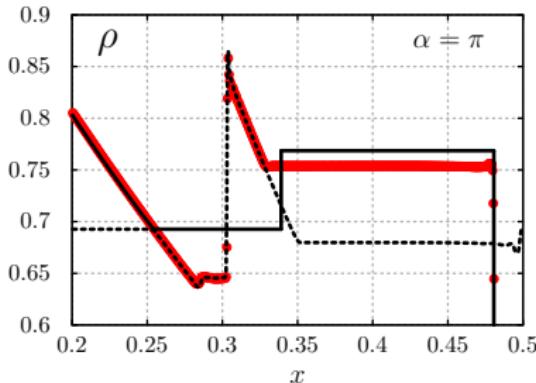
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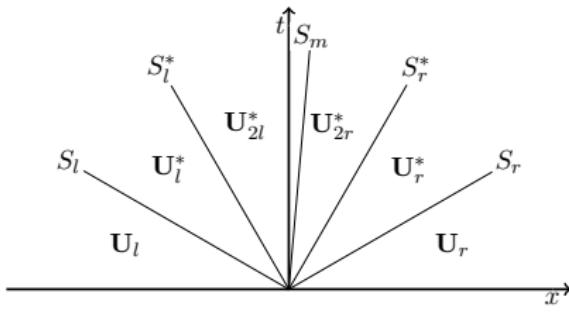
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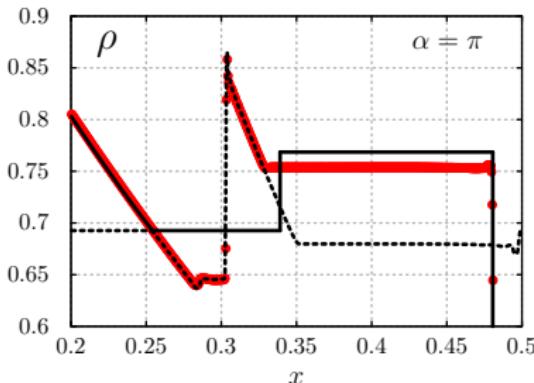


- Need to reduce numerical diffusion.
- $\rho$  and  $B_t$  should remain constant across the rotational discontinuity  $x = 0.303$ .
- Limit flux associated with the compound wave.

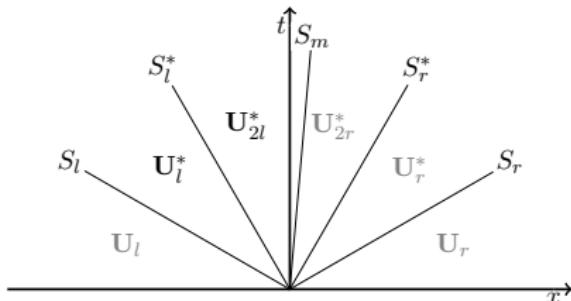
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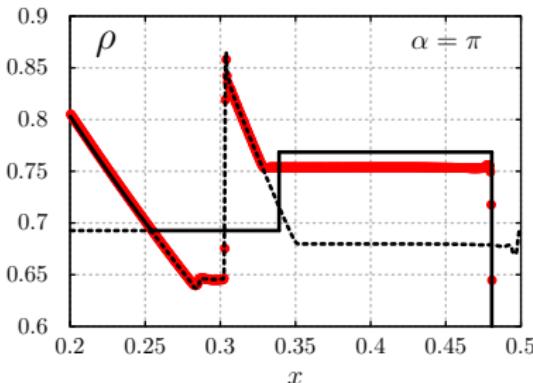
- Use HLLD to approximate intermediate states upstream and downstream of rotational discontinuity, i.e.,  $\mathbf{U}_l^*$  and  $\mathbf{U}_{2l}^*$ .



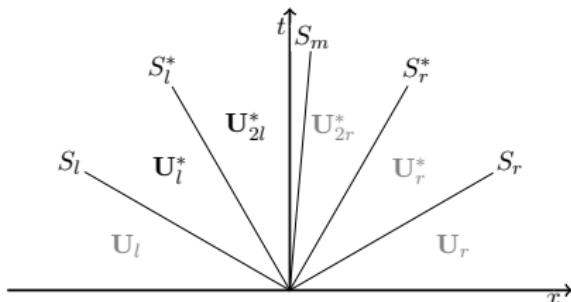
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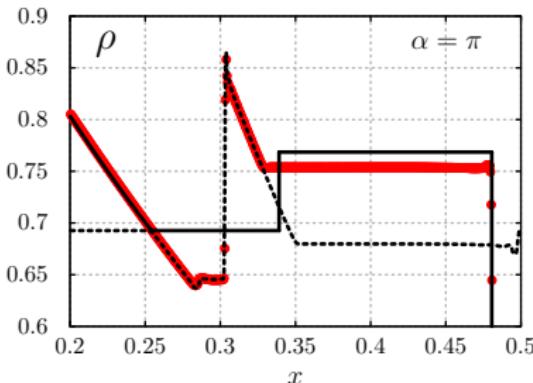
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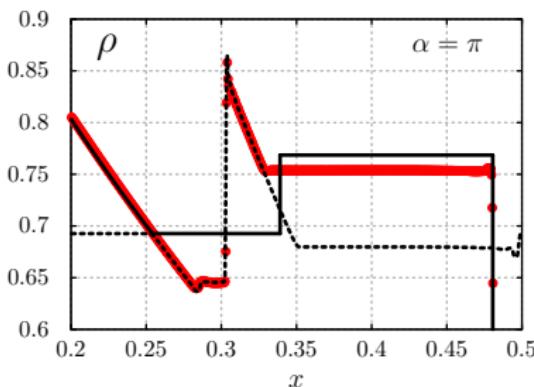
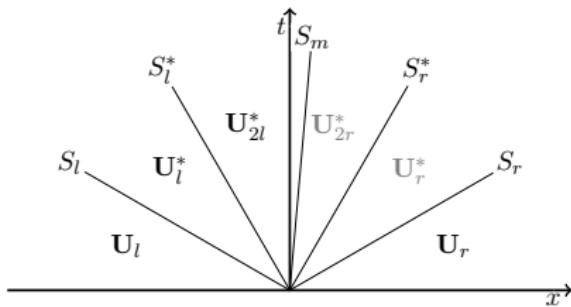
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- Calculate flux  $\mathbf{F}^c$  between  $\mathbf{U}_l^*$  and  $\mathbf{U}_{2l}^*$ .
- Reduce the contribution of  $\mathbf{F}^c = \mathbf{F}_{hlld}(\mathbf{U}_l^*, \mathbf{U}_{l2}^*)$  to the total flux.

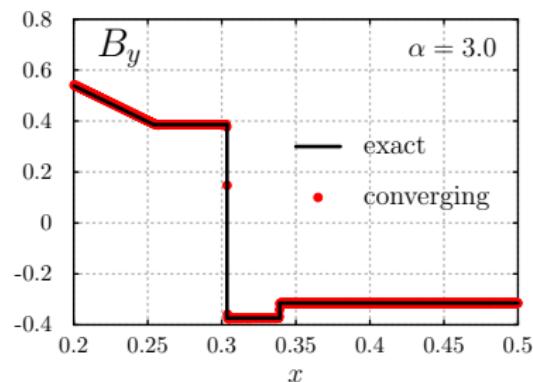
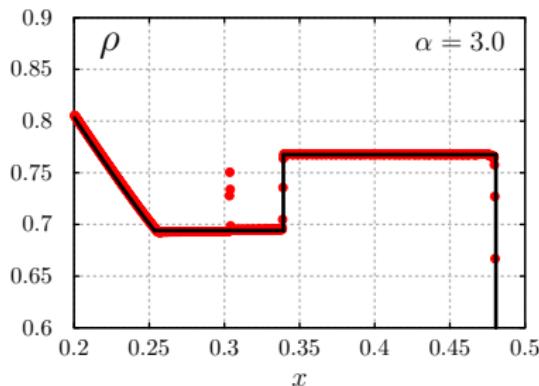


# Compound Wave modification



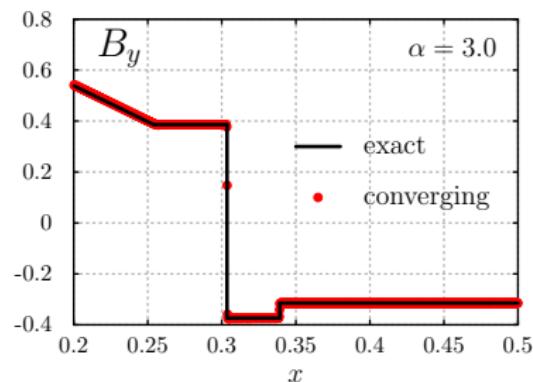
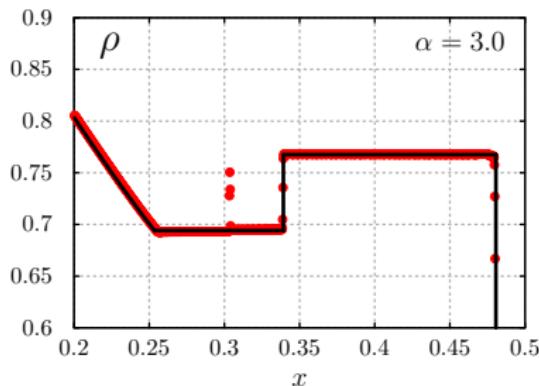
- Use HLLD to approximate intermediate states upstream and downstream of rotational discontinuity, i.e.,  $\mathbf{U}_l^*$  and  $\mathbf{U}_{2l}^*$ .
- Calculate flux  $\mathbf{F}^c$  between  $\mathbf{U}_l^*$  and  $\mathbf{U}_{2l}^*$ .
- Reduce the contribution of  $\mathbf{F}^c = \mathbf{F}_{hlld}(\mathbf{U}_l^*, \mathbf{U}_{l2}^*)$  to the total flux.
- $\mathbf{F}_{cwm} = \mathbf{F}_{hlld}(\mathbf{U}_l, \mathbf{U}_r) - A\mathbf{F}^c$ , where  $A < 0.5$ .

# CWM solution



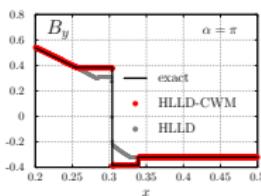
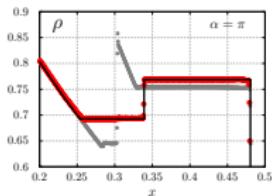
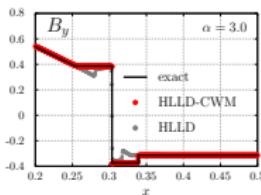
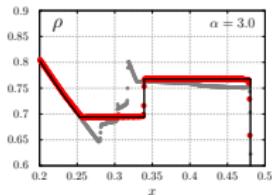
- CWM recovers the correct solution upstream and downstream of rotational discontinuity.
- Transition across rotational discontinuity is unresolved.
- Resolve it?

## CWM solution



- CWM recovers the correct solution upstream and downstream of rotational discontinuity.
- Transition across rotational discontinuity is unresolved.
- Resolve it?
- Simple but non-conservative.

# CWM Resolving the transition



- Jump conditions in Lagrangian mass coordinates,  $V = 1/\rho$ ,  $W$  is wave speed.
- Brackets denote difference across discontinuity.

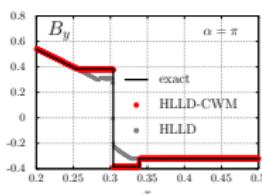
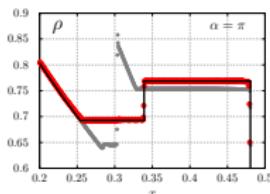
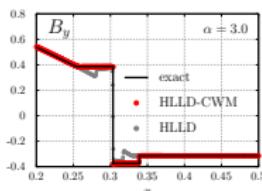
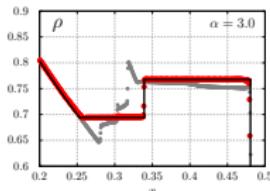
$$W[V] = -[v_n],$$

$$W[v_n] = -[P - B_n^2],$$

$$W[\mathbf{v}_t] = -B_n[\mathbf{B}_t],$$

$$W[V\mathbf{B}_t] = -B_n[\mathbf{v}_t],$$

# CWM Resolving the transition



- Across rotational discontinuity

$$[V] = 0,$$

$$[v_n] = 0,$$

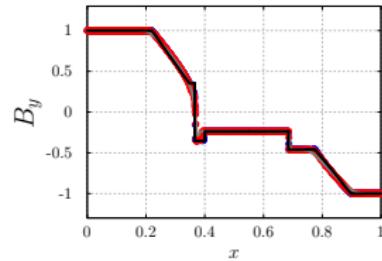
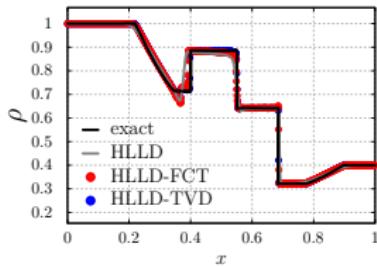
$$[p_g] = 0,$$

$$[B_t] = 0,$$

$$W[\mathbf{v}_t] = -B_n[\mathbf{B}_t],$$

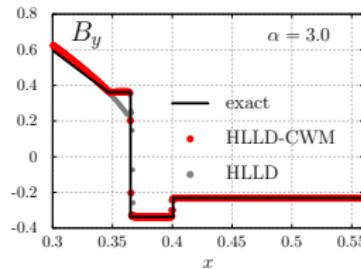
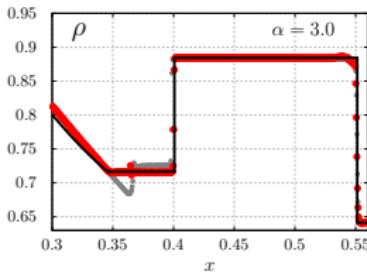
- $W = \sqrt{\rho}B_n$  is Lagrangian speed of linear wave.

# Examples



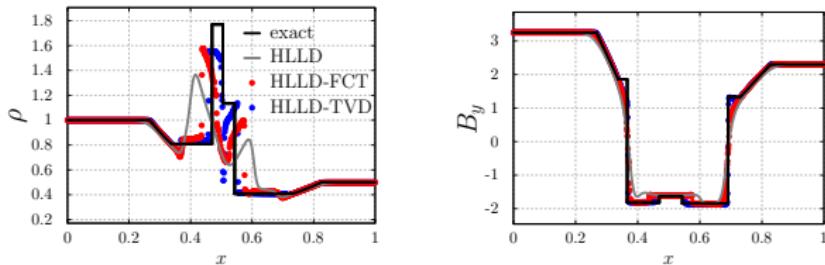
- Near coplanar initial conditions.
- Fast compound wave at  $x = 0.365$

# Examples



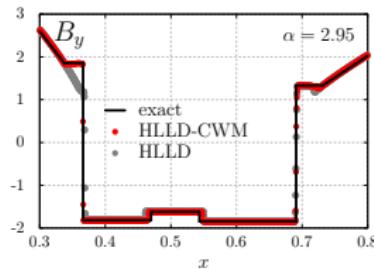
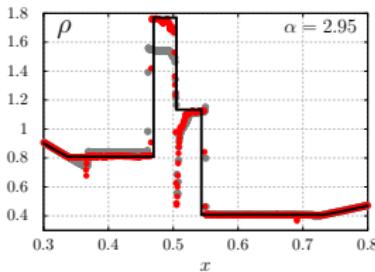
- Near coplanar initial conditions.
- Fast compound wave at  $x = 0.365$
- Small deviation for weak intermediate shocks.

# Examples



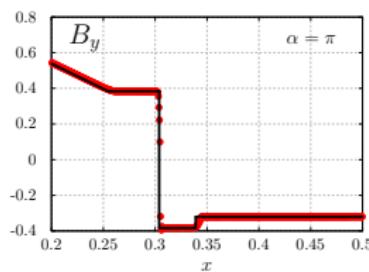
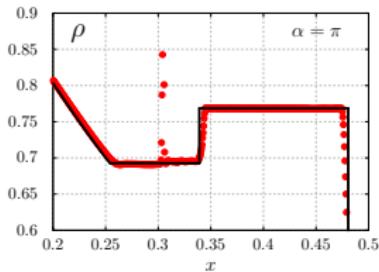
- Non-planar initial conditions.
- Fast compound waves at  $x = 0.366$  and  $x = 0.691$

# Examples



- Non-planar initial conditions.
- Fast compound waves at  $x = 0.366$  and  $x = 0.691$
- Small deviation for weak intermediate shocks.

# Examples



- Works with FCT!
- At rotation, set antidiffusion = CWM.
- Larger Cour. No. without additional diffusion downstream.
- Slow shock downstream poorly resolved, but weak.

# Outline

Introduction

Shocks in space plasma

Overview

Riemann problems of ideal MHD

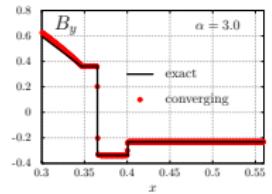
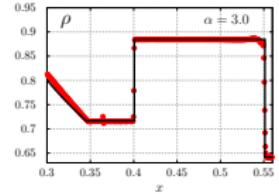
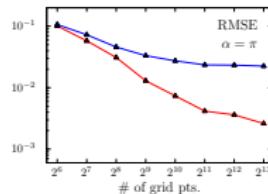
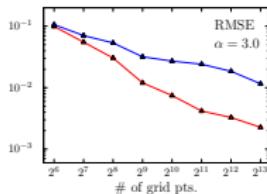
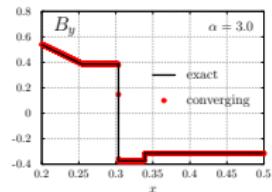
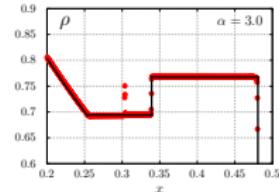
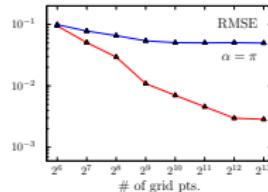
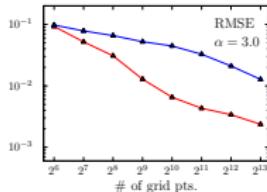
Compound wave formation in ideal MHD

Removing compound wave formation in ideal MHD

Convergence results using new modification

Shared memory parallelism

# Error analysis



- Error calculation without applying the correction at the rotational discontinuity.
- Without CWM, the compound wave starts to break apart between  $2^{10}$  and  $2^{11}$ .
- CWM produces convergence at low grid resolutions.
- $\approx 10$  times faster than exact Riemann solver.

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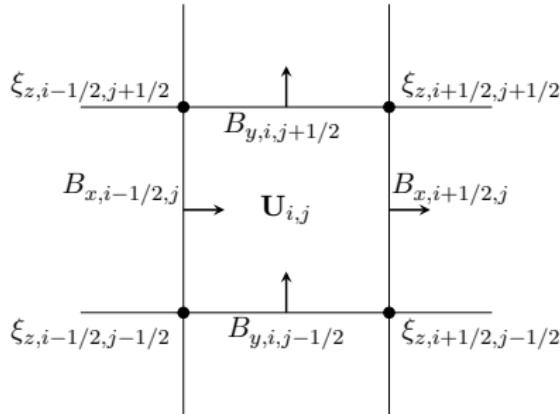
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# Higher dimensions

Maintaining  $\nabla \cdot \mathbf{B} = 0$  with constrained transport [4].

- Staggered grid.
- Hydrodynamical variables at cell centers.
- Magnetic field at interface.
- $\mathbf{E} = -\mathbf{v} \times \mathbf{B}$  at corners.
- Denote z-component of the emf as  $\xi_z$ .



Finite area integration of interface  $\mathbf{B}$

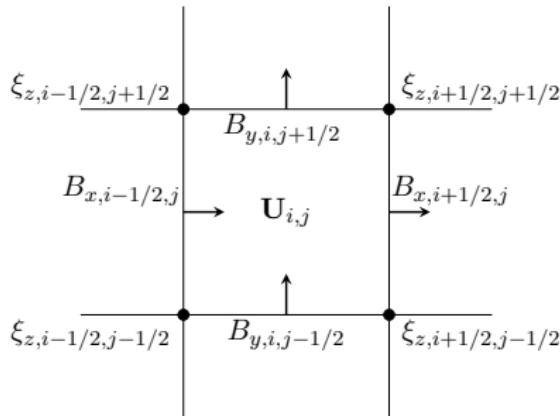
$$B_{x,i+1/2,j}^{n+1} = B_{x,i+1/2,j}^n - \frac{\delta t}{\delta y} (\xi_{z,i+1/2,j+1/2} - \xi_{z,i+1/2,j-1/2})$$

$$B_{y,i,j+1/2}^{n+1} = B_{y,i,j+1/2}^n + \frac{\delta t}{\delta x} (\xi_{z,i+1/2,j+1/2} - \xi_{z,i-1/2,j-1/2})$$

# Higher dimensions

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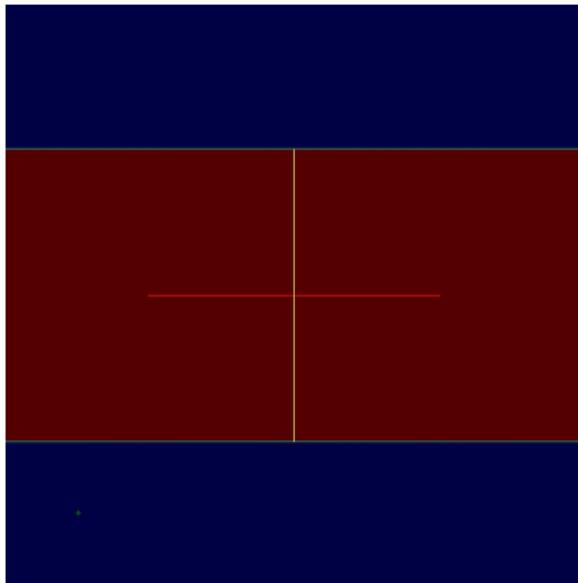
- Staggered grid.
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- $\mathbf{E} = -\mathbf{v} \times \mathbf{B}$  at corners.
- Denote z-component of the emf as  $\xi_z$ .



Due to perfect cancellation, the numerical divergence in the cell remains zero to machine precision.

$$(\nabla \cdot \mathbf{B})_{i,j} = \frac{1}{\delta x} (B_{x,i+1/2,j} - B_{x,i-1/2,j}) + \frac{1}{\delta y} (B_{y,i,j+1/2} - B_{y,i,j-1/2})$$

# Performance Comparison

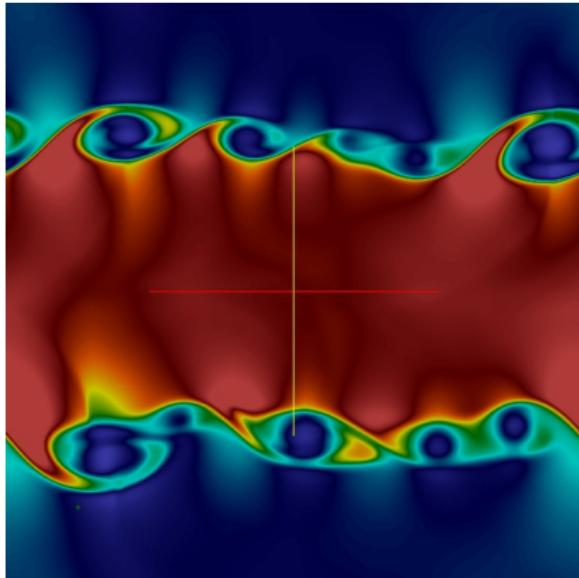


Performance comparison for Kelvin-Helmholtz Instability.

grid size	GPU/CPU
$64 \times 64$	5
$128 \times 128$	19
$256 \times 256$	58
$512 \times 512$	75
$1024 \times 1024$	81

- GPU GeForce GTX TITAN and CPU Intel Xeon E5645 @ 2.40 Ghz.
- Factor of three increase of speed ratio from  $128 \times 128$  to  $256 \times 256$ .

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# Conclusion

- Compound wave modification:
  - ▶ Produces rotational discontinuity for coplanar problems.
  - ▶ Removes pseudo-convergence for near coplanar problems.
  - ▶ Does not require exact solver.
  - ▶ FAST! HLLD intermediate states are already calculated.
  - ▶ Produces the correct result when other numerical inaccuracies are present.
- Released a nonlinear solver for ideal MHD.
- Released a high-order multi-dimensional fluid solver.
  - ▶ General geometry on unstructured grids.
  - ▶ Capable of shared memory parallelism on GPU and CPU.
  - ▶ Can be used as blueprint or benchmark by anyone in computational physics and space weather communities wishing to increase performance.

# Bibliography I

- [1] J. P. Boris and D. L. Book. “Flux-Corrected Transport I. SHASTA, A Fluid Transport Algorithm That Works”. In: *J. Comp. Phys.* 11 (1973), pp. 38–69.
- [2] H. de Sterck, B. C. Low, and S. Poedts. “Complex magnetohydrodynamic bow shock topology in field-aligned low- $\beta$  flow around a perfectly conducting cylinder”. In: *Physics of Plasmas* 5 (Nov. 1998), pp. 4015–4027.
- [3] B. Einfeldt. “On Godunov-Type Methods for Gas Dynamics”. In: *SIAM J. Numer. Anal.* 25 (1988), pp. 294–318.
- [4] C. R. Evans and J. F. Hawley. “Simulation of magnetohydrodynamic flows - A constrained transport method”. In: *ApJ* 332 (Sept. 1988), pp. 659–677.

## Bibliography II

- [5] A. Harten. "High resolution schemes for hyperbolic conservation laws". In: *J. Comp. Phys.* 49 (1983), pp. 357–393.
- [6] Jared Hoberock and Nathan Bell. *Thrust: A Parallel Template Library*. Version 1.7.0. 2010. URL: <http://thrust.github.io/>.
- [7] L. D. Landau, E. M. Lifshitz, and L. P. Pitaevskii. *Electrodynamics of continuous media*. 3rd. 1984.
- [8] T. Miyoshi and K. Kusano. "A multi-state HLL approximate Riemann solver for ideal MHD". In: *J. Comp. Phys.* 208 (May 2005), pp. 315–344.
- [9] S. A. Orszag and C.-M. Tang. "Small-scale structure of two-dimensional magnetohydrodynamic turbulence". In: *Journal of Fluid Mechanics* 90 (Jan. 1979), pp. 129–143.

## Bibliography III

- [10] *Spasce Weather.* [http://now.uiowa.edu/files/now.uiowa.edu/styles/prim\\_horizontal\\_640/public/sun-earth-640.jpg?itok=ESKvx0GJ](http://now.uiowa.edu/files/now.uiowa.edu/styles/prim_horizontal_640/public/sun-earth-640.jpg?itok=ESKvx0GJ).
- [11] J. Stone, T. Gardner, and P. Teuben. *Athena MHD Code Project*. <https://trac.princeton.edu/Athena/>. Dec. 2010.
- [12] E. F. Toro, M. Spruce, and W. Speares. “Restoration of the contact surface in the HLL-Riemann solver”. In: *Shock Waves* 4 (Mar. 1994), pp. 25–34.
- [13] M. Torrilhon. “Non-uniform convergence of finite volume schemes for Riemann problems of ideal magnetohydrodynamics”. In: *J. Comp. Phys.* 192 (Nov. 2003), pp. 73–94.