High-Order Finite Difference Schemes for computational MHD

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Outline

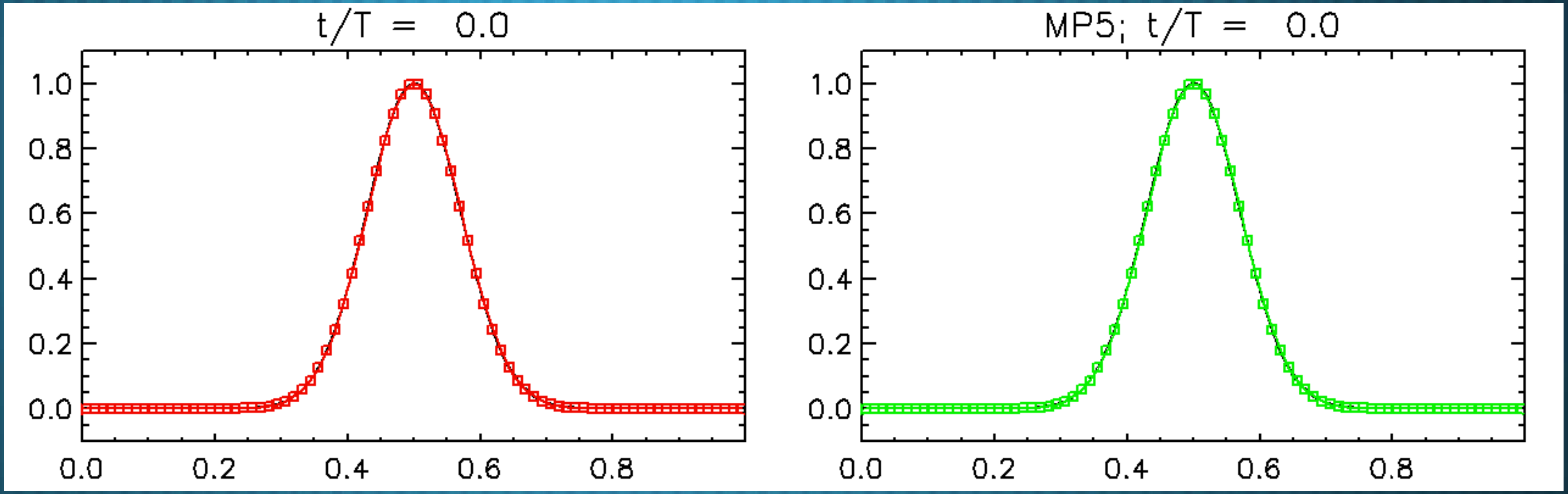
- Motivations for high-order cell-centered schemes;
- Selected formulation → GLM-MHD equations
- Finite Difference framework:
  - Numerical Formulation
  - Third & Fifth order reconstruction techniques
- Numerical Results
- Conclusion & Future Developments

Motivations

- Why High order ?
  - reduce intrinsical numerical dissipation
  - Achieving the same accuracy with fewer number of points
  - more practical for large scale simulations:
    - ✓ Complex flow / multiple waves interactions
    - ✓ Long time evolution
    - ✓ Steady state applications
- Why Cell centered ?
  - Conceptually easier
  - facilitate extension to AMR
  - adaptation to more complex physics

Motivations:

- TVD schemes may intodoce excessive numerical dissipation:



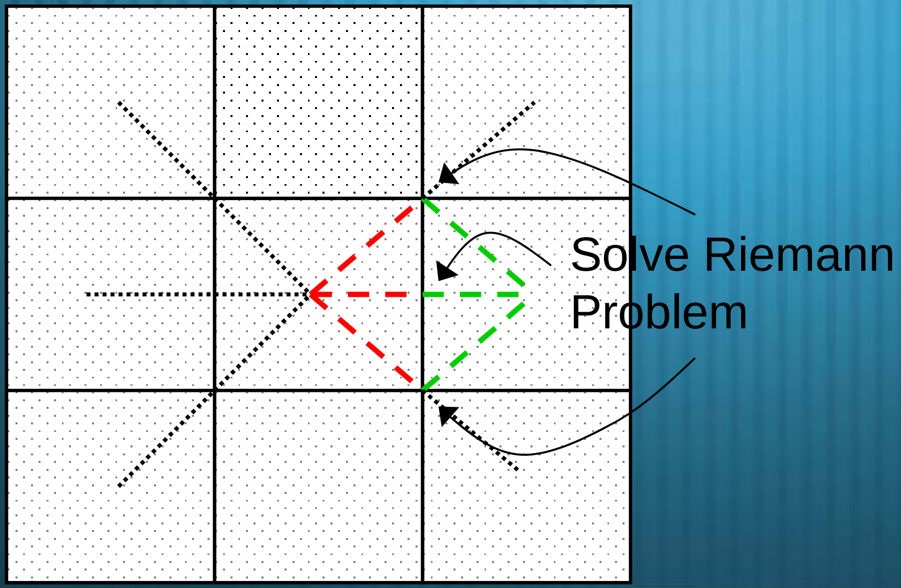
- Low accuracy (2nd), smearing, clipping,squaring
- → limit the largest achievable Reynold numbers

High Order:
Finite Volume vs Finite Difference

FV:

$$\frac{d\langle \mathbf{U}\rangle_{ij}}{dt} = -\frac{1}{\Delta\mathcal{V}_{ij}}\oint_{\partial_{ij}} \mathbf{F}\cdot d\mathbf{S}$$

- Evolve average values
- multi-D interpolation/ multiple Riemann problem solutions
- Complex to code/CPU-Expensive
- General meshes



High Order: Finite Volume vs Finite Difference

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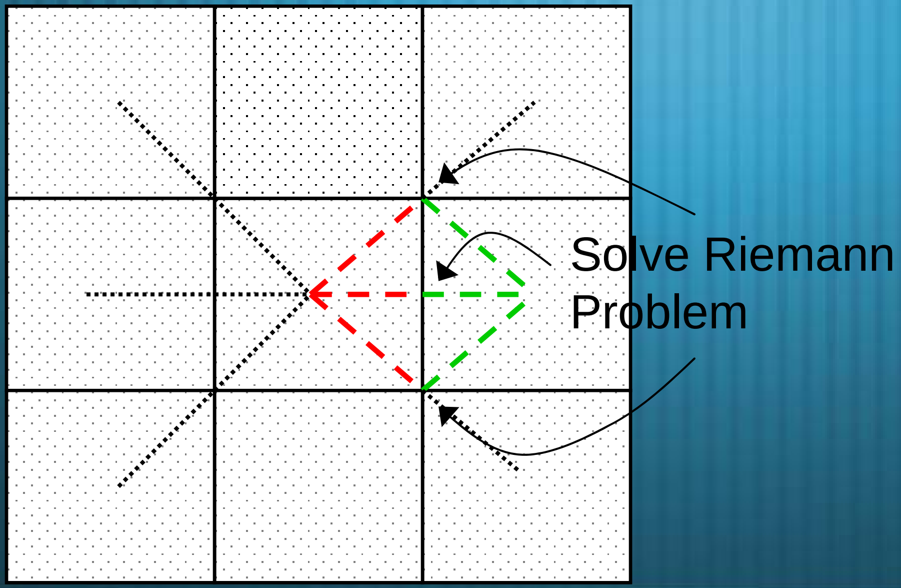
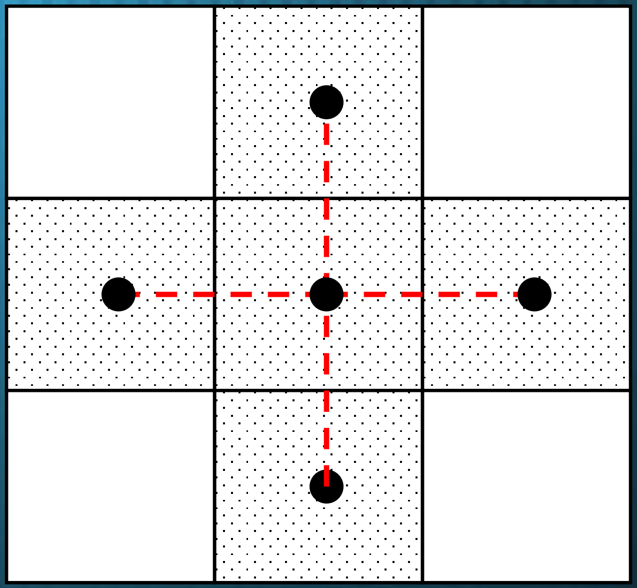
FD:

$$\frac{d\mathbf{U}_{ij}}{dt} = -\left(\nabla\cdot\mathbf{F}\right)_{ij}$$

- Evolve point-values
- 1-D stencils
- Easy and faster to code
- Limited to uniform meshes





Cell-Centered GLM-MHD Equations

- In [D2] the $\nabla \bullet B=0$ constraint is enforced by introducing a new scalar field function or Generalized Lagrange Multiplier (GLM):

$$\left\{\begin{array}{rcl} \nabla\cdot\mathbf{B} & = & 0\,, \\ \dfrac{\partial\mathbf{B}}{\partial t} & = & \nabla\times(\mathbf{v}\times\mathbf{B})\,, \end{array}\right. \quad\Longrightarrow\quad \left\{\begin{array}{rcl} \mathcal{D}(\psi)+\nabla\cdot\mathbf{B} & = & 0\,, \\ \dfrac{\partial\mathbf{B}}{\partial t}+\nabla\psi & = & \nabla\times(\mathbf{v}\times\mathbf{B})\,, \end{array}\right.$$

- $\mathcal{D}(\psi)$ is a differential operator:
  - $\mathcal{D}(\psi) = 0$: Elliptic Correction → $\Delta\psi = 0$
  - $\mathcal{D}(\psi) = \psi/c^2_p$: Parabolic Correction → $\partial_t B + \nabla\cdot(vB - Bv) = c_p^2\nabla(\nabla\cdot B)$

    (errors decay in time)
  - $\mathcal{D}(\psi) = \partial_t\psi/c^2_h$: Hyperbolic correction → $\partial_t\psi + c_h^2\nabla\cdot B = 0$

    (errors propagate at the max admissible speed)

[D2]: Dedner et al., "Hyperbolic Divergence Cleaning for the MHD equations", JCP (2002) 175, 645

Cell-Centered GLM-MHD Equations

- Mixed hyperbolic/parabolic correction:
  - Offers propagation *and* dissipation of divergence errors;
  - Avoid accumulation at stagnation points;
  - preserve full conservation
  - Explicit scheme → no need for iterative solvers

$$
\begin{aligned}
\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v}) &= 0\,,\\
\frac{\partial(\rho\mathbf{v})}{\partial t} + \nabla\cdot\left[\rho\mathbf{v}\mathbf{v}^T - \mathbf{B}\mathbf{B}^T + \mathsf{I}\left(p + \frac{\mathbf{B}^2}{2}\right)\right] &= 0\,,\\
\frac{\partial\mathbf{B}}{\partial t} + \nabla\cdot\left(\mathbf{v}\mathbf{B}^T - \mathbf{B}\mathbf{v}^T\right) + \nabla\psi &= 0\,,\\
\frac{\partial E}{\partial t} + \nabla\cdot\left[\left(E + p + \frac{\mathbf{B}^2}{2}\right)\mathbf{v} - (\mathbf{v}\cdot\mathbf{B})\,\mathbf{B}\right] &= 0\,,\\
\frac{\partial\psi}{\partial t} + c_h^2\nabla\cdot\mathbf{B} &= -\frac{c_h^2}{c_p^2}\psi\,,
\end{aligned}
$$

- The system has 9 real eigenvalues

$$
\lambda^{1,9} = \mp c_h\,,\quad \lambda^{2,8} = v_x \mp c_f\,,\quad \lambda^{3,7} = v_x \mp c_a\,,\quad \lambda^{4,6} = v_x \mp c_s\,,\quad \lambda^5 = v_x
$$

- where

$$
c_{f,s} = \sqrt{\frac{1}{2\rho}\left(\Gamma p + |\mathbf{B}|^2 \pm \sqrt{\left(\Gamma p + |\mathbf{B}|^2\right)^2 - 4\Gamma p B_x^2}\right)}\,,\qquad c_a = \frac{|B_x|}{\sqrt{\rho}}
$$

- c_h: is chosen to be the maximum compatible speed: $c_h = \frac{C_a}{\Delta t^n}\min(\Delta x, \Delta y, \Delta z)$
- See MT09 for an unsplit 2nd order implementation

[MT09]: Mignone, Tzeferacos, “A 2nd-order unsplit Godunov Scheme for cell-centered MHD: the CTU-GLM scheme”, sub. JCP

Finite Difference Formulation

- Method of lines, RK time stepping:

$$\frac{d\mathbf{U}}{dt} = \mathcal{L}\left(\mathbf{U}\right) \approx -\frac{\partial \mathbf{F}_x}{\partial x} - \frac{\partial \mathbf{F}_y}{\partial y} - \frac{\partial \mathbf{F}_z}{\partial z}$$

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- Identify point values of $\mathbf{F}_i$ as cell averages of $\hat{\mathbf{F}}(x)$

$$\mathbf{F}_i = \frac{1}{\Delta x}\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \hat{\mathbf{F}}(\xi)d\xi = \frac{1}{\Delta x}\left[\mathbf{H}(x_{i+\frac{1}{2}}) - \mathbf{H}(x_{i-\frac{1}{2}})\right]$$

H(x) is the primitive function:

$$\mathbf{H}(x) = \int_{-\infty}^{x} \hat{\mathbf{F}}(\xi)d\xi$$

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- Differentiation leads to

$$\frac{\partial \mathrm{F}}{\partial x} = \frac{1}{\Delta x}\left(\hat{\mathbf{F}}_{i+\frac{1}{2}} - \hat{\mathbf{F}}_{i-\frac{1}{2}}\right)$$

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- Differentiation leads to

$$\frac{\partial \mathbf{F}}{\partial x} = \frac{1}{\Delta x}\left(\hat{\mathbf{F}}_{i+\frac{1}{2}} - \hat{\mathbf{F}}_{i-\frac{1}{2}}\right)$$

- *Problem*: find high-order interface values $\hat{\mathbf{F}}_{i+\frac{1}{2}}$ knowing undivided differences of primitive function ΔH → Same as F.V. reconstructions

$$\hat{\mathbf{F}}_{i+\frac{1}{2}} = \mathcal{R}\left(\mathbf{F}_s\right), \quad s = i-S, \dots, i+S+1$$

Finite difference schemes

- Reconstruction step better carried using characteristic variables to ensure robustness and oscillation-free results
- Split the flux into negative and positive contributions:

$$\begin{cases} V^{\kappa,+}_{[i+\frac{1}{2}],s} & = & \mathbf{L}^{\kappa}_{i+\frac{1}{2}} \cdot \left(\mathbf{F}_s + \alpha^{\kappa}\mathbf{U}_s\right) \\ V^{\kappa,-}_{[i+\frac{1}{2}],s} & = & \mathbf{L}^{\kappa}_{i+\frac{1}{2}} \cdot \left(\mathbf{F}_{s'} - \alpha^{\kappa}\mathbf{U}_{s'}\right) \end{cases}$$

- Reconstruct each characteristic field $\hat{V}^{\kappa,\pm}_{i+\frac{1}{2}} \equiv \mathcal{R}\left(V^{\kappa,\pm}_{[i+\frac{1}{2}],s}\right)$
- On 1-D stencils, Bx and ψ decouple from the remaining equations and can be solved preliminary;
- Use the 7x7 standard MHD wave decomposition;
- → FD formulation available in future releases of the PLUTO code [M07].

[M07]: Mignone et al., “PLUTO:A numerical code fo computational Astrophysics”, ApJS (2007), 170,228

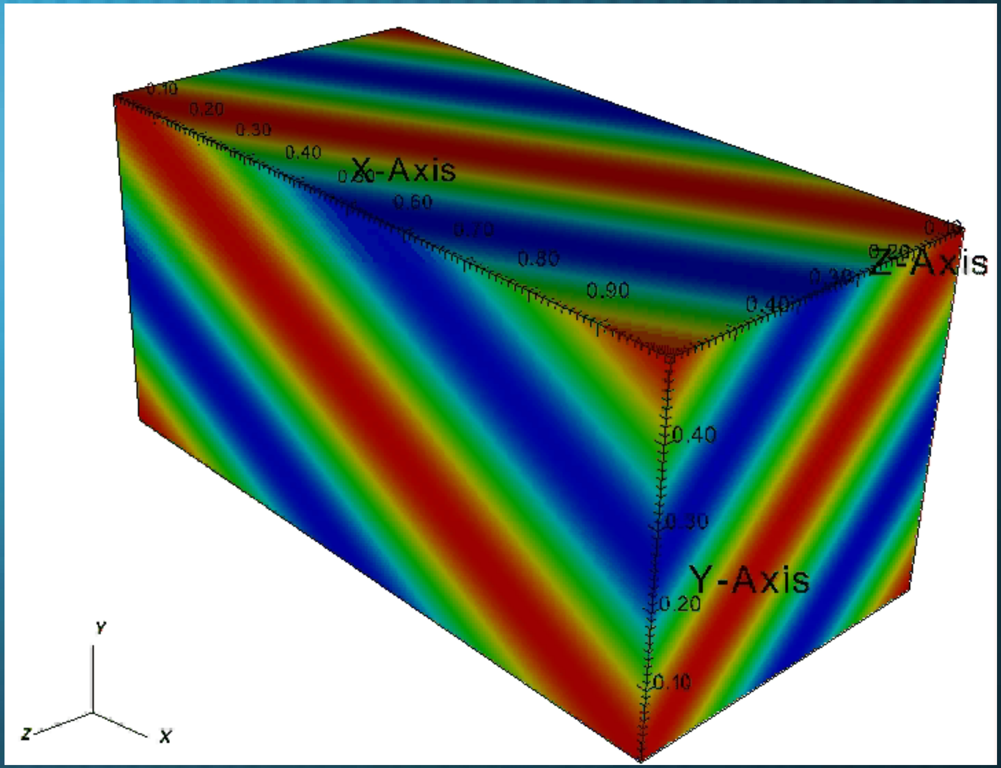
3rd and 5th-order Accurate Schemes

- Third-order: based on a 3 point local stencil:
  - *WENO+3*: 3rd order WENO with new weights [YC] providing faster convergence and improved accuracy near critical points,
  - *LimO3*: New third-order limited polynomial reconstruction by Cada Torrilhon [CT] based on nonlinear functions
- Fifth-order: based on a 5 point local stencil:
  - *WENO-Z*: 5th order WENO with improved weights [BCCD] providing less dissipation and higher resolution than the classical 5th order method;
  - *MP5*: Monotonicity Preserving (MP) fifth-order scheme of Suresh-Huynh [SH]: interface value must lie in a certain interval to preserve monotonicity near discontinuities and accuracy in smooth regions;

[YC]: Yamaleev & Carpenter, "Third-order energy stable WENO scheme", JCP (2009), 228, 3025
[CT]: Cada & Torrilhon, "Compact third-order limiter functions for finite volume methods", JCP (2009), 228, 4118
[BCCD]: Borges, Carmona, Costa & Don, "An improved WENO scheme for hyperbolic conservation laws", JCP (2008), 227, 3191
[SH]: Suresh & Huynh, "Accurate Monotonicity Preserving Schemes with Runge-Kutta Time Stepping", JCP (1997),136, 83

Circularly Polarized Alfven Waves

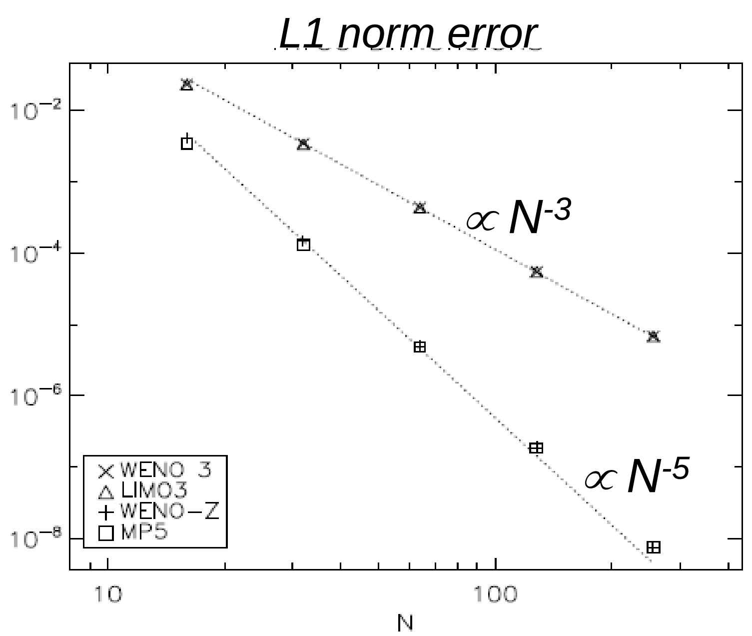
- CP Alfven waves propagate oscillations of the transverse components of velocity vector and magnetic induction;
- CP waves are exact nonlinear solutions of the MHD equations;
- Useful benchmark in 1, 2 and 3D using rotated configurations

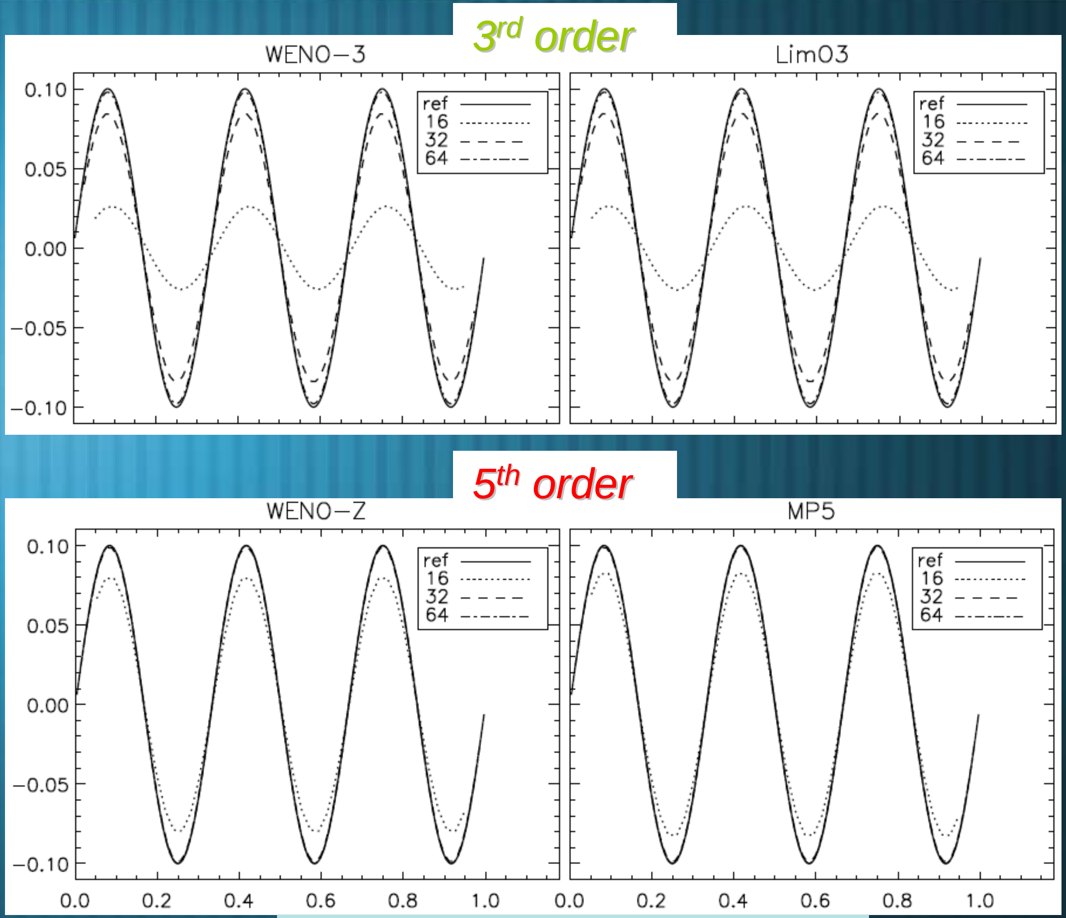


Circularly Polarized Alfven Waves

3D Propagation [GS08]

- $k_y / k_x = k_z / k_x = 2$
- ability to retain planar sym
- Order of accuracy



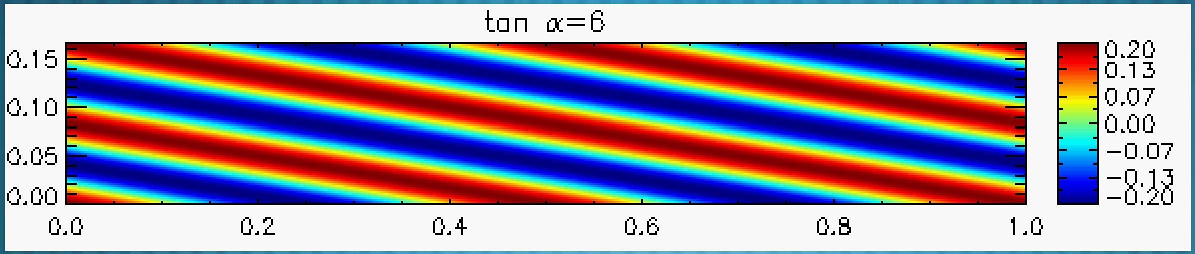


Scatter plot: $B_2(i,j,k)[x_1(i,j,k)]$

[GS08]: Gardiner & Stone, "An unsplit Godunov method for ideal MHD via constrained transport in 3D", JCP (2008), 227, 4123

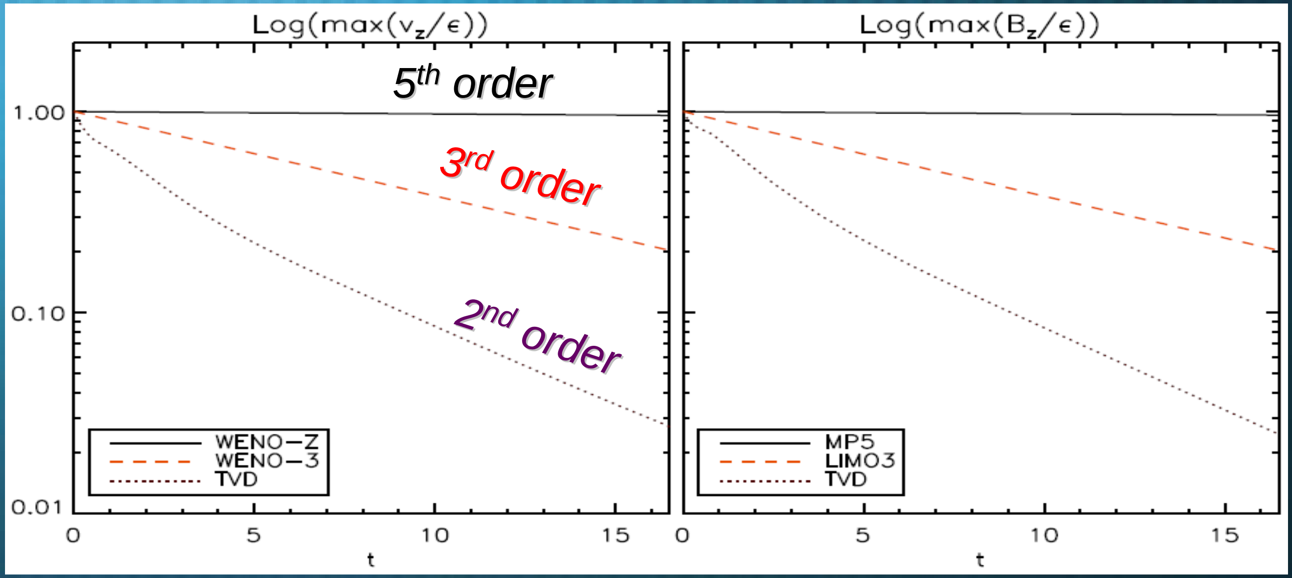
Dissipation & Long Term Decay in 2D

- Long term propagation (100 wave periods) in a 2D domain



small inclination angle, tan α = 6 [B04]

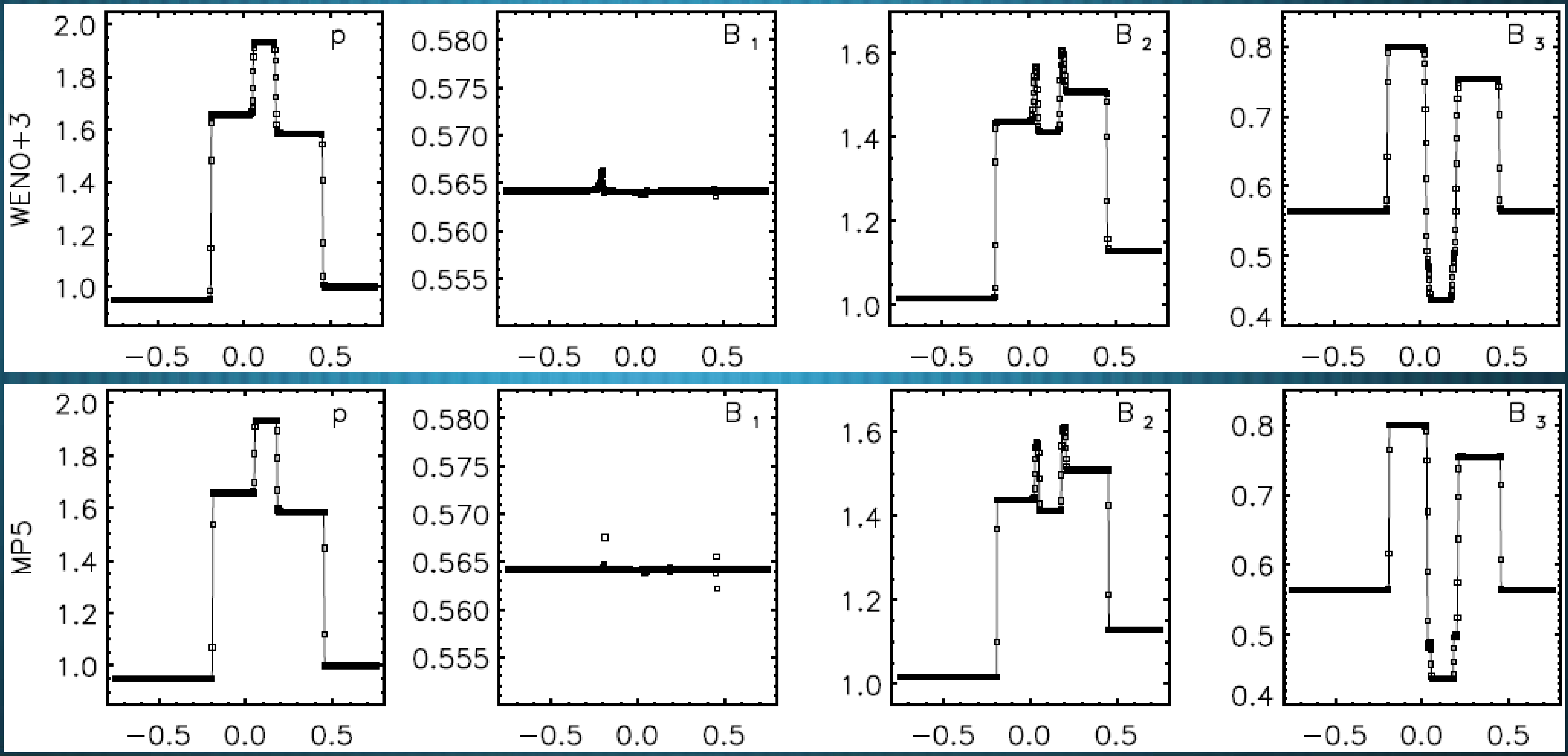
- dissipation mechanism is solely numerical in nature → direct measure of numerical resistivity [RJF95]



[B04]: Balsara, "Second-order-accurate schemes for MHD with divergence-free reconstruction", ApJ (2004), 151,149
[RJF95]: Ryu, Jones & Frank, "Numerical MHD in Astrophysics: algorithm and tests for multi-D flows", ApJ (1995), 452:785

Rotated Shock Tubes

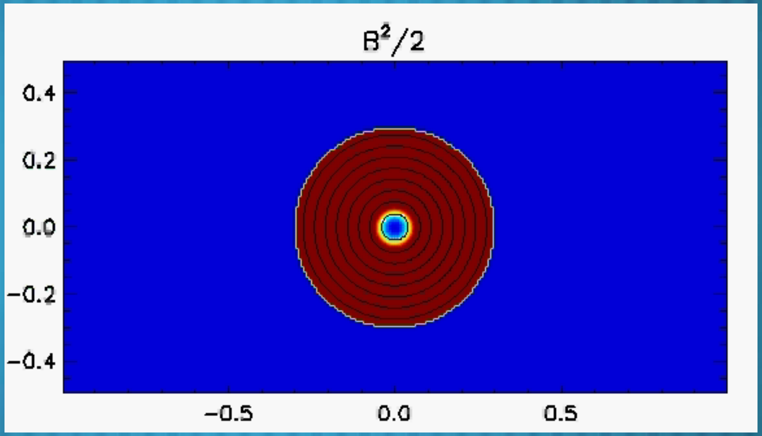
- Riemann problem involving propagation of discontinuities, [GS08];



[GS08]: Gardiner & Stone, "An unsplit Godunov method for ideal MHD via constrained transport in 3D", JCP (2008), 227, 4123

Field Loop Advection

- Advection of a weakly magnetized field loop traversing the computational domain diagonally [GS05, LD09];



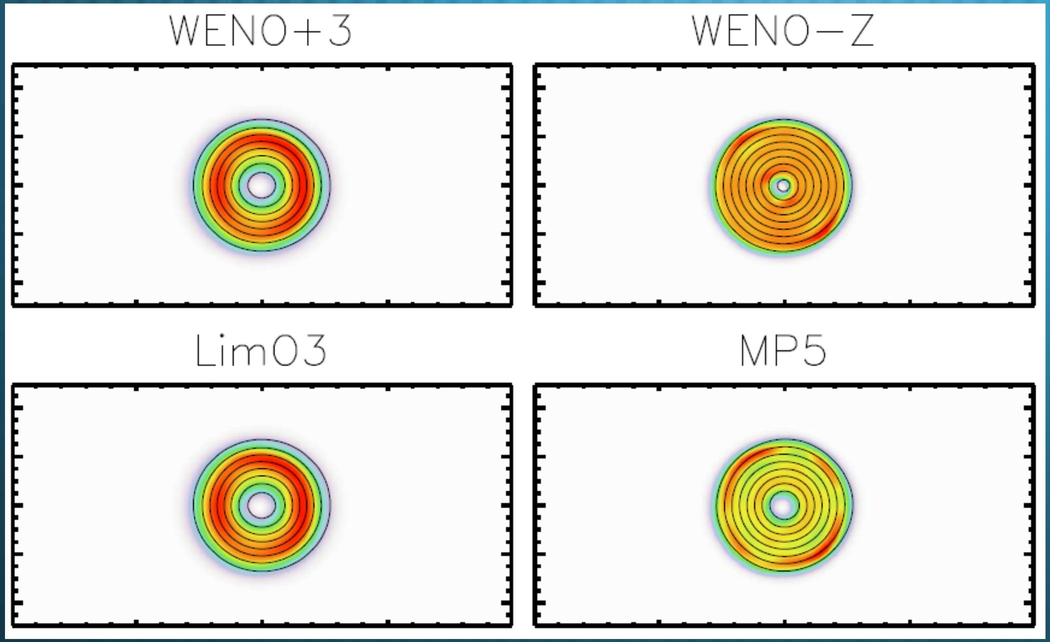
- For β >> 1 → equivalent to advection of a passive scalar;
- Check the correct discretization of multi-D term in the numerical method;
- I.C.

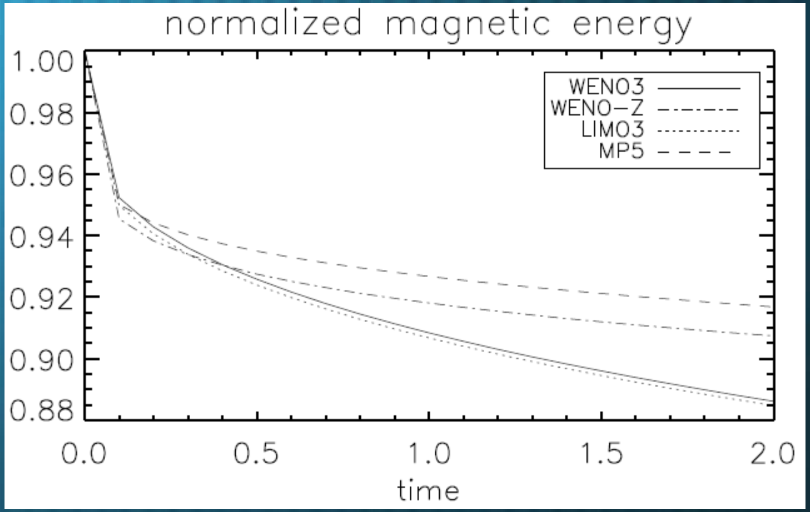
$$A_z = \begin{cases} a_0 + a_2 r^2 & \text{if} \quad 0 \le r \le R_1\,, \\ A_0(R-r) & \text{if} \quad R_1 < r \le R\,, \\ 0 & \text{if} \quad r > R\,, \end{cases} \quad \Longrightarrow \quad B_\phi = \begin{cases} -2a_2 r^2 & \text{if} \quad 0 \le r \le R_1\,, \\ A_0 & \text{if} \quad R_1 < r \le R\,, \\ 0 & \text{if} \quad r > R\,, \end{cases}$$

[GS05]: Gardiner & Stone, "An unsplit Godunov method for ideal MHD via constrained transport", JCP (2005), 205,509
[LD09]: Lee, Deane, "An unsplit staggered mesh scheme for multidimensional MHD", JCP (2009), 228, 952

Field Loop Advection

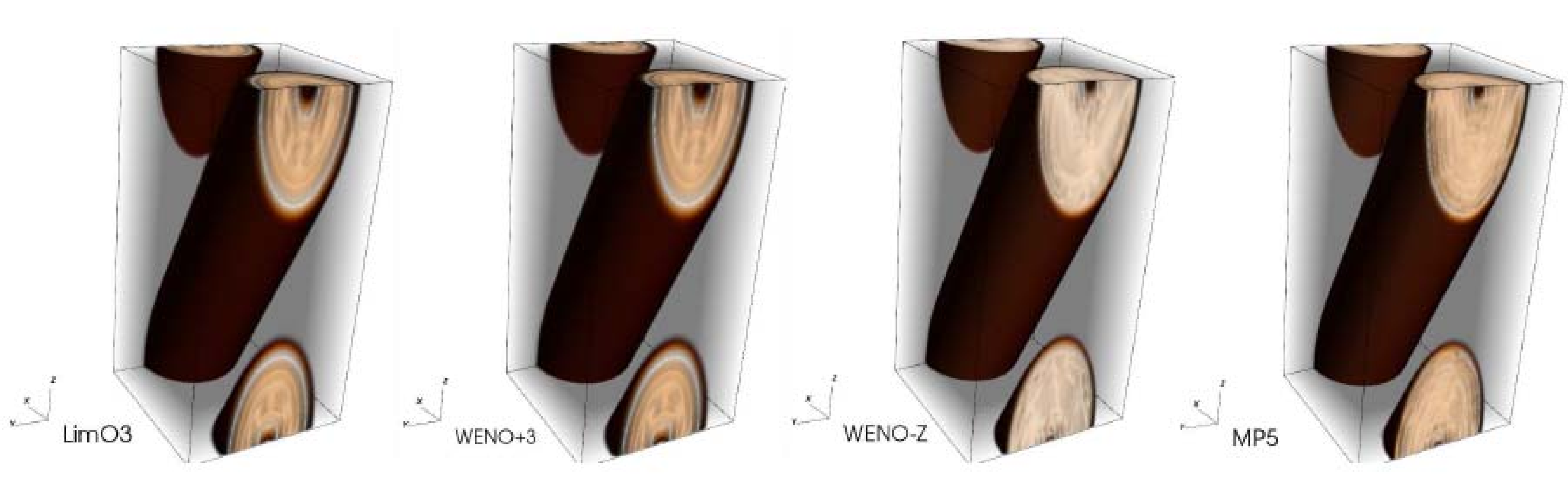
- Results at t=2 (two loop periods) for 128x64 grid points;
- Third-order schemes show more dissipation;
- All reconstruction preserve the circular shape of the loop;





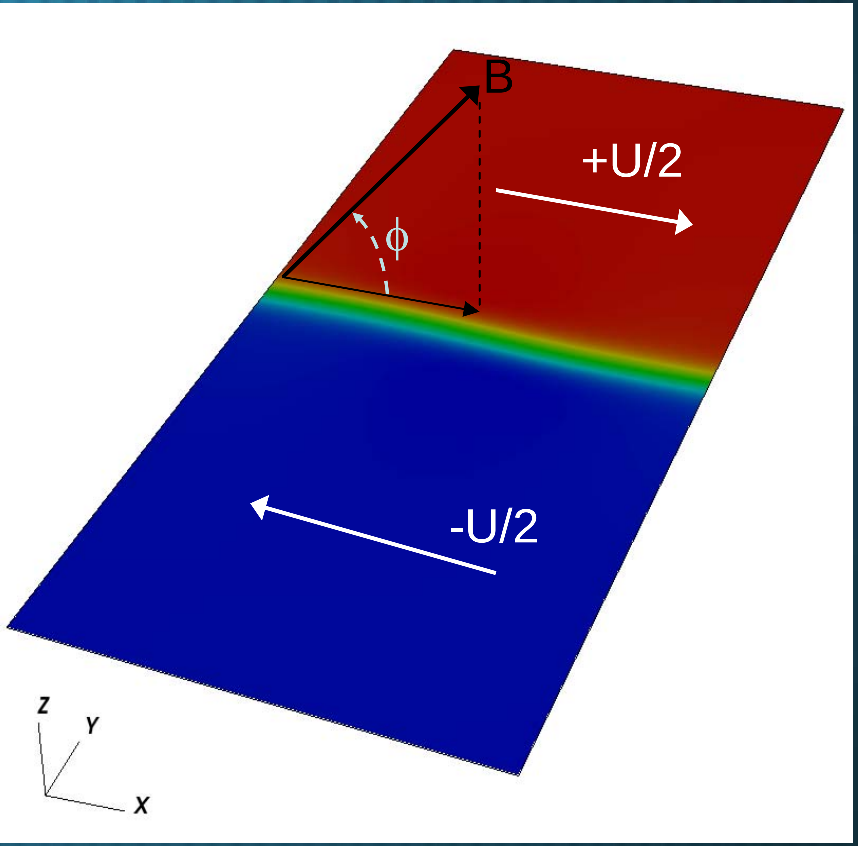
3D Field Loop Advection

- 3D oblique propagation, res = 128x128x256 grid points



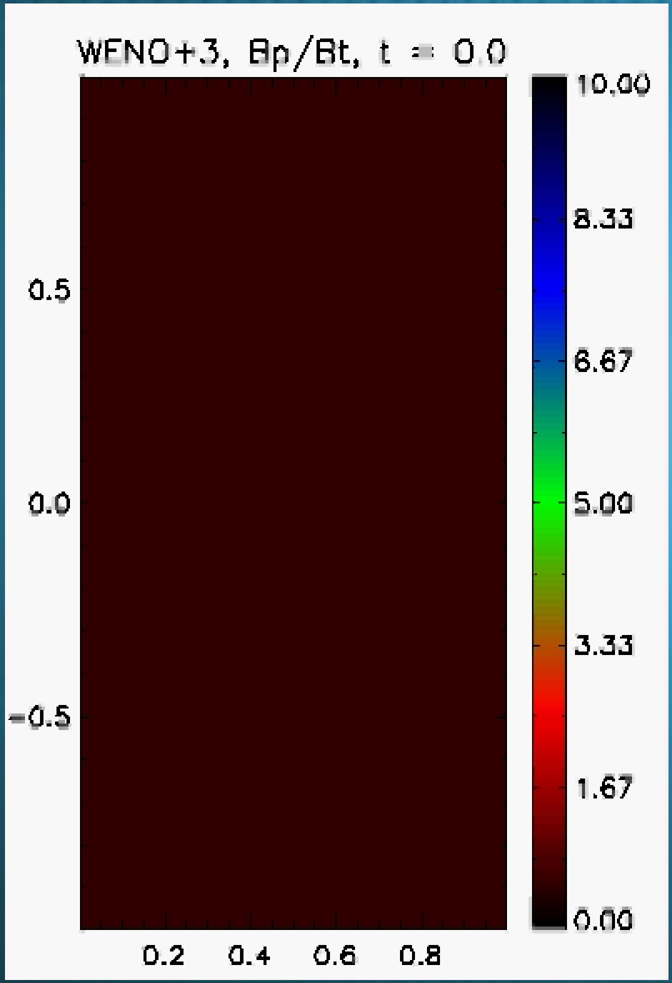
Kelvin-Helmholtz Unstable Flow

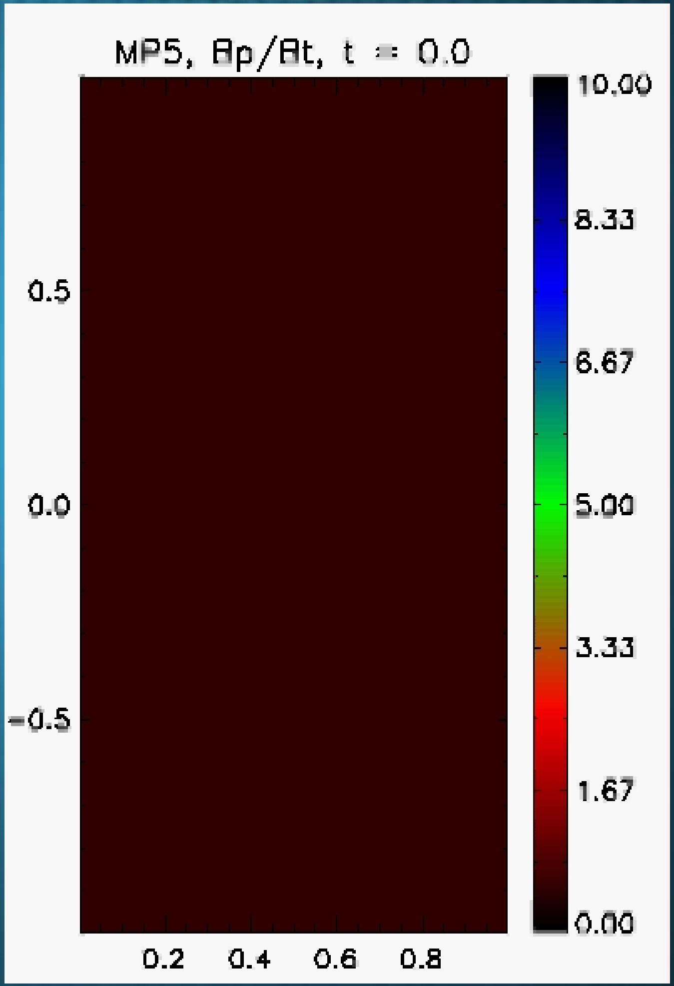
- Single magnetized planar velocity shear layer [J97];
- 2.5 Dimensions;
- $\Delta M_s = 1$, $\Delta M_A = 20$, $\phi=\pi/3$;
- Scheme & Resolution study:
  - 64x128
  - 128x256
  - 256x512



[J97]: Jones et al, “MHD KH Instability. II. The roles of a weak and oblique fields in planar flows”, ApJ (1997), 482:230

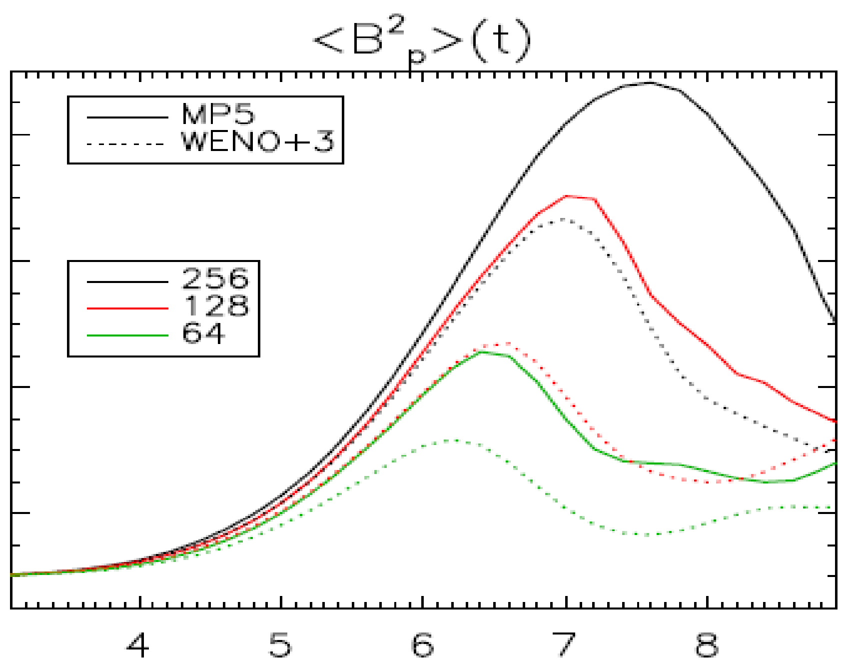
Kelvin-Helmholtz Unstable Flow

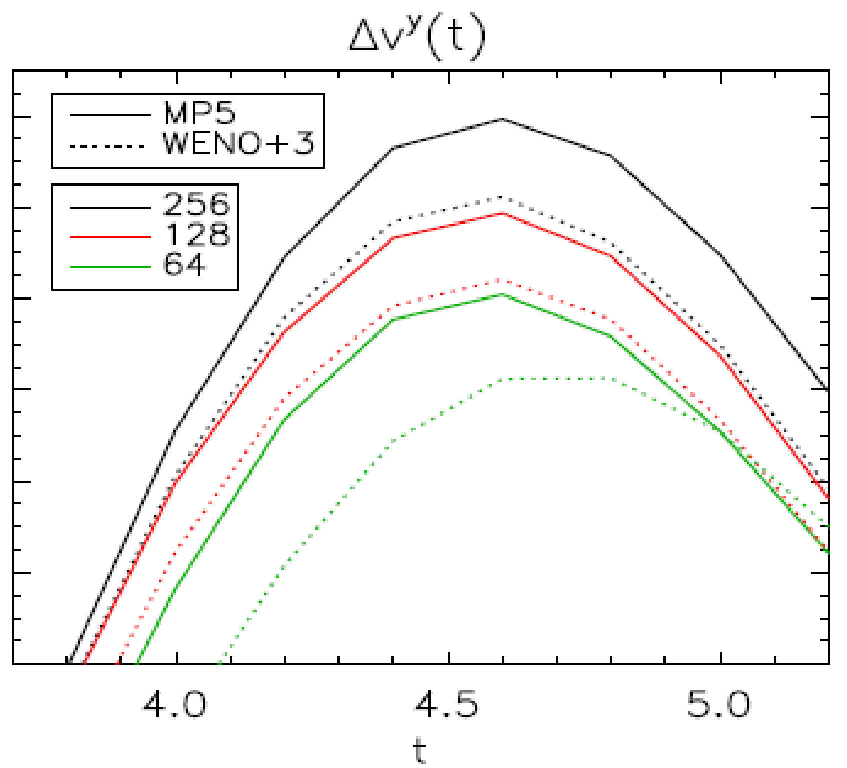




Kelvin-Helmholtz Unstable Flow

- Field amplification proceed faster for smaller numerical resistivity
- For t > 8 tearing mode instabilities lead to reconnection event → prevent field amplification





- Growth rate computed as $\Delta v^y = (v_{y,max} - v_{y,min})/2$, related to poloidal field amplification

CPU cost

	WENO+3	LimO3	WENO-Z	MP5	PPM-CT
KH (256x128)	3.09	2.89	3.83	3.44	-
CP3D ($128x64^2$)	2.26	2.04	2.70	2.30	-
OT3D (48^3)	3.02	2.92	4.08	3.58	1.49

- WENO-Z most expensive
- Small additional cost (~10-20 %) when moving from 3rd→ 5th order
  → Better off going to higher order !
- FD schemes are ~2.4-3 slower than second-order TVD/PPM schemes

Conclusions & Perspectives

- FD, Cell-centered schemes offer simplicity and ease of implementation;
- Results show high level of accuracy for both smooth and discontinuous flow features
- Preferred Scheme: MP5
- More accurate and less dissipative than traditional 2nd order Godunov schemes;
- Cost-effective, easy to incorporate additional physics (e.g. viscosity)
- More convenient in terms of accuracy vs. CPU time, specially for 3D problems;

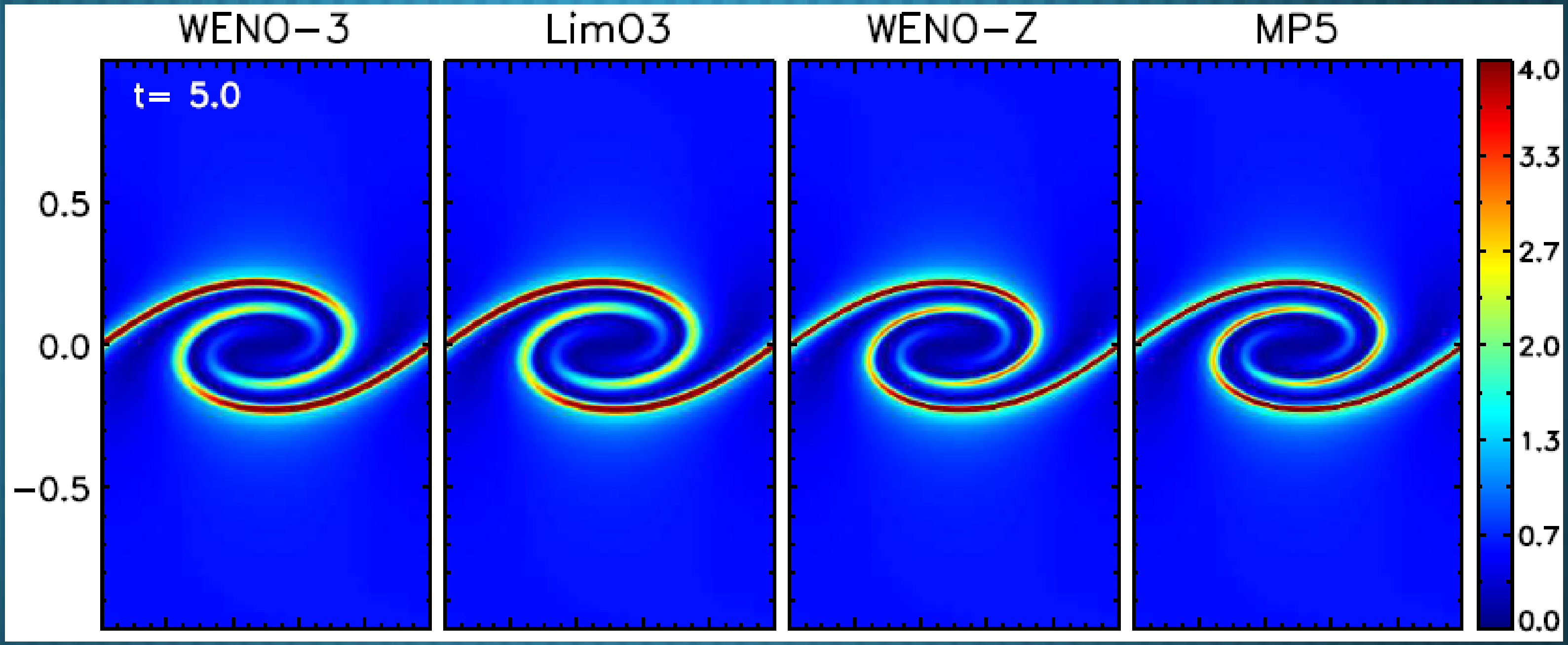
  → Comparison with F.V. schemes

  → Extension to higher accuracy in time

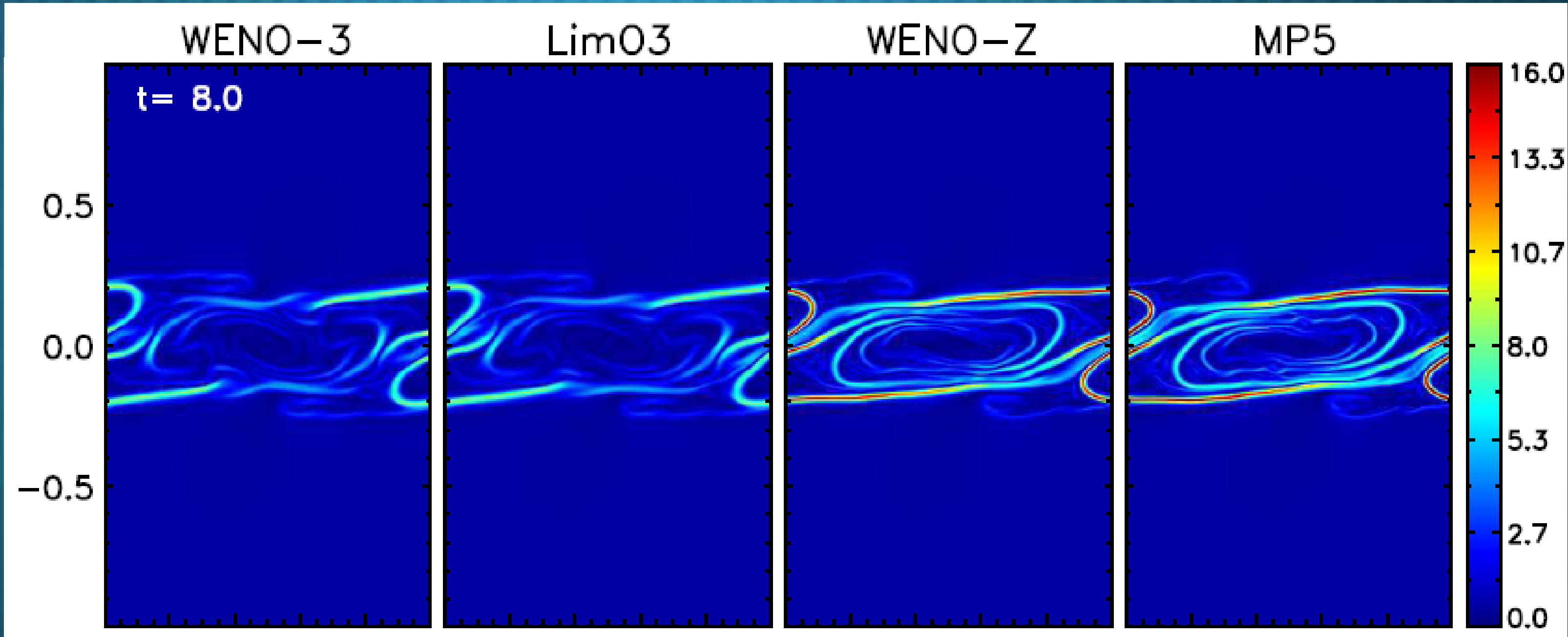
  → Applications to turbulence (Molecular cloud fragmentation, MRI, etc…)
- Available in next releases of the PLUTO code.

~ THANK YOU ~

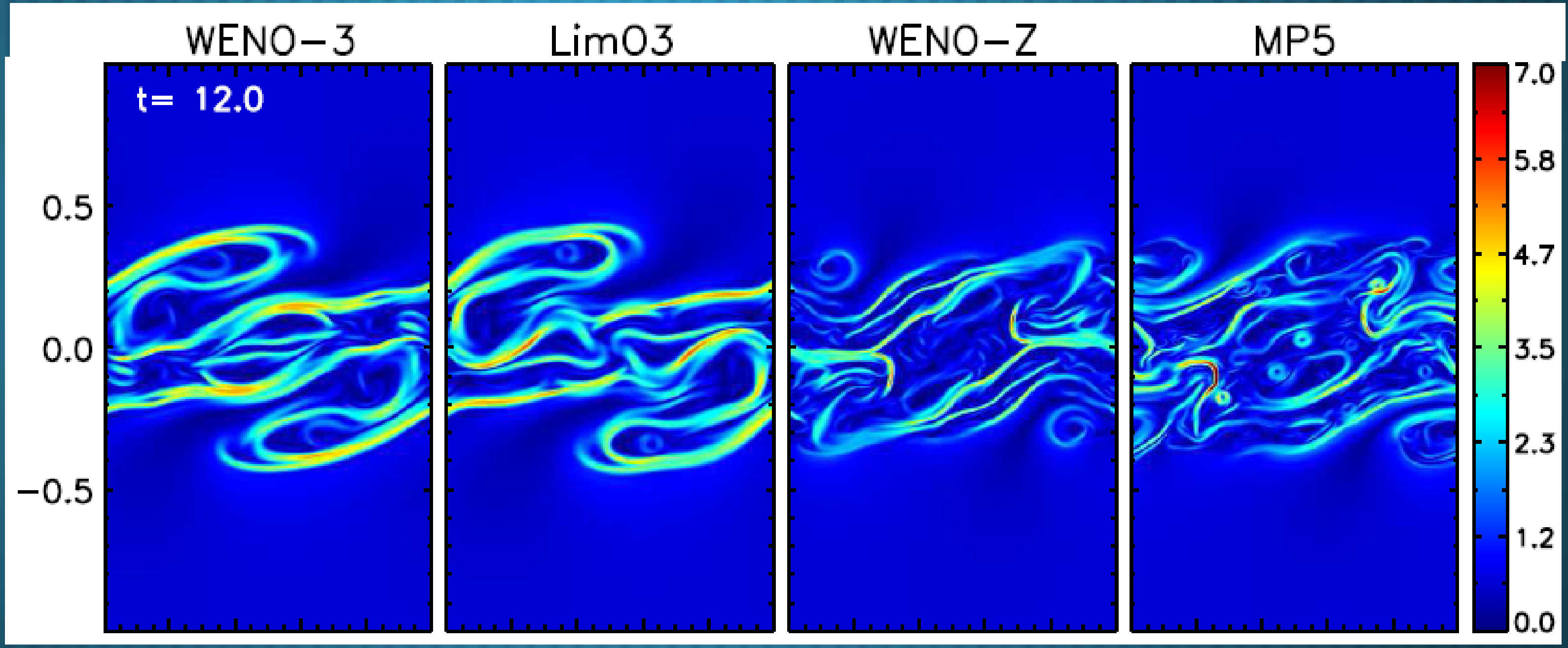
Kelvin-Helmholtz Unstable Flow



Kelvin-Helmholtz Unstable Flow



Kelvin-Helmholtz Unstable Flow



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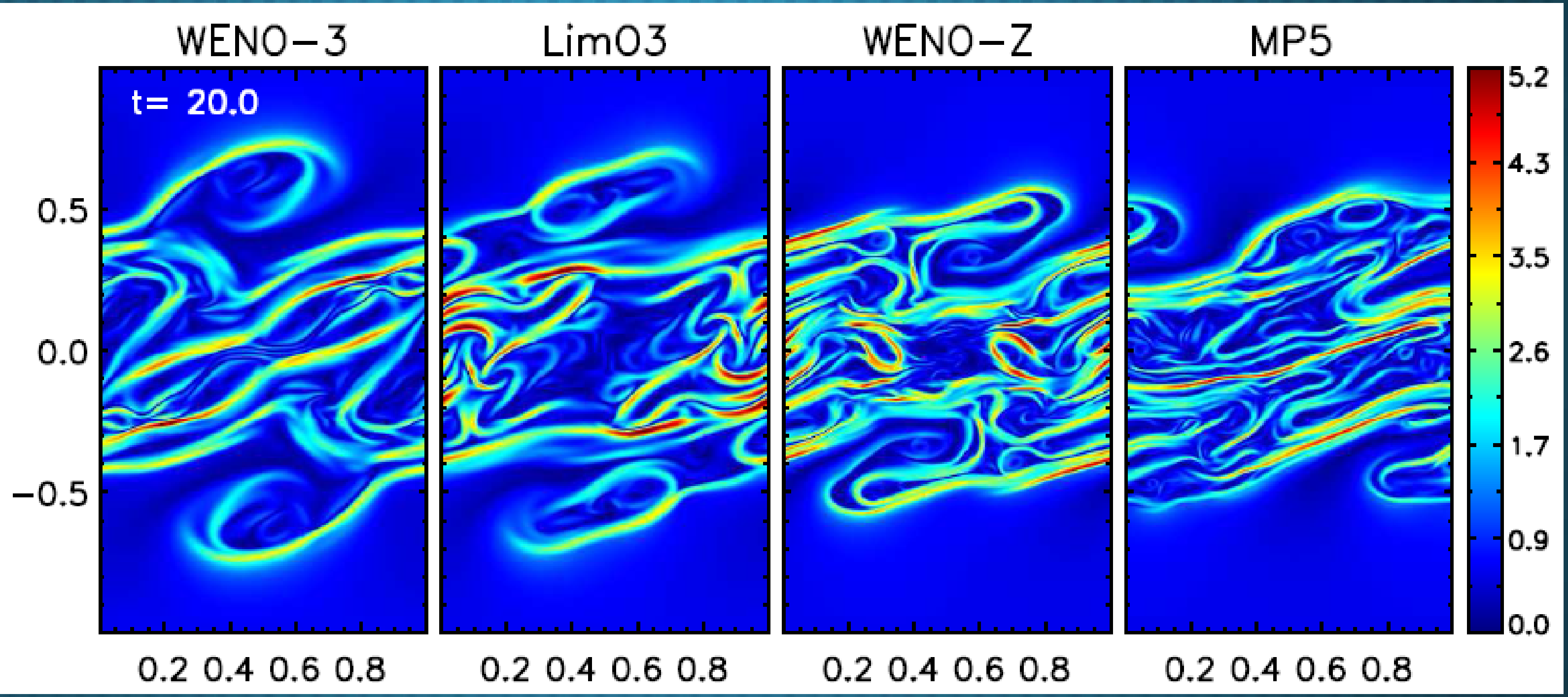

Divergence of B

- In time for KH ?
- For ST ?
- As integral average ?

Third-order accurate schemes

- Based on a 3 point local stencil:
  - *WENO+3*: 3rd order WENO with new weights [YC] providing faster convergence and improved accuracy near critical points,

$$\mathcal{R}(f_s) = \omega_0 \frac{f_i + f_{i+1}}{2} + \omega_1 \frac{-f_{i-1} + 3f_i}{2}$$

  - *LimO3*: New third-order limited polynomial reconstruction by Cada Torrilhon [CT]

$$\mathcal{R}(f_s) = f_i + \frac{\Delta_{i+\frac{1}{2}}}{2}\left[P_3(\theta) + \alpha\left(\hat{\phi}(\theta) - P_3(\theta)\right)\right] \qquad \theta = \Delta_{i-\frac{1}{2}}/\Delta_{i+\frac{1}{2}}$$

based on the accuracy and shape-preserving third-order limiter

$$\hat{\phi}(\theta) = \begin{cases} \max\left[0, \min\left(P_3(\theta), 2\theta, 1.6\right)\right] & \text{if} \quad \theta \geq 0 \\ \max\left[0, \min\left(P_3(\theta), -\frac{\theta}{2}\right)\right] & \text{if} \quad \theta < 0 \end{cases}$$

[YC]: Yamaleev & Carpenter, “Third-order energy stable WENO scheme”, JCP (2009), 228, 3025
[CT]: Cada & Torrilhon, “Compact third-order limiter functions for finite volume methods”, JCP (2009), 228, 4118

Fifth-order accurate schemes

- Based on a 5 point local stencil:
  - *WENO-Z*: 5th order WENO [JS] with improved weights [BCCD] providing faster convergence and improved accuracy near critical points,

$$\mathcal{R}(f_s) = \omega_0 P^{(3)}_{i-1} + \omega_1 P^{(3)}_{i} + \omega_2 P^{(3)}_{i+1}$$

  - *MP5*: Monotonicity Preserving (MP) fifth-order scheme of Suresh-Huynh [SH]:

$$f_{i+\frac{1}{2}} = \frac{2f_{i-2} - 13f_{i-1} + 47f_i + 27f_{i+1} - 3f_{i+2}}{60}$$

    interface value must lie in a certain interval to preserve monotonicity near discontinuities and accuracy in smooth regions:

$$\mathcal{R}\left(f_s\right) = \begin{cases} f_{i+\frac{1}{2}} & \text{if} \quad (f_{i+\frac{1}{2}} - f_i)(f_{i+\frac{1}{2}} - f^{\mathrm{MP}}) < 0\,, \\ \mathrm{Median}\left(f^{\min}, f_{i+\frac{1}{2}}, f^{\max}\right) & \text{otherwise} \end{cases}$$

[JS]: Jiang, Wu, "Efficient Implementation of WENO schemes", JCP (1996), 126, 202
[BCCD]: Borges, Carmona, Costa & Don, "An improved WENO scheme for hyperbolic conservation laws", JCP (2008), 227, 3191
[SH]: Suresh & Huynh, "Accurate Monotonicity Preserving Schemes with Runge-Kutta Time Stepping", JCP (1997),136, 83