Numerical Methods for Magnetogasdynamics

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Requirements

Compressible: Waves and shocks \Rightarrow need algorithm that can cope with this.

Solenoidal Constraint: Need to do something about the condition $\nabla \cdot \mathbf{B} = 0$.

Stiffness: Equations might include source terms due to heating/cooling etc. These can sometimes make the equations stiff (small timescales).

Adaptive mesh refinement: Sometimes have a large range of length and timescales \Rightarrow need adaptive mesh refinement (AMR).

Non-ideal MHD: These involve diffusive terms \Rightarrow small timesteps with explicit schemes.

Most effective methods are conservative and upwind: conservative to capture shocks; upwind to ensure clean solutions (no oscillations at shocks etc).

Basic Equations

The equations are the usual Euler equations + magnetic terms and induction equation

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

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} + p_g I) = \mathbf{J} \wedge \mathbf{B} = -\nabla \cdot (\frac{1}{2} I B^2 - \mathbf{B} \mathbf{B}) \quad (I \text{ identity matrix}),$$

$$\frac{\partial e}{\partial t} + \nabla \cdot [\mathbf{v}(e + p_g + \frac{1}{2}\rho v^2)] = \mathbf{v} \cdot (\mathbf{J} \wedge \mathbf{B}) = -\nabla \cdot [\mathbf{v} \cdot (\frac{1}{2}IB^2 - \mathbf{B}\mathbf{B})],$$

 $\mathbf{J} = \nabla \wedge \mathbf{B}$ no displacement current, $\nabla \cdot \mathbf{B} = 0$,

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \wedge \mathbf{E} = \nabla \wedge (\mathbf{v} \wedge \mathbf{B}) = \nabla \cdot (\mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v})$$
 ideal, but see later.

$$e = \rho U + \frac{1}{2}\rho v^2 + \frac{1}{2}B^2$$
 total energy (U is internal energy/unit mass).

Integral Conservation Law

Write these as

$$\frac{\partial Q_i}{\partial t} + \nabla \cdot (F_i, G_i, H_i) = S_i \quad i = 1 \dots 8 \quad *$$

where the Q_i are the conserved variables (ρ etc) and F_i , G_i , H_i are their fluxes in the x, y, and z directions.

Now integrate the equations over a fixed volume, V, with surface S.

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{V} Q_i \, \mathrm{d}V + \int_{S} (F_i, G_i, H_i) \cdot \mathrm{d}\mathbf{S} = \int_{V} S_i \, \mathrm{d}V.$$

This is the fundamental law. If solution is smooth, can write it as

$$\int_{V} \left[\frac{\partial Q_i}{\partial t} + \nabla \cdot (F_i, G_i, H_i) - S_i \right] dV = 0$$

Since V is arbitrary, the integrand must vanish $\Rightarrow *$.

Conservative Equations

Write in the form

$$\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} + \frac{\partial \mathbf{G}}{\partial y} + \frac{\partial \mathbf{H}}{\partial z} = \mathbf{S}$$
 where $\mathbf{Q} = [\rho, \rho \mathbf{v}, \mathbf{B}, e]^t$ are conserved quantities.

$$\mathbf{F} = \begin{bmatrix} \rho v_{x} \\ p_{t} + \rho v_{x}^{2} - B_{x}^{2} \\ \rho v_{x} v_{y} - B_{x} B_{y} \\ \rho v_{x} v_{z} - B_{x} B_{z} \\ 0 \\ B_{y} v_{x} - B_{x} v_{y} \\ B_{z} v_{x} - B_{x} v_{z} \\ v_{x}(e + p_{t}) - B_{x}(\mathbf{B} \cdot \mathbf{v}) \end{bmatrix} \quad \mathbf{G} = \begin{bmatrix} \rho v_{y} \\ \rho v_{x} v_{y} - B_{x} B_{y} \\ \rho v_{x} v_{y} - B_{x} B_{y} \\ \rho v_{y} v_{z} - B_{y} B_{z} \\ B_{x} v_{y} - B_{y} v_{x} \\ 0 \\ B_{z} v_{y} - B_{y} v_{z} \\ v_{x}(e + p_{t}) - B_{y}(\mathbf{B} \cdot \mathbf{v}) \end{bmatrix}$$

$$\mathbf{H} = \begin{bmatrix} \rho v_z \\ \rho v_x v_z - B_x B_z \\ \rho v_y v_z - B_y B_z \\ p_t + \rho v_z^2 - B_z^2 \\ B_x v_z - B_z v_x \\ B_y v_z - B_z v_y \\ 0 \\ v_z(e+p_t) - B_z(\mathbf{B} \cdot \mathbf{v}) \end{bmatrix} \quad p_t = p_g + B^2/2 \; \text{total pressure}$$

$$\mathbf{S} \; - \; \text{heating/cooling, non-ideal MHD, gravity etc.}$$

$$p_t = p_g + B^2/2$$
 total pressure

Conservative Finite Volume Scheme

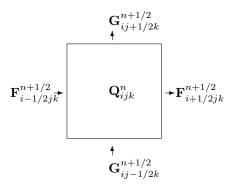
A conservative finite volume scheme takes the form

$$\frac{1}{\Delta t} (\mathbf{Q}_{ijk}^{n+1} - \mathbf{Q}_{ijk}^{n}) = \frac{1}{\Delta X} (\mathbf{F}_{i-1/2jk}^{n+1/2} - \mathbf{F}_{i+1/2jk}^{n+1/2}) + \frac{1}{\Delta Y} (\mathbf{G}_{i-1/2jk}^{n+1/2} - \mathbf{G}_{i+1/2jk}^{n+1/2})
+ \frac{1}{\Delta Z} (\mathbf{H}_{i-1/2jk}^{n+1/2} - \mathbf{H}_{i+1/2jk}^{n+1/2}) + \mathbf{S}_{ijk}^{n+1/2}$$

 \mathbf{Q}_{ijk}^n — cell averaged numerical solution in the ijk cell at timestep n

 $\mathbf{F}_{i+1/2jk}^{n+1/2}$ etc – approximations to time average of interface fluxes

 $\mathbf{S}_{ijk}^{n+1/2}$ – approximation to time average of source term



Upwind Schemes (Godunov)

Determine fluxes at interfaces from solution to a Riemann problem: one-dimensional problem with initial data

$$\mathbf{Q}(x,0) = \mathbf{Q}_0(x) = \begin{cases} \mathbf{Q}_l = \text{const.} & \text{for } x < 0 \\ \mathbf{Q}_r = \text{const.} & \text{for } x > 0 \end{cases}$$

Approximate time average at interface $\mathbf{F}_{i+1/2jk}^{n+1/2}$ etc by $\mathbf{F}(\mathbf{Q}^*)$.

 \mathbf{Q}^* is state at $x = x_{i+1/2jk}$ in Riemann problem with $\mathbf{Q}_l = \mathbf{Q}_{i-1jk}^n$, $\mathbf{Q}_r = \mathbf{Q}_{ijk}^n$.

Exact Riemann Solver

Gas dynamics with ideal equation of state – **Easy**

Gas dynamics with non-ideal equation of state – **Not much fun**

Relativistic gas dynamics with ideal equation of state – Even less fun

MHD with ideal equation of state – **Ghastly**

Relativistic MHD with ideal equation of state – **Beyond belief**

Most Riemann problems are linear. Rarely, if ever, need an exact Riemann solver.

Can use approximate solutions (with some care).

(See Riemann Solvers and Numerical Methods for Fluid Dynamics by E. F. Toro, 2009)

Linear Riemann Problem

Write one dimensional equations in the form

$$\mathbf{Q}_t + \mathbf{F}_x = \mathbf{Q}_t + J\mathbf{Q}_x = 0$$

where $J = \frac{\partial \mathbf{F}}{\partial \mathbf{\Omega}} = J(\mathbf{Q}_l, \mathbf{Q}_r) = \text{const}$ is the Jacobian of \mathbf{F} w.r.t. \mathbf{Q} (linear problem).

Let \mathbf{r}_i , \mathbf{l}_i be left/right eigenvectors of J with eigenvalue λ_i ($J\mathbf{r}_i = \lambda_i\mathbf{r}_i$, $\mathbf{l}_iJ = \lambda_i\mathbf{l}_i$). These are bi-orthogonal: $\mathbf{l}_i \cdot \mathbf{r}_j = \delta_{ij}$ (provided Jordan form of J is diagonal).

Write solution as $\mathbf{Q} = \sum_{i=1}^{n} v_i(x,t) \mathbf{r}_i$ $(v_i = \mathbf{l}_i \cdot \mathbf{Q})$.

Substituting into the equation gives $\sum_{i=1}^{n} \left(\frac{\partial v_i}{\partial t} + \lambda_i \frac{\partial v_i}{\partial x} \right) \mathbf{r}_i = 0$

Multiplying by l_j and using the bi-othorgonality property gives

$$\frac{\partial v_j}{\partial t} + \lambda_j \frac{\partial v_j}{\partial x} = 0$$
 $(j = 1 \cdots n)$ linear advection equations

Solution is $v_j(x,t) = \mathbf{l}_j \cdot \mathbf{Q}_0(x - \lambda_j t)$ if initial data is $\mathbf{Q}(x,0) = \mathbf{Q}_0(x)$.

Hence complete solution is $\mathbf{Q} = \sum_{i=1}^{n} \mathbf{l}_i \cdot \mathbf{Q}_0(x - \lambda_i t) \mathbf{r}_i$.

i.e. n waves moving with speeds $\lambda_i^{i=1} \Rightarrow$ these are the wavespeeds.

At
$$x = 0$$
, solution is $\mathbf{Q} = \mathbf{Q}^* = \sum_{i=1}^n \mathbf{l}_i \cdot \mathbf{Q}_0(-\lambda_i t) \mathbf{r}_i = \sum_{\lambda_i > 0} \mathbf{l}_i \cdot \mathbf{Q}_l \mathbf{r}_i + \sum_{\lambda_i < 0} \mathbf{l}_i \cdot \mathbf{Q}_r \mathbf{r}_i$

$$= \sum_{i=1}^n \mathbf{l}_i \cdot \mathbf{Q}_l \mathbf{r}_i - \sum_{\lambda_i < 0} \mathbf{l}_i \cdot \mathbf{Q}_l \mathbf{r}_i + \sum_{\lambda_i < 0} \mathbf{l}_i \cdot \mathbf{Q}_r \mathbf{r}_i = \mathbf{Q}_l + \sum_{\lambda_i < 0} \mathbf{l}_i \cdot (\mathbf{Q}_r - \mathbf{Q}_l) \mathbf{r}_i$$

$$\mathbf{F}(\mathbf{Q}^*) = J\mathbf{Q}^* = J\left[\mathbf{Q}_l + \sum_{\lambda_i < 0} \mathbf{l}_i \cdot (\mathbf{Q}_r - \mathbf{Q}_l) \mathbf{r}_i\right] = \mathbf{F}_l + \sum_{\lambda_i < 0} \lambda_i \mathbf{l}_i \cdot (\mathbf{Q}_r - \mathbf{Q}_l) \mathbf{r}_i$$

$$= J \left[\mathbf{Q}_r + \sum_{\lambda > 0} \mathbf{l}_i \cdot (\mathbf{Q}_l - \mathbf{Q}_r) \mathbf{r}_i \right] = \mathbf{F}_r + \sum_{\lambda > 0} \lambda_i \mathbf{l}_i \cdot (\mathbf{Q}_l - \mathbf{Q}_r) \mathbf{r}_i,$$

which gives

$$\mathbf{F}(\mathbf{Q}^*) = \frac{1}{2} \left| \mathbf{F}_l + \mathbf{F}_r - \sum_{i=1}^{n} |\lambda_i| \mathbf{l}_i \cdot (\mathbf{Q}_r - \mathbf{Q}_l) \mathbf{r}_i \right|$$
 i.e. average plus extra term.

We have

$$rac{\partial \mathbf{F}}{\partial x} \simeq rac{1}{\Delta x} (\mathbf{F}_{j+1/2} - \mathbf{F}_{j-1/2}) = rac{J}{\Delta x} [\mathbf{Q}^*(\mathbf{Q}_{j+1}, \mathbf{Q}_j) - \mathbf{Q}^*(\mathbf{Q}_j, \mathbf{Q}_{j-1})]$$

$$= \frac{J}{2\Delta x} \left[\mathbf{Q}_{j+1}^k + \mathbf{Q}_j^k - \sum_{i=1}^n \operatorname{sign}(\lambda_i) \mathbf{l}_i \cdot (\mathbf{Q}_{j+1}^k - \mathbf{Q}_j^k) \mathbf{r}_i \right]$$

$$-\mathbf{Q}_j^k - \mathbf{Q}_{j-1}^k + \sum_{i=1}^n \operatorname{sign}(\lambda_i) \mathbf{l}_i \cdot (\mathbf{Q}_j^k - \mathbf{Q}_{j-1}^k) \mathbf{r}_i \right]$$

$$= \frac{J}{2\Delta x} \sum_{i=1}^n \mathbf{l}_i \cdot \left[\mathbf{Q}_{j+1}^k - \operatorname{sign}(\lambda_i) (\mathbf{Q}_{j+1}^k - \mathbf{Q}_j^k) - \mathbf{Q}_{j-1}^k + \operatorname{sign}(\lambda_i) (\mathbf{Q}_j^k - \mathbf{Q}_{j-1}^k) \right] \mathbf{r}_i$$

$$= \frac{J}{\Delta x} \left[\sum_{\mathbf{k} \in \mathcal{Q}} \mathbf{l}_i \cdot (\mathbf{Q}_{j+1}^k - \mathbf{Q}_j^k) + \sum_{\mathbf{k} \in \mathcal{Q}} \mathbf{l}_i \cdot (\mathbf{Q}_j^k - \mathbf{Q}_{j-1}^k) \right] \mathbf{r}_i$$

This means that we have a right difference for waves with $\lambda_i < 0$ and a left difference for $\lambda_i > 0$ i.e. and upwind scheme. This is equivalent to diagonalising the equations and using an upwind scheme on each equation.

In some sense this is the "best" 1st order scheme for linear advection (stable scheme with highest accuracy).

MHD Waves (x direction)

Fast Waves: $\lambda_{1,7} = v_x \mp c_f$. Magnetic field does not rotate. Magnetic field increases when gas pressure increases. Genuinely non-linear (speed not constant across wave).

Alfvén Waves: $\lambda_{2,6} = v_x \mp c_a$ Magnetic field rotates with constant magnitude. p_t , ρ , v_x constant. Linearly degenerate: speed constant across wave.

Slow Waves: $\lambda_{3,5} = v_x \mp c_s$. Magnetic field does not rotate. Magnetic field decreases when gas pressure increases. Genuinely non-linear.

Entropy Wave: $\lambda_4 = v_x$. p_t , ρ , \mathbf{v} , \mathbf{B} constant. Only ρ changes. Linearly degenerate.

Alfvén speed:
$$c_a = \frac{B_x}{\rho^{1/2}}$$

Slow/Fast speeds:
$$c_{s,f} = \frac{1}{2} \left[a^2 + \frac{B^2}{\rho} \mp \left\{ \left(a^2 + \frac{B^2}{\rho} \right)^2 - \frac{4a^2 B_x^2}{\rho} \right\}^{1/2} \right]$$

$$a = \sqrt{\left(\frac{\gamma p_g}{\rho}\right)}$$
 is the sound speed.

Note $c_s < c_a < c_f$.

Only 7 waves since must have $B_x = \text{const.}$ in 1D because of $\nabla \cdot \mathbf{B} = 0$.

Magnetohydrodynamic Shock Types

In shock frame $s = 0 \Rightarrow [\mathbf{F}] = 0$, which gives $(\mathbf{B}_t, \mathbf{v}_t$ - transverse field and velocity)

a)
$$[\rho v_x] = 0$$
, b) $[p_t + \rho v_x^2] = 0$,

c)
$$\frac{\rho v_x}{B_x}[\mathbf{v}_t] = [\mathbf{B}_t]$$
, d) $[\mathbf{B}_t v_x] = B_x[\mathbf{v}_t]$, e) $[(e + p_t)v_x - B_x(\mathbf{B} \cdot \mathbf{v})] = 0$.

Contact Discontinuity $v_x = 0$

a), b), c), d)
$$\Rightarrow$$
 [p_t] = [v_t] = [B_t] = 0, [ρ] arbitrary.

Alfvén Shock
$$(c_a^2 - v_x^2)_l = (c_a^2 - v_x^2)_r = 0$$

a), b)
$$\Rightarrow$$
 $[v_x] = [\rho] = [p_t] = [|B_t|] = 0$,

c), d)
$$\Rightarrow$$
 f) $[\mathbf{B}_t(c_a^2 - v_x^2)] = 0 \Rightarrow \mathbf{B}_t$ can rotate by an arbitrary amount.

a)
$$[\rho v_x] = 0$$
, b) $[p_t + \rho v_x^2] = 0$,

c)
$$\frac{\rho v_x}{B_x}[\mathbf{v}_t] = [\mathbf{B}_t],$$
 d) $[\mathbf{B}_t v_x] = B_x[\mathbf{v}_t],$ e) $[(e + p_t)v_x - B_x(\mathbf{B} \cdot \mathbf{v})] = 0.$

$$f)[\mathbf{B}_t(c_a^2 - v_x^2)] = 0$$

Slow/Fast Shocks $sign\{(c_a^2 - v_x^2)_l\} = sign\{(c_a^2 - v_x^2)_r\}$

f) \Rightarrow $(\mathbf{B}_t)_l$ is parallel to $(\mathbf{B}_t)_r$ and has the same sign i.e. no rotation of transverse field.

Intermediate Shocks $sign\{(c_a^2 - v_x^2)_l\} \neq sign\{(c_a^2 - v_x^2)_r\}$

f) \Rightarrow B_t changes sign i.e. transverse field rotates by π .

Not evolutionary: an Alfvén wave incident from downstream gets trapped in shock \Rightarrow transverse field rotates across shock \Rightarrow violates shock conditions.

Exact MHD Riemann Problem (Ryu & Jones 1995; Falle, Komissarov & Joarder 1998)

J is not constant. No length scale \Rightarrow solution of the form $\mathbf{Q} = \mathbf{Q}(x/t)$.

 \Rightarrow Still have n waves moving at constant speeds: can be discontinuities (shocks, Alfvén waves, entropy waves) or simple waves (rarefaction waves).

Linear Approximations

Solve linear problem with appropriate (?) $J = J(\mathbf{Q}_l, \mathbf{Q}_r)$.

Roe Matrix

 $J(\mathbf{Q}_l, \mathbf{Q}_r)$ has the properties

- A) Real eigenvalues and a complete set of eigenvectors.
- B) $J(\mathbf{Q}, \mathbf{Q}) = J(\mathbf{Q})$ i.e. consistent.
- C) $\mathbf{F}(\mathbf{Q}_r) \mathbf{F}(\mathbf{Q}_l) = J(\mathbf{Q}_r \mathbf{Q}_l) \Rightarrow \text{exact solution for single discontinuity.}$

Neat way to do this for gas dynamics, more complicated for MHD. Preserves stationary contacts.

Flaws

Generates rarefaction shocks in transonic rarefactions. Needs entropy fix to avoid this (extra dissipation).

Carbuncles and Quirk instability (see later).

Arithmetic Mean Matrix (Falle, Komissarov & Joarder 1998)

Better to work with primitive variables, $\mathbf{P} = [\rho, \mathbf{v}, p_g, \mathbf{B}]^t$ i.e. solve $\frac{\partial \mathbf{P}}{\partial t} + A \frac{\partial \mathbf{P}}{\partial x} = 0$.

Define mean matrix by $A = A[\mathbf{P}_m]$ with $\mathbf{P}_m = \frac{1}{2}(\mathbf{P}_l + \mathbf{P}_r)$

This ensures that A is computed from a physical state (e.g. $p_q > 0$).

Solve linear Riemann problem with A. Obtain flux from

$$\mathbf{F}^* = \frac{1}{2} \left[\mathbf{F}_l + \mathbf{F}_r - C \sum_{i=1}^7 |\lambda_i| \mathbf{l}_i \cdot (\mathbf{P}_r - \mathbf{P}_l) \mathbf{r}_i \right] \quad \text{where } C_{ij} = \frac{\partial Q_i}{\partial P_j} \text{ (in state } \mathbf{P}_m).$$

 λ_i , \mathbf{l}_i , \mathbf{r}_i eigenvalues and eigenvectors of A.

Add artificial viscous, conductive and resistive fluxes of the form

$$\alpha_v s_m \rho_m (\mathbf{v}_l - \mathbf{v}_r)$$
 Viscous flux $\alpha_e s_m \rho_m (T_l - T_r)$ Thermal flux $\alpha_m s_m (\mathbf{B}_l - \mathbf{B}_r)$ Resistive flux

 $s_m = max[c_f(\mathbf{Q}_l), c_f(\mathbf{Q}_r)]$ (magnetosonic fast speed)

 ho_m mean density

$$\alpha_v = \alpha_e = \alpha_m = 0.2$$
 is fine

Must normalise eigenvectors carefully because of degeneracies (Roe & Balsara 1996).

Fast, robust, no rarefaction shocks or other nasties. Preserves stationary contacts.

Reduced Wave Riemann Solvers

Only consider some of the waves (HLL, HLLC, etc). For HLL the flux is

If $s_l < 0$ and $s_r < 0$, then $\mathbf{F} = \mathbf{F}(\mathbf{Q_l})$.

If $s_l > 0$ and $s_r > 0$, then $\mathbf{F} = \mathbf{F}(\mathbf{Q_r})$.

Otherwise

$$\mathbf{F} = \frac{s_r \mathbf{F}_l - s_l \mathbf{F}_r + s_l s_r (\mathbf{Q_r} - \mathbf{Q}_l)}{s_r - s_l}.$$

Here s_l is the smallest wave speed in left state, s_r the largest wave speed in the right state.

Fast and robust. Note that it is upwind in some sense. Does not preserve stationary contacts (HLLC does).

Kurganov-Tadmor Central Scheme

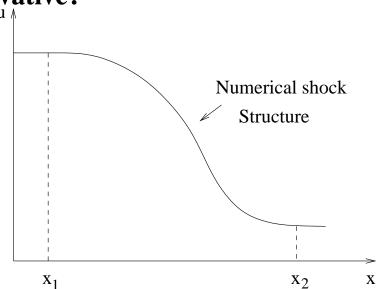
Flux is given by

$$\mathbf{F} = \frac{1}{2} [\mathbf{F} (\mathbf{Q}_{i-1jk}^n + \mathbf{F} (\mathbf{Q}_{ijk}^n) - s[\mathbf{Q}_{ijk}^n - \mathbf{Q}_{i-1jk}^n]]$$

s is the maximum absolute value of the wave speed in the cells (i-1,j,k) and (i,j,k).

Simple to implement and works quite well. Note that it is not upwind and does not preserve stationary contacts.

Why Conservative?



Apply conservation to $[x_1, x_2]$. If numerical shock structure is steady, then satisfies shock relations exactly.

In practice numerical shock structure is quasi-periodic. But OK if shock speed changes slowly on shock structure crossing time.

Second Order (Falle 1991)

Scheme first order if use Q_{ijk}^n , Q_{i-1jk}^n etc. A simple way to get second order is as follows: Use the first order scheme to compute a solution $Q_{ijk}^{n+1/2}$ at the half time.

Use linear extrapolation to get \mathbf{Q}_l , \mathbf{Q}_r

$$\mathbf{Q}_{l}^{n+1/2} = \mathbf{Q}_{i-1jk}^{n+1/2} + \frac{1}{2} \left(\frac{\partial \mathbf{Q}}{\partial x} \right)_{i-1jk}^{n+1/2}, \quad \mathbf{Q}_{r}^{n+1/2} = \mathbf{Q}_{ijk}^{n+1/2} - \frac{1}{2} \left(\frac{\partial \mathbf{Q}}{\partial x} \right)_{ijk}^{n+1/2},$$

where the gradients are

$$\left(\frac{\partial \mathbf{Q}}{\partial x}\right)_{ijk}^{n+1/2} = av\left(\frac{\mathbf{Q}_{i+1jk}^{n+1/2} - \mathbf{Q}_{ijk}^{n+1/2}}{\Delta x}\right), \left(\frac{\mathbf{Q}_{ijk}^{n+1/2} - \mathbf{Q}_{i-1jk}^{n+1/2}}{\Delta x}\right).$$

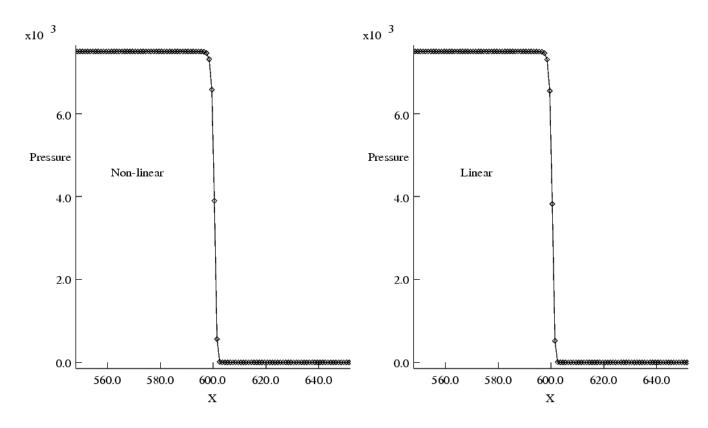
Here av(a,b) is an averaging function which reduces to (a+b)/2 if a, b are nearly equal, but otherwise is biased towards the smaller absolute value e.g.

$$av(a,b) = \frac{b^2a + a^2b}{a^2 + b^2}$$
 (van Leer 1977).

Compute fluxes with \mathbf{Q}_l , \mathbf{Q}_r and use these to advance solution through a full timestep with term computed from $\mathbf{Q}_{ijk}^{n+1/2}$.

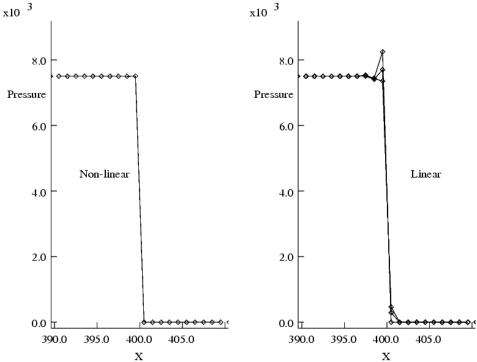
Lots of other ways to do this (see e.g. Toro 2009).

Moving Strong Gas Dynamic Shock



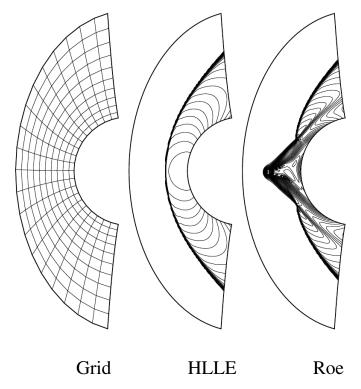
Linear Riemann solver works fine.

Stationary Strong Gas Dynamic Shock



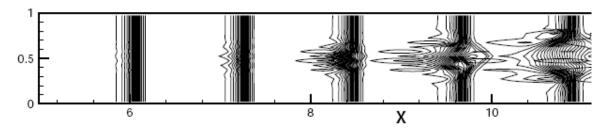
Shock stationary at a cell edge. For exact solver $\mathbf{F}^* = \mathbf{F}(\mathbf{Q}_l) = \mathbf{F}(\mathbf{Q}_r)$ \Rightarrow preserves solution. Linear solver does not.

Carbuncle (Quirk 1994)



Temperature contours in steady Mach 10 flow past a cylinder (Robinet et al. 2000)

Quirk Instability (Quirk 1994)



Density Contours in a slightly perturbed plane shock (Robinet et al. 1999).

This is very insidious since it grows slowly (Jordan mode \Rightarrow grows like t).

Carbuncle and Quirk instability are related in the sense that if a scheme suffers from one of them, then it suffers from the other.

Get these even with an exact Riemann solver.

Due to lack of numerical dissipation in certain cases.

Artificial Dissipation (Falle et al. 1998)

This is all to do with numerical dissipation: entropy fix in Roe method just adds dissipation; HLL method is more dissipative etc.

Why not just add it explicitly in Riemann solver?

Let $a_m = max[a(\mathbf{Q}_l), a(\mathbf{Q}_r)]$ (max sound speed).

Add viscous momentum flux $\mathbf{F}_v = \alpha_p max[\rho(\mathbf{Q}_l), \rho(\mathbf{Q}_r)])a_m(\mathbf{v}_l - \mathbf{v}_r)$.

Add conduction energy $F_e = \alpha_e max[\rho(\mathbf{Q}_l), \rho(\mathbf{Q}_r)])a_m(T_l - T_r)$ (T is temperature).

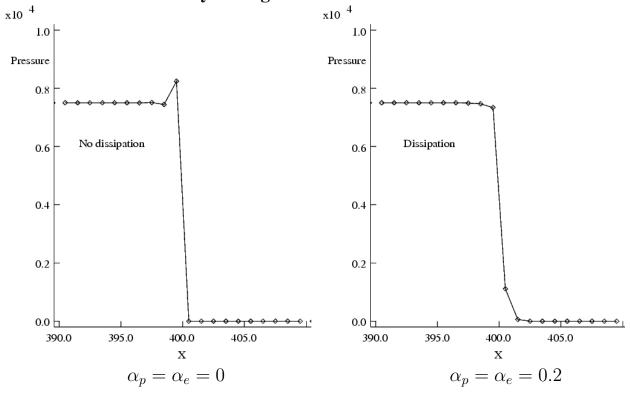
Add magnetic diffusion $\mathbf{F}_B = \alpha_m max[\rho(\mathbf{Q}_l), \rho(\mathbf{Q}_r)])a_m(\mathbf{v}_l - \mathbf{v}_r).$

$$\alpha_p$$
, α_e , α_m are parameters ($\alpha_p = \alpha_e = \alpha_m = 0.2$ is fine).

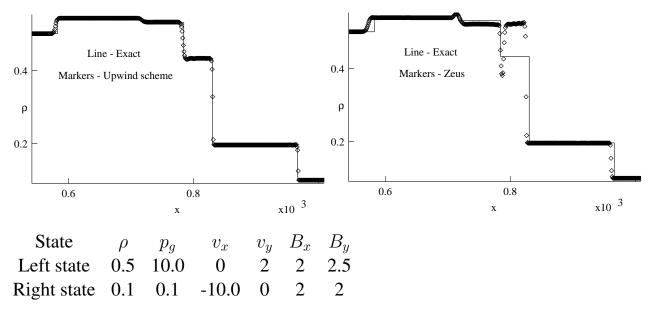
Cures carbuncles and Quirk instabilities.

Doesn't change order of scheme since dissipative terms are $O(\Delta x)$ in smooth regions.

Linear Solver for Stationary Strong Shock



MHD Riemann Problem (Falle 2002)

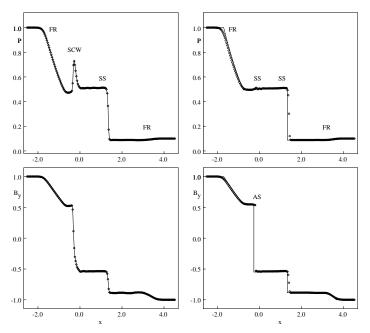


Waves are: Fast shock; slow rarefaction; entropy; slow shock; fast shock.

No Alfvén waves (velocity and field co-planar).

Zeus is neither conservative nor upwind.

Brio & Wu Problem (Brio & Wu 1988)



Standard upwind conservative scheme

→ intermediate shockwith compound wave.

Random choice (Glimm 1965) with exact Riemann solver.

→ Alfvén shock

Solenoidal Constraint

Take the divergence of the induction equation

$$\nabla \cdot \left(\frac{\partial \mathbf{B}}{\partial t} - \nabla \wedge (\mathbf{v} \wedge \mathbf{B}) \right) = \frac{\partial \nabla \cdot \mathbf{B}}{\partial t} = 0 \quad \text{since} \ \nabla \cdot [\nabla \wedge (\mathbf{v} \wedge \mathbf{B})] \equiv 0.$$

For exact equations $\nabla \cdot \mathbf{B} = 0$ if it is so initially. But not necessarily true for numerical approximation.

Constrained Transport (Evans & Hawley 1988)

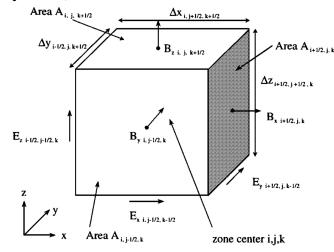
Use integral form of induction equation on faces

$$\int_{S} \frac{\partial \mathbf{B}}{\partial t} \cdot d\mathbf{S} = \oint_{C} (\mathbf{v} \wedge \mathbf{B}) \cdot d\mathbf{r}$$
$$= -\oint_{C} \mathbf{E} \cdot d\mathbf{r}$$

Field defined at cell faces.

Neatest version in Toth 2000.

But complicated and has big stencil



 \Rightarrow messy for AMR, but no worse than ambi-polar diffusion.

Eight Wave (Powell 1996)

Allow $\nabla \cdot \mathbf{B} \neq 0$ (monopoles), but add extra terms to ensure Galilean invariance

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v} + p_g I) = \mathbf{J} \wedge \mathbf{B} = -\nabla \cdot (\frac{1}{2} I B^2 - \mathbf{B} \mathbf{B}) - \mathbf{B} \nabla \cdot \mathbf{B}$$

$$\frac{\partial e}{\partial t} + \nabla \cdot [\mathbf{v}(e + p_g + \frac{1}{2}\rho v^2)] = \mathbf{v} \cdot (\mathbf{J} \wedge \mathbf{B}) = -\nabla \cdot [\mathbf{v} \cdot (\frac{1}{2}IB^2 - \mathbf{B}\mathbf{B})] - (\mathbf{v} \cdot \mathbf{B})\nabla \cdot \mathbf{B}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \cdot (\mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v}) - \mathbf{v}\nabla \cdot \mathbf{B}$$

Taking the divergence of the induction equation gives

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

i.e. Monopoles advected with fluid velocity (hence "eight wave").

Not conservative \Rightarrow not brilliant at shocks, which is where monopoles are densest.

Projection (see Toth 2000)

Advance B in time with as usual to get B^* .

Define auxiliary scalar function ψ by $\nabla^2 \psi = \nabla \cdot \mathbf{B}^*$.

Final field is $\mathbf{B} = \mathbf{B}^* - \nabla \psi$, which is divergence free.

Solution to Poisson equation cheap: $\nabla \cdot \mathbf{B}^*$ dominated by short wavelengths.

Divergence Cleaning (Dedner et al. 2002)

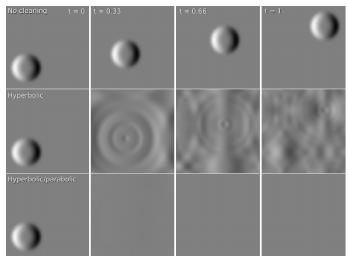
Induction equation is
$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v}) + \nabla \psi = 0 \text{ with } \frac{\partial \psi}{\partial t} + c_h^2 \nabla \cdot \mathbf{B} = -\frac{c_h^2}{c_p^2} \psi.$$

Then
$$\frac{\partial \nabla \cdot \mathbf{B}}{\partial t} + \nabla^2 \psi = 0$$
,

$$\frac{\partial^2 \psi}{\partial t^2} + \frac{c_h^2}{c_n^2} \frac{\partial \psi}{\partial t} = c_h^2 \nabla^2 \psi,$$

 ψ is advected with speed c_h and damped with coefficient c_h^2/c_p^2 .

Advection of a circle of $\nabla \cdot \mathbf{B}$ with SPH (Tricco et al 2016).



Adaptive Mesh Refinement (AMR)

Basic idea of AMR is to refine mesh where solution varies rapidly e.g. shocks, dense clumps etc.

Hierarchical AMR

Hierarchy of grids – solution computed on all grids

Quadrilateral grid in 2D, hexahedral in 3D i.e. not triangles and tetrahedra

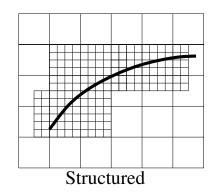
Ingredients

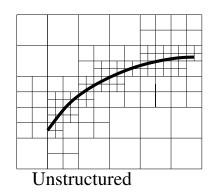
Criterion for mesh refinement – ideally based on error estimates

Procedure for coarse-fine grid boundaries

Different timesteps for different grids

Structured versus Unstructured





Structured codes: Chombo, Pluto, Flash, Enzo, Astrobear, AMRVAC.

Unstructured: Ramses, MG.

Efficiency

For D dimensional calculation

Uniform grid Unstructured AMR

Memory cost
$$\propto (1/\Delta x)^D \propto (1/\Delta x)^{D-1}$$

CPU time
$$\propto 1/\Delta x)^{D+1} \propto (1/\Delta x)^D$$

if regions requiring high resolution are sheets.

Refinement control

Grids $G^0 \cdots G^N$ with mesh spacing on $G^n \Delta x_0/2^n$.

 G^0 , G^1 cover whole domain, finer grids need not do so.

For each cell on G^n compare solutions on G^n and G^{n-1} .

If error exceeds a given tolerance, refine G^n cell to G^{n+1}

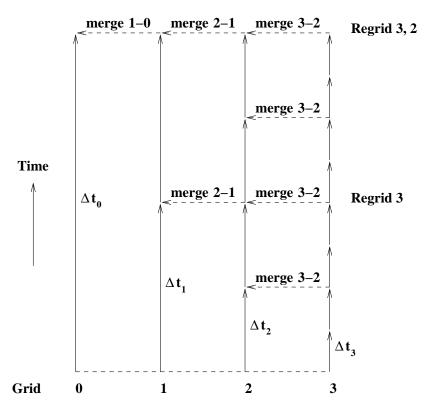
Integration Algorithm

```
integrate(n)
                            Integrate grid n
  step(n)
                            Advance grid n by one step
                            Increment grid n time
  t[n] += dt[n]
                            Finer grids exist
  if (n < N)
     while (t[n+1] < t[n])
       integrate(n+1)
                            Integrate to grid n+1 to grid n time
    regrid(n)
                            Compare solutions on grids n and n-1
                            \rightarrow decide grid n+1 refinement
                            Project n+1 solution onto grid n
     merge(n)
  return
```

Then

integrate(0) integrates all grids through one coarse grid timestep

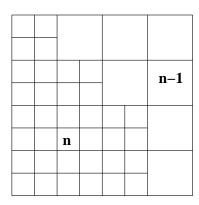
Integration of 4 level Grid



Note that each grid has its own timestep. Important for Courant number matching at coarse-fine boundaries.

Coarse-fine Grid Boundaries

Boundary of G^n grid



Need boundary condition for grid G^n at coarse-fine boundary

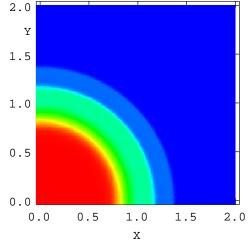
Already have solution on G^{n-1} at advanced time

Use this to construct space-time interpolant for solution at boundary

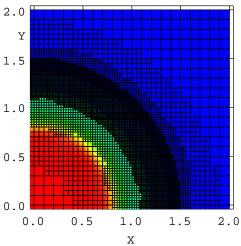
Flux at coarse-fine boundary used to update G^{n-1} different from flux used for G^n . \Rightarrow Must correct solution on G^{n-1} to ensure conservation at coarse-fine boundary.

5 Level Calculation of Circular Sod Problem

Density



Grid



Multifluid MHD

N fluids with equations $(i = 1 \cdots N)$

$$\frac{\partial \rho_i}{\partial t} + \frac{\partial \rho_i v_{ix}}{\partial x} = \sum_{i \neq i} S_{ij} \quad S_{ij} \quad \text{rate of conversion of } i \text{ to } j,$$

$$\frac{\partial \rho_i \mathbf{v}_i}{\partial t} + \nabla \cdot (\rho_i \mathbf{v}_i \mathbf{v}_i + p_i I) = \alpha_i \rho_i (\mathbf{E} + \mathbf{v}_i \wedge \mathbf{B}) + \sum_{i \neq 1} \mathbf{f}_{ij}$$

 $\mathbf{f}_{ij} = K_{ij}\rho_i\rho_j(\mathbf{v}_j - \mathbf{v}_i)$ – force exerted on i by j, α_i – charge to mass ratio

$$\frac{\partial e_i}{\partial t} + \nabla \cdot \left[\mathbf{v_i} (\frac{1}{2} \rho_i v_i^2 + p_i) \right] = H_i + \sum_{i \neq i} G_{ij}$$

 H_i – energy loss rate for i, G_{ij} – energy transfer rate from j to i

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \wedge \mathbf{E}, \quad \nabla \wedge \mathbf{B} = \mathbf{J} = \sum_{i} \alpha_{i} \rho_{i} \mathbf{v}_{i}$$

Species 1 - neutral ($\alpha_1 = 0$), Species $2 \cdots N$ charged.

Define Hall parameter
$$\beta_i = \frac{\alpha_i B}{\rho_1 K_{i1}}$$

 $\beta_i \gg 1 \Rightarrow$ Species i tied to field lines $\alpha_i \rho_i(\mathbf{E} + \mathbf{v}_i \wedge \mathbf{B})$ dominates, $\beta_i \ll 1 \Rightarrow$ Species i tied to neutrals $\sum_{j \neq 1} \mathbf{f}_{ij}$ dominates.

Two Fluid

 $\beta_i \gg 1$ for all $i > 1 \Rightarrow$ have neutral and single perfectly conducting fluid.

Neutral Fluid

Conducting Fluid

$$\frac{\partial \mathbf{U}_n}{\partial t} + \frac{\partial \mathbf{F}_n}{\partial x} = \mathbf{S}_n$$

$$\frac{\partial \mathbf{U}_c}{\partial t} + \frac{\partial \mathbf{F}_c}{\partial x} = \mathbf{S}_c$$

$$\mathbf{U}_n = \begin{bmatrix} \rho_n \\ \rho_n v_{nx} \\ \rho_n v_{ny} \end{bmatrix}$$

$$\mathbf{U}_c = \left[egin{array}{c}
ho_c v_{cx} \
ho_c v_{cy} \ B_y \end{array}
ight]$$

$$\mathbf{F}_n = \begin{bmatrix} \rho_n v_{nx} \\ a_n^2 \rho_n + \rho_n v_{nx}^2 \\ \rho_n v_{nx} v_{ny} \end{bmatrix}$$

$$\mathbf{F}_{n} = \begin{bmatrix} \rho_{n}v_{nx} \\ a_{n}^{2}\rho_{n} + \rho_{n}v_{nx}^{2} \\ \rho_{n}v_{nx}v_{ny} \end{bmatrix} \qquad \mathbf{F}_{c} = \begin{bmatrix} \rho_{c}v_{cx} \\ a_{c}^{2}\rho_{c} + B_{y}^{2}/2 + \rho_{c}v_{cx}^{2} \\ \rho_{c}v_{cx}v_{cy} - B_{x}B_{y} \\ v_{cx}B_{y} - v_{cy}B_{x} \end{bmatrix}$$

$$\mathbf{S}_n = \left[\begin{array}{c} 0 \\ \mathbf{f} \end{array} \right]$$

$$\mathbf{S}_c = \left[egin{array}{c} 0 \ -\mathbf{f} \ 0 \end{array}
ight]$$

Note this is isothermal for simplicity.

Can use upwind scheme for each fluid.

But

Must have all Hall parameters $\beta_i \gg 1$.

In ISM true for ions and electrons, but not for grains.

In accretion discs may not be true for ions.

If density of conducting fluid \ll total density

- ⇒ conducting fluid wavespeeds ≫ equilibrium wavespeeds
- ⇒ small timestep with explicit scheme

Multi-Fluid (Falle 2003)

Some species with $\beta_i \simeq 1$, total density of charged species \ll total density \Rightarrow neglect inertia of charged species (otherwise equations are stiff)

Get single fluid with induction equation

$$\begin{split} \frac{\partial \mathbf{B}}{\partial t} &= -\nabla \wedge \mathbf{E} = \nabla \wedge (\mathbf{v} \wedge \mathbf{B}) \quad \text{hyperbolic} \\ &- \nabla \wedge \big[\nu_0 \frac{(\mathbf{J} \cdot \mathbf{B})}{B^2} \mathbf{B} \big] \quad \text{conduction parallel to field} \\ &- \nabla \wedge \big[\nu_1 \frac{(\mathbf{J} \wedge \mathbf{B})}{B} \big] \quad \text{Hall effect} \\ &- \nabla \wedge \big[\nu_2 \frac{(\mathbf{J} \wedge \mathbf{B})}{B^2} \wedge \mathbf{B} \big] \quad \text{ambipolar diffusion} \\ \text{Conductivities:} \quad \sigma_0 &= \frac{1}{B} \sum_i \alpha_i \rho_i \beta_i, \quad \sigma_1 &= \frac{1}{B} \sum_i \frac{\alpha_i \rho_i \beta_i}{(1 + \beta_i^2)}, \quad \sigma_2 &= -\frac{1}{B} \sum_i \frac{\alpha_i \rho_i}{(1 + \beta_i^2)} \\ \text{Resistivities:} \quad \nu_0 &= \frac{1}{\sigma_0} \quad \nu_1 &= -\frac{\sigma_2}{(\sigma_1^2 + \sigma_2^2)} \quad \nu_2 &= -\frac{\sigma_1}{(\sigma_1^2 + \sigma_2^2)} \end{split}$$

Note $|\nu_1| \ll 1$ if all $\beta_i \gg 1$ i.e. no Hall effect

Momentum equations for charged species reduce to

$$\frac{\beta_i}{B}(\mathbf{E} + \mathbf{v}_i \wedge \mathbf{B}) + (\mathbf{v}_1 - \mathbf{v}_i) = 0 \quad i = 2 \cdots N$$

(Neglecting inertia and collisions between charged species) Also have

$$\mathbf{J} = \nabla \wedge \mathbf{B} = \sum_{i} \alpha_{i} \rho_{i} \mathbf{v}_{i}$$

These N equations determine E and the \mathbf{v}_i for $i = 2 \cdots N$.

Given the v_i , determine the ρ_i from the continuity equations \Rightarrow Resistivities.

Subtleties

If not isothermal, must include Lorentz force, $J \wedge B$ as source term in momentum and energy equations to get correct relations across a gas dynamic shock.

Hall term dispersive with $\omega^2 = \nu_1^2 \cos^2 \theta k^4$ (θ is angle between field and x axis) i.e. phase and group velocity $\to \infty$ as wavelength $\to 0$ (whistler waves).

Might suppose that group velocity, $2\nu_1\cos\theta k$, is effective wavespeed and Δx is smallest wavelength

 \Rightarrow stable timestep for explicit scheme $\Delta t = \Delta x^2/4\pi\nu_1$.

True if careful (see O'Sullivan & Downes 2006)

Efficiency

Even if we use an explicit scheme for field, the multi-fluid scheme is faster for low ionisation fraction, X_i :

Multi-fluid scheme

Shock width $L \propto \text{resistivity } \nu_2 \propto \frac{1}{X_i}$, mesh spacing $\Delta x \propto L$

Time step
$$\Delta t \propto \frac{\Delta x^2}{\nu_2} \propto L^2 X_i$$

Flow time $\propto L$

$$\Rightarrow$$
 No of steps in a flow time $\propto \frac{L}{\Delta t} \propto \frac{1}{LX_i}$ – independent of X_i

Two-Fluid Scheme

Conducting fluid wavespeed
$$c_i \propto \frac{1}{X_i^{1/2}}$$

Time step
$$\Delta t \propto \frac{\Delta x}{c_i} \propto L X_i^{1/2}$$

$$\Rightarrow$$
 No of steps in a flow time $\propto \frac{L}{\Delta t} \propto \frac{1}{X_i^{1/2}}$ – increases as X_i decreases

Shock Structure with Large Hall Parameters

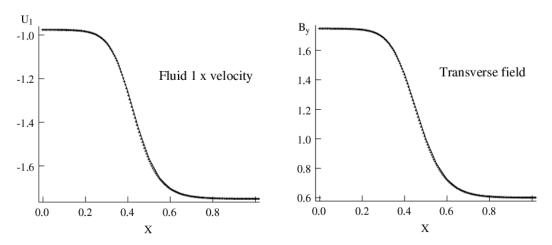
Two charged species: $\beta_2 = -5.8 \ 10^6$ (electrons), $\beta_3 = 5.8 \ 10^3$ (ions)

Preshock state: $B_x = 1.0$, $B_y = 0.6$, Fast Mach No = 1.5

 $\nu_0 = 1.7 \ 10^{-12}, \, \nu_1 = 10^{-5}, \, \nu_2 = -0.058$ (Hall effect negligible)

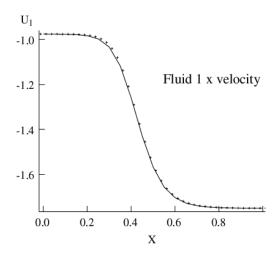
Isothermal – neutral pressure negligible.

High Resolution ($\Delta x = 5 \ 10^{-3}$)



Line – Integration of steady equations, markers – Numerical scheme No rotation – Z component of field $\simeq 10^{-4}$

Low Resolution ($\Delta x = 2.5 \ 10^{-2}$)



Line – Integration of steady equations, markers – Numerical scheme

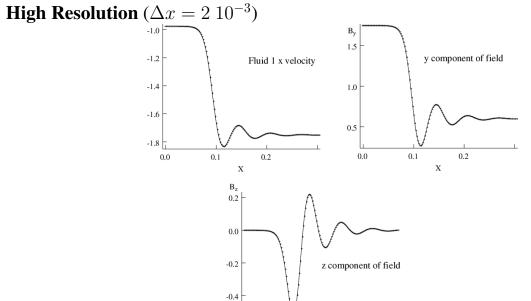
Shock Structure with Strong Hall Effect

Two charged species: $\beta_2 = -5.8 \ 10^6$ (electrons), $\beta_3 = 0.233$ (grains).

Preshock: $B_x = 1.0$, $B_y = 0.6$, Fast Mach No = 1.5

 $\nu_0 = 1.7 \ 10^{-9}, \, \nu_1 = 0.01, \, \nu_2 = 0.0023$ (Significant Hall effect)

Isothermal – neutral pressure negligible.



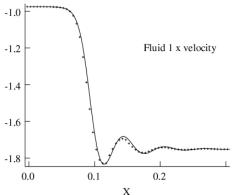
Line – Integration of steady equations, markers – Numerical scheme

0.1

0.2

0.0

Low Resolution ($\Delta x = 5 \ 10^{-3}$)



Line – Integration of steady equations, markers – Numerical scheme

Shock Structure with Neutral Subshock

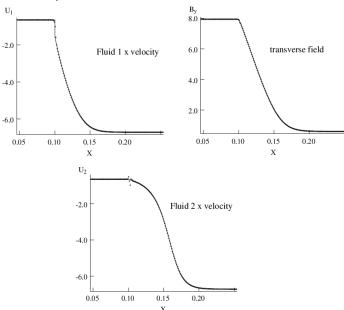
Two charged species: $\beta_2 = -5.8 \ 10^6$ (electrons), $\beta_3 = 5.8 \ 10^3$ (ions)

Preshock state: $B_x = 1.0$, $B_y = 0.6$, Fast Mach No = 5

 $\nu_0 = 1.7 \ 10^{-12}, \, \nu_1 = 10^{-5}, \, \nu_2 = -0.058$ (Hall effect negligible)

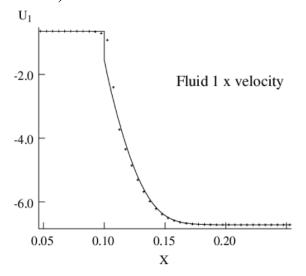
Isothermal – neutral sound speed a = 1.

High Resolution ($\Delta x = 10^{-3}$)



Line – Integration of steady equations, markers – Numerical scheme

Low Resolution ($\Delta x = 5 \ 10^{-3}$)



Line – Integration of steady equations, markers – Numerical scheme

Efficiency Revisited

Non-ideal terms are diffusive \Rightarrow time step $\propto \Delta x^2$.

Can get unconditionally stable scheme with implicit 1st order step followed by explicit 2nd order step

Resistive terms contain cross-derivatives ⇒ implicit scheme messy

But: Treat cross-derivatives explicitly and only use implicit approximation for diagonal terms:

$$\frac{\partial^2 B_y}{\partial x^2}$$
, $\frac{\partial^2 B_x}{\partial y^2}$ etc

Does not change stability properties. Cheap: just have tridiagonal matrices to invert.

Super time stepping (O'Sullivan & Downes 2006; O'Sullivan 2015)

Use a set of steps, some with time steps larger than stability limit, some smaller ⇒ can get larger effective time step (Alexiades et al. 1996).

Works for parabolic problems, such as this. Easy to implement.

Can use such schemes for:

- 1. Multifluid shocks
- 2. Ambipolar diffusion in star forming regions.
- 3. Ambipolar diffusion and Hall effect in discs
- 4. etc

Further Reading

Alexiades V., Amiez G., Gremaud P. Super-time-stepping acceleration of explicit schemes for parabolic problems. Com. Num. Meth. Eng., 12, 31, 1996.

Brio, M., Wu, C. C. An Upwind Differencing Scheme for the Equations of Ideal Magnetohydrodynamics.JCP, 75, 400, 1988.

Crockett, R.K., Colella, P., Fisher, R.T., Klein, R.I., McKee, C.F. An unsplit Godunov method for ideal MHD. JCP, 203, 422, 2005.

Dedner, A., Kemm, F., Kroner, D., Munz, C.-D., Schnitzer, T., Wesenberg, M. Hyperbolic divergence cleaning for the MHD equations. JCP, 175, 645, 2002.

Evans, C. R., Hawley, J. F. Simulation of Magnetohydrodynamic Flows: a Constrained Transport Method. ApJ, 332, 659, 1988.

Falle, S.A.E.G. Self-similar Jets. MNRAS,250,581,1991.

Falle, S.A.E.G. Rarefaction Shocks, Shock Errors, and Low Order of Accuracy in ZEUS. ApJ, 577, L123, 2002.

Falle, S.A.E.G. A numerical scheme for multifluid magnetohydrodynamics. MNRAS, 344, 1210, 2003.

Falle, S.A.E.G., Komissarov, S.S., Joarder, P. A multidimensional upwind scheme for magnetohydrodynamics. MNRAS, 297, 265, 1998.

Falle, S.A.E.G., Komissarov, S.S. On the Inadmissibility of Non-evolutionary Shocks. J. Plasma Physics, 65, 29, 2001.

Glimm, J. Solutions in the large for nonlinear hyperbolic systems of equations, Comm. Pure App. Math., 18,697715, 1965.

Jeffrey, A., Taniuti, T. Nonlinear wave propagation. Academic Press, New York, 1964.

LeVeque R. J. Finite volume methods for hyperbolic problems, CUP, 2003.

O'Sullivan, S., Downes, T.P., An explicit scheme for multifluid magnetohydrodynamics. MNRAS,366, 1329, 2006.

Quirk, J.J. A contribution to the great Riemann solver debate. International Journal of Numerical Methods in Fluids, 23, 125, 1994.

Roe, P.L., Balsara, D.S. Notes on the eigensystem of magnetohydrodynamics. , SIAM J. Appl. Math, 56, 57, 1996

Ryu, D., Jones, T.W. Numerical magnetohydrodynamics in astrophysics: algorithms and tests for one dimensional flow, ApJ, 442, 228, 1995.

Toth, G. The Div B = 0 constraint in shock-capturing magnetohydrodynamics codes. JCP, 161,605,2000.

Toro, E. F. Riemann solvers and numerical methods for fluid dynamics. Third Edition, Springer, 2009.

Tricco, T.S., Price, D.J., Bate, M.R. Constrained hyperbolic divergence cleaning in smoothed particle magnetohydrodynamics with variable cleaning speeds. JCP, 322, 326, 2016.

Also see lectures by Toro and Toth on www.jetset2007.ph.unito.it