Hydro and MHD Solvers in FLASH: How to use them

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FLASH Tutorial
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Outline

- Broad Ranges of Applications
  - Astrophysics and HEDP

- Algorithms and mathematics
  - Governing equations, difference equations of PDEs
  - Dimensionally Split vs. Unsplit formulations
  - Hydro and MHD solvers
    - High-order Reconstructions, Riemann problems, physical units
  - Explicit vs. Implicit schemes
  - Beyond the hyperbolic system (diffusion, source terms, Biermann battery, etc)

- Examples: setting up problems, how to use various features and switches

- Summary
Coupling Hydro/MHD with Astrophysics and HEDP

- Single-fluid description Hydrodynamics, MHD, RHD
  - Multitemperature extension for hydro/MHD
- Equations of State
  - Gamma law, multigamma, Helmholtz, relativistic ideal gamma
  - Multitemperature (gamma, multigamma, tabulated, multitype)
- Nuclear physics and source terms
  - Burn, ionization, stir, gravity
  - Laser energy deposition, heat exchange, Biermann battery
- Active and passive particles
- Material properties
  - Thermal conductivity, magnetic diffusivity, viscosity
  - Opacity, operator split (semi) implicit solver for diffusive terms
- Cosmology
- Radiative transfer: multigroup diffusion
Astrophysical Applications

Cosmological cluster formation

Supersonic MHD turbulence decay

Type 1a SN

Ram pressure stripping

Galaxy Cluster sloshing

Laser-driven shock instabilities

RT Instabilities

Magnetic RT

MHD Vortex

Gravitational Collapse
HEDP Applications

Shot 27, 2w | sphere | Ar @ 0.5 mbar | t = 100.0 ns

R_bubble = 4.32 mm

No radiation
Radiation

Density (g/cm³)

Mass Density
Mag. Field (G)
Two Excellent Books

E.F. Toro
Riemann Solvers and Numerical Methods for Fluid Dynamics
A Practical Introduction
2nd Edition
Springer

Finite-Volume Methods for Hyperbolic Problems
RANDALL J. LEVEQUE
FLASH’s hydro/MHD solves conservation laws using a finite-volume (FV) approach

- Highly compressible flows with shocks and discontinuities
- Differential (smooth) form of PDE becomes invalid
- Integral form of PDE relaxes the smoothness assumptions and seeks for weak solutions over control volumes and their boundaries

Basics of FV formulation (1D):

\[
Q^n_i \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x, t_n) \, dx \equiv \frac{1}{\Delta x} \int_{C_i} q(x, t_n) \, dx, \quad F^n_{i-1/2} \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2}, t)) \, dt.
\]
integral form of PDE:

\[ \int_{C_i} q(x, t_{n+1}) \, dx - \int_{C_i} q(x, t_n) \, dx = \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2}, t)) \, dt - \int_{t_n}^{t_{n+1}} f(q(x_{i+1/2}, t)) \, dt. \]

volume averaged cell centered quantity and time averaged flux:

\[ Q_i^n \approx \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x, t_n) \, dx \equiv \frac{1}{\Delta x} \int_{C_i} q(x, t_n) \, dx, \]

\[ F_{i-1/2}^n \approx \frac{1}{\Delta t} \int_{t_n}^{t_{n+1}} f(q(x_{i-1/2}, t)) \, dt. \]

finite wave speed in hyperbolic system:

\[ F_{i-1/2}^n = \mathcal{F}(Q_{i-1}^n, Q_i^n) \]

* high-order reconstruction in space & time
* riemann problems at each interface

general difference equation in conservation form:

\[ Q_i^{n+1} = Q_i^n - \frac{\Delta t}{\Delta x} (F_{i+1/2}^n - F_{i-1/2}^n). \]
Multidimensional hyperbolic system in conservation laws:

\[ Q_{ij}^n \approx \frac{1}{\Delta x \Delta y} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} q(x, y, t_n) \, dx \, dy. \]

\[ F_{i-1/2,j}^n \approx \frac{1}{\Delta t \Delta y} \int_{t_n}^{t_{n+1}} \int_{y_{j-1/2}}^{y_{j+1/2}} f(q(x_{i-1/2}, y, t)) \, dy \, dt, \]

\[ G_{i,j-1/2}^n \approx \frac{1}{\Delta t \Delta x} \int_{t_n}^{t_{n+1}} \int_{x_{i-1/2}}^{x_{i+1/2}} g(q(x, y_{j-1/2}, t)) \, dx \, dt. \]

2D discrete form:

\[ Q_{ij}^{n+1} = Q_{ij}^n - \frac{\Delta t}{\Delta x} [F_{i+1/2,j}^n - F_{i-1/2,j}^n] - \frac{\Delta t}{\Delta y} [G_{i,j+1/2}^n - G_{i,j-1/2}^n], \]

Two approaches:
- Directionally “split”
- Directionally “unsplit”
Directionally split (1\textsuperscript{st} order Godunov; 2\textsuperscript{nd} order Strang splitting)

\[
PDE : \quad U_t + F(U)_x + G(U)_y = 0 , \\
IC : \quad U(x, y, t^n) = U^n .
\]

\[
\begin{align*}
PDEs : & \quad U_t + F(U)_x = 0 \quad \Rightarrow \quad U^{n+\frac{1}{2}} \\
ICs : & \quad U^n
\end{align*}
\]

\[
\begin{align*}
PDEs : & \quad U_t + G(U)_y = 0 \quad \Rightarrow \quad U^{n+1} \\
ICs : & \quad U^{n+\frac{1}{2}}
\end{align*}
\]

- **1\textsuperscript{st} order:**
  
  \[
  U^{n+1} = \mathcal{Y}(\Delta t) \mathcal{X}(\Delta t)(U^n) \quad \text{or} \quad U^{n+1} = \mathcal{X}(\Delta t) \mathcal{Y}(\Delta t)(U^n)
  \]

- **2\textsuperscript{nd} order:**

  \[
  U^{n+1} = \frac{1}{2} \left[ \mathcal{X}(\Delta t) \mathcal{Y}(\Delta t) + \mathcal{Y}(\Delta t) \mathcal{X}(\Delta t) \right](U^n)
  \]

Directional splitting scheme is easy to implement to extend 1D to multidimensional scheme. It is robust and accurate in general.
Unsplit Formulations

- Directionally unsplit (1\textsuperscript{st} order Donor Cell; 2\textsuperscript{nd} order Corner-Transport-Upwind)
  - 1\textsuperscript{st} order Donor cell vs. 2\textsuperscript{nd} order CTU

\begin{align*}
|\frac{u \Delta t}{\Delta x}| + |\frac{v \Delta t}{\Delta y}| &\leq 1. \\
\max \left(\left|\frac{u \Delta t}{\Delta x}\right|, \left|\frac{v \Delta t}{\Delta y}\right| \right) &\leq 1.
\end{align*}
Unsplit Formulations

- Directionally unsplit (1\textsuperscript{st} order Donor Cell; 2\textsuperscript{nd} order Corner-Transport-Upwind)

- 1\textsuperscript{st} order Donor cell vs. 2\textsuperscript{nd} order CTU

- **Stencil:**

\[
Q^{n+1}_{i,j} = Q^n_{i,j} - \frac{u \Delta t}{\Delta x} [Q^n_{i,j} - Q^n_{i-1,j}] - \frac{v \Delta t}{\Delta y} [Q^n_{i,j} - Q^n_{i,j-1}]
\]

\[
Q^{n+1}_{i,j} = Q^n_{i,j} - \frac{u \Delta t}{\Delta x} [Q^n_{i,j} - Q^n_{i-1,j}] - \frac{v \Delta t}{\Delta y} [Q^n_{i,j} - Q^n_{i,j-1}]
+ \frac{\Delta t^2}{2} \left\{ \frac{u}{\Delta x} \left[ \frac{v}{\Delta y} (Q^n_{i,j} - Q^n_{i-1,j}) - \frac{v}{\Delta y} (Q^n_{i-1,j} - Q^n_{i-1,j-1}) \right] 
+ \frac{v}{\Delta y} \left[ \frac{u}{\Delta x} (Q^n_{i,j} - Q^n_{i,j-1}) - \frac{u}{\Delta x} (Q^n_{i,j-1} - Q^n_{i-1,j-1}) \right] \right\}
\]
Hydro Comparison between Split vs. Unsplit


- Top: split schemes
  - PLM (2\textsuperscript{nd} order)
  - PPM + old slope limiter (3\textsuperscript{rd} order)
  - PPM + new slope limiter (3\textsuperscript{rd} order)
  - high-wavenumber instability grows due to experiencing high compression and expansion in each directional sweep

- Bottom: unsplit schemes
  - PLM
  - PPM + old slope limiter
  - PPM + new slope limiter
  - High-wavenumber instabilities are suppressed
Weakly magnetized Field loop advection in 2.5D
Gardiner & Stone 2005 (JCP); Lee and Deane 2009 (JCP)
MHD Comparison between Split vs. Unsplit

- 8-wave split MHD scheme (Powell et al. 1999) at t=2.0
- Unsplit staggered mesh MHD scheme (Lee and Deane, 2009) at t=2.0
What is wrong with the split formulation for MHD?

In the split formulation, you cannot correctly include terms proportional to $\nabla \cdot B$

Gardiner and Stone (2005)

Dynamics of in-plane magnetic fields in $x$ and $y$ directions are ruined from erroneous growth of magnetic field in $z$ direction:

$$\frac{\partial B_z}{\partial t} + B_z \frac{\partial u}{\partial x} - B_x \frac{\partial w}{\partial x} - w \frac{\partial B_x}{\partial x} + u \frac{\partial B_z}{\partial x} + B_z \frac{\partial v}{\partial y} - B_y \frac{\partial w}{\partial y} - w \frac{\partial B_y}{\partial y} + v \frac{\partial B_z}{\partial y} = 0$$

$$w \nabla \cdot B = w(\Delta B_{x,i}/\Delta x + \Delta B_{y,j}/\Delta y).$$
Lax equivalence theorem (for linear problem; 1956)

- The only convergent schemes are those that are both consistent and stable!
- Hard to show that the numerical solution converges to the original solution of the PDE; relatively easy to show consistency and stability of numerical schemes

In practice, non-linear problems adopts the linear theory as guidance

- Analytical solution if any
- Grid resolution (self-convergent) test
Grid resolution test for smooth solution

![Graphs showing convergence rate for standing and traveling waves.](image)

(a) Convergence rate for the standing wave solutions at $t = 1.0$

(b) Convergence rate for the traveling wave solutions at $t = 1.0$

Fig. 8. The circularly polarized Alfvén wave convergence rate for both the standing and traveling wave problems. PPM is used along with the HLLD Riemann solver.
Comparison with exact solution

(a) Scatter image of $B_2$ plotted with respect to $x_1$ - axis at time $t = 5$.

(b) Scatter image of $B_2$ plotted with respect to $x_1$ - axis at time $t = 5$.

Fig. 10. Plot of $B_2$ versus $x_1$ for the traveling wave using (a) the full 3D CTU scheme with CFL=0.95, and (b) the reduced 3D CTU scheme with CFL=0.475. The initial condition using $N = 64$ is also plotted.
The Riemann problem:

\[ PDEs: \quad U_t + A U_x = 0, \quad -\infty < x < \infty, \quad t > 0, \]
\[ IC: \quad U(x,0) = U^{(0)}(x) = \begin{cases} U_L & x < 0, \\ U_R & x > 0 \end{cases} \]

Two cases:

\[ u_L \quad u_R \]
\[ x \]

Fig. 2.13. (a) Compressive discontinuous initial data (b) picture of characteristic (c) solution on \( x-t \) plane

\[ u_L \quad u_R \]
\[ x \]

Fig. 2.16. Centred rarefaction wave: (a) expansive discontinuous initial data (b) picture of characteristics (c) entropy satisfying (rarefaction) solution on \( x-t \) plane
The Riemann fan:
Godunov’s innovative method (1959) to solve non-linear conservative system using the exact solution of the Riemann problem at intercell boundaries.

Fig. 6.1. Piece-wise constant distribution of data at time level n, for a single component of the vector $U$. 
Godunov’s innovative method (1959) to solve non-linear conservative system using the exact solution of the Riemann problem at intercell boundaries.
Godunov’s “order-barrier” theorem (1959) says:

- If an advection scheme (of PDE) preserves the monotonicity of the solution it is at most first-order accurate!

- Second or higher order schemes are NOT monotone and will generate oscillations

- Discouraging and seems to be doomed to improve any advection scheme of PDE!

- Linear theory is assumed!

Good! High-resolution scheme became possible using non-linear schemes

- 70’s and 80’s: Boris, van Leer, Zalesak, Woodward, Colella, Harten, Shu, Engquist, etc.

- Use of slope limiters (e.g., Koren, van Leer)

- MUSCL-Hancock, Piecewise Parabolic Method (PPM), ENO, WENO, etc.
Fig. 6.5. Grid values $Q^a$ and reconstructed $\tilde{q}^a(t_n)$ using (a) minmod slopes, (b) superbee or MC slopes. Note that these steeper slopes can be used and still have the TVD property.
Godunov Theorem and high-order schemes

- **Slope limiters:**

- **Examples:**
  - Minmod, van Leer, MC, Superbee
Riemann Solvers

- **Exact Riemann solvers**
  - Involves iterations for pressure to seek for a solution over the Riemann fan
  - Very accurate in general but it can be defective without converging

- **Approximate Riemann solvers**
  - No iterations needed
  - Rusanov (local Lax-Friedrichs)
  - HLL*-type (HLLE, H LLC for hydro/MHD; HLLD for MHD)
  - Roe solver
  - Hybrid method (e.g., HLL + Roe; HLL + HLLD)
  - Plays a crucial role to determine solution stability and accuracy!
Riemann Solvers

Fig. 6.16. The Lax-Friedrichs method applied to Test 4, with $x_0 = 0.4$. Numerical (symbol) and exact (line) solutions are compared at the output time 0.035 units.

Fig. 10.8. Godunov's method with HLLC Riemann solver applied to Test 4, with $x_0 = 0.4$. Numerical (symbol) and exact (line) solutions are compared at time 0.035.

Fig. 10.13. Godunov's method with HLL Riemann solver applied to Test 4, with $x_0 = 0.4$. Numerical (symbol) and exact (line) solutions are compared at time 0.035.

Fig. 11.7. Godunov's method with Roe's Riemann solver applied to Test 4, with $x_0 = 0.4$. Numerical (symbol) and exact (line) solutions are compared at time 0.035.
Fact:

\[ \Delta t_{\text{Diffusion}} \approx \Delta x^2; \quad \Delta t_{\text{Advection}} \approx \Delta x \]

Diffusive time scale dominates as refinement level increases

The need of overcoming small diffusive time scale:
- Explicit super-time-stepping algorithm
- Operator split semi-implicit (using HYPRE)
- Fully implicit time stepping (Jacobian-Free Newton-Krylov) algorithms
Fully Implicit JFNK Solver in FLASH

- NSF Grant award (PHY-0903997) for fiscal years 2009 – 2011, $400K
  - Dongwook Lee (PI), Shravan Gopal

- Jacobian-Free Newton-Krylov implicit scheme (e.g., Knoll and Keys 2004; Toth et al. 2006)
  - 2\textsuperscript{nd} order accurate in space and time to solve \( Ax = b \)
  - GMRES iteration to seek solutions in Krylov subspace
  - Hybrid method of using both Explicit/Implicit blocks in a computational domain
  - Requires load balancing between two different explicit/implicit types of blocks

- Schwarz-type preconditioner
  - Preconditioner to accelerate convergence rates for iterative solution
  - Off-processor data may be needed
  - Schwarz-type preconditioner minimizes the need for off-processor data
  - Efficient approach in FLASH’s block-structured AMR

- The implicit solver will extend FLASH’s capability to overcome small diffusive time scales in both astrophysical and HEDP applications
Anisotropic Heat Conduction Test for HEDP

- MHD Rotor test with $\chi_c = 5 \times 10^7$ for a cold plasma regime

- For hot plasmas, a full Spitzer conductivity can be used
1D Sinusoidal Wave Advection

\[ \frac{\partial \chi}{\partial t} + u \frac{\partial \chi}{\partial x} = 0, \quad a = 1 \]

<table>
<thead>
<tr>
<th>CFL=10 (2 iter with PC)</th>
<th>u=1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Red</td>
<td>t=0</td>
</tr>
<tr>
<td>Blue</td>
<td>t=2</td>
</tr>
<tr>
<td>Green</td>
<td>t=4</td>
</tr>
<tr>
<td>Magenta</td>
<td>t=6</td>
</tr>
<tr>
<td>Black</td>
<td>t=8</td>
</tr>
<tr>
<td>Red</td>
<td>t=10</td>
</tr>
</tbody>
</table>
1D Thermal Conduction

<table>
<thead>
<tr>
<th>Scheme</th>
<th>CFL</th>
<th>steps</th>
</tr>
</thead>
<tbody>
<tr>
<td>Explicit (Red)</td>
<td>0.8</td>
<td>19,256</td>
</tr>
<tr>
<td>Implicit (Blue)</td>
<td>0.8</td>
<td>19,256</td>
</tr>
<tr>
<td>Implicit (pink)</td>
<td>10</td>
<td>1556</td>
</tr>
<tr>
<td>Implicit (black)</td>
<td>100</td>
<td>174</td>
</tr>
<tr>
<td>Implicit (green)</td>
<td>1000</td>
<td>39</td>
</tr>
</tbody>
</table>
2D Thermal Conduction (4 blocks)

Implicit JFNK, GMRES with ILU(0)
L2 Error Norm: 1.95319e-3

HYPRE with PCG and ILU(0)
L2 Error Norm: 1.95318e-3
Cosmic magnetic fields are ubiquitous, but their origins remain unclear.

Biermann battery term is important in recreating cosmic conditions within the lab and in computations.

Magnetic fields are important because they modify transport process, accelerate particles and exert body forces.

Battery term can play an important role in seeding magnetic fields in HEDP simulations:

\[-\frac{\partial B}{\partial t} = \nabla \times (U \times B) + c \frac{\nabla n_e \times \nabla p_e}{n_e^2 e}\]

In FLASH’s single-fluid radiation-hydro model with 3T, a simple battery approximation is available (Kulsrud 2004; Xu 2008) assuming:

- Charge neutrality, LTE, a constant degree of ionization in space
- For more complicated HEDP described by non-LTE, two-fluid model is required
The (yet simplified) generalized Ohm’s law can be written assuming high collisions in MHD single fluid theory and dropping the electron inertia term

\[
E = -\frac{u \times B}{c} + \frac{j}{\sigma} + \frac{j \times B}{cn_e e} - \frac{\nabla p_e}{n_e e}
\]

- **Induction Term**\( -\frac{u \times B}{c} \)
- **Ohmic Term**\( \frac{j}{\sigma} \)
- **Hall Term**\( \frac{j \times B}{cn_e e} \)
- **Battery Term**\( -\frac{\nabla p_e}{n_e e} \)

- Ideal MHD uses IT only (magnetic flux freezing, both ions and electrons are glued to the low-frequency fluid-like field lines)
- OT can be ignored for large magnetic Reynolds number
- Both Hall and Battery terms can be dropped if the Lamor gyration radius of ions is much smaller than the length scale (therefore no charge separation)
- HT becomes more important than BT for high plasma beta:

\[
\frac{|BT|}{|HT|} = \frac{\nabla p_e / e n_e}{|j \times B / e n_e|} \approx \beta \frac{L_B}{L_p}
\]
The default unit in FLASH is cgs for physical variables such as density, pressure, etc.

For electromagnetic variables, FLASH has a convenient unit in that magnetic permeability, electric permittivity, the speed of light and the factor 4pi are absorbed into the physical variables

<table>
<thead>
<tr>
<th>Quantity</th>
<th>FLASH’s None</th>
<th>Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>magnetic field</td>
<td>B</td>
<td>$\frac{B}{\sqrt{4\pi}}$</td>
</tr>
<tr>
<td>electric field</td>
<td>E</td>
<td>$\frac{cE}{\sqrt{4\pi}}$</td>
</tr>
<tr>
<td>current density</td>
<td>j</td>
<td>$\sqrt{4\pi}j$</td>
</tr>
<tr>
<td>vector potential</td>
<td>A</td>
<td>$\frac{A}{\sqrt{4\pi}}$</td>
</tr>
<tr>
<td>magnetic diffusivity</td>
<td>$\eta$</td>
<td>$\frac{c^2}{4\pi} \eta$</td>
</tr>
</tbody>
</table>

Table 4. Conversion table for electrodynamics quantities from FLASH’s none to Gaussian.

To simulate in gaussian cgs, FLASH needs to:

- **Initialize**: $B_{\text{none}} \rightarrow B_{\text{none}}/\sqrt{4\pi}$
- **Visualize**: $B_{\text{chk}} \rightarrow \sqrt{4\pi} B_{\text{chk}}$, where $B_{\text{chk}} = B_{\text{none}}/\sqrt{4\pi}$
The FLASH Code: Hydro Unit in FLASH
An unsplit staggered mesh scheme for multidimensional magneto-hydrodynamics

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\textbf{A B S T R A C T}

We introduce a total variation diminishing (TVD) second-order MHD scheme for multidimensional magneto-hydrodynamics. The schemes use a single, high-resolution smoothness indicator to limit the transport upwind by the AUSM method. The schemes use linear polynomial fluxes and dissipative elements. The schemes are monotonic and dissipative. The scheme is a variant of the 3D unsplit CTU method by Saltzman [J. Saltzman, An unsplit 3D upwind method for hyperbolic conservation laws, J. Comput. Phys. 115 (1994) 153–168] for hyperbolic conservation laws. The key novelty in our approach is that the TVD methods for 3D hyperbolic conservation laws are used for the MHD equations, whereas previously the schemes were designed for 2D cases only.

\textbf{RéSUMÉ}

Unsplit Staggered Mesh (USM) MHD Solver

- Shock-capturing high-order Godunov Riemann solver (Lee & Deane, JCP, 2009; Lee 2012, submitted)
- Finite volume method, adaptive mesh refinement, uniform grid
- New data reconstruction-evolution algorithm for high-order accuracy
- 1st order Godunov, 2nd order MUSCL-Hancock, 3rd order PPM, 5th Order WENO
- Approximate Riemann solvers: Roe, HLL, HLLC, HLLD, Marquina, modified Marquina, Local Lax-Friedrichs
- Monotonicity preserving upwind PPM slope limiter for MHD (Lee, 2010, Astronum)
- Divergence of magnetic fields is numerically controlled on a staggered grid, using a constrained transport (CT) method (Evans & Hawley, 1998)
- Wide ranges of plasma flows, extended to HEDP
- Full Courant stability limit (CFL ~ 1 for 3D) using corner-transport-upwind (CTU)
MHD Governing Equations

- MHD system of equations:
  
  \[
  \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0, \\
  \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho uu - BB) + \nabla p_{\text{tot}} = 0, \\
  \frac{\partial B}{\partial t} + \nabla \cdot (uB - Bu) = 0, \\
  \frac{\partial E}{\partial t} + \nabla \cdot (uE + up_{\text{tot}} - BB \cdot u) = 0.
  \]

- This can be written in a simple matrix form:

  \[
  \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} + \frac{\partial H}{\partial z} = 0,
  \]
MHD Governing Equations

Conservative variables and fluxes:

\[
U = \begin{pmatrix} 
\rho \\
\rho u \\
\rho v \\
\rho w \\
B_x \\
B_y \\
B_z \\
E 
\end{pmatrix}, \quad 
F = \begin{pmatrix} 
\rho u \\
\rho u^2 + p_{tot} - B_x^2 \\
\rho uv - B_y B_x \\
\rho uw - B_z B_x \\
0 \\
u B_y - v B_x (-= -E_z) \\
u B_z - w B_x (-= E_y) \\
(E + p_{tot}) u - B_x (u B_x + v B_y + w B_z) 
\end{pmatrix}, \quad (7)
\]

\[
G = \begin{pmatrix} 
\rho v \\
\rho vu - B_x B_y \\
\rho v^2 + p_{tot} - B_y^2 \\
\rho vw - B_z B_y \\
v B_x - u B_y (= E_z) \\
0 \\
v B_z - w B_y (-= -E_x) \\
(E + p_{tot}) v - B_y (u B_x + v B_y + w B_z) 
\end{pmatrix}, \quad 
H = \begin{pmatrix} 
\rho w \\
\rho wu - B_x B_z \\
\rho wv - B_y B_z \\
\rho w^2 + p_{tot} - B_z^2 \\
w B_x - u B_z (= -E_y) \\
w B_y - v B_z (= E_x) \\
0 \\
(E + p_{tot}) w - B_z (u B_x + v B_y + w B_z) 
\end{pmatrix} \ . (8)
\]
General Features

- New approach of using characteristic tracing for BOTH normal predictor and transverse corrector

- Reduced 3D CTU
  - A direct extension of 2D CTU to 3D
  - Requires 3 Riemann solves for 3D (6-ctu needs 6 Riemann solves)
  - Only including second cross derivatives
  - CFL limit ~ 0.5

- Full 3D CTU
  - Full considerations of accounting for third cross derivatives
  - Requires 3 Riemann solves for 3D (12-ctu needs 12 Riemann solves)
  - CFL limit ~ 1.0
  - 20% relative performance gain compared to reduced 3D CTU
Divergence-Free fields: Constrained Transport (CT) MHD
CT scheme by Balsara and Spicer, 1998:

\[
E^{n+1/2}_{z,i+1/2,j+1/2,k} = \frac{1}{4} \left( E^{*,n+1/2}_{z,i+1/2,j,k} + E^{*,n+1/2}_{z,i+1/2,j+1,k} + E^{*,n+1/2}_{z,i+1,j+1/2,k} + E^{*,n+1/2}_{z,i+1,j+1/2,k} \right)
\]
Constraint Transport Method: Recall...

- Conservative variables and fluxes:

\[
U = \begin{pmatrix}
\rho \\
\rho u \\
\rho v \\
\rho w \\
B_x \\
B_y \\
B_z \\
E
\end{pmatrix}, \quad F = \begin{pmatrix}
\rho u \\
\rho u^2 + p_{\text{tot}} - B_x^2 \\
\rho uv - B_y B_x \\
\rho uw - B_z B_x \\
0 \\
(B + p_{\text{tot}})u - B_x(u B_x + v B_y + w B_z)
\end{pmatrix}.
\]  

\[
G = \begin{pmatrix}
\rho v \\
\rho vu - B_x B_y \\
\rho v^2 + p_{\text{tot}} - B_y^2 \\
vB_x - uB_y(= -E_z) \\
0 \\
vB_z - wB_y(= -E_x)
\end{pmatrix}, \quad H = \begin{pmatrix}
\rho w \\
\rho wu - B_x B_z \\
\rho vw - B_y B_z \\
wB_x - uB_z(= -E_y) \\
wB_y - vB_z(= E_x) \\
0 \\
(E + p_{\text{tot}})w - B_z(u B_x + v B_y + w B_z)
\end{pmatrix}.
\]
A New Upwind Constraint Transport Method

- New upwind biased modified electric field construction (upwind-MEC), Lee 2012:

\[
E_{z,i+1/2,j+1/2,k}^{n+1/2} = \alpha \left[ \nu_P \left( E_{z,i+1/2,j+1/2,k}^{*,n+1/2} + \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial y^2} \right) + \right]
\]

\[
\nu_N \left( E_{z,i+1/2,j+1/2,k}^{*,n+1/2} - \frac{\Delta y}{2} \frac{\partial E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial y} + \frac{\Delta y^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial y^2} \right) + \right]
\]

\[
u_P \left( E_{z,i+1/2,j+1/2,k}^{*,n+1/2} + \frac{\Delta x}{2} \frac{\partial E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) + \]

\[
u_N \left( E_{z,i+1/2,j+1/2,k}^{*,n+1/2} - \frac{\Delta x}{2} \frac{\partial E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial x} + \frac{\Delta x^2}{8} \frac{\partial^2 E_{z,i+1/2,j+1/2,k}^{*,n+1/2}}{\partial x^2} \right) \right].
\]

\[u_P = \frac{1}{2} (1 + \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})|,
\]

\[u_N = \frac{1}{2} (1 - \text{sign}(u_{i+1/2,j+1/2}))|\text{sign}(u_{i+1/2,j+1/2})|,
\]

\[v_P = \frac{1}{2} (1 + \text{sign}(v_{i+1/2,j+1/2}))|\text{sign}(v_{i+1/2,j+1/2})|,
\]

\[v_N = \frac{1}{2} (1 - \text{sign}(v_{i+1/2,j+1/2}))|\text{sign}(v_{i+1/2,j+1/2})|,
\]

\[\text{sign}(x) = \begin{cases} 
 1 & \text{if } x > 0, \\
 0 & \text{if } x = 0, \\
 -1 & \text{if } x < 0.
\end{cases}
\]
A New Upwind Constraint Transport Method

Small angle advection of the 2D field loop:

(a) $B_p$ with the standard CT at $t = 0.1$

(b) $B_p$ with the standard CT at $t = 2$

(c) $B_p$ with the upwind-MEC at $t = 0.1$

(d) $B_p$ with the upwind-MEC at $t = 2$
A New Upwind Constraint Transport Method

- Small angle advection of the 3D field loop:

(a) $B_p$ using the standard CT at $t = 2$.
(b) $B_p$ using the standard MEC at $t = 2$.
(c) $B_p$ using the upwind MEC at $t = 2$. 
Three CT schemes discussed:

- **Standard CT scheme by Balsara and Spicer, 1998:**
  - Takes a simple arithmetic averaging
  - Lacks numerical diffusion for magnetic fields advection

- **Modified electric field construction (MEC) scheme by Lee and Deane, 2009:**
  - 3rd order accurate in space
  - Not enough numerical diffusion for field advection

- **Upwind biased MEC (upwind-MEC) scheme by Lee, 2012 (submitted):**
  - Upwind scheme of MEC
  - Added numerical diffusion to stabilize field advection
Numerical Tests

Fig. 11. Density plots of the Oszag-Tang problem at a resolution of $128^3$ using the Roe Riemann solver.
Numerical Tests

(a) Density and magnetic pressure at $t = 0.0$

(b) Density and magnetic pressure at $t = 0.02$

(c) Density and magnetic pressure at $t = 0.04$

(d) Density and magnetic pressure at $t = 0.06$
Numerical Tests

Fig. 17. Results of the blast problem simulation with \( B_0 = 50/\sqrt{\pi} \) using a hybrid Riemann solver. In (a), density (denoted as "den" in the legend) is plotted at the top half. Magnetic pressure (denoted as "magy" in the legend) is plotted at the bottom half. In (b), 40 contour lines are plotted.
# Runtime Parameters

# (1) Interpolation, reconstruction, slope limiter:

- **PARAMETER order**: INTEGER 2  # Order of scheme: 1st/2nd/3rd/5th order
- **PARAMETER transOrder**: INTEGER 1  # Order of transverse flux: 1st order. 3rd order is experimental.
- **PARAMETER slopeLimiter**: STRING "vanLeer"  # Slope limiter for Riemann state
- **PARAMETER charLimiting**: BOOLEAN TRUE  # Turn on/off characteristic/primitive limiting
- **PARAMETER LimitedSlopeBeta**: REAL 1.0  # Any real value specific for the Limited Slope
- **PARAMETER use_steepeening**: BOOLEAN FALSE  # Turn on/off PPM contact steepeening
- **PARAMETER use_flattening**: BOOLEAN FALSE  # Turn on/off flattening
- **PARAMETER use_avisc**: BOOLEAN FALSE  # Turn on/off artificial viscosity
- **PARAMETER cvisc**: REAL 0.1  # artificial viscosity constant
- **PARAMETER use_upwindTVD**: BOOLEAN FALSE  # Turn on/off upwinding TVD slopes

# (2) For 3D CTU

- **PARAMETER use_3dFullCTU**: BOOLEAN TRUE  # FALSE will give the simpler CTU without corner upwind coupling

# (3) Riemann solvers

- **PARAMETER RiemannSolver**: STRING "Roe"  # Approximate Riemann solver:
  - Roe (default), HLL, HLLC, Marquina, MarquinaMod, Hybrid
  - or local Lax-Friedrichs, plus HLLD for MHD
- **PARAMETER entropy**: BOOLEAN FALSE  # Turn on/off an entropy fix routine
- **PARAMETER entropyFixMethod**: STRING "HartenHyman"  # Entropy fix method for the Roe Riemann solver:
  - Harten or HartenHyman
- **PARAMETER shockDetect**: BOOLEAN FALSE  # Turn on/off a shock detecting switch
- **PARAMETER EOSforRiemann**: BOOLEAN FALSE  # Turn on/off EOS calls for the Riemann states
- **PARAMETER addThermalFlux**: BOOLEAN TRUE  # Add/don't add thermal fluxes to hydro fluxes

# (4) Gravity updates

- **PARAMETER use_gravHalfUpdate**: BOOLEAN FALSE  # Include gravitational accelerations to hydro coupling at n+1/2
- **PARAMETER use_gravConsv**: BOOLEAN FALSE  # Use conservative variables for gravity coupling at n+1/2
- **PARAMETER use_GravPotUpdate**: BOOLEAN FALSE  # Parameter for half timestep update of gravitational potential
# Runtime Parameters for unsplit USM-MHD solver

<table>
<thead>
<tr>
<th>PARAMETER</th>
<th>TYPE</th>
<th>VALUE</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>killDivb</td>
<td>BOOLEAN</td>
<td>TRUE</td>
<td>Turn on/off DivB cleaning</td>
</tr>
<tr>
<td>E_modification</td>
<td>BOOLEAN</td>
<td>TRUE</td>
<td>Turn on/off electric field modification</td>
</tr>
<tr>
<td>E_upwind</td>
<td>BOOLEAN</td>
<td>FALSE</td>
<td>Turn on/off upwind update for induction equations</td>
</tr>
<tr>
<td>energyFix</td>
<td>BOOLEAN</td>
<td>FALSE</td>
<td>Turn on/off an energy correction for CT scheme</td>
</tr>
<tr>
<td>ForceHydroLimit</td>
<td>BOOLEAN</td>
<td>FALSE</td>
<td>Turn on/off a hydro limiting switch</td>
</tr>
<tr>
<td>facevar2ndOrder</td>
<td>BOOLEAN</td>
<td>TRUE</td>
<td>Turn on/off a 2nd order facevar update</td>
</tr>
<tr>
<td>use_Biermann</td>
<td>BOOLEAN</td>
<td>FALSE</td>
<td>Biermann Battery Term</td>
</tr>
<tr>
<td>use_Biermann1T</td>
<td>BOOLEAN</td>
<td>FALSE</td>
<td>1T Biermann Battery Term</td>
</tr>
<tr>
<td>hy_biermannSource</td>
<td>BOOLEAN</td>
<td>FALSE</td>
<td>Enable Battery Source (vs. flux)</td>
</tr>
<tr>
<td>hy_bier1TZ</td>
<td>REAL</td>
<td>-1.0</td>
<td>Zbar value for 1T Biermann Battery Term</td>
</tr>
<tr>
<td>hy_bier1TA</td>
<td>REAL</td>
<td>-1.0</td>
<td>Abar value for 1T Biermann Battery Term</td>
</tr>
<tr>
<td>prolMethod</td>
<td>STRING</td>
<td>&quot;INJECTION_PROL&quot;</td>
<td>Prolongation method: injection_prol/Balsara_prol</td>
</tr>
<tr>
<td>hy_biermannCoef</td>
<td>REAL</td>
<td>1.0</td>
<td>Coefficient of Biermann Battery flux</td>
</tr>
</tbody>
</table>

# Number of guard cells at each boundary

USESETUPVARS SupportWeno, SupportPpmUpwind

IF SupportWeno
    GUARDCELLS 6 # the Unsplit Hydro/MHD solver requires 6 guard cells to support WENO!
ELSEIF SupportPpmUpwind
    GUARDCELLS 6 # the Unsplit Hydro/MHD solver requires 6 guard cells to support PPM Upwind!
ELSE
    GUARDCELLS 4 # the Unsplit Hydro/MHD solver requires 4 guard cell layers!
ENDIF
Intermediate Summary II

- Verification tests for the reduced/full 3D CTU schemes:
  - CFL=0.95 for all 3D simulations using the full CTU scheme
  - CFL=0.475 for the reduced CTU scheme
  - They both converge in 2\textsuperscript{nd} order
  - 20\% performance gain in using the full CTU scheme:
    \[
    \frac{CPU_{F-ctu}}{CPU_{R-ctu}} \approx 0.8
    \]
  - Various choices in runtime parameters
Outline & Conclusion

- Broad Ranges of Applications
  - Astrophysics and HEDP

- Algorithms and mathematics
  - Governing equations, difference equations of PDEs
  - Dimensionally Split vs. Unsplit formulations
  - Hydro and MHD solvers
    - High-order Reconstructions, Riemann problems, physical units
  - Explicit vs. Implicit schemes
  - Beyond the hyperbolic system (diffusion, source terms, Biermann battery, etc)

- Examples: setting up problems, how to use various features and switches

- Summary
Thank You

Questions?
New Upwind PPM for Slowly Moving Shock

- Standard PPM
- Standard PPM with increasing By
- Upwind PPM
- 5th order WENO
New Upwind PPM for Slowly Moving Shock

Lee, 2010, 5\textsuperscript{th} Astronum Proceeding;

Lee, 2011, in preparation

Standard PPM

Standard PPM with increasing By

Upwind PPM

5\textsuperscript{th} order WENO

larger By
Mesh package can be selected at configuration time

The basic abstraction is a block of interior cells surrounded by guard cells

Grid unit makes sure that blocks are self contained before being given to the solvers
Take a deep breath!
A primitive form:

\[ \mathbf{V} = (\rho, u, v, w, B_x, B_y, B_z, \rho)^T, \quad \frac{\partial \mathbf{V}}{\partial t} + \mathbf{A}_x \frac{\partial \mathbf{V}}{\partial x} + \mathbf{A}_y \frac{\partial \mathbf{V}}{\partial y} + \mathbf{A}_z \frac{\partial \mathbf{V}}{\partial z} = 0. \]

where the coefficient matrix is

\[
\mathbf{A}_x = \begin{pmatrix}
    u & \rho & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & u & 0 & 0 & -\frac{B_x}{\rho} & \frac{B_y}{\rho} & \frac{B_z}{\rho} & 1 \\
    0 & 0 & u & 0 & -\frac{B_y}{\rho} & -\frac{B_z}{\rho} & 0 & 0 \\
    0 & 0 & 0 & u & 0 & 0 & -\frac{B_x}{\rho} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & B_y & -B_x & 0 & -v & u & 0 & 0 \\
    0 & B_z & 0 & -B_x & -w & 0 & u & 0 \\
    0 & \gamma p & 0 & 0 & -k u \cdot \mathbf{B} & 0 & 0 & u
\end{pmatrix},
\]
Corner Transport Upwind (CTU)

\[ V_{i,j+1,S}^{n+1/2} \]
\[ V_{i,j,N}^{n+1/2} \]
\[ V_{i,j,E}^{n+1/2} \]
\[ V_{i,j,W}^{n+1/2} \]
\[ *(i,j) \]
\[ V_{i+1,j,W}^{n+1/2} \]
\[ V_{i-1,j,E}^{n+1/2} \]
\[ V_{i,j-1,N}^{n+1/2} \]

Linear system in 3D

\[ V_{i,j,k,E,W}^{n+1/2} = V_{i,j,k}^{n} + \frac{1}{2} \left[ \pm I - \frac{\Delta t}{\Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^{n} - \frac{\Delta t}{2\Delta y} A_y(V_{i,j,k}^{n}) \Delta_j^{n} - \frac{\Delta t}{2\Delta z} A_z(V_{i,j,k}^{n}) \Delta_k^{n} \right] \]

\[ V_{i,j,k,N,S}^{n+1/2} = V_{i,j,k}^{n} - \frac{\Delta t}{2\Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^{n} + \frac{1}{2} \left[ \pm I - \frac{\Delta t}{\Delta y} A_y(V_{i,j,k}^{n}) \Delta_j^{n} - \frac{\Delta t}{2\Delta z} A_z(V_{i,j,k}^{n}) \Delta_k^{n} \right] \]

\[ V_{i,j,k,T,B}^{n+1/2} = V_{i,j,k}^{n} - \frac{\Delta t}{2\Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^{n} - \frac{\Delta t}{2\Delta y} A_y(V_{i,j,k}^{n}) \Delta_j^{n} + \frac{1}{2} \left[ \pm I - \frac{\Delta t}{\Delta z} A_z(V_{i,j,k}^{n}) \Delta_k^{n} \right] \]
## Corner Transport Upwind (CTU)

### Linear system in 3D

<table>
<thead>
<tr>
<th>Normal predictor</th>
<th>Transverse corrector</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_{i,j,k,E,W}^{n+1/2} = V_{i,j,k}^{n} + \frac{1}{2} \left[ \pm 1 - \frac{\Delta t}{\Delta x} A_x(V_{i,j,k}^{n}) \right] \Delta_i^n )</td>
<td>( \frac{\Delta t}{2\Delta y} A_y(V_{i,j,k}^{n}) \Delta_j^n - \frac{\Delta t}{2\Delta z} A_z(V_{i,j,k}^{n}) \Delta_k^n )</td>
</tr>
<tr>
<td>( V_{i,j,k,N,S}^{n+1/2} = V_{i,j,k}^{n} - \frac{\Delta t}{2\Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^n + \frac{1}{2} \left[ \pm 1 - \frac{\Delta t}{\Delta y} A_y(V_{i,j,k}^{n}) \right] \Delta_j^n - \frac{\Delta t}{2\Delta z} A_z(V_{i,j,k}^{n}) \Delta_k^n )</td>
<td>( \frac{\Delta t}{2\Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^n - \frac{\Delta t}{2\Delta y} A_y(V_{i,j,k}^{n}) \Delta_j^n + \frac{1}{2} \left[ \pm 1 - \frac{\Delta t}{\Delta z} A_z(V_{i,j,k}^{n}) \right] \Delta_k^n )</td>
</tr>
<tr>
<td>( V_{i,j,k,T,B}^{n+1/2} = V_{i,j,k}^{n} - \frac{\Delta t}{2\Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^n - \frac{\Delta t}{2\Delta y} A_y(V_{i,j,k}^{n}) \Delta_j^n + \frac{1}{2} \left[ \pm 1 - \frac{\Delta t}{\Delta z} A_z(V_{i,j,k}^{n}) \right] \Delta_k^n )</td>
<td>( \frac{\Delta t}{2\Delta z} A_z(V_{i,j,k}^{n}) \Delta_k^n )</td>
</tr>
</tbody>
</table>
**Corner Transport Upwind (CTU)**

<table>
<thead>
<tr>
<th>$V_{i,j}^{n+1/2}$</th>
<th>$V_{i,j}^{n+1/2}$</th>
<th>$V_{i,j}^{n+1/2}$</th>
<th>$V_{i,j}^{n+1/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{i-1,j,E}^{n+1/2}$</td>
<td>$V_{i,j,W}^{n+1/2}$</td>
<td>$*(i,j)$</td>
<td>$V_{i-1,j,W}^{n+1/2}$</td>
</tr>
<tr>
<td>$V_{i,j}^{n+1/2}$</td>
<td>$V_{i,j}^{n+1/2}$</td>
<td>$V_{i,j,S}^{n+1/2}$</td>
<td>$V_{i,j-1,N}^{n+1/2}$</td>
</tr>
</tbody>
</table>

- **Normal predictor**
  
  $V_{i,j,k,E,W}^{n+1/2} = V_{i,j,k}^{n} + \frac{1}{2} \left[ \pm I - \frac{\Delta t}{\Delta x} A_x(V_{i,j,k}^{n}) \right] \Delta_i^n$

  $V_{i,j,k,N,S}^{n+1/2} = V_{i,j,k}^{n} - \frac{\Delta t}{2 \Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^n + \frac{1}{2} \left[ \pm I - \frac{\Delta t}{\Delta y} A_y(V_{i,j,k}^{n}) \right] \Delta_j^n - \frac{\Delta t}{2 \Delta z} A_z(V_{i,j,k}^{n}) \Delta_k^n$

  $V_{i,j,k,T,B}^{n+1/2} = V_{i,j,k}^{n} - \frac{\Delta t}{2 \Delta x} A_x(V_{i,j,k}^{n}) \Delta_i^n - \frac{\Delta t}{2 \Delta y} A_y(V_{i,j,k}^{n}) \Delta_j^n + \frac{1}{2} \left[ \pm I - \frac{\Delta t}{\Delta z} A_z(V_{i,j,k}^{n}) \right] \Delta_k^n$

- **Transverse corrector**

  - Traditional approach (Colella 1990; Saltzman 1994)
  - Characteristic tracing for the normal predictor
  - Subsequent calls to Riemann solvers for transverse corrector

**Linear system in 3D**
### Corner Transport Upwind (CTU)

<table>
<thead>
<tr>
<th></th>
<th>( \mathbf{V}_{i,j+1,S}^{n+1/2} )</th>
<th>( \mathbf{V}_{i,j,N}^{n+1/2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \mathbf{V}_{i,j,E}^{n+1/2} )</td>
<td>( \mathbf{V}_{i,j,W}^{n+1/2} )</td>
<td>( \mathbf{V}_{i,j,E}^{n+1/2} )</td>
</tr>
</tbody>
</table>
| \( \mathbf{V}_{i,j,S}^{n+1/2} \) | \( \mathbf{V}_{i,j-1,N}^{n+1/2} \)

#### Linear system in 3D

**Normal predictor**

\[
\mathbf{V}_{i,j,k,E,W}^{n+1/2} = \mathbf{V}_{i,j,k}^{n} + \frac{1}{2} \left[ \pm \mathbf{I} - \frac{\Delta t}{\Delta x} \mathbf{A}_x(\mathbf{V}_{i,j,k}^{n}) \right] \Delta_i^n - \frac{\Delta t}{2\Delta y} \mathbf{A}_y(\mathbf{V}_{i,j,k}^{n}) \Delta_j^n - \frac{\Delta t}{2\Delta z} \mathbf{A}_z(\mathbf{V}_{i,j,k}^{n}) \Delta_k^n
\]

**Transverse corrector**

\[
\mathbf{V}_{i,j,k,N,S}^{n+1/2} = \mathbf{V}_{i,j,k}^{n} - \frac{\Delta t}{2\Delta x} \mathbf{A}_x(\mathbf{V}_{i,j,k}^{n}) \Delta_i^n + \frac{1}{2} \left[ \pm \mathbf{I} - \frac{\Delta t}{\Delta y} \mathbf{A}_y(\mathbf{V}_{i,j,k}^{n}) \right] \Delta_j^n - \frac{\Delta t}{2\Delta z} \mathbf{A}_z(\mathbf{V}_{i,j,k}^{n}) \Delta_k^n
\]

**New approach (Lee and Deane 2009):**

- Characteristic tracing for BOTH normal predictor and transverse corrector!
A primitive form:
\[
\mathbf{V} = (\rho, u, v, w, B_x, B_y, B_z, \mathcal{p})^T, \quad \frac{\partial \mathbf{V}}{\partial t} + \mathbf{A}_x \frac{\partial \mathbf{V}}{\partial x} + \mathbf{A}_y \frac{\partial \mathbf{V}}{\partial y} + \mathbf{A}_z \frac{\partial \mathbf{V}}{\partial z} = 0.
\]

where the coefficient matrix is
\[
\mathbf{A}_x = \begin{pmatrix}
    u & \rho & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & u & 0 & 0 & -\frac{B_x}{\rho} & \frac{B_z}{\rho} & \frac{B_z}{\rho} & 1 \\
    0 & 0 & u & 0 & -\frac{B_y}{\rho} & \frac{B_y}{\rho} & \frac{B_x}{\rho} & 0 \\
    0 & 0 & 0 & u & -\frac{B_x}{\rho} & 0 & -\frac{B_x}{\rho} & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
    0 & B_y & -B_x & 0 & -v & u & 0 & 0 \\
    0 & B_z & 0 & -B_x & -w & 0 & u & 0 \\
    0 & \gamma \mathcal{p} & 0 & 0 & -k \mathbf{u} \cdot \mathbf{B} & 0 & 0 & u
\end{pmatrix}
\]

First consider the evolution in the x-normal direction and treat the normal magnetic field separately from the other variables:
\[
\begin{bmatrix}
    \mathbf{\hat{V}}_{x_{i,j,k}} \\
    B_{x_{i,j,k}}
\end{bmatrix}_{n+1/2, i,j,k,E,W} = \begin{bmatrix}
    \mathbf{\hat{V}}_{x_{i,j,k}} \\
    B_{x_{i,j,k}}
\end{bmatrix}_n + \frac{1}{2} \left( \pm \begin{bmatrix}
    \hat{\mathbf{i}} & 0 \\
    0 & 1
\end{bmatrix} - \frac{\Delta t}{\Delta x} \begin{bmatrix}
    \mathbf{\hat{A}}_x & \mathbf{A}_{Bx}
\end{bmatrix}_n \right) \begin{bmatrix}
    \mathbf{\bar{A}}_{x_i} \\
    \mathbf{\bar{A}}_{x_i}
\end{bmatrix}_n.
\]

\[
\mathbf{\bar{V}}_x = \begin{bmatrix}
    \mathbf{\hat{V}}_x \\
    B_x
\end{bmatrix} \quad \text{and} \quad \mathbf{\bar{A}}_x = \begin{bmatrix}
    \mathbf{\hat{A}}_x & \mathbf{A}_{Bx}
\end{bmatrix}.
\]
\[
\mathbf{A}_{Bx} = \begin{bmatrix}
    0, -\frac{B_x}{\rho}, -\frac{B_y}{\rho}, -\frac{B_z}{\rho}, -v, -w, -k \mathbf{u} \cdot \mathbf{B}
\end{bmatrix}^T.
\]
### Single-step data Reconstruction-evolution in USM

**Normal Predictor**

\[
\begin{align*}
\hat{V}^{n+1/2}_{x,i,j,k,E,W} &= \hat{V}^{n}_{x,i,j,k,E} + \frac{1}{2} \left( \pm \hat{I} - \frac{\Delta t}{\Delta x} \hat{A}_{x} \right)^{n}_{i,j,k} \hat{A}_{i}^{n} - \frac{\Delta t}{2\Delta x} \left( A_{B_{x}} \right)_{i,j,k}^{n} A^{n}_{B_{x},i}, \\
(B_{x})^{n+1/2}_{i,j,k,E,W} &= B^{n}_{x,i,j,k} \pm \frac{1}{2} A^{n}_{B_{x},i},
\end{align*}
\]

**Characteristic Tracing**

\[
\hat{V}^{n+1/2}_{x,i,j,k,E} = \hat{V}^{n}_{x,i,j,k} + \frac{1}{2} \sum_{k; \lambda_{i,j,k}^{k} > 0} \left( 1 - \frac{\Delta t}{\Delta x} \lambda_{i,j,k}^{k} \right) r_{x,i,j,k}^{k} \hat{A}_{i}^{n} - \frac{\Delta t}{2\Delta x} \left( A_{B_{x}} \right)_{i,j,k}^{n} A^{n}_{B_{x},i},
\]
Characteristic tracing for Transverse corrector

- A jump relationship:

\[ \hat{A}_y \hat{V}_l + \sum_{m=1}^{m_0-1} \lambda^m r^m \tilde{\Delta} \alpha = \hat{A}_y \hat{V}_r - \sum_{m=m_0}^{7} \lambda^m r^m \tilde{\Delta} \alpha. \]  

(42)

The property of conservation across discontinuities of the Roe matrix \( \hat{A}_y \) (see (11) and (16)) \([36, 56]\) gives

\[ \hat{A}_y \Delta = \hat{A}_y (\hat{V}_r - \hat{V}_l) = G(\hat{V}_r) - G(\hat{V}_l) = G_{i,j+1/2} - G_{i,j-1/2}. \]  

(43)

From (42) and (43), the upwind flux gradient can be replaced by

\[ G_{i,j+1/2} - G_{i,j-1/2} = \sum_{m=1}^{7} \lambda^m r^m \tilde{\Delta} \alpha, \]

(44)

where the first-order upwind slope limiter \( \tilde{\Delta} \) is applied to each characteristic variable \( \alpha \) by

\[ \tilde{\Delta} \alpha = \begin{cases} 
I^m \cdot \hat{\Delta}^n_+ & \text{if } \lambda^m < 0, \\
I^m \cdot \hat{\Delta}^n_- & \text{if } \lambda^m > 0.
\end{cases} \]  

(45)
Reduced 3D CTU in USM

\[
\hat{\mathbf{V}}^{n+1/2}_{x,i,j,k,E} = \hat{\mathbf{V}}^n_{x,i,j,k} + \frac{1}{2} \sum_{k_i, \lambda^k_{i,j,k} > 0} \left( 1 - \frac{\Delta t}{\Delta x} \lambda^k_{i,j,k} \right) \mathbf{r}^k_{x,i,j,k} \hat{\alpha}^n_i - \frac{\Delta t}{2\Delta x} (A_{Bx})^n_{i,j} \Delta B^n_{x,i},
\]

\[
\hat{\alpha}^n_i = TVD\_Limiter \left[ \mathbf{I}^k_{x,i,j,k} \cdot \hat{\alpha}^n_{i,+}, \mathbf{I}^k_{x,i,j,k} \cdot \hat{\alpha}^n_{i,-} \right].
\]

\[
\hat{\mathbf{V}}^{n+1/2}_{y,i,j,k,E,W} = \hat{\mathbf{V}}^{n+1/2}_{i,j,k,E,W} - \frac{\Delta t}{2\Delta y} A_y(\mathbf{V}^n_{i,j,k,E}) \Delta j,
\]

\[
\hat{\mathbf{V}}^{n+1/2}_{z,i,j,k,E,W} = \hat{\mathbf{V}}^{n+1/2}_{i,j,k,E,W} - \frac{\Delta t}{2\Delta z} A_z(\mathbf{V}^n_{i,j,k,E}) \Delta j,
\]

\[
\hat{\mathbf{V}}^{n+1/2}_{y,i,j,k,E,W} = \hat{\mathbf{V}}^{n+1/2}_{y,i,j,k,E,W} - \frac{\Delta t}{2\Delta y} \sum_{k=1}^7 \lambda^k_{y,i,j,k} \mathbf{r}^k_{y,i,j,k} \hat{\alpha}^n_{y,j} - \frac{\Delta t}{2\Delta y} (A_{By})^n_{i,j,k} \Delta B^n_{y,j},
\]

\[
\hat{\alpha}^n_{y,j} = Upwinding \left[ \mathbf{I}^k_{y,i,j,k} \cdot \hat{\alpha}^n_{y,j,+}, \mathbf{I}^k_{y,i,j,k} \cdot \hat{\alpha}^n_{y,j,-} \right].
\]
\[ \hat{\mathbf{v}}_{x,i,j,k}^{n+1/2} = \hat{\mathbf{v}}_{x,i,j,k}^n + \frac{1}{2} \sum_{k; \lambda_{x,i,j,k}^k > 0} \left( 1 - \frac{\Delta t}{\Delta x} \lambda_{x,i,j}^k \right) \mathbf{r}_{x,i,j,k}^k \Delta \alpha_i^n - \frac{\Delta t}{2\Delta x} (A_{Bx})_{i,j,k}^n \Delta B_{x,i}^n, \]

\[ \hat{\Delta} \alpha_i^n = \text{TVD Limiter} \left[ I_{x,i,j,k}^n \cdot \hat{\Delta} n_{i,+}^n, I_{x,i,j,k}^n \cdot \hat{\Delta} n_{i,-}^n \right]. \]