The Use of M3D-C^1 Vector Representation in the HiFi Code

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Key Points

- Goal: fast, scalable parallel solver for the HiFi code.
- Physics-Based Preconditioning + Algebraic Multigrid
  Works well for ideal MHD waves, but Newton convergence is much slower for the GEM Challenge magnetic reconnection problem.
- Quiet initial conditions and improved graphic diagnostics help to identify the cause of the problem: since the tearing mode growth rate is much less than sound and Alfven frequencies, there is approximate cancellation in the flux-normal components of the force terms **J**x**B** - grad p, leaving noise.
- The M3D-C^1 representation of velocity and field vectors eliminates such cancellations analytically.
- The separation of application and solver modules in the HiFi facilitates adaptation of the M3D-C^1 representation to HiFi. The use of C^0 rather than C^1 in HiFi requires the use of auxiliary variables.
- Equations have been derived and coded up but not yet fully tested.

GEM Magnetic Reconnection Problem

Equilibrium

$$x \in \frac{1}{2}(-l_x, l_x), \quad y \in \frac{1}{2}(-l_y, l_y), \quad z \in \frac{1}{2}(-l_z, l_z)$$

Periodic in x and z, conducting wall in y

$$A_x = -B_0 y, \quad A_y = 0, \quad A_z = -\lambda \ln\cosh\left(\frac{y}{\lambda}\right)$$

$$B_x = \tanh\left(\frac{y}{\lambda}\right), \quad B_z = B_0$$

$$p = nT = p_0 + \operatorname{sech}^2\left(\frac{y}{\lambda}\right), \quad T = \frac{1}{2} \quad \rho v_x = \rho v_y = \rho v_z = 0$$

Parameters

$$l_x = 25.6, \quad l_y = 12.8, \quad l_z = 6.4, \quad \lambda = \frac{1}{2}, \quad p_0 = .2, \quad B_0 = 0$$

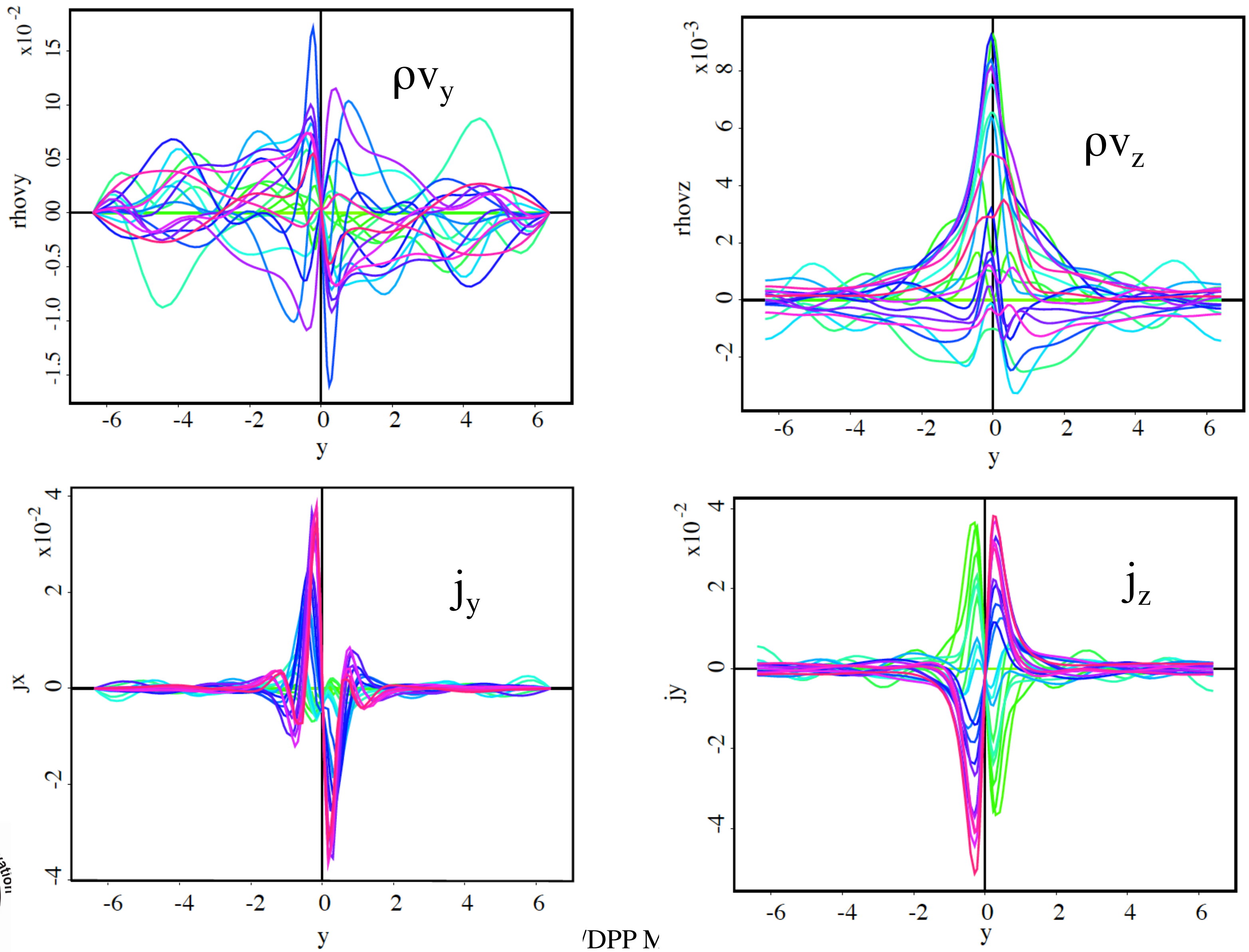
$$\eta = 10^{-3}, \quad \mu = \kappa = 10^{-2}$$

Noisy Initial Conditions

$$\tilde{A}_z = \delta \cos(k_x x)\cos(k_z z)\exp(-y^2/\lambda^2)$$

Smooth perturbation, but out of balance.

Noisy Start



Quiet Initial Conditions

Flux-Source Form

$$\frac{\partial u_i}{\partial t} + \nabla \cdot \mathbf{F}_i = S_i, \quad \mathbf{F}_i = \mathbf{F}_i(t, \mathbf{x}, u_j, \nabla u_j), \quad S_i = S_i(t, \mathbf{x}, u_j, \nabla u_j)$$

Galerkin Expansion, Spatial Discretization

$$u_i(\mathbf{x}, t) = u_{ij}(t)\alpha_j(\mathbf{x})$$

$$(\alpha_i, \alpha_j)\dot{u}_j = \int_\Omega d\mathbf{x}\,(S\alpha_i + \mathbf{F} \cdot \nabla\alpha_i) - \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{F}\alpha_i$$

$$\mathbf{M}\dot{\mathbf{u}} = \mathbf{r}(\mathbf{u})$$

1D Static Equilibrium + Linearization

$$u_i(x, y, z, t) = u_{i0}(y) + u_{i1}(y)\exp\left[i(k_x + k_z z) + st\right]$$

$$\frac{\partial}{\partial t} \to s, \quad \nabla \to \left(ik_x, \frac{\partial}{\partial y}, ik_z\right), \quad J_{ij} = \left.\frac{\partial r_j}{\partial u_i}\right|_{u=u0}$$

Expand in 1D spectral elememts in y

Generalized 1D Eigenvalue Problem

$$\mathbf{A}\mathbf{u} = s\mathbf{B}\mathbf{u}$$

SLEPc

- Scalable Library for Eigenvalue Problem Computations
  http://www.grycap.upv.es/slepc/documentation/manual.htm

- Developed as an extension of PETSc
  by Jose Román *et al* at the University of Valencia, Spain

- Solution of large sparse eigenproblems on parallel computers.

- Advanced iterative solution procedures.

- Allows selection of a portion of the spectrum
  e.g. largest real eigenvalues

- Accurate solution of 1D complex eigenvalue problem in a few seconds
  on one processor.

Grid Packing: Equations

Grid Packing Function

$$y(\xi,\lambda) = \ln\left(\frac{1+\lambda\xi}{1-\lambda\xi}\right) \Big/ \ln\left(\frac{1+\lambda}{1-\lambda}\right)$$

$$\lim_{\lambda\to 0} y(\xi,\lambda) = \xi$$

Center and Edge Grid Densities

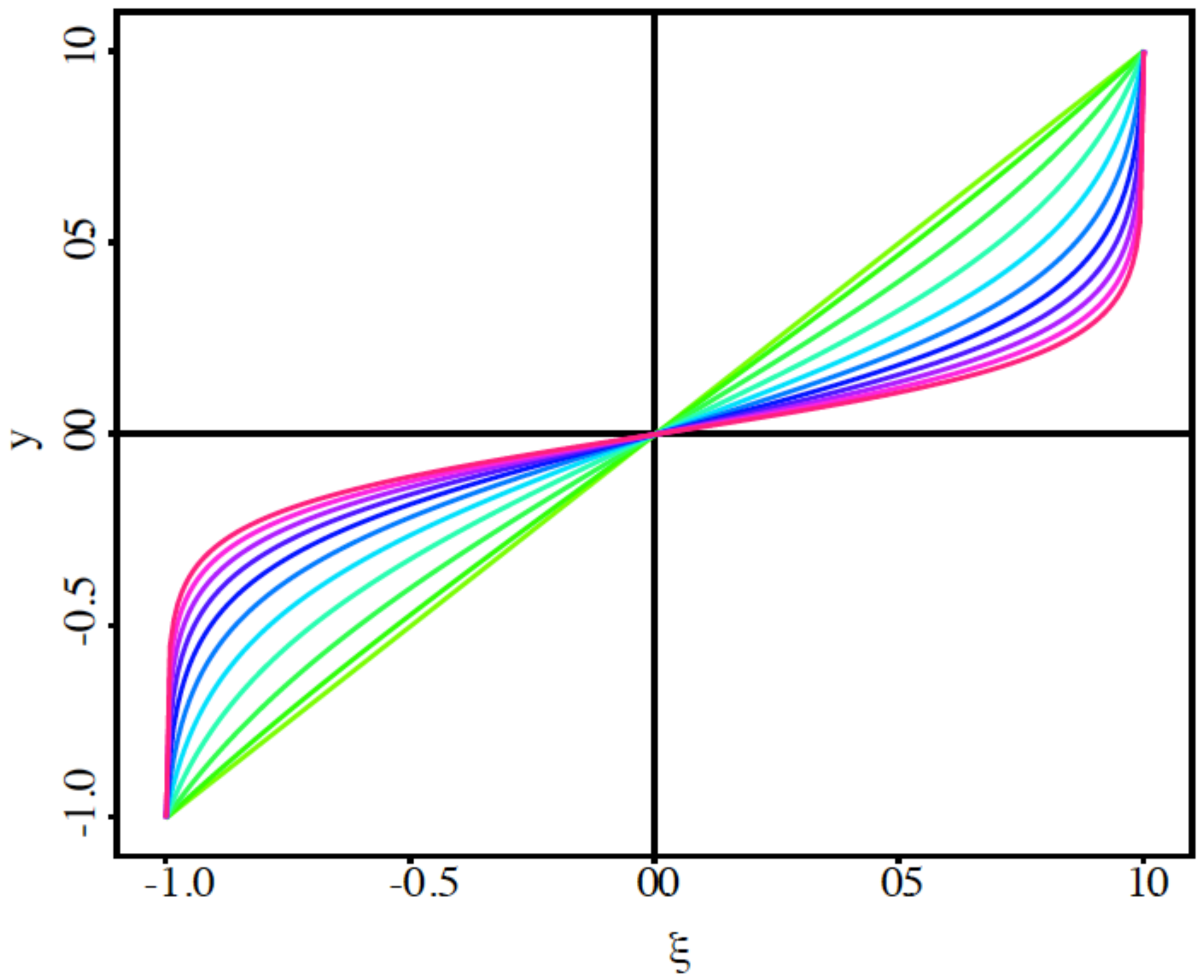
$$\frac{\partial y}{\partial \xi} = \frac{2\lambda}{1-\lambda^2\xi^2}, \quad \left.\frac{\partial y}{\partial \xi}\right|_{\xi=0} = 2\lambda, \quad \left.\frac{\partial y}{\partial \xi}\right|_{\xi=\pm 1} = \frac{2\lambda}{1-\lambda^2}$$

Packing Ratio

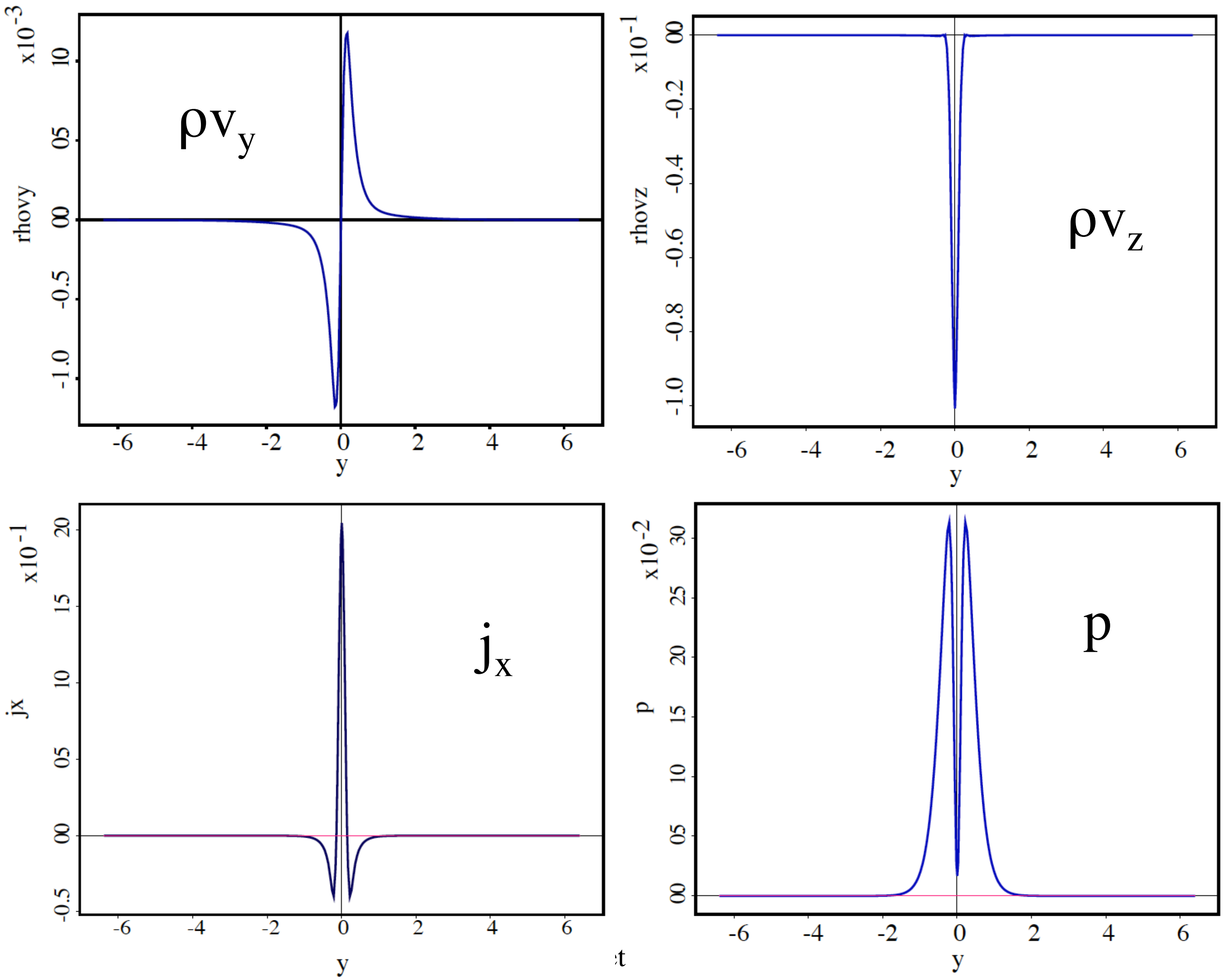
$$P(\lambda) \equiv \frac{\partial y/\partial\xi|_{\xi=0}}{\partial y/\partial\xi|_{\xi=\pm 1}} = 1-\lambda^2$$

$$\lambda = (1-P)^{1/2}$$

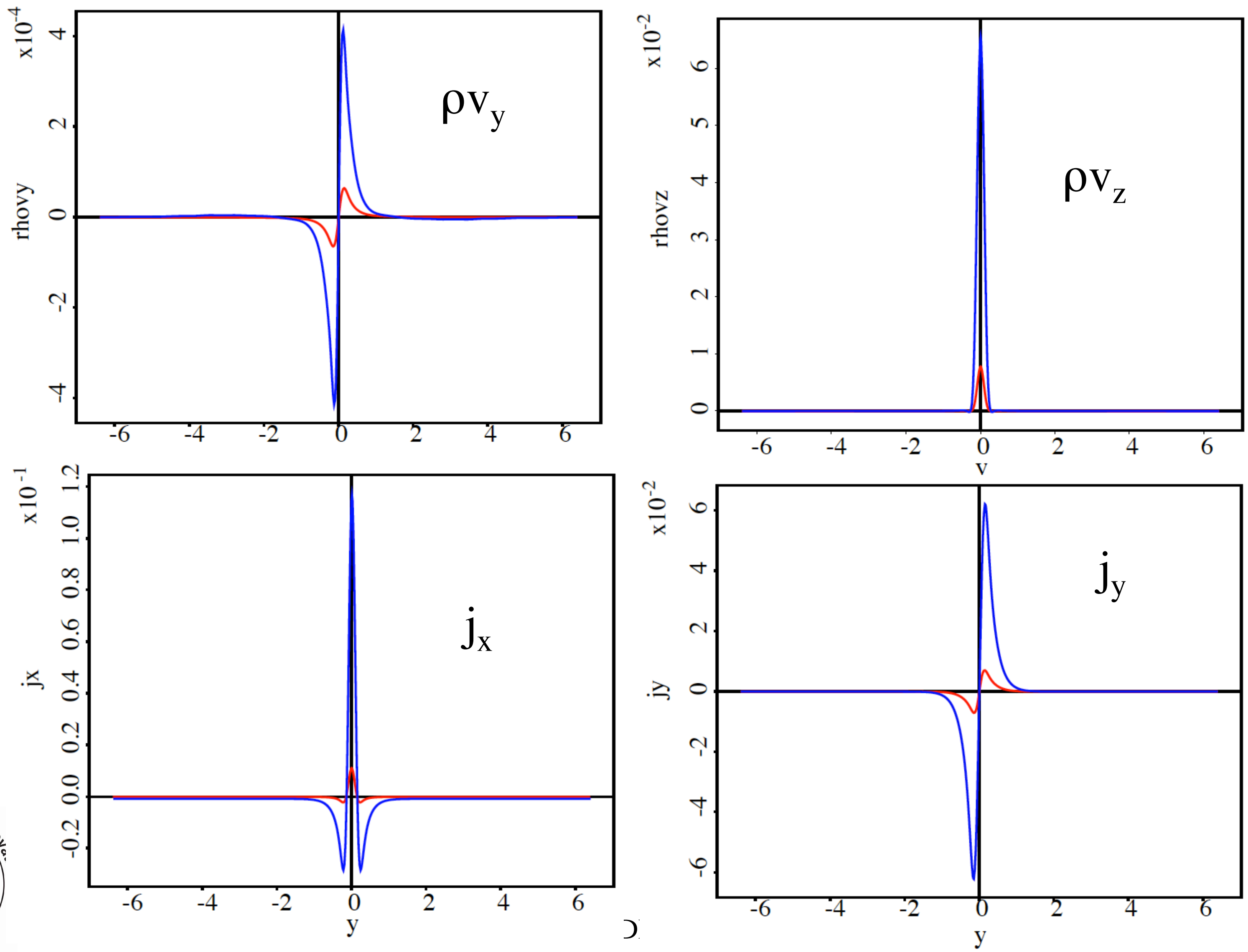
Grid Packing: Graphs



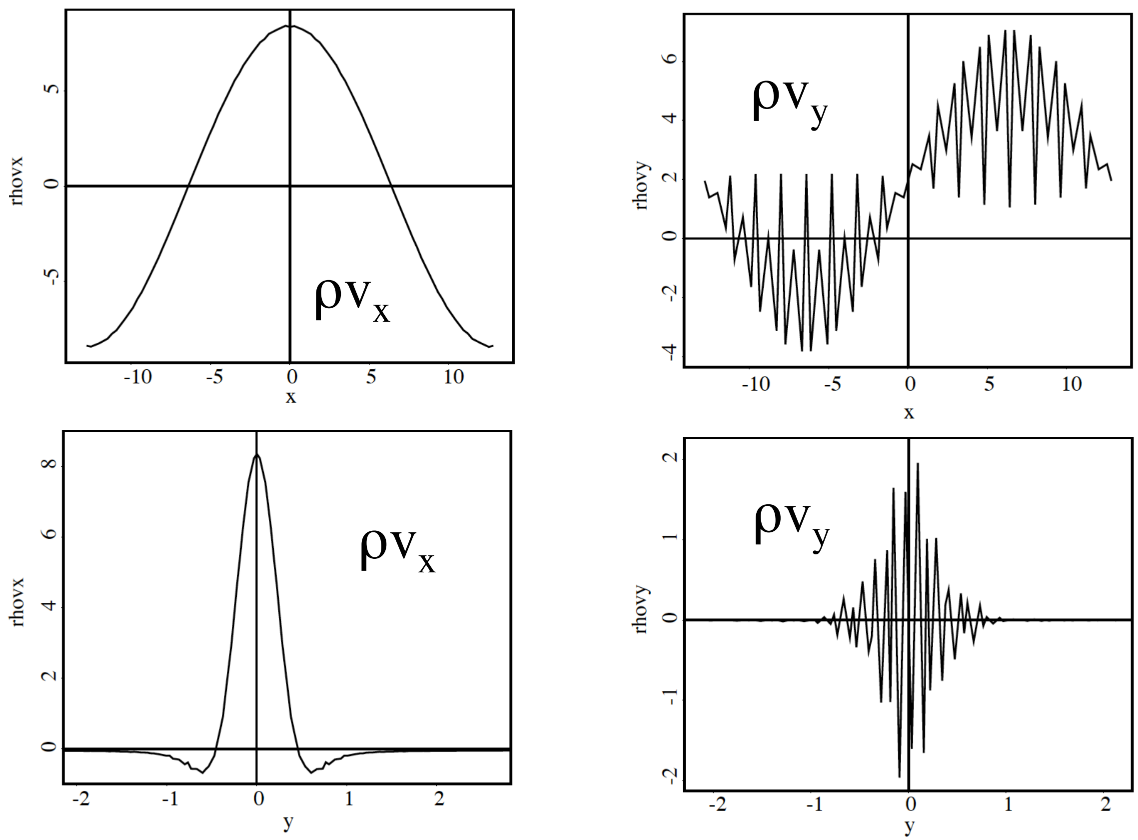
Eigenfunctions



Quiet Start



Cancellation in JxB – grad p Causes Noise



- The noise is in the time derivative *d(rho*vy)/dt* of the component of the momentum normal to the flux surfaces. It is caused by approximate cancellation of the force terms **JxB** – **grad** p.
- The noise inhibits Newton convergence when used with Physics-Based Preconditioning.
- The M3D-C^1 velocity (momentum) representation avoids numerical cancellation by using the curl to annihilate the pressure terms.

M3D-C¹ Representation: Momentum Equation

Cartesian Momentum Representation

$$\rho\mathbf{v} = \nabla_\perp\chi + \nabla z \times \nabla U + \rho v_z \nabla z$$

Annihilators

$$\begin{aligned}
\text{fast}: &\quad \mathbf{L}_1 \cdot \rho\mathbf{v} \equiv \nabla_\perp \cdot \rho\mathbf{v} = \nabla_\perp^2 \chi \\
\text{shear}: &\quad \mathbf{L}_2 \cdot \rho\mathbf{v} \equiv \nabla z \cdot \nabla \times \rho\mathbf{v} = \nabla_\perp^2 U \\
\text{slow}: &\quad \mathbf{L}_3 \cdot \rho\mathbf{v} \equiv \nabla z \cdot \rho\mathbf{v} = \rho v_z
\end{aligned}$$

Vector Momentum Equation

$$\frac{\partial}{\partial t}(\rho\mathbf{v}) + \nabla \cdot \mathsf{T} = \mathbf{J} \times \mathbf{B} - \nabla p, \quad \mathsf{T} \equiv \rho\mathbf{v}\mathbf{v} + \pi = \mathsf{T}^T$$

Scalar Momentum Equations

$$\frac{\partial}{\partial t}\nabla_\perp^2\chi + \nabla_\perp \cdot (\nabla \cdot \mathsf{T}) = \nabla_\perp \cdot (\mathbf{J} \times \mathbf{B} - \nabla p)$$

$$\frac{\partial}{\partial t}\nabla_\perp^2 U + \nabla_\perp \cdot [(\nabla \cdot \mathsf{T}) \times \nabla z] = \nabla_\perp \cdot [(\mathbf{J} \times \mathbf{B}) \times \nabla z]$$

$$\frac{\partial}{\partial t}(\rho v_z) + \nabla z \cdot \nabla \cdot \mathsf{T} = \nabla z \cdot (\mathbf{J} \times \mathbf{B} - \nabla p)$$

M3D-C¹ Representation: Electromagnetic Fields

Cartesian Field Representation

$$\mathbf{A} = \nabla z \times \nabla f + \psi \nabla z - F_0 y \nabla x + \nabla \Lambda, \quad \nabla F_0 = 0, \quad \varphi = 0$$

$$\mathbf{B} = \nabla \times \mathbf{A} = \nabla \psi \times \nabla z - \nabla f' + F \nabla z$$

$$\mathbf{J} = \nabla \times \mathbf{B} = \nabla F \times \nabla z + \nabla \psi' - \nabla^2 \psi \nabla z$$

$$f' \equiv \frac{\partial f}{\partial z}, \quad F \equiv F_0 + \nabla^2 f = F_0 + \nabla_\perp^2 f + f''$$

Annihilators

$$\mathbf{L}_1 \cdot \mathbf{A} \equiv \nabla z \cdot \nabla \times \mathbf{A} = F_0 + \nabla_\perp^2 f$$

$$\mathbf{L}_2 \cdot \mathbf{A} \equiv \nabla z \cdot \mathbf{A} = \psi + \Lambda', \quad \mathbf{L}_3 \cdot \mathbf{A} \equiv \nabla_\perp \cdot \mathbf{A} = \nabla_\perp^2 \Lambda$$

Vector Potential Equation

$$\frac{\partial \mathbf{A}}{\partial t} = \mathbf{v} \times \mathbf{B} - \eta \mathbf{J}$$

Scalar Component Equations

$$\frac{\partial}{\partial t}(F_0 + \nabla_\perp^2 f) = \nabla \cdot [(\mathbf{v} \times \mathbf{B} - \eta \mathbf{J}) \times \nabla z]$$

$$\frac{\partial}{\partial t}(\psi + \Lambda') = \nabla z \cdot (\mathbf{v} \times \mathbf{B} - \eta \mathbf{J})$$

$$\frac{\partial}{\partial t} \nabla_\perp^2 \Lambda = \nabla_\perp \cdot (\mathbf{v} \times \mathbf{B} - \eta \mathbf{J})$$

Density and Pressure Equations

Density Equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial z}(\rho v_z) = -\nabla_\perp^2 \chi$$

Pressure Equation

$$\begin{aligned}
\frac{\partial p}{\partial t} &= -\,\gamma p \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \nabla p \\
&= -\,\nabla \cdot (\gamma p \mathbf{v}) + (\gamma - 1)\mathbf{v} \cdot \nabla p \\
&= -\,\frac{\partial}{\partial z}(\gamma p v_z) - \nabla_\perp \cdot \left(\frac{\gamma p}{\rho} \rho \mathbf{v}\right) + (\gamma - 1)\mathbf{v} \cdot \nabla p
\end{aligned}$$

$$\begin{aligned}
\frac{\partial p}{\partial t} + \frac{\partial}{\partial z}(\gamma p v_z) &= -\frac{\gamma p}{\rho} \nabla_\perp^2 \chi - \rho \mathbf{v} \cdot \nabla_\perp \left(\frac{\gamma p}{\rho}\right) + (\gamma - 1)\mathbf{v} \cdot \nabla p \\
&= \frac{\gamma p}{\rho} \left(\mathbf{v}_\perp \cdot \nabla \rho - \nabla_\perp^2 \chi\right) - \mathbf{v}_\perp \cdot \nabla p + (\gamma - 1) v_z \frac{\partial p}{\partial z}
\end{aligned}$$

Scalar Dependent Variables

Density and Pressure

$$u_1 = \rho, \quad u_2 = p$$

Momentum

$$u_3 = \chi, \quad u_4 = U, \quad u_5 = \rho v_z, \quad u_6 = \nabla_\perp^2 \chi, \quad u_7 = \nabla_\perp^2 U$$

Fields

$$u_8 = f, \quad u_9 = f', \quad u_{10} = f'', \quad u_{11} = \psi, \quad u_{12} = \psi', \quad u_{13} = \Lambda$$

$$u_{14} = \nabla_\perp^2 f, \quad u_{15} = \nabla_\perp^2 \psi, \quad u_{16} = \nabla_\perp^2 \Lambda$$

Stress Tensor

$$u_{17} = T_{11}, \quad u_{18} = T_{20}, \quad u_{19} = T_{33}$$

$$u_{20} = T_{12}, \quad u_{21} = T_{22}, \quad u_{22} = T_{31}$$

Conclusions and Future Work

- For slow-growing instabilities, approximate numerical cancellation in the equation for the flux-normal velocity causes large numerical error.
- The M3D-C1 vector representations for momentum and fields are used to analytically eliminate such cancellations.
- The structure of the HiFi code enables relatively simple adaptation of this representation, modifying only the application module and not the solver.
- The use of C^0 finite elements in HiFi, compared to C^1 elements in M3D-C1, requires the use of auxiliary dependent variables.
- Doubling the number of dependent variables is offset by the use of sparse and iterative solvers and improved convergence.
- Equations have been derived and coded up but not yet fully tested.
- Imitation is the sincerest form of flattery.