Computational MHD: Tutorial

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Outline

- Primitive vs. Conservative MHD Equations
- Rusanov Scheme and Limiters
- Adaptive Mesh Refinement
- div B = 0 constraint
- Semi-relativistic MHD
- Implicit time stepping
- Going beyond ideal MHD with BATSRUS
- Summary

Resistive MHD Equations: Primitive form

- **Mass conservation:** $$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v})$$
- **Force equation:** $$\rho \frac{\partial \mathbf{v}}{\partial t} = -\rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla p + \mathbf{J} \times \mathbf{B}$$
- **Pressure equation:** $$\frac{\partial p}{\partial t} = -\nabla \cdot (\mathbf{v} p) - (\gamma - 1)(p \nabla \cdot \mathbf{v} - \eta \mathbf{J}^2)$$
- **Induction equation:** $$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} = \nabla \times (\mathbf{v} \times \mathbf{B} - \eta \mathbf{J})$$
- **Conservation of div B:** $$\frac{\partial (\nabla \cdot \mathbf{B})}{\partial t} = -\nabla \cdot (\nabla \times \mathbf{E}) = 0$$

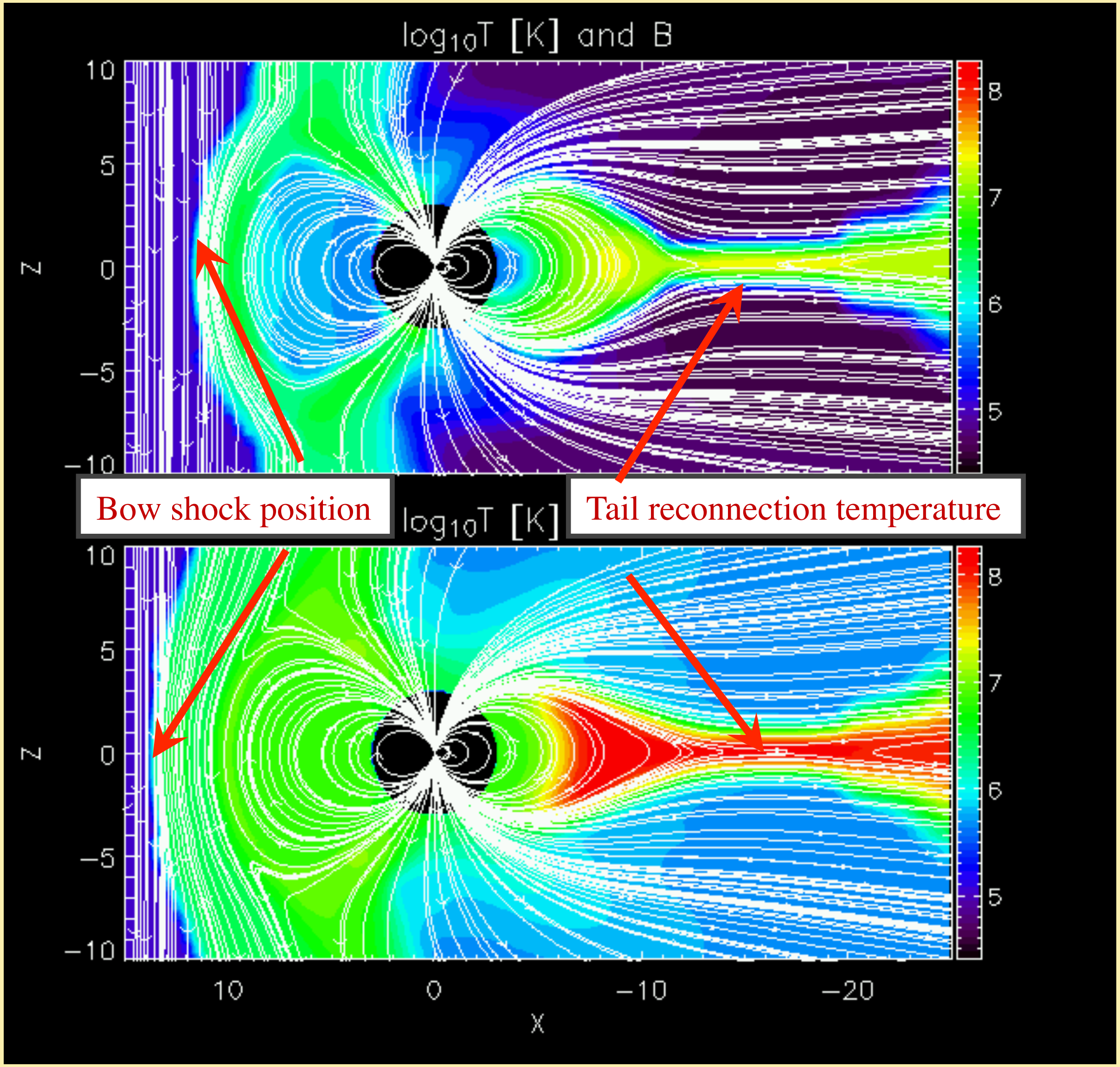
Discontinuous/Weak Solutions

- To obtain correct weak solutions, the MHD equations have to be rewritten into conservation form, and the numerical scheme also has to be conservative.

- Numerical diffusion can produce magnetic reconnection even in an ideal MHD model. Energy conservation will be violated by a non-conservative ideal MHD scheme because Joule heating is neglected.

- Note: reconnection is not very well modeled either by ideal or by resistive MHD. One needs to include more physics, e.g. Hall MHD and/or go to really high grid resolution so that small scale instabilities can develop.

Non-Conservative vs. Conservative



Magnetosphere solutions with B_Z = -5nT, U_X = -400km/s

Resistive MHD Equations in Conservative Form

- **Mass conservation:** $$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{v})$$
- **Momentum cons.:** $$\frac{\partial \rho \mathbf{v}}{\partial t} = -\nabla \cdot \left(\mathbf{v}\rho\mathbf{v} + \bar{I}p + \bar{I}\frac{\mathbf{B}^2}{2} - \mathbf{B}\mathbf{B}\right)$$
- **Energy cons.:** $$\frac{\partial e}{\partial t} = -\nabla \cdot \left[\mathbf{v}(e+p) + \mathbf{v}\cdot\left(\bar{I}\frac{\mathbf{B}^2}{2} - \mathbf{B}\mathbf{B}\right) - \mathbf{B}\times\eta\mathbf{J}\right]$$
- **Induction equation:** $$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} = \nabla \times (\mathbf{v}\times\mathbf{B} - \eta\mathbf{J})$$
- **Energy density:** $$e = \frac{p}{\gamma - 1} + \frac{\rho \mathbf{v}^2}{2} + \frac{\mathbf{B}^2}{2}$$

System of Conservation Laws

$$\mathbf{U} = (\rho, \rho\mathbf{v}, e, \mathbf{B})^T$$

$$\mathbf{F} = \left(\rho\mathbf{v}, \mathbf{v}\rho\mathbf{v} + \bar{I}(p + \mathbf{B}^2/2) - \mathbf{B}\mathbf{B}, \mathbf{v}(e + p + \mathbf{B}^2/2) - \mathbf{v}\cdot\mathbf{B}\mathbf{B}, \mathbf{v}\mathbf{B} - \mathbf{B}\mathbf{v}\right)^T$$

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

So can one use any of the numerical schemes developed for general conservation laws?

Essentially YES!

Numerical Schemes used in Computational MHD

- Lax-Wendroff scheme with artificial viscosity
- Finite differences with artificial viscosity
- Flux Corrected Transport (FCT)
- TVD/MUSCL scheme with Lax-Friedrichs (Rusanov), HLL, HLLC, HLLD, or Roe flux
- PPM, ENO, WENO
- Pseudo-spectral
- Finite Elements
- Spectral Elements
- Discontinuous Galerkin (DG)
- and many more ...

Finite Volume Rusanov Scheme

- Conservative update:

$$U_i^{n+1} = U_i^n - \Delta t \frac{F_{i+1/2} - F_{i-1/2}}{\Delta x} + \Delta t S_i$$

- Rusanov flux uses maximum wave speed:

$$F_{i+1/2} = \frac{F(U^R_{i+1/2}) + F(U^L_{i+1/2})}{2} - \frac{1}{2}|\lambda_{\rm max}|(U^R_{i+1/2} - U^L_{i+1/2})$$

- Right and left face values:

$$U^R_{i+1/2} = U_{i+1} - \frac{1}{2}\bar{\Delta} U_{i+1} \qquad U^L_{i+1/2} = U_i + \frac{1}{2}\bar{\Delta} U_i$$

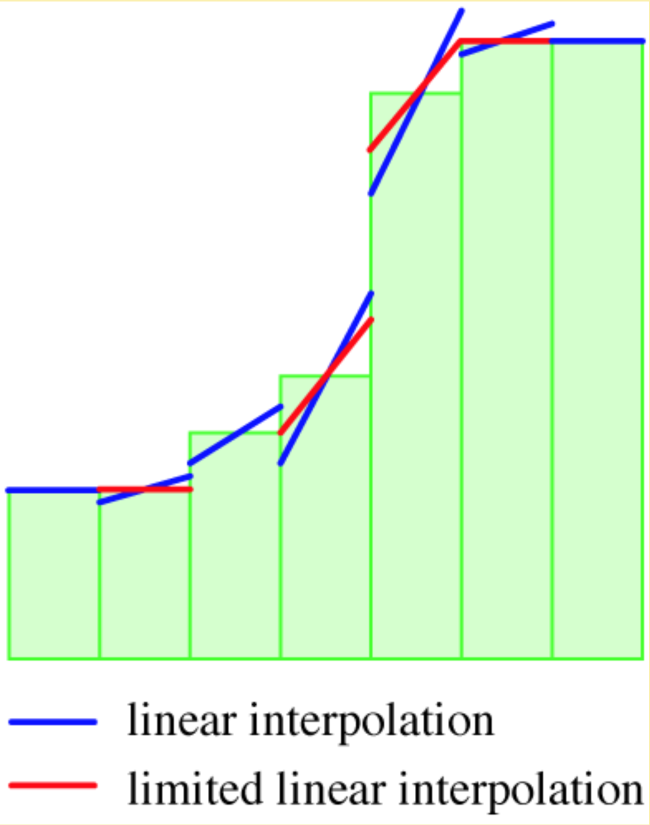
- Limited slope with monotonized central (MC) limiter:

$$\bar{\Delta} U_i = \mathrm{minmod}[\beta(U_{i+1} - U_i), \beta(U_i - U_{i-1}), (U_{i+1} - U_{i-1})/2]$$

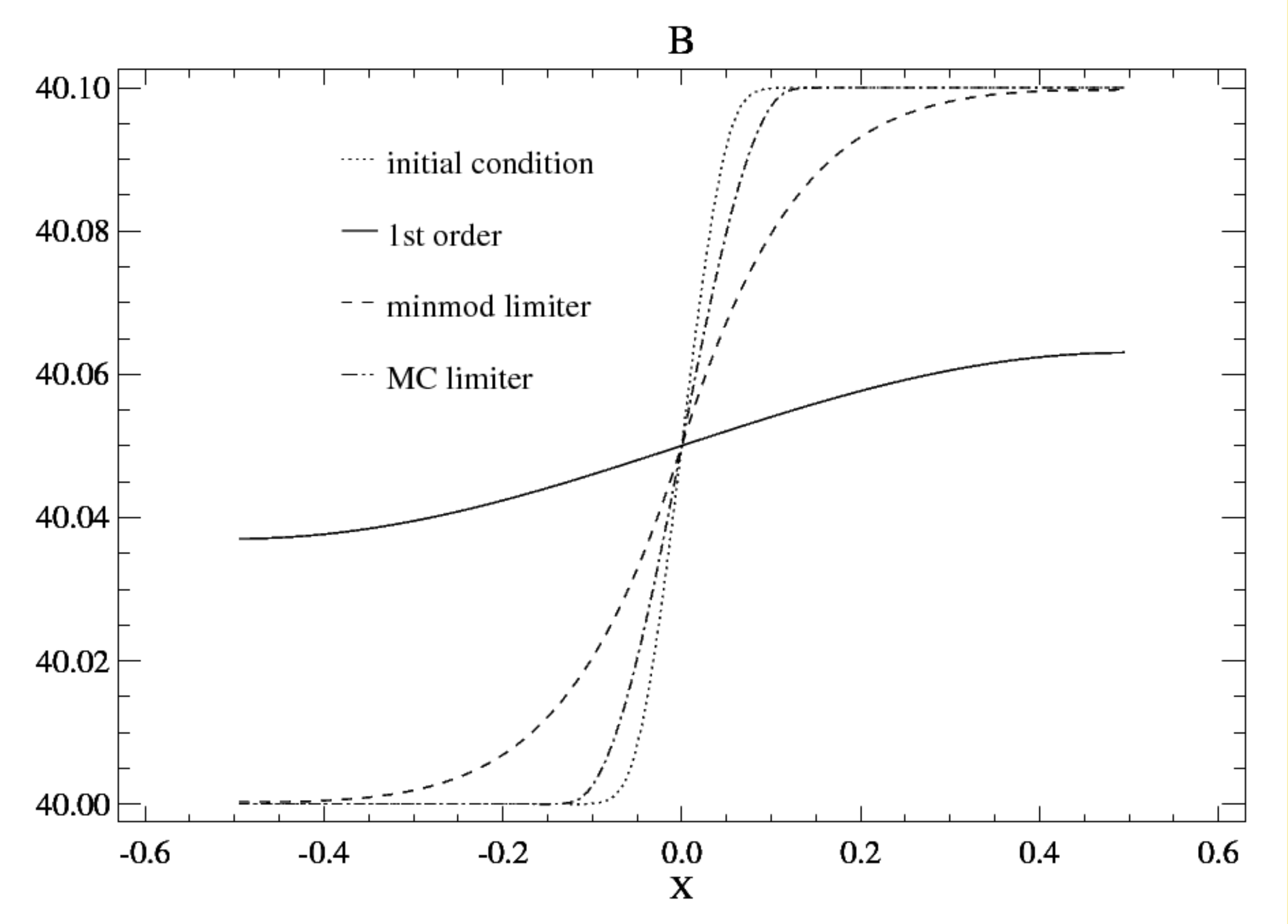
Limited Reconstruction: Total Variation Diminishing Schemes

- Unlimited reconstruction process can introduce new extrema. Need to limit the slopes so that reconstructed values are bounded by cell-center values.

- TVD schemes are first order near discontinuities and at local extrema, second or third order in monotonic smooth regions. Overall second order for smooth problems.



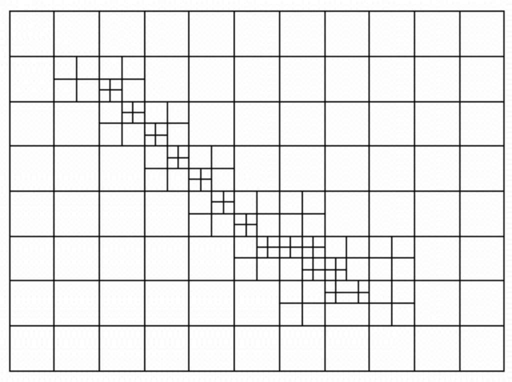
Effect of Various Slope Limiters on Numerical Diffusion

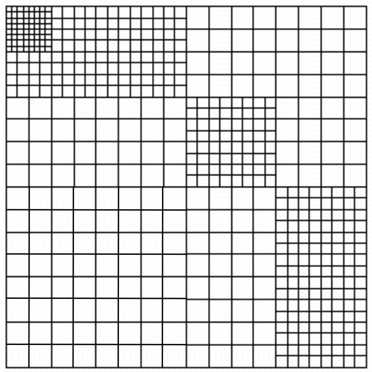


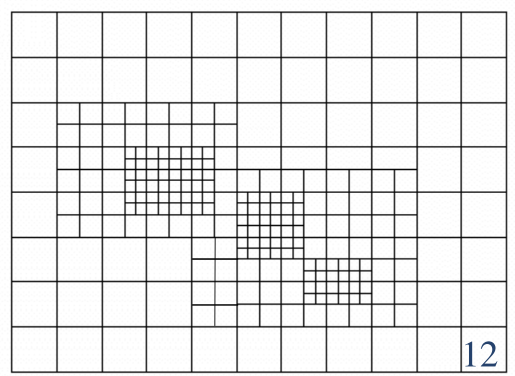
Initial condition: jump in the transverse magnetic field balanced by thermal pressure. Results are obtained with the Rusanov scheme.

Adaptive Mesh Refinement: Cell, Block and Patch Based

- **Cell based AMR**
  - Each cell can be refined.
  - Resolution changes by factors of 2.
- **Block based AMR**
  - Each block can be refined.
  - Resolution changes by factors of 2 or more.
- **Patch based AMR**
  - Blocks of variable size.
  - Resolution changes by factors of 2 or more.
- **Other possibilities**
  - unstructured grids, non-Cartesian grids

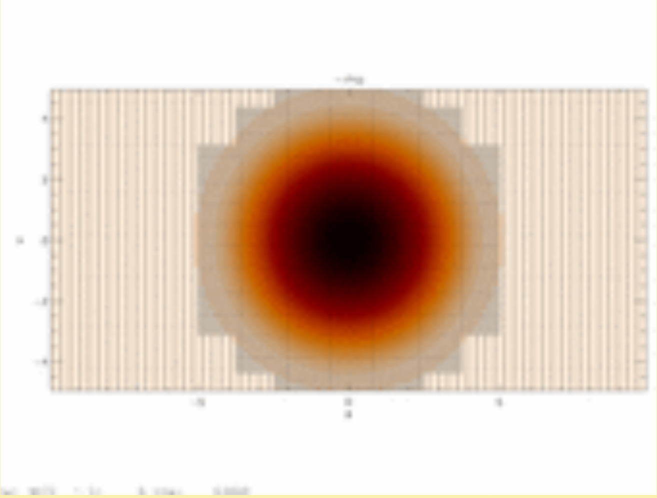






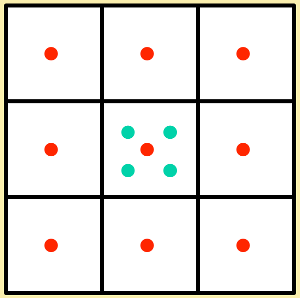
Grid Adaptation Strategies

- **Based on error estimates**
  - Compare solutions on two different grid levels, refine if difference is large.
  - Coarsen if difference is below some threshold.
- **Based on smoothness, gradients, curls etc.**
  - Calculate some quantities that indicate interesting features.
  - Use thresholds to flag regions fore refinement and coarsening.
- **Based on geometrical criteria**
  - Define regions to be refined/coarsened based on location and time.

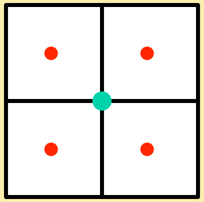


Prolongation and Restriction

- **Prolongation**
  - When a grid cell is refined, the solution is interpolated to a finer grid.
  - Conservation is important for shock capturing schemes.
  - Oscillation free prolongation is preferred for positivity.
  - Spatial order of accuracy should match the order of the scheme.



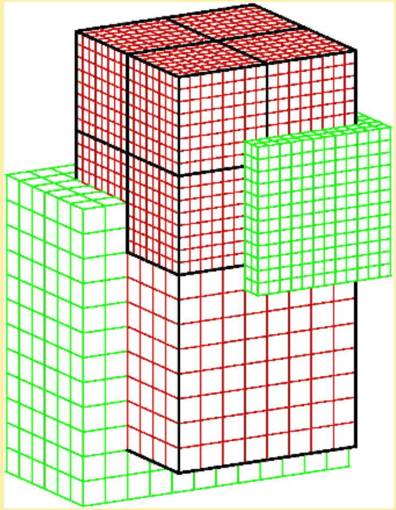
- **Restriction**
  - Re-grid solution to a coarser grid.
  - Simple averaging of fine cells is conservative, positive, oscillation free, and exact in the finite volume sense.



- **Proper nesting**
  - Refinement can only change by one level at any interface (edge/corner).

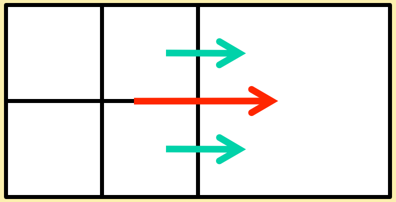
Resolution Changes

Ghost Cells



- Blocks/patches typically communicate through ghost cells.
- At resolution changes the ghost cell values are obtained by prolongation and restriction of neighboring physical cells.
- Conservative prolongation/restriction is not necessary.
- Oscillation free discretization can be important.
- Spatial order of accuracy should match the order of scheme.
- Special care needed for second order spatial derivatives!

Flux correction for conservative schemes

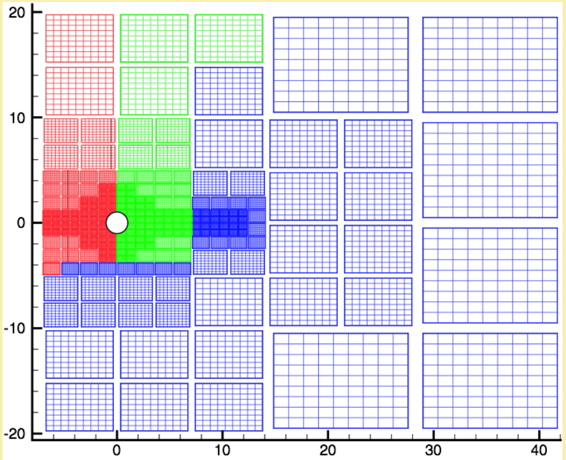


- Fluxes going into the coarse cell should be overwritten by the sum of fine fluxes.

Time Stepping in a block-AMR grid

- **Global explicit time step**
  - + very simple, easy load balancing
  - + works well if cells with the smallest allowed time step dominate
  - - wasteful if the time step is controlled by a small fraction of cells
- **Explicit time step proportional to cell size**
  - + efficient if wave speed does not vary much and the smallest cells do not dominate
  - - fairly complicated algorithm, load balancing is not easy
  - - far from optimal if time step is controlled by wave speed (not cell size) variation
- **Explicit time step proportional to CFL condition**
  - + simple and often very efficient choice for steady state calculations
  - - transient to steady state is non-conservative, div B is generated
  - - complicated for time accurate problems (but see DES, Omelchenko etc)
- **Global implicit time step**
  - + efficient for really stiff problems (accurate time step > 100 explicit steps)
  - + may be done on a subset of blocks
  - - complicated algorithm, scaling is not easy
  - - large amount of memory required

Parallel AMR



- **Load balancing**
  - Distribute grid among many processors.
  - Keep load equal as much as possible.
  - Order with space filling curves.
- **Message passing**
  - Ghost cells need to be filled in from data stored on other processors.
  - It is not easy to write an efficient message passing algorithm.
- **Time stepping**
  - Implicit time stepping requires global communication.
  - Efficient parallel implicit solvers are very difficult to obtain.

How to Get an Adaptive MHD Code?

- **Use existing AMR MHD codes (http://astro-sim.org/)**
  - BATSRUS (block), FLASH (block), MPIAMRVAC (block)
  - NIRVANA (blocks with clustering), PLUTO (patch), RAMSES (cell)
  - + no development effort, high quality software, support
  - - may not do exactly what you want
- **Use an AMR library**
  - ~~PARAMESH~~ (block-based), CHOMBO, GrACe, SAMRAI (patch-based)
  - + much less work than starting from scratch, efficient and flexible
  - - requires writing/adapting simulation code
- **Develop your own AMR code (not really…)**
  - + Good training, and it will do exactly what you want **if** you succeed
  - - takes a lot of time and requires a lot of algorithmic knowledge

What is Different in Computational MHD from Hydrodynamics?

- **Div B = 0 constraint.**
- **Exact Riemann solvers are costly (no analytic solution).**
  - Approximate Riemann solvers.
- **Total energy can be dominated by magnetic energy.**
  - Splitting the magnetic field as $B_0 + B_1$.
  - Hybrid method: solve both energy and pressure equations
- **Alfvén speed can be huge.**
- **Extra physics**
  - Resistivity, Hall MHD, field-aligned heat conduction, **….**

div B = 0

All components of B have some error in a numerical model.

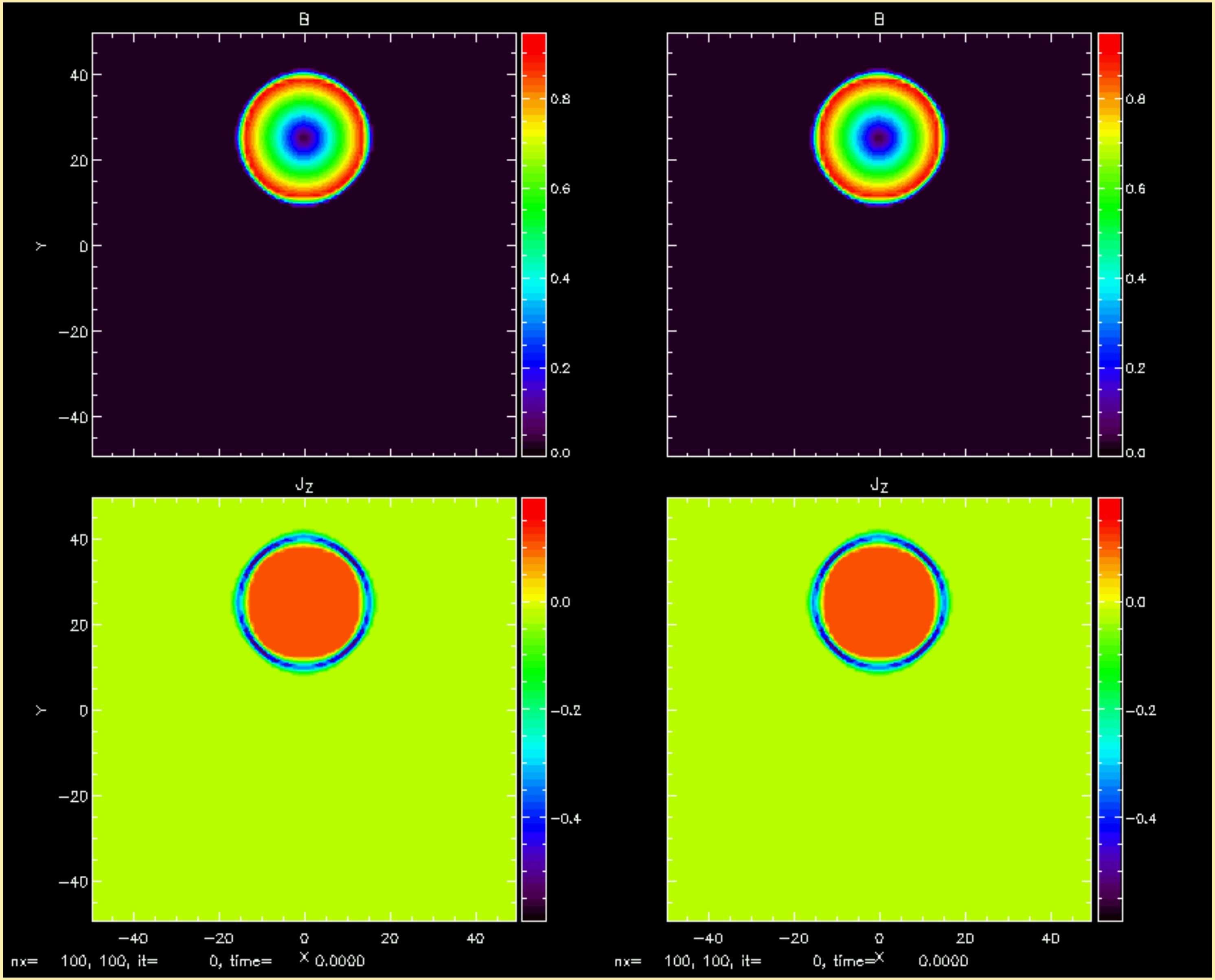
Why should we care about the numerical error in div B?

- To improve accuracy
- To improve robustness
- To make theoreticians happy

No div B control vs. 8-wave scheme

B

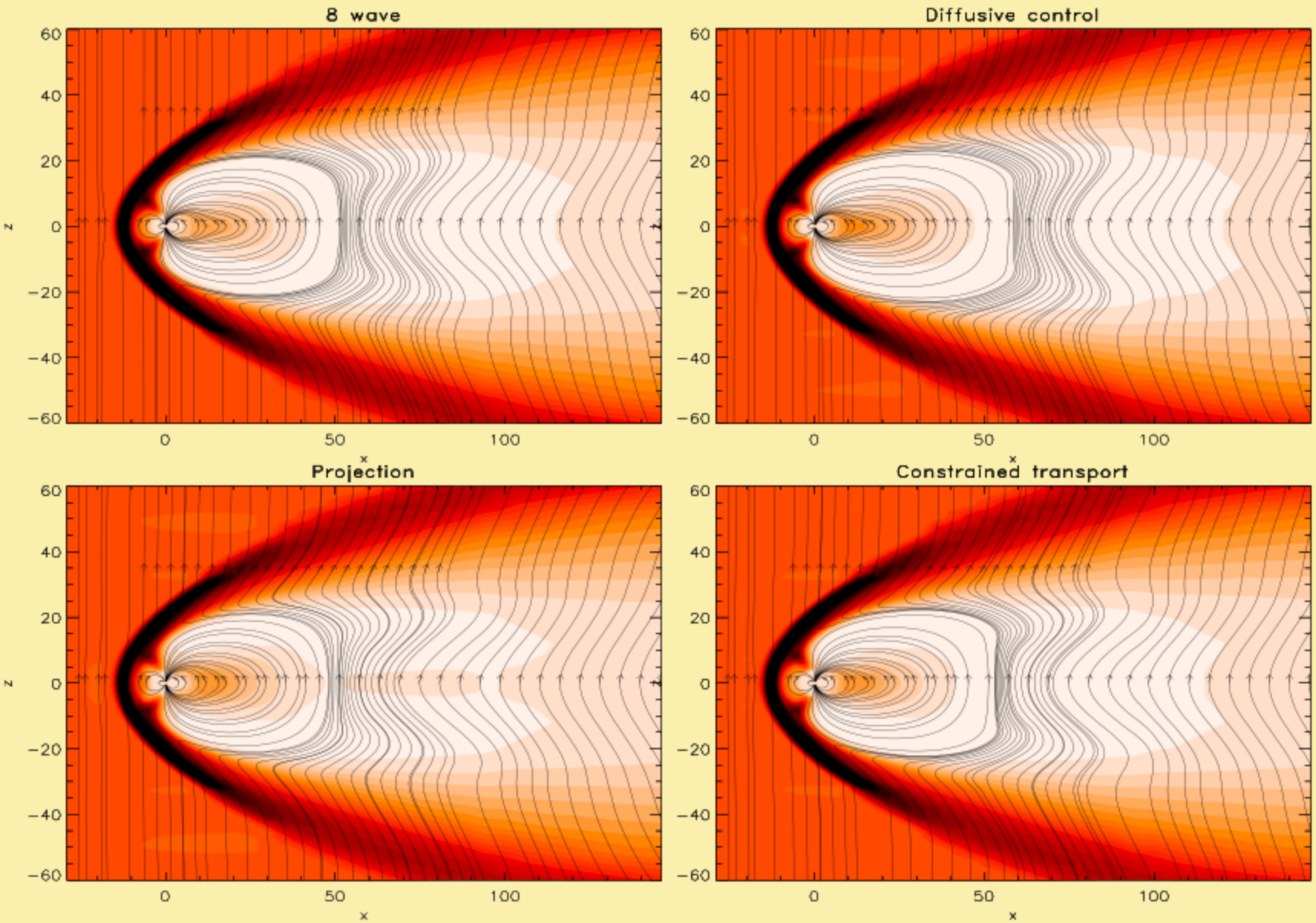
J_Z



Summary of div B Control Schemes

- **Projection scheme** (Brackbill and Barnes)
  - Solve a Poisson equation to remove div B after each time step.
  - \+ Accurate scheme. - Expensive, especially with AMR.
- **8-Wave scheme** (Godunov, Powell, also Janhunen, Dellar)
  - Modify MHD equations for non-zero divergence so it is advected.
  - \+ Simple, fast and robust. - Div B may not be very small. Not conservative.
- **Hyperbolic/parabolic cleaning** (Dedner et al.)
  - Add a scalar field coupled to div B to advect and diffuse div B away.
  - \+ Simple and fast. More effective than 8-wave. Fully conservative.
- **Central Difference Scheme** (Tóth)
  - Use central differences for induction equation to conserve div B.
  - \+ Simple, fast and accurate. - It does not generalize to AMR grids.
- **Constrained Transport** (Balsara, Dai, Ryu, Tóth, Gardiner ...)
  - Use staggered (face centered) grid for the magnetic field to conserve div B.
  - \+ Fast and accurate. - Very complicated, especially for AMR grids.

Effect of Div B Control Scheme



Magnetosphere solutions for Northward B_Z.
Field lines and density (colors) are shown.
Note the lack of differences.

Large Alfvén speed: Semi-Relativistic MHD

Classical Alfvén speed $B/\sqrt{\rho}$ is not limited by speed of light c.

Semi-relativistic case: $c_A \approx c$, $v << c$

Keep displacement current (Boris 1970) in $\mathbf{J} = \nabla \times \mathbf{B} - \frac{1}{c^2}\frac{\partial E}{\partial t}$

Semi-relativistic MHD equations in conservative form:

$$\mathbf{U} = \left[\rho, \rho\mathbf{v} + \frac{1}{c^2}(\mathbf{E}\times\mathbf{B}), \frac{1}{2}\rho\mathbf{v}^2 + \frac{p}{\gamma-1} + \frac{1}{2}\mathbf{B}^2 + \frac{1}{2c^2}\mathbf{E}^2, \mathbf{B}\right]^T$$

$$\mathbf{F} = \left[\begin{array}{c} \rho\mathbf{v} \\ \mathbf{v}\rho\mathbf{v} + \bar{I}\left(p + \mathbf{B}^2/2 + E^2/(2c^2)\right) - \mathbf{BB} - \mathbf{EE}/c^2 \\ \mathbf{v}\left(\rho\mathbf{v}^2/2 + \gamma p/(\gamma-1)\right) + \mathbf{E}\times\mathbf{B} \\ \mathbf{vB} - \mathbf{Bv} \end{array}\right]$$

The Alfvén wave speed is now bound by c (see Gombosi et al 2002).

Lowering the Speed of Light

- **Semi-relativistic MHD is used to model Jupiter and Saturn where classical Alfven speed can be larger than c.**
- **Semi-relativistic MHD is also used in combination with an artificially lowered speed of light for simulating the magnetosphere of the Earth**
  - Allows larger explicit time steps
  - Reduces numerical diffusion which is proportional to the fastest wave speed for most numerical schemes.
  - Converges to the correct solution for (quasi-)steady problems only.
- **Implicit Scheme with Limited Numerical Dissipation (ISLND) [Toth et al, JGR 2011] is an alternative**
  - In the Rusanov scheme use $\lambda'_{max} = \min(\lambda_{max}, \Lambda)$

Fully Implicit Jacobian-Free Newton-Krylov Scheme (JFNKS)

- Solve the non-linear semi-discretized PDE $\dfrac{\partial \mathbf{U}}{\partial t} = \mathbf{R}(\mathbf{U})$
- **BDF2** scheme for variable time step:

$$\mathbf{U}^{n+1} = \mathbf{U}^n + \Delta t_n \left[\beta \mathbf{R}(\mathbf{U}^{n+1}) + (1-\beta)\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t_{n-1}}\right]$$

- **Linearize** (non-linear and linear systems are both 2nd order in time):

$$\left[I - \Delta t_n \beta \frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right] \cdot (\mathbf{U}^{n+1} - \mathbf{U}^n) = \Delta t_n \left[\beta \mathbf{R}(\mathbf{U}^n) + (1-\beta)\frac{\mathbf{U}^n - \mathbf{U}^{n-1}}{\Delta t_{n-1}}\right]$$

- **Use spatially first order scheme for Jacobian.** The scheme is still 2nd order accurate. Upwind scheme helps with diagonal dominance.
- **Jacobian-free evaluation of matrix-vector products:**

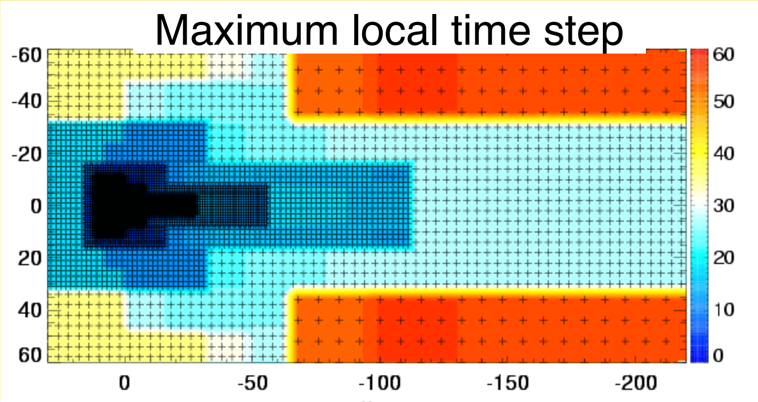
$$\left[I - \Delta t_n \beta \frac{\partial \mathbf{R}}{\partial \mathbf{U}}\right] \Delta \mathbf{U} = \Delta \mathbf{U} - \Delta t_n \beta \frac{\mathbf{R}(\mathbf{U}^n + \epsilon \Delta \mathbf{U}) - \mathbf{R}(\mathbf{U}^n)}{\epsilon} + \mathcal{O}(\epsilon)$$

Preconditioned Krylov Solvers

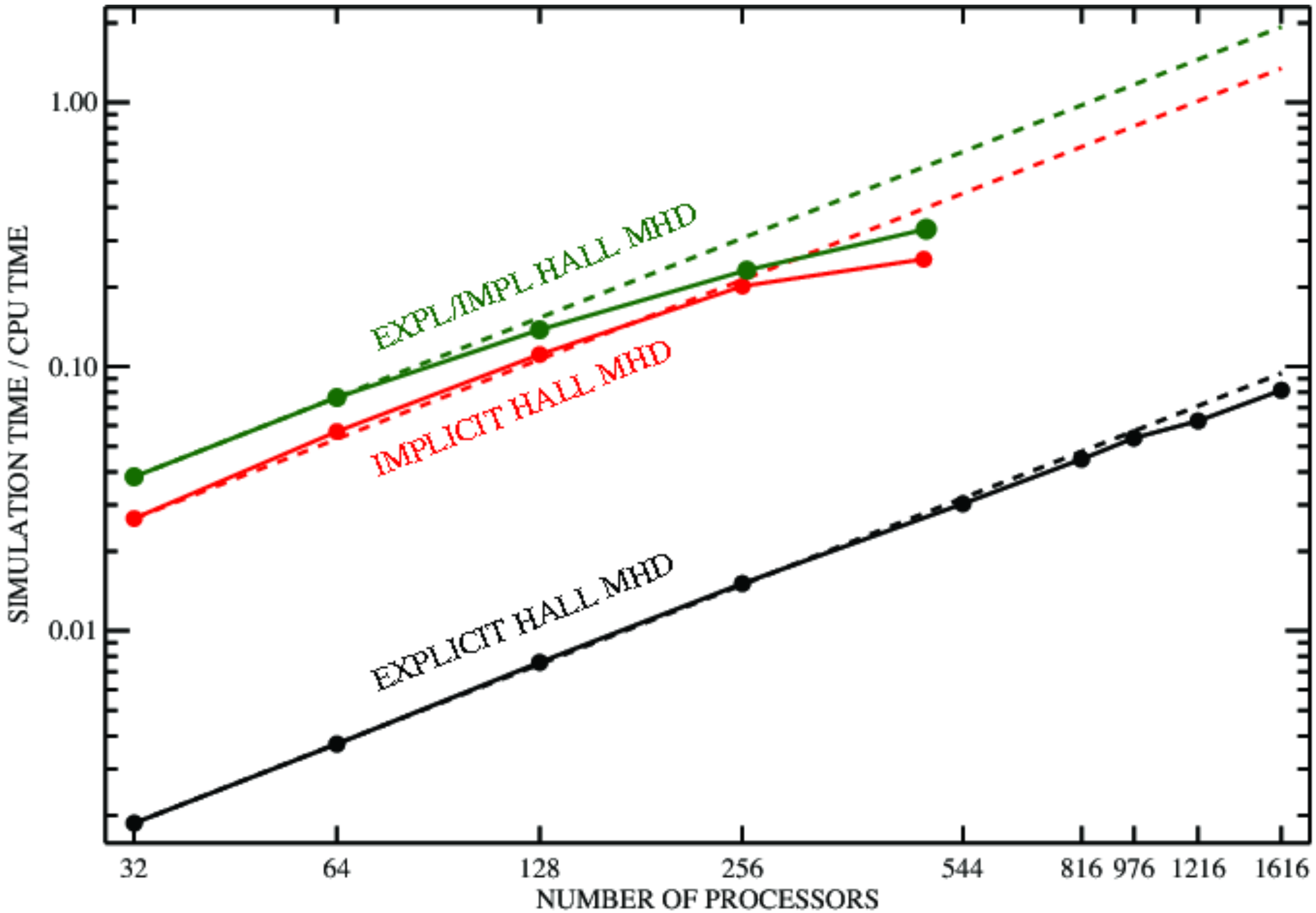
- **Krylov solvers (GMRES, BiCGSTAB) with preconditioning are robust and efficient for solving large linear systems.**
- **Schwarz preconditioning uses local data only (BILU / grid block)**
  - Natural choice for block adaptive grid: simple Jacobian matrix
  - Is overlap necessary? Not for the applications I tried.
  - The preconditioner is based on the first order Rusanov scheme and it is evaluated with numerical derivatives of flux and source functions. Additional terms are added as needed.
- **Multi-level preconditioning based on algebraic multigrid solver**
  - Optimal for elliptic source terms
  - Scales better than Schwarz preconditioning

Explicit/Implicit Scheme

- **Fully implicit scheme has no CFL limit, but each iteration is expensive (memory and CPU)**
- **Fully explicit is inexpensive for one iteration, but CFL limit may mean a very small Δt**
- **Set optimal Δt limited by accuracy requirement:**
  - Solve blocks with unrestrictive CFL explicitly
  - Solve blocks with restrictive CFL implicitly
  - Load balance explicit and implicit blocks separately

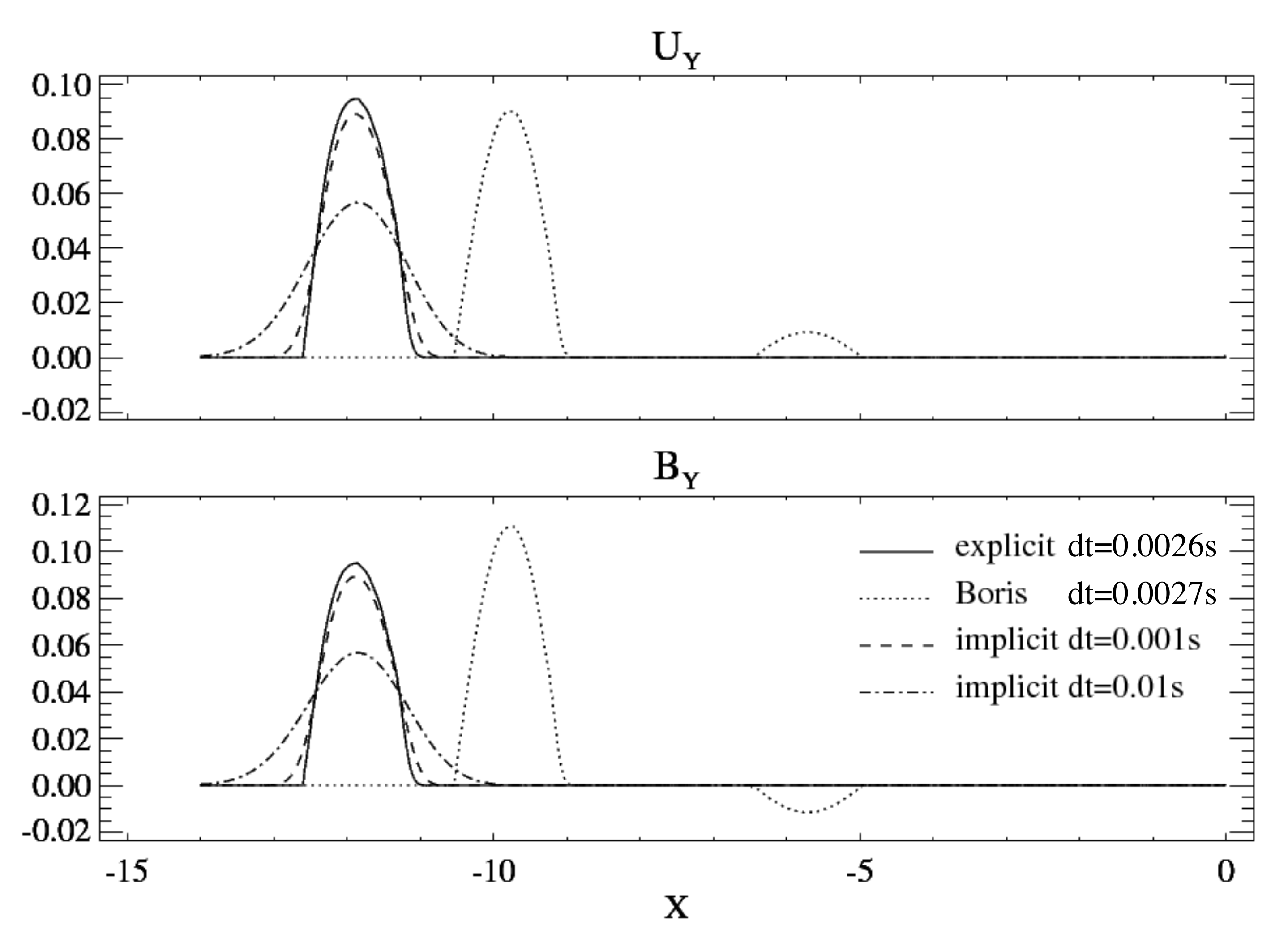


Strong Scaling of Explicit, Implicit and Explicit/Implicit Schemes



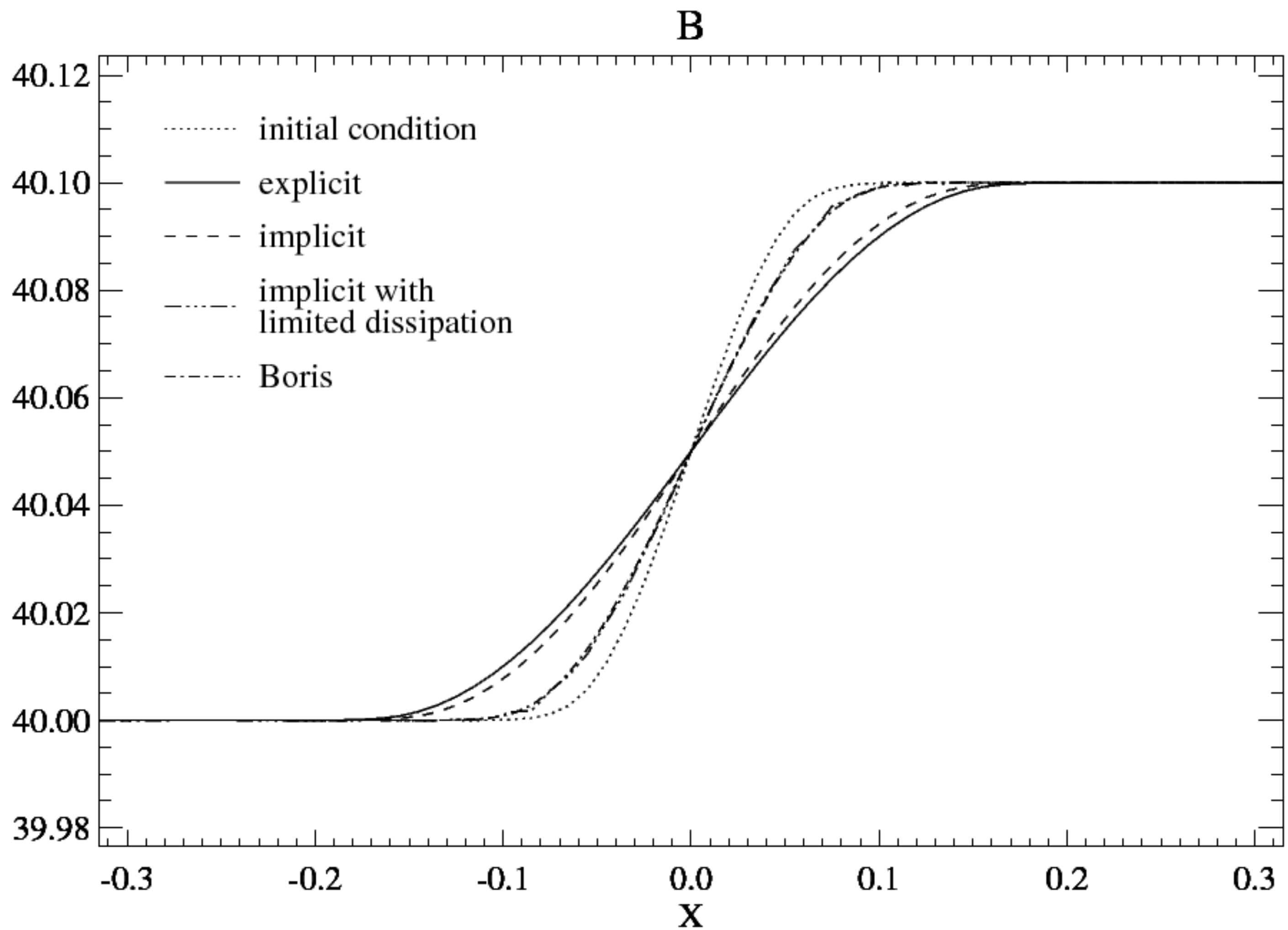
Grid: 4848 blocks with 8x8x8 cells (2.5 million cells)
Simulations done on an SGI Altix machine.

Boris Correction vs. Implicit Scheme for propagating Alfven waves



- Boris scheme gives wrong speed and amplitude
- Implicit scheme gives diffusive solution for large dt

Boris Correction vs. ISLND Scheme for Steady State Problem

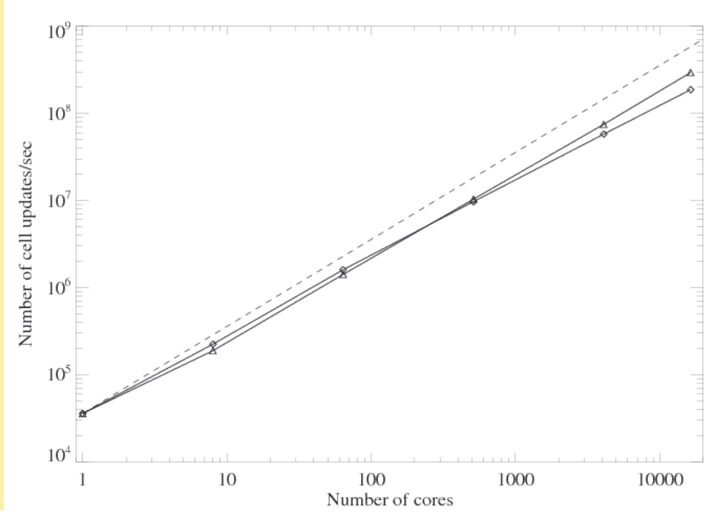


Numerical diffusion of sharp gradient in the transvers magnetic field.

Going Beyond Ideal MHD with BATS-R-US

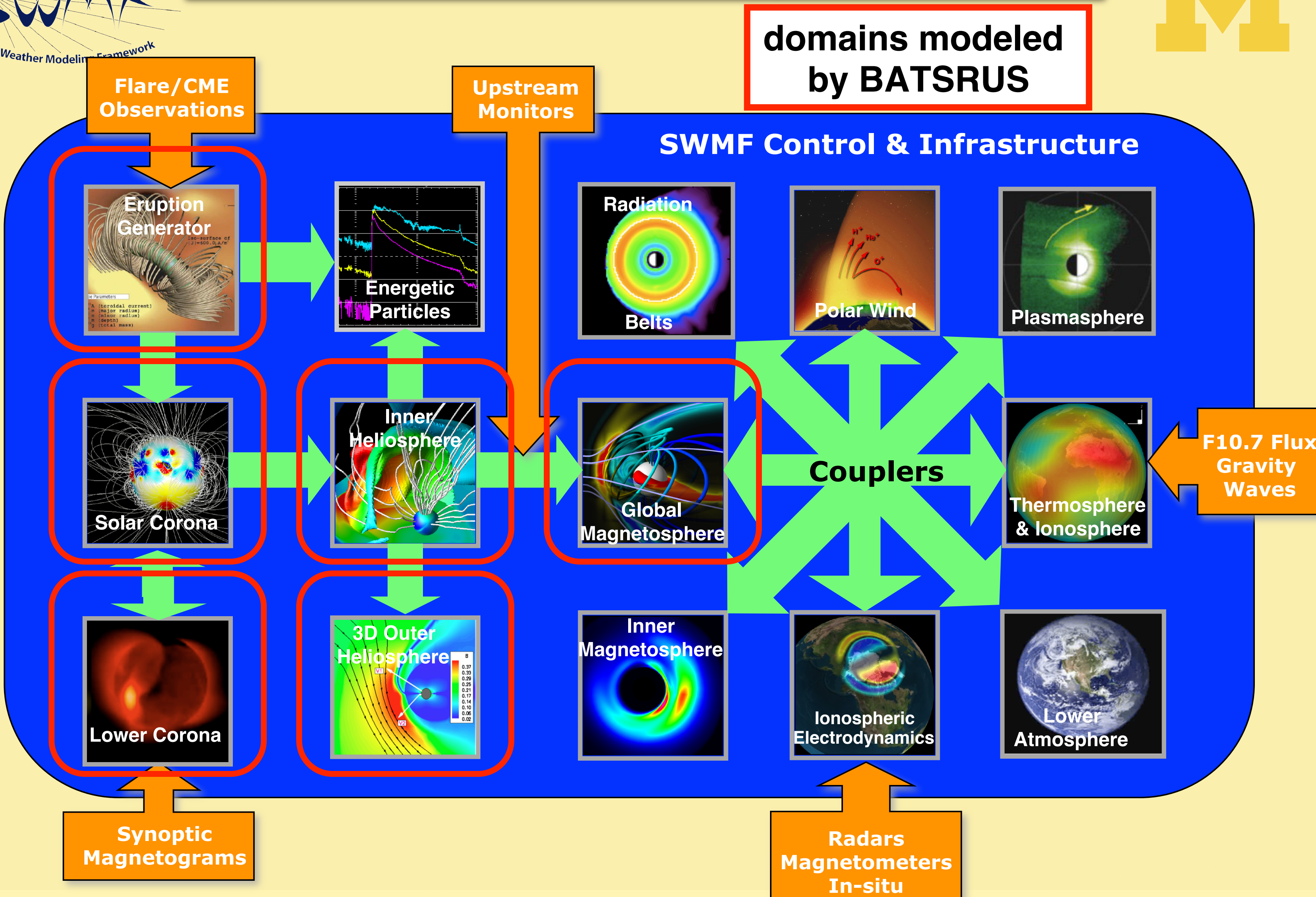
Block Adaptive Tree Solar-wind Roe Upwind Scheme

- **Physics**
  - Classical, semi-relativistic and Hall MHD
  - Multi-species, multi-fluid, anisotropic pressure
  - Radiation hydrodynamics multigroup diffusion
  - Multi-material, non-ideal equation of state
  - Solar wind turbulence, Alfven wave heating
- **Numerics**
  - Conservative finite-volume discretization
  - Parallel block-adaptive grid
  - Cartesian and generalized coordinates
  - Splitting the magnetic field into $B_0 + B_1$
  - Divergence B control: 8-wave, CT, projection, parabolic/hyperbolic
  - Shock-capturing TVD schemes: Rusanov, HLLE, AW, Roe, HLLD
  - Explicit, point-implicit, semi-implicit, fully implicit time stepping
- **Applications**
  - Sun, heliosphere, magnetospheres, planets, moons, comets…
- **100,000+ lines of Fortran 90 code with MPI parallelization**
- **Freely available as part of the SWMF at http://csem.engin.umich.edu**



Weak scaling from 1 to 16,384 cores

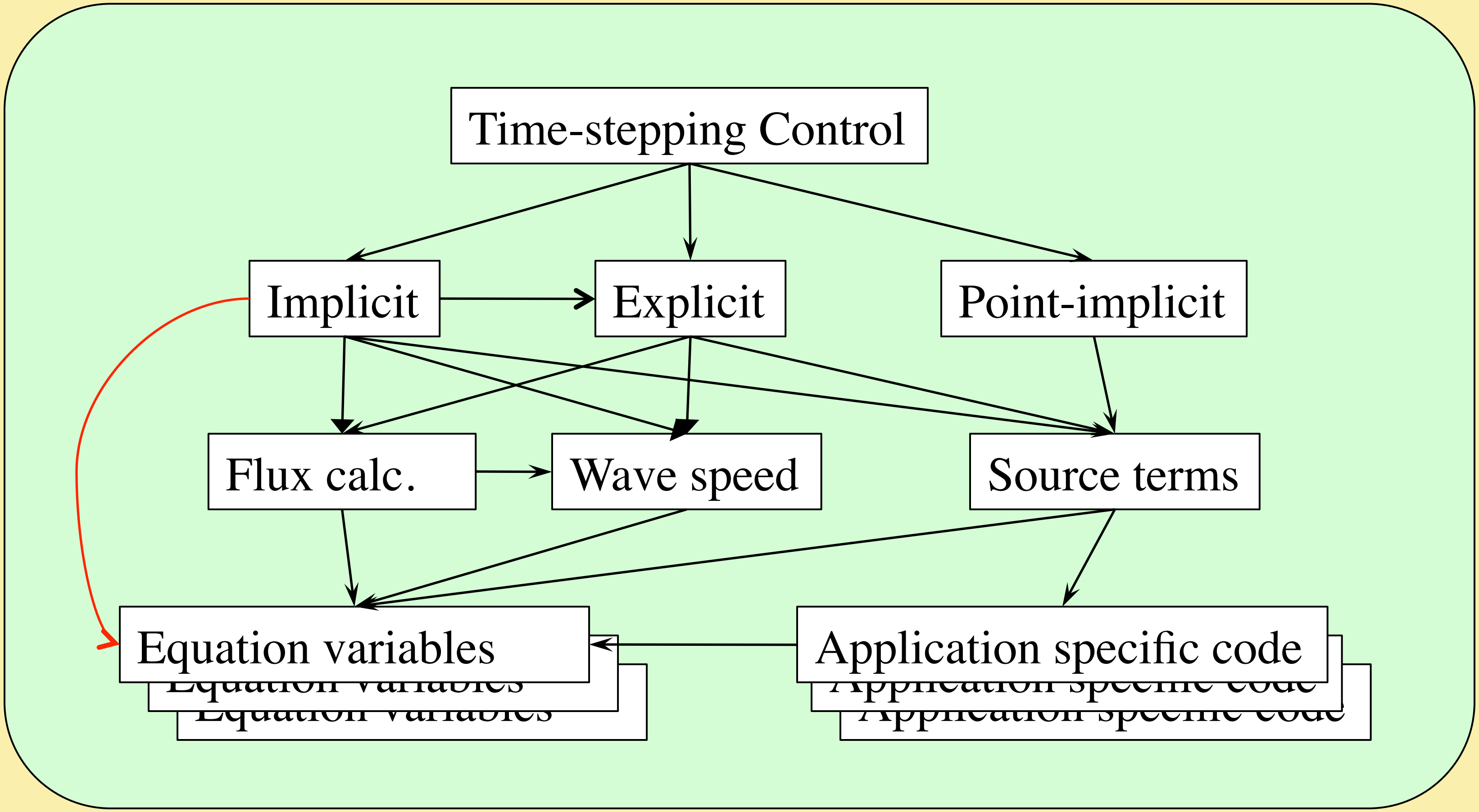
Space Weather Modeling Framework



SWMF is freely available at http://csem.engin.umich.edu and via CCMC

Layered Software Design

Goal: **maximum efficiency of schemes for maximum number of applications with minimum amount of code development.**



Hall MHD Equations

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

$$\frac{\partial \rho \mathbf{v}}{\partial t} = -\nabla \cdot (\mathbf{v}\rho\mathbf{v} + \bar{I}p + \bar{I}\mathbf{B}^2/2 - \mathbf{B}\mathbf{B})$$

$$\frac{\partial e}{\partial t} = -\nabla \cdot \left[\mathbf{v}\left(\frac{\gamma p}{\gamma - 1} + \frac{\rho \mathbf{v}^2}{2}\right) + (\mathbf{v} + \mathbf{v}_H) \cdot (\bar{I}\mathbf{B}^2 - \mathbf{B}\mathbf{B})\right]$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} = \nabla \times [(\mathbf{v} + \mathbf{v}_H) \times \mathbf{B}]$$

$$v_H = -\frac{\mathbf{J}}{ne} = -\frac{\nabla \times \mathbf{B}}{ne}$$

$$e = \frac{p}{\gamma - 1} + \frac{\rho \mathbf{v}^2}{2} + \frac{\mathbf{B}^2}{2}$$

- Electron inertia is neglected.
- Gradient of electron pressure is implemented (not shown).

Algorithmic Challenges in Hall MHD

- The fastest wave speed is the Whistler wave speed, estimated as

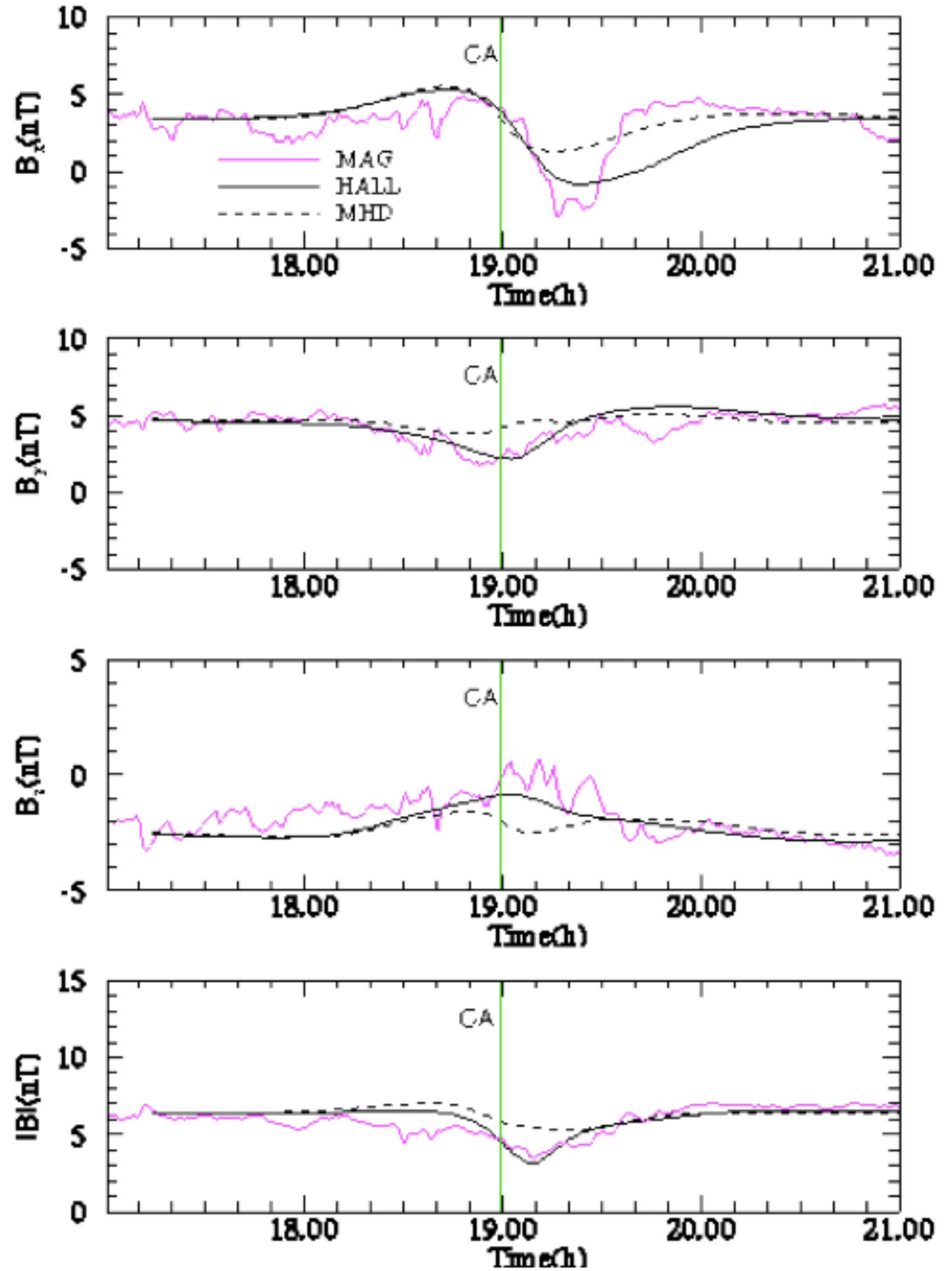
$$c_w = c_f + \frac{|B|\,\pi}{e\,n\,\Delta x}$$

- The CFL condition becomes:

$$\Delta t < \frac{\Delta x}{|u| + c_w} \propto \Delta x^2$$

- Implicit time integration is very beneficial if Whistler waves are not important in the dynamics. Note: **the numerical dissipation must be reduced in the implicit scheme** [Chacon and Knoll]

Comparison of Measured and Modeled Magnetic Fields for Cassini Titan T9 flyby
(Ma et al, GRL 2007)



- **Steady state simulation on spherical grid with multi-species (Hall) MHD.**
- **Hall MHD result (solid line) matches observations (magenta line) significantly better than ideal MHD simulation (dashed line).**

http://csem.engin.umich.edu

Multi-Fluid MHD

- **Multi-fluid MHD has many space physics applications**
  - ionospheric outflow, Earth magnetosphere, Martian ionosphere, outer heliosphere interaction with interstellar medium, etc.
- **BATS-R-US now contains a general multi-fluid solver with arbitrary number of ion and neutral fluids.**
- **Each fluid has separate densities, velocities and temperatures.**
- **One ion fluid + neutrals can be solved as MHD for ions, and HD for neutrals.**
- **Ions and neutrals are coupled by charge exchange and chemical reactions.**
- **Neutrals are coupled by collisions and chemical reactions.**
- **Coupling source terms can be evaluated point-implicitly.**

Multi-Ion MHD Derived

Momentum equations for ion fluids s with charge q_s and electrons with charge $-e$

$$\frac{\partial \rho_s \mathbf{u}_s}{\partial t} + \nabla \cdot \left(\rho_s \mathbf{u}_s \mathbf{u}_s + I p_s\right) = + n_s q_s \left(\mathbf{E} + \mathbf{u}_s \times \mathbf{B}\right) + S_{\rho_s \mathbf{u}_s}$$

$$\cancel{\frac{\partial \rho_e \mathbf{u}_e}{\partial t}} + \nabla \cdot \left(\cancel{\rho_e \mathbf{u}_e \mathbf{u}_e} + I p_e\right) = - n_e e \left(\mathbf{E} + \mathbf{u}_e \times \mathbf{B}\right) + S_{\rho_e \mathbf{u}_e}$$

Express electric field from electron momentum equation neglecting small terms:

$$\mathbf{E} = -\mathbf{u}_e \times \mathbf{B} - \frac{1}{e n_e} \nabla p_e + \eta \mathbf{J}$$

Obtain electron density from charge neutrality and electron velocity from current:

$$n_e = \frac{1}{e} \sum_s n_s q_s$$

$$\mathbf{u}_e = -\frac{\mathbf{J}}{e n_e} + \mathbf{u}_+$$ where the charge averaged ion velocity is $$\mathbf{u}_+ = \frac{\sum_s n_s q_s \mathbf{u}_s}{e n_e}$$

The electron pressure p_e is either a fixed fraction of total ion pressure, or we solve

$$\frac{\partial p_e}{\partial t} + \nabla \cdot \left(p_e \mathbf{u}_e\right) = -\left(\gamma - 1\right) p_e \nabla \cdot \mathbf{u}_e + S_{p_e}$$

Multi-Ion MHD

For each ion fluid *s* we obtain (neglecting resistive terms):

Cannot be written in conservative form

Gyration of ions around each other. Can be stiff.

$$\frac{\partial \rho_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s) = S_{\rho_s}$$

$$\frac{\partial \rho_s \mathbf{u}_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + I p_s) = \frac{n_s q_s}{n_e e}(\mathbf{J} \times \mathbf{B} - \nabla p_e) + n_s q_s (\mathbf{u}_s - \mathbf{u}_+) \times \mathbf{B} + S_{\rho_s \mathbf{u}_s}$$

$$\frac{\partial p_s}{\partial t} + \nabla \cdot (p_s \mathbf{u}_s) = -(\gamma - 1) p_s \nabla \cdot \mathbf{u}_s + S_{p_s}$$

We can also solve for *hydro* energy density $e_s = \rho_s \mathbf{u}_s^2/2 + p_s/(\gamma - 1)$

$$\frac{\partial e_s}{\partial t} + \nabla \cdot [(e_s + p_s)\mathbf{u}_s] = \mathbf{u}_s \cdot \left[\frac{n_s q_s}{n_e e}(\mathbf{J} \times \mathbf{B} - \nabla p_e) + n_s q_s (\mathbf{u}_s - \mathbf{u}_+) \times \mathbf{B}\right] + S_{e_s}$$

Finally the induction equation with or without the Hall term becomes

$$\frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u}_e \times \mathbf{B}) = 0 \quad \text{or} \quad \frac{\partial \mathbf{B}}{\partial t} - \nabla \times (\mathbf{u}_+ \times \mathbf{B}) = 0$$

Two-Stream Instability

- **Perpendicular ion velocities are coupled through the magnetic field**
- **Parallel ion velocities are not coupled by the multi-ion MHD equations.**
- Two-stream instability restricts the velocity differences parallel to **B**
  - We cannot resolve the two-stream instability
  - Use a simple ad-hoc friction source term in the momentum equations:

$$S^{friction}_{\rho \mathbf{u}_s} = \frac{1}{\tau_c} \sum_{q \neq s} \min(\rho_s, \rho_q)(\mathbf{u}_q - \mathbf{u}_s) \left(\frac{|\mathbf{u}_s - \mathbf{u}_q|}{u_c} \right)^{\alpha_c}$$

  - Using the minimum of the two densities makes the friction uniformly effective in regions of low and high densities.
  - τ_C is the time scale, u_C is the cut-off velocity, α_C is the cut-off exponent
  - Currently we use fixed parameters.
  - We will explore physics based parameter setting and formulas in the future.

Positivity

- **Positivity is difficult to maintain in empty regions where some of the fluids do not occur.**
- **For *minor* fluids**
  - Density is set to a small fraction ($\sim 10^{-4}$) of the total ion density.
  - Velocity and temperature are set to the same as for the total ion fluid.
  - This is a physically meaningful state that can interact properly with the truly multifluid regions.

Stability

- Naïve explicit scheme is unconditionally unstable.
- Fully implicit scheme can be slow due to many variables.
- We can combine explicit scheme with **point-implicit source terms:**

$$
(\rho_s \mathbf{u}_s)^{n+1} = (\rho_s \mathbf{u}_s)^n - \Delta t \nabla \cdot \mathbf{F}^n + \Delta t S^{n+1}_{\rho \mathbf{u}_s}
$$

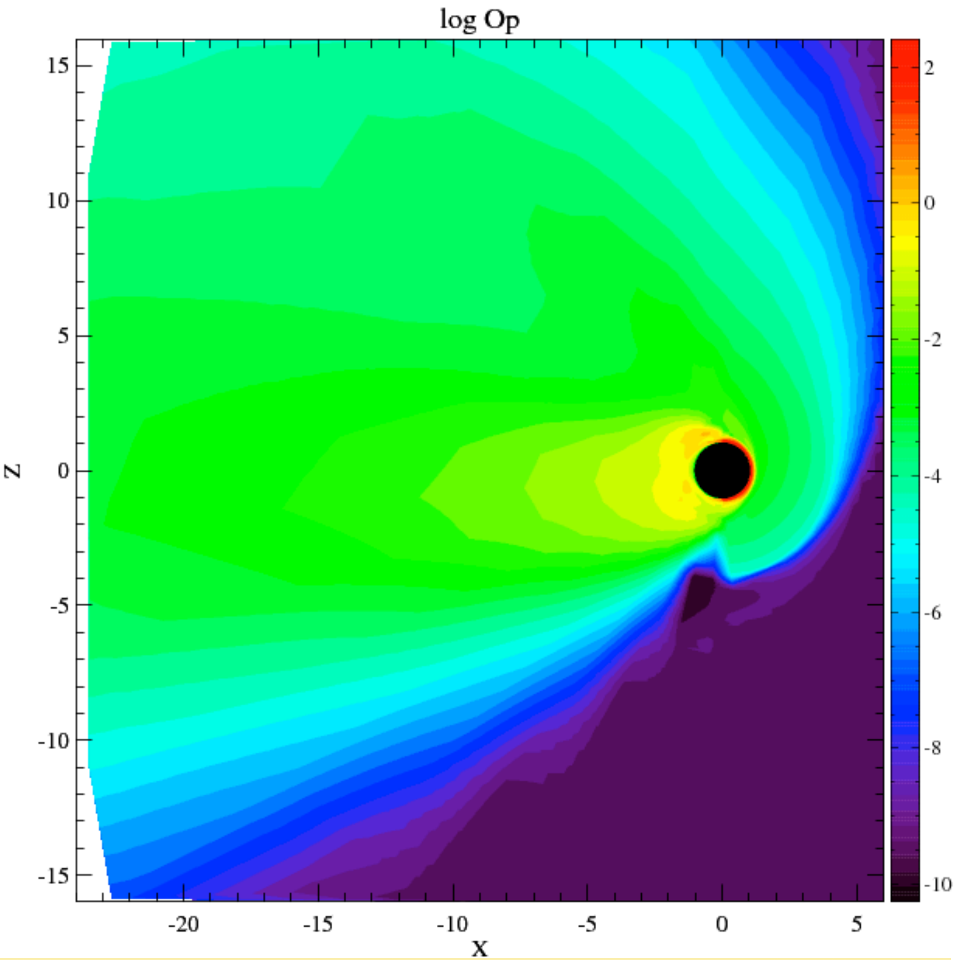
$$
+\Delta t \left[\frac{q_s}{M_s} (\rho_s \mathbf{u}_s - \rho_s \mathbf{u}_+)^{n+1} \times \mathbf{B}^n + \frac{n_s^n q_s}{n_e^n e} (\mathbf{J}^n \times \mathbf{B}^n - \nabla p_e^n) \right]
$$

where M_S is the mass of ion s.

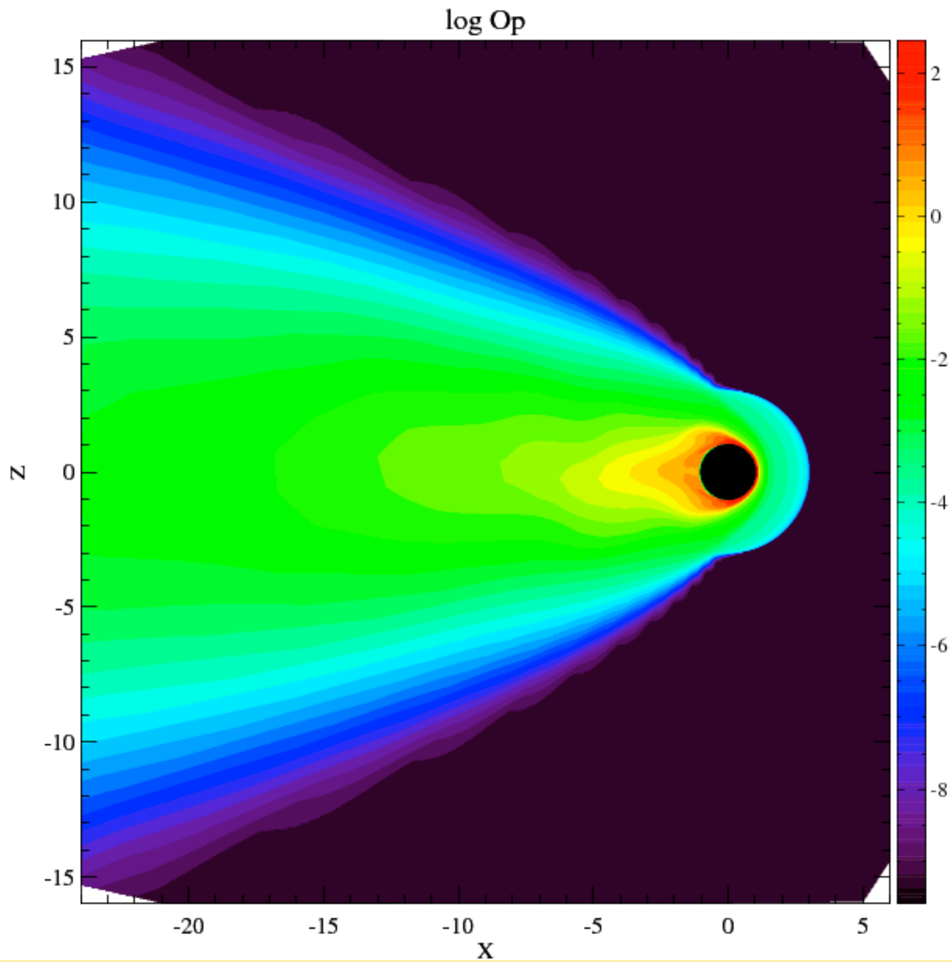
- The linear equations can be solved in every grid cell independently.
- The unknowns are the momenta of the ion fluids.
- The three spatial components are coupled by the artificial friction term.
- We use an analytic Jacobian matrix for sake of efficiency and accuracy.

O+ Escape from Mars Ionosphere

Multi-fluid MHD



Multi-species MHD



Point-Implicit Scheme Example: Multi-Ion MHD

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Momentum equation for each ion fluid s :

Gyration of ions around each other. Can be stiff.

Chemistry, charge exchange, recombination, etc. Stiff.

$$\frac{\partial \rho_s \mathbf{u}_s}{\partial t} + \nabla \cdot (\rho_s \mathbf{u}_s \mathbf{u}_s + I p_s) = \frac{n_s q_s}{n_e e}(\mathbf{J} \times \mathbf{B} - \nabla p_e) + n_s q_s (\mathbf{u}_s - \mathbf{u}_+) \times \mathbf{B} + S_{\rho_s \mathbf{u}_s}$$

$$\mathbf{u}_+ = \frac{\sum_s n_s q_s \mathbf{u}_s}{e n_e}$$

Point-implicit discretization is needed to make the scheme stable

$$(\rho_s \mathbf{u}_s)^{n+1} = (\rho_s \mathbf{u}_s)^n - \Delta t \nabla \cdot \mathbf{F}^n + \Delta t S^{n+1}_{\rho \mathbf{u}_s}$$
$$+ \Delta t \left[\frac{q_s}{M_s} (\rho_s \mathbf{u}_s - \rho_s \mathbf{u}_+)^{n+1} \times \mathbf{B}^n + \frac{n_s^n q_s}{n_e^n e} (\mathbf{J}^n \times \mathbf{B}^n - \nabla p_e^n) \right]$$

Numerical Jacobian for flexibility and/or analytic Jacobian for speed.

Anisotropic MHD

- **In a collisionless plasma**
  - Different pressures parallel and perpendicular to the magnetic field
- **Where does it matter in space physics?**
  - Reconnection
  - Magnetosphere
  - Inner magnetosphere
  - Solar wind heating

Resistive MHD with electrons and anisotropic ion pressure

Mass conservation: $$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0$$

Momentum: $$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u}\mathbf{u} + P) = \mathbf{J} \times \mathbf{B}$$

$$P = (p_\perp + p_e) I + (p_\parallel - p_\perp)\mathbf{b}\mathbf{b} \qquad p = \frac{2p_\perp + p_\parallel}{3}$$

Induction: $$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

Pressure: $$\frac{\partial p_\perp}{\partial t} + \nabla \cdot (p_\perp \mathbf{u}) = \frac{1}{3\tau}(p_\parallel - p_\perp) + \frac{2}{\tau_{ie}}(p_e - p) - p_\perp \nabla \cdot \mathbf{u} + p_\perp \mathbf{b} \cdot (\nabla \mathbf{u}) \cdot \mathbf{b}$$

$$\frac{\partial p_\parallel}{\partial t} + \nabla \cdot (p_\parallel \mathbf{u}) = \frac{2}{3\tau}(p_\perp - p_\parallel) + \frac{2}{\tau_{ie}}(p_e - p) - 2p_\parallel \mathbf{b} \cdot (\nabla \mathbf{u}) \cdot \mathbf{b}$$

$$\tau_{ie} = \frac{2}{3}\frac{M_i}{\eta e^2 n_e}$$

Electron pressure:

$$\frac{\partial p_e}{\partial t} + \nabla \cdot (p_e \mathbf{u}) = (\gamma - 1)\left[-p_e \nabla \cdot \mathbf{u} + \eta \mathbf{J}^2 + \nabla \cdot (\kappa \mathbf{b}\mathbf{b} \cdot \nabla T_e)\right] + \frac{2}{\tau_{ie}}(p - p_e)$$

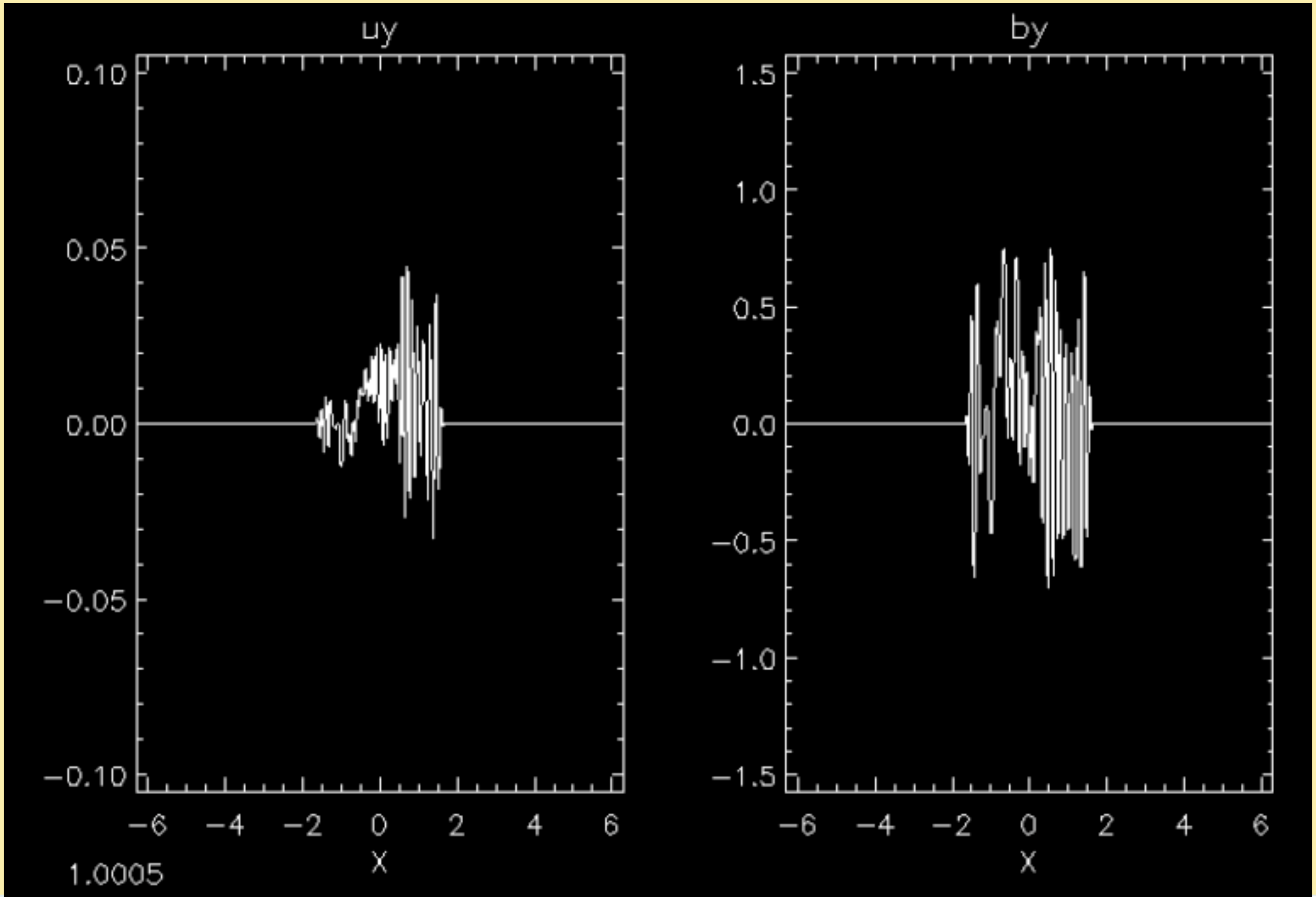
Electric field: $$\mathbf{E} = -\mathbf{u} \times \mathbf{B} + \eta \mathbf{J} \qquad \mathbf{b} = \mathbf{B}/B$$

Current: $$\mathbf{J} = \nabla \times \mathbf{B}$$

Alfven waves with anisotropic pressure

Circularly polarized Alfven wave propagates at $v_A = \sqrt{(\mathbf{B}^2 + p_\perp - p_\parallel)/\rho}$

This can become unstable if the parallel pressure is large enough!

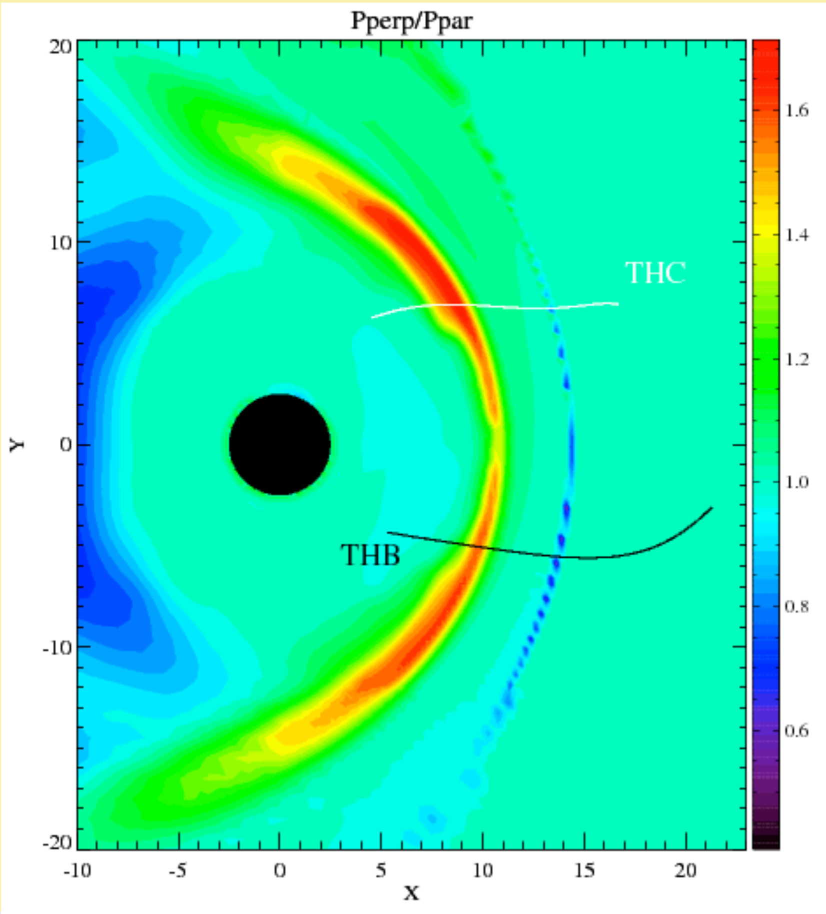


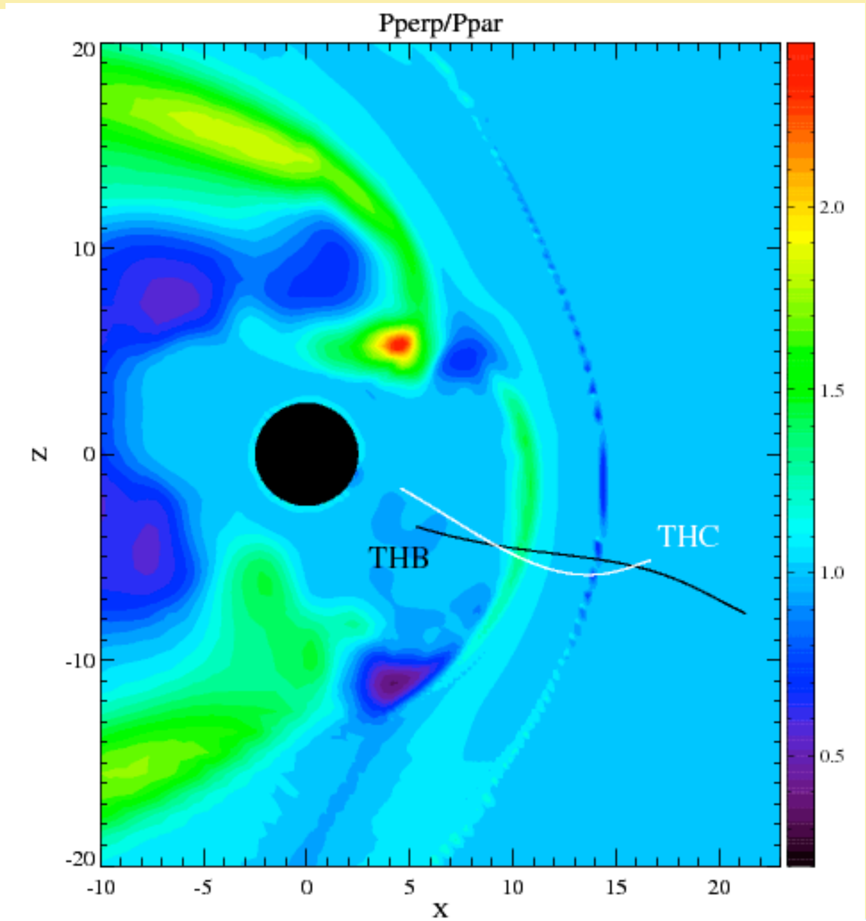
Limiting the Anisotropy

- **Instabilities**
  - Fire-hose: $$\frac{p_\parallel}{p_\perp} > 1 + \frac{B^2}{p_\perp}$$
  - Mirror: $$\frac{p_\perp}{p_\parallel} > 1 + \frac{B^2}{2p_\perp}$$
  - Proton cyclotron: $$\frac{p_\perp}{p_\parallel} > 1 + 0.847\left(\frac{B^2}{2p_\parallel}\right)^{0.48}$$
  - In unstable regions, we relax anisotropy towards stable state
- **Ion-ion, ion-electron and/or wave-ion interactions:**
  - Push ion pressure towards isotropic distribution with time rate τ

Quiet Time Magnetosphere Run

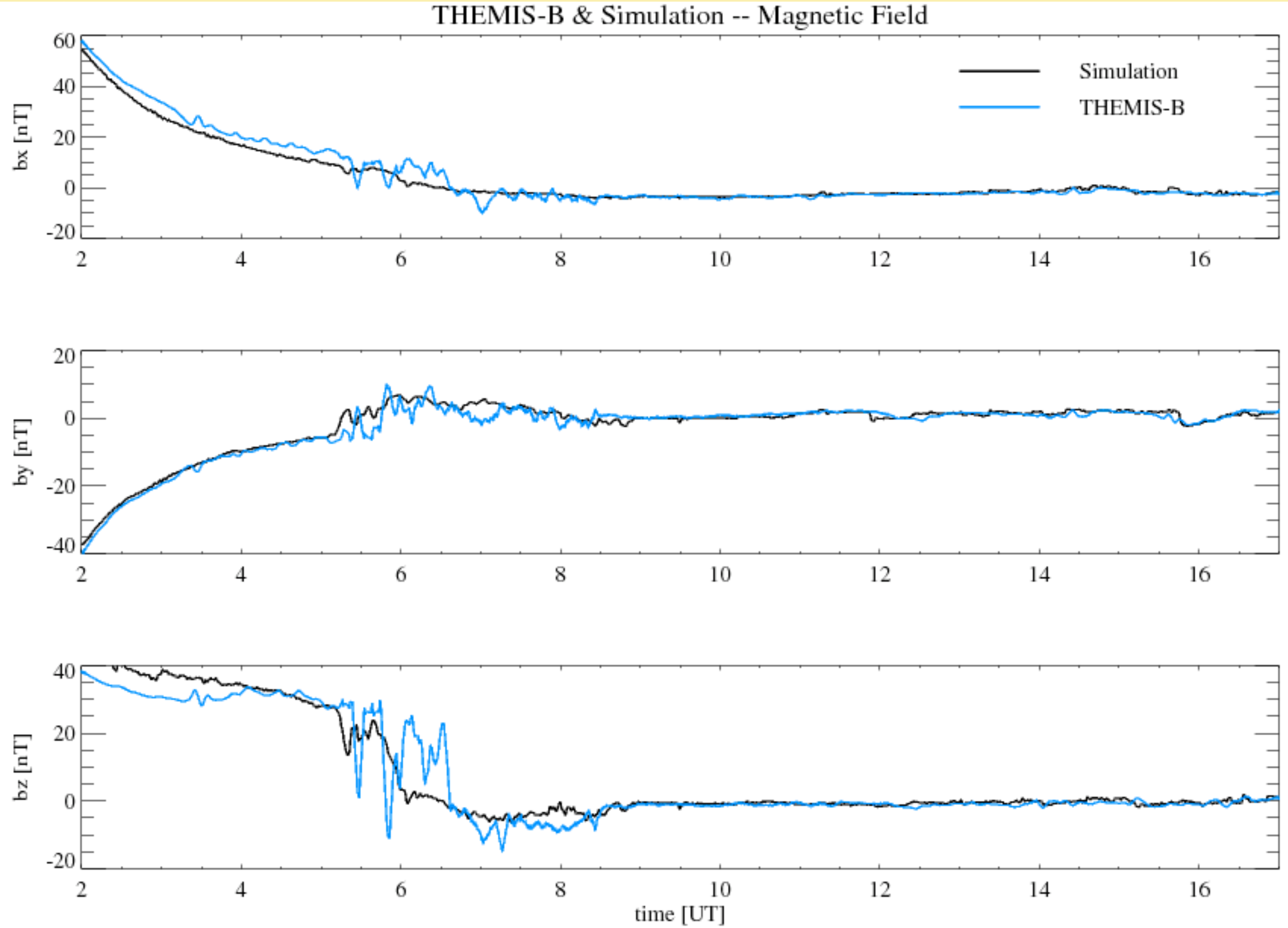
- Driven by ACE satellite data for 02-17UT, July 29, 2008
  - ≈ 370km/s, 3-6 amu/cc, B_x, B_y, B_z ≈ 2nT
- BATS-R-US + RIM + RCM, relaxation with τ=1s for R < 4Re
- Compare with Themis B and C data





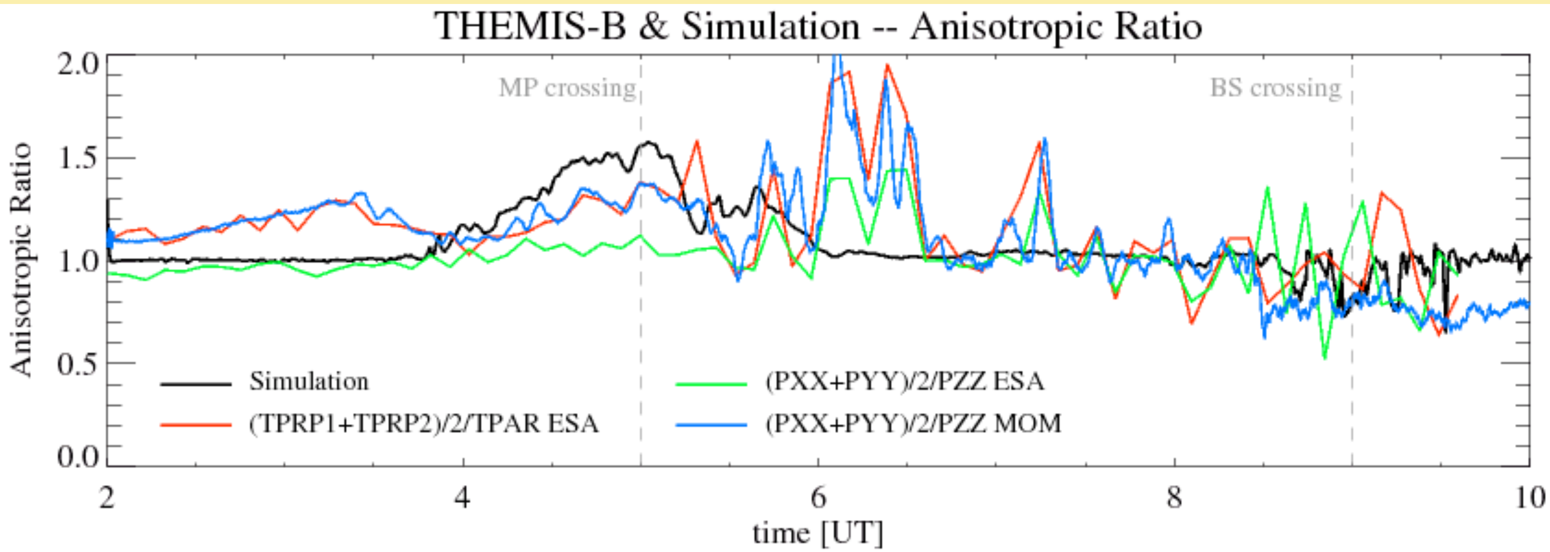
Quiet Time Magnetosphere Run

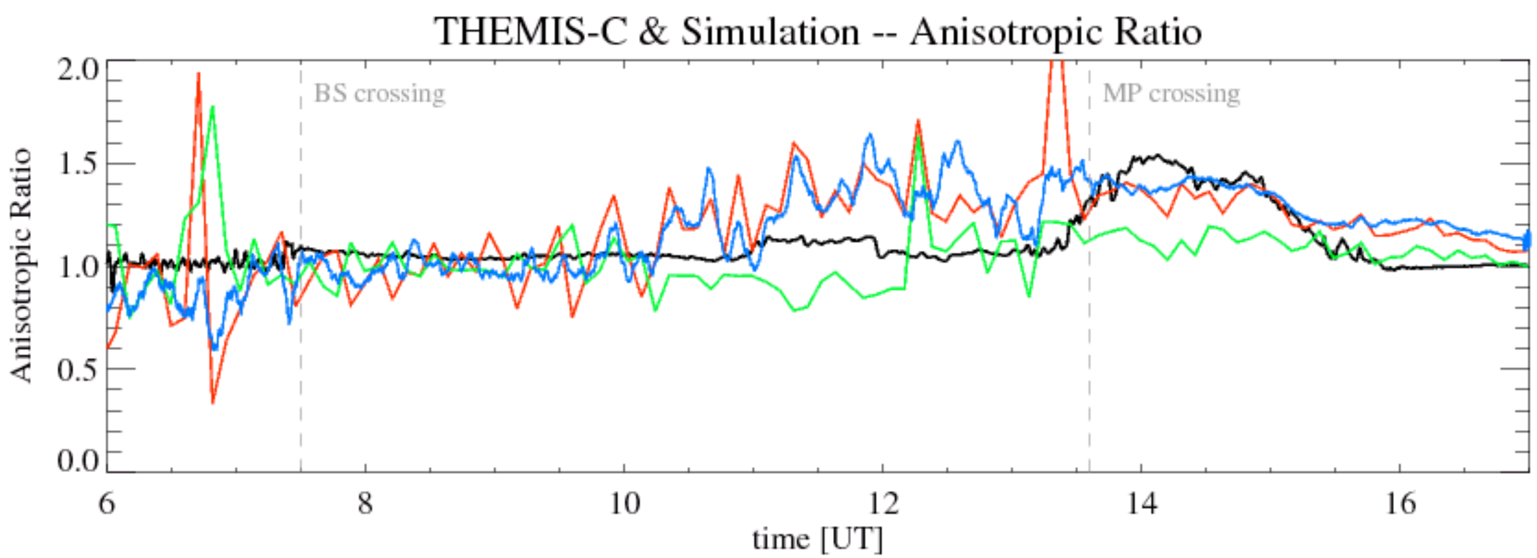
Simulated magnetic field agrees well with Themis data



Quiet Time Magnetosphere Run

- Simulated anisotropy shows similarities with data.
- Different instruments do not agree with each other.





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Conclusions

- Computational MHD is a dynamically evolving field.
- There is no point to be ‘religious’ about certain attributes, like exact conservation, strict positivity, or div B = 0.
- Different applications require different numerical schemes.
- Numerical schemes should be compared for their accuracy, robustness, efficiency, and flexibility for applications of interest.
- Adaptive mesh refinement and implicit time stepping can improve efficiency.
- Going beyond ideal MHD creates new algorithmic challenges.
- Large simulation codes require more than a good algorithm: good software development practices, testing, coupling of heterogeneous models, good visualization tools, user-friendly interface, documentation, etc.
- Good simulations require more than a good code: good understanding of the limitations of physics and numerics.
- Without a grid convergence study, a numerical solution cannot be trusted.

For more detail please read our 2011 JCP review paper:
Adaptive Numerical Algorithms in Space Weather Modeling