Adaptive Mesh Algorithm and GEM benchmark with SEL code.

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CEMM Pre-APS Meeting on October 29th, 2006

SEL Code Features

- High order spectral elements: exponential convergence of spatial truncation error + adaptable grid + parallelization.
- Time step: fully implicit, 2^{nd}-order accurate, Newton iteration, static condensation preconditioning.
- Efficient parallel operation with MPI and PETSc.
- Grid adaptation to concentrate the grid where spatial convergence is the worst + alignment with evolving magnetic field.
- Flux-source form: simple, general problem setup.

Flux-Source Formulation

$$\frac{\partial U^k}{\partial t} + \nabla \cdot \mathbf{F^k} = S^k \quad => \quad \mathcal{J}\frac{\partial U^k}{\partial t} + \frac{\partial}{\partial \xi_i}(\mathcal{J}\mathbf{F^k} \cdot \nabla \xi_i) = \mathcal{J} S^k$$

$$\mathbf{F^k} = \mathbf{F^k}(t, \bar{x}, U^l, U^l_x, U^l_y), \quad S = S(t, \bar{x}, U^l, U^l_x, U^l_y),$$

U^k is a set of dependent variables, $U^k_x \equiv (\partial U^k / \partial x)$,

$\{\xi\}_i = \{\xi, \eta\}$ is an arbitrary (LOGICAL) coordinate system in which calculations are performed: $\{\xi, \eta\} \in [0,1] \times [0,1]$;

$\{x\}_j = \{x, y\}$ is the fixed (PHYSICAL) coordinate system in which fluxes and sources are expressed;

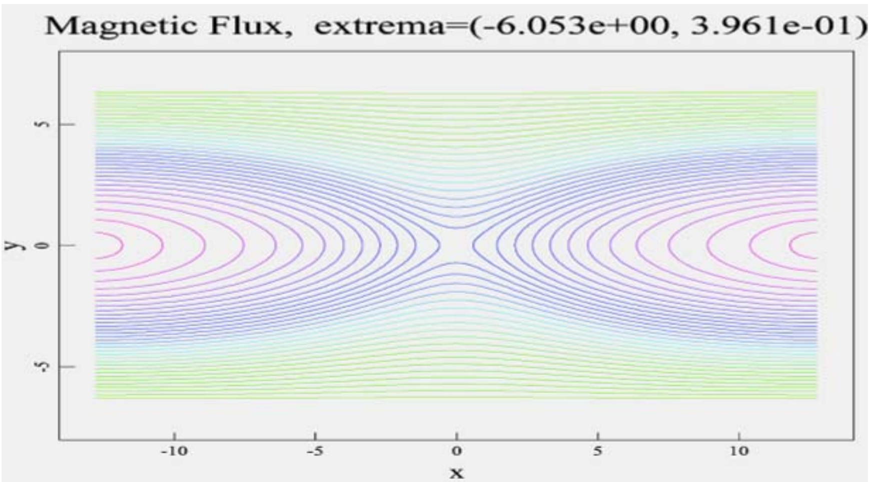
$\mathcal{J}(\xi, \eta) \equiv \frac{(\hat{z} \cdot \nabla x \times \nabla y)}{(\hat{z} \cdot \nabla \xi \times \nabla \eta)}$ is the jacobian of the transformation between the coordinate systems.

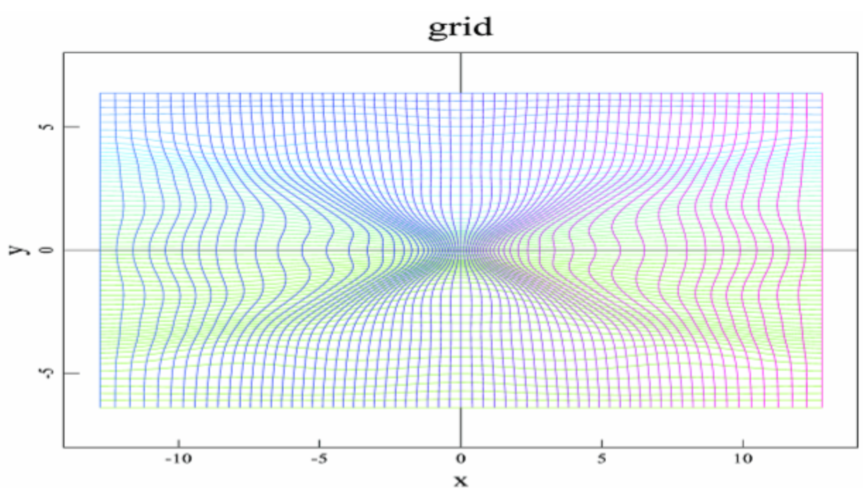
Assume that $x = x(\xi, \eta)$ and $y = y(\xi, \eta)$ are known.
The coordinate transformation is $\nabla \xi_i = (\partial \xi_i / \partial x_j) \nabla x_j$:

$$\nabla \xi = \frac{\partial \xi}{\partial x} \nabla x + \frac{\partial \xi}{\partial y} \nabla y, \qquad \nabla \eta = \frac{\partial \eta}{\partial x} \nabla x + \frac{\partial \eta}{\partial y} \nabla y,$$

Representation on Curvilinear Logically Rectangular Grid

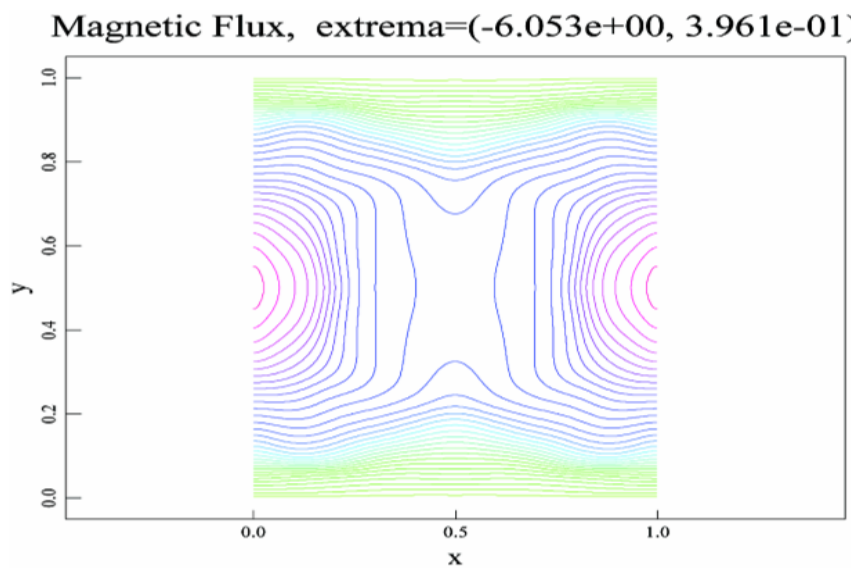
Physical Space





Logical Space

(Uniform Orthogonal Grid)



Harmonic Grid Generation

- Harmonic mapping of a logical grid onto a curvilinear physical grid with some boundaries.
- Usually, but not necessarily, use a conformal structured logical grid of a fixed size.
- Allows for both static and dynamic regrid.
- Implicit or explicit time-stepping.
- Ability to approximately align the physical grid with magnetic field (or achieve any other desired property) within the constraints of a given logical grid topology.

Adaptive Field-Aligned Grid Generation

Variational Principle

$$\mathcal{L} = \frac{1}{2}\int_\Omega \frac{1}{w\sqrt{g}}\mathbf{g} : \nabla\xi^i \nabla\xi^i d\mathbf{x}$$

Euler-Lagrange Equation

$$\nabla \cdot \left(\frac{1}{w\sqrt{g}}\mathbf{g} \cdot \nabla\xi^i \right) = 0$$

Expressed in Logical Coordinates (Chacon)

$$\frac{1}{\mathcal{J}}\frac{\partial}{\partial\xi^j}\left(\frac{\mathcal{J}}{w\sqrt{g}} g^{kl} \frac{\partial\xi^i}{\partial x^k}\frac{\partial\xi^j}{\partial x^l} \right) = 0, \quad \frac{\partial\xi^i}{\partial x^j} \to \frac{\partial x^i}{\partial\xi^j}$$

Metric Tensor Used for Alignment

$$\mathbf{g} = \mathbf{B}_1\mathbf{B}_1 + \mathbf{B}_2\mathbf{B}_2 + \epsilon\mathbf{I}, \quad \mathbf{B}_1 \equiv \hat{\mathbf{z}} \times \nabla\psi, \quad \mathbf{B}_2 = k\hat{\mathbf{z}} \times \mathbf{B}^1$$

- Alignment of the grid is controlled by **g** tensor; Want to have contours of constant ξ^i be parallel to **B** – minimize $\mathbf{B}\cdot\nabla\xi^i$;

- Grid density (adaptation) is controlled by the weight function ω, which is determined from a measure of spatial convergence.

SEL with Static Regrid (adaptation only)

1. a) Smooth initial mapping from logical to physical grid: $x = x(\xi, \eta)$ and $y = y(\xi, \eta)$
   b) Initial condition of the simulation: $U(x, y) \rightarrow U(\xi, \eta) = U_i \alpha_i(\xi, \eta)$

2. Evaluate spatial convergence of the solution in both directions along the logical grid to get two smooth functions of space ($C_\xi(\xi, \eta)$, $C_\eta(\xi, \eta)$).

3. IF MAXVAL(C_ξ, C_η) $\geq G_{tol}$ (ELSE skip to Step (6)):

   a) Rescale ($C_\xi(\xi, \eta)$, $C_\eta(\xi, \eta)$):

$$C_\xi \rightarrow 1 + \Phi * \frac{C_\xi}{MAXVAL(C_\xi, C_\eta)} \qquad C_\eta \rightarrow 1 + \Phi * \frac{C_\eta}{MAXVAL(C_\xi, C_\eta)}$$

   b) Calculate $\omega(\xi, \eta) = \mathrm{MAX}(C_\xi, C_\eta)$ and $\mathbf{g} = \left\{\begin{matrix} C_\xi & 0 \\ 0 & C_\eta \end{matrix}\right\}$

4. Use SEL machinery to solve the Beltrami Equation with given ω and **g** for the "old" logical coordinates {ξ, η} in terms of the "new" {ξ`, η`}.

5. From {ξ(ξ`, η`), η (ξ`, η`)}, {x(ξ, η), y (ξ, η)} and U(ξ, η), we interpolate the physical coordinates {x, y} and the solution vector U onto the new logical grid to find {x(ξ`, η`), y (ξ`, η`)} and U(ξ`, η`).

6. Continue the calculation of the physical problem at hand using the new logical-to-physical grid mapping, reevaluating spatial convergence every time step until MAXVAL(C_ξ, C_η) ≥ Gtol => return to Step 3.

SEL with Static Regrid: Schematic

If $\mathrm{MAXVAL}(C_\xi, C_\eta) \geq G_{tol}$
Calculate $\omega(\xi, \eta)$, and $\mathbf{g}\,(\xi, \eta)$

Solve a system of coupled non-linear "Physics" PDEs

(Ex.: Nonlinear Heat Eq.,
Reduced MHD,
Hall MHD,
Extended 2-fluid MHD, …)

Evaluate (C_ξ, C_η)

Solve Beltrami Eqs.:

In 2D, a system of two coupled PDEs for

$\xi(\xi`, \eta`), \eta\,(\xi`, \eta`)$

Interpolate to find $x(\xi`, \eta`)$, $y\,(\xi`, \eta`)$ and $U(\xi`, \eta`)$.
$(\xi`, \eta`) \rightarrow (\xi, \eta)$

GEM Hall MHD Benchmark:
SEL (vs. NIMROD vs. M3D-C1)

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v_i}) = 0 \tag{1}$$

$$\begin{aligned}\frac{\partial (\rho \mathbf{v_i})}{\partial t} &+ \nabla \cdot \Big[\rho \mathbf{v_i} \mathbf{v_i} + p\bar{\mathbf{I}} + (B^2/2)\bar{\mathbf{I}} - \mathbf{BB} \\ &- \bar{\mu}(\nabla \mathbf{v_i} + \nabla \mathbf{v_i}^T) - \bar{\nu}\nabla(v_{ez}\hat{z})\Big] = 0\end{aligned} \tag{2}$$

$$\mathbf{E} = -\mathbf{v_e} \times \mathbf{B} - \frac{d_i}{\rho}\nabla p_e + \bar{\eta}\mathbf{J} + \frac{d_i}{\rho}\bar{\nu}\nabla^2(v_{ez}\hat{z}) \tag{3}$$

$$\begin{aligned}\frac{1}{\gamma - 1}\frac{\partial p}{\partial t} &+ \nabla \cdot \left(\frac{\gamma}{\gamma - 1} p \mathbf{v_i} - \bar{\kappa_\perp}\nabla_\perp T - \bar{\kappa_{||}}\nabla_{||} T\right) \\ &= \mathbf{v_i} \cdot \nabla p + \bar{\eta}|\mathbf{J}|^2 + \bar{\mu}(\nabla \mathbf{v_i} + \nabla \mathbf{v_i}^T) : \nabla \mathbf{v_i} + \bar{\nu}|\nabla v_{ez}|^2\end{aligned} \tag{4}$$

$$d_i \nabla \times \mathbf{B} = d_i \mathbf{J} = \rho \mathbf{v_i} - \rho \mathbf{v_e} \tag{5}$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} \tag{6}$$

$$p = p_i + p_e = \rho T = \rho(T_i + T_i), \quad \frac{T_e}{T_i} = \alpha = const, \tag{7}$$

Benchmark parameter values:

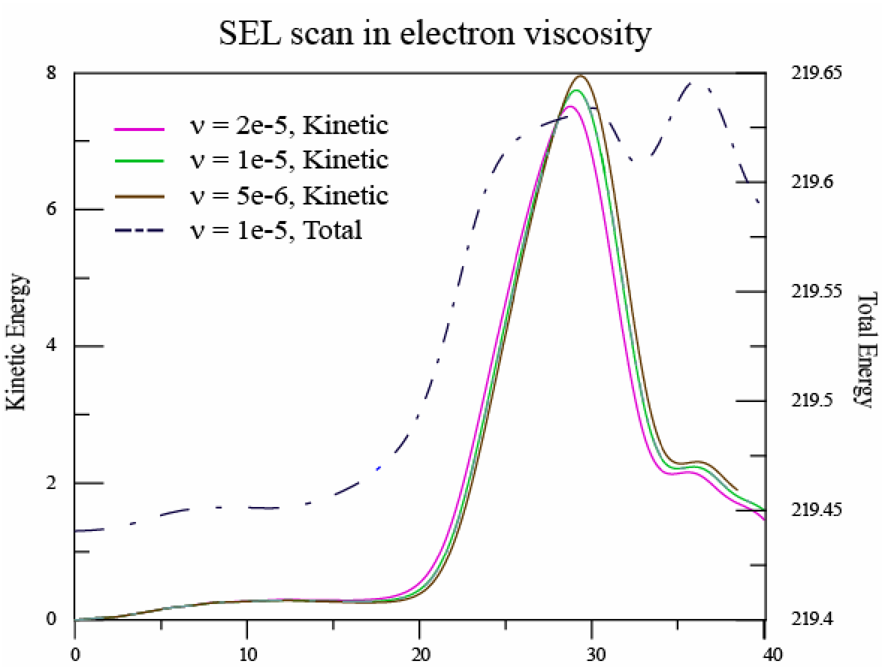
d_i

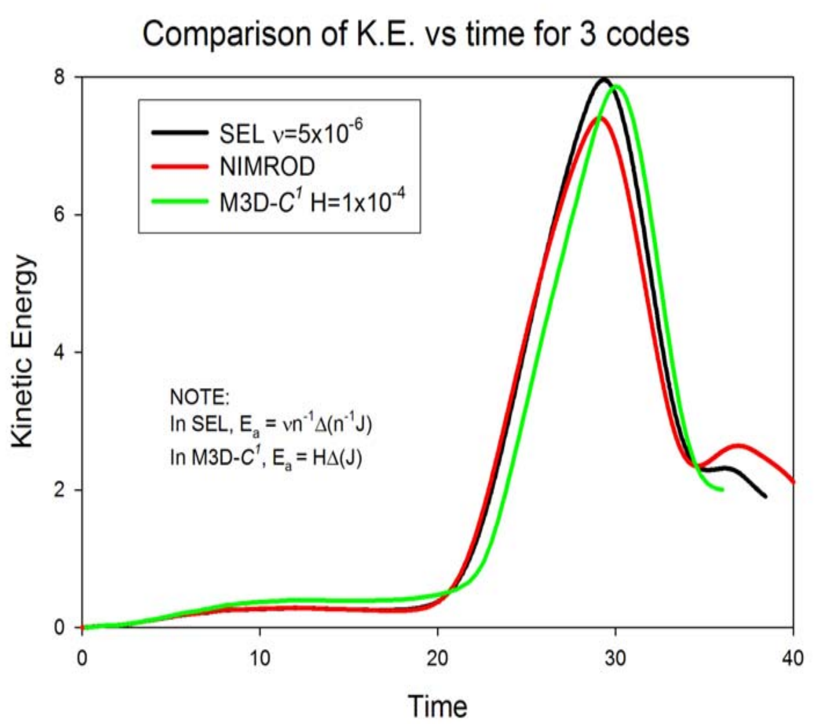
GEM Hall MHD Benchmark

Initial and boundary conditions as in the original GEM challenge
(Birn, *et. al.*, J. Geophys. Res. **106**, 3715 (2001)):

$B_x = B_0 \tanh(y/\lambda)$, $\rho = \rho_0(1/\cosh^2(y/\lambda) + .2)$, $\mathbf{v_i} = 0$, zero guide field, uniform temperature;

$\lambda = d_i/2$; box size: $[lx, ly] = [25.6d_i, 12.8d_i]$, periodic in x, perfectly conducting walls in y.

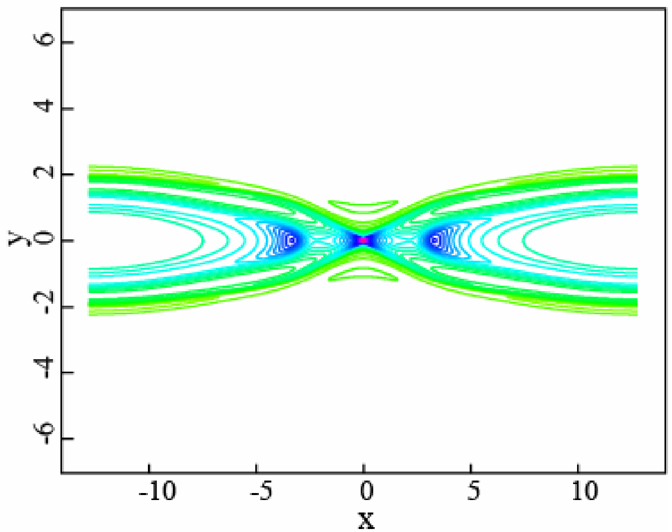




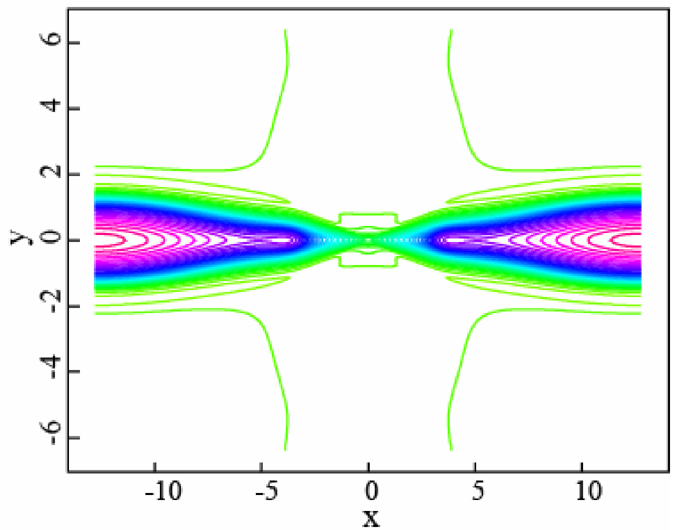
<u>*Comparison results as of late August, 2006.*</u>
(For more on Hall reconnection dependence on electron viscosity,
see poster VP1.00076 on Thursday afternoon)

GEM Hall MHD Benchmark

Electron z-momentum at t = 20.0625



Density at t = 20.0625



<u>$\nu = 1*10^{-5}$</u>

Logical grid:
[nx, ny, np] = [40, 40, 8]

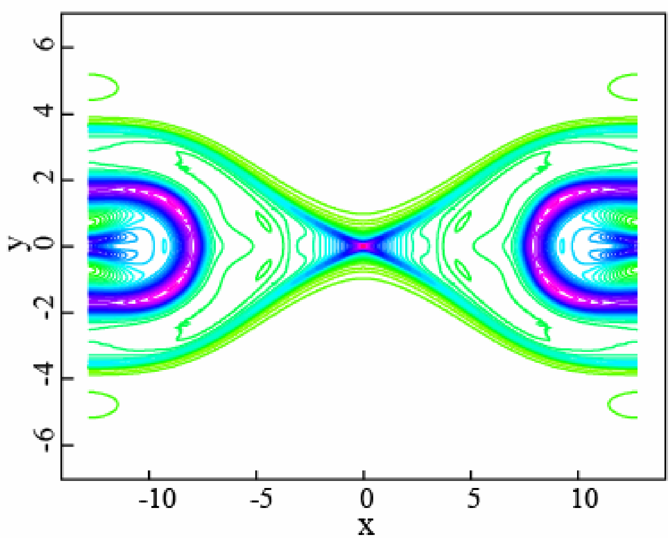
# of time-steps = 419
dt = .0625 → .25

# of grid remappings = 18

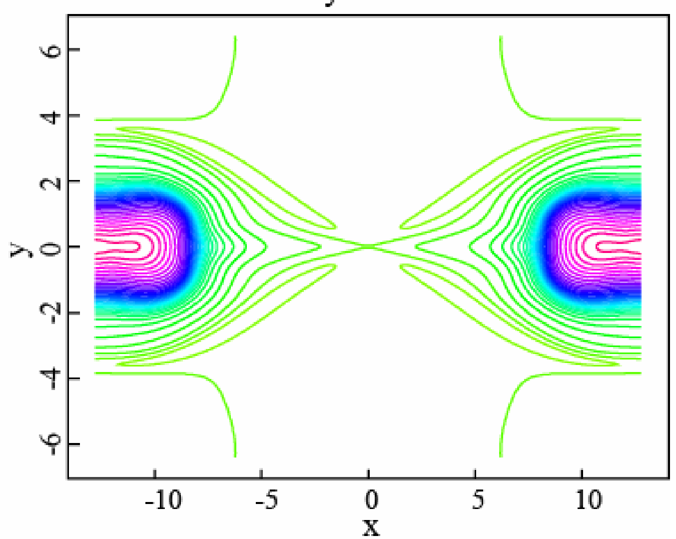
Computed on Bassi
4 nodes × 8 processors

Wallclock time = 9 hours
=> cpu time = 288 hours

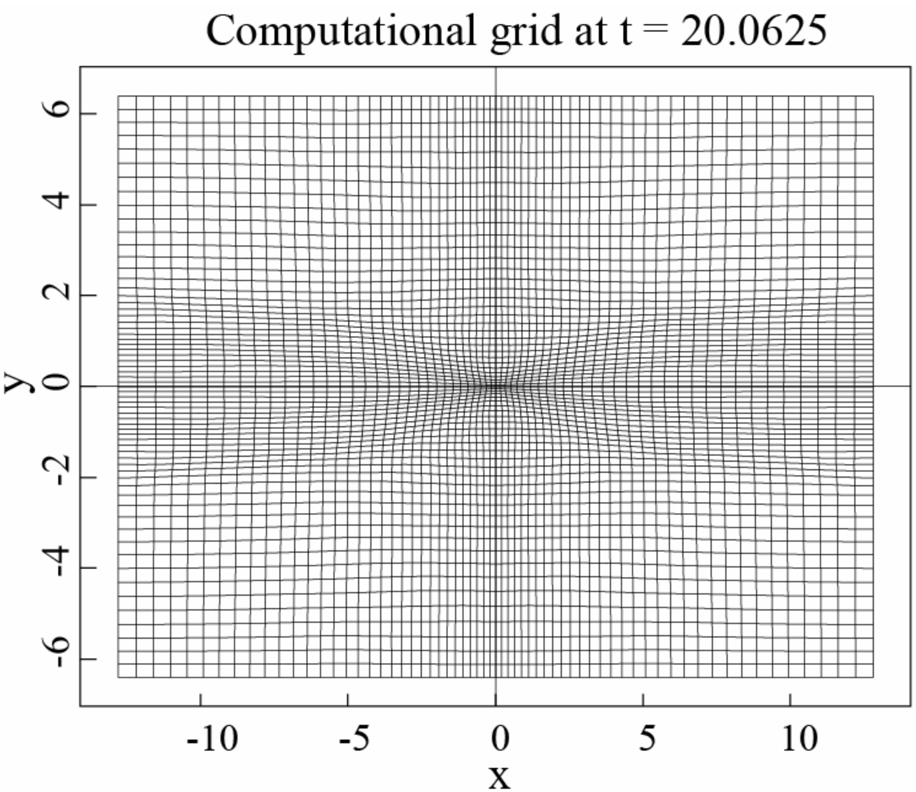
Electron z-momentum at t = 29.125

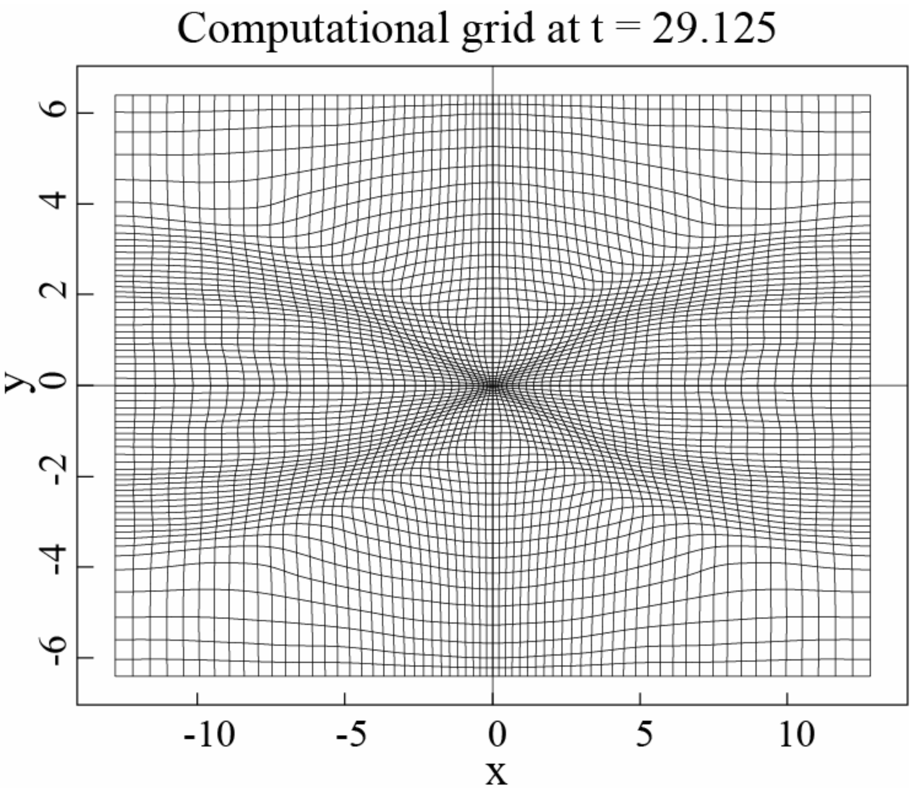


Density at t = 29.125



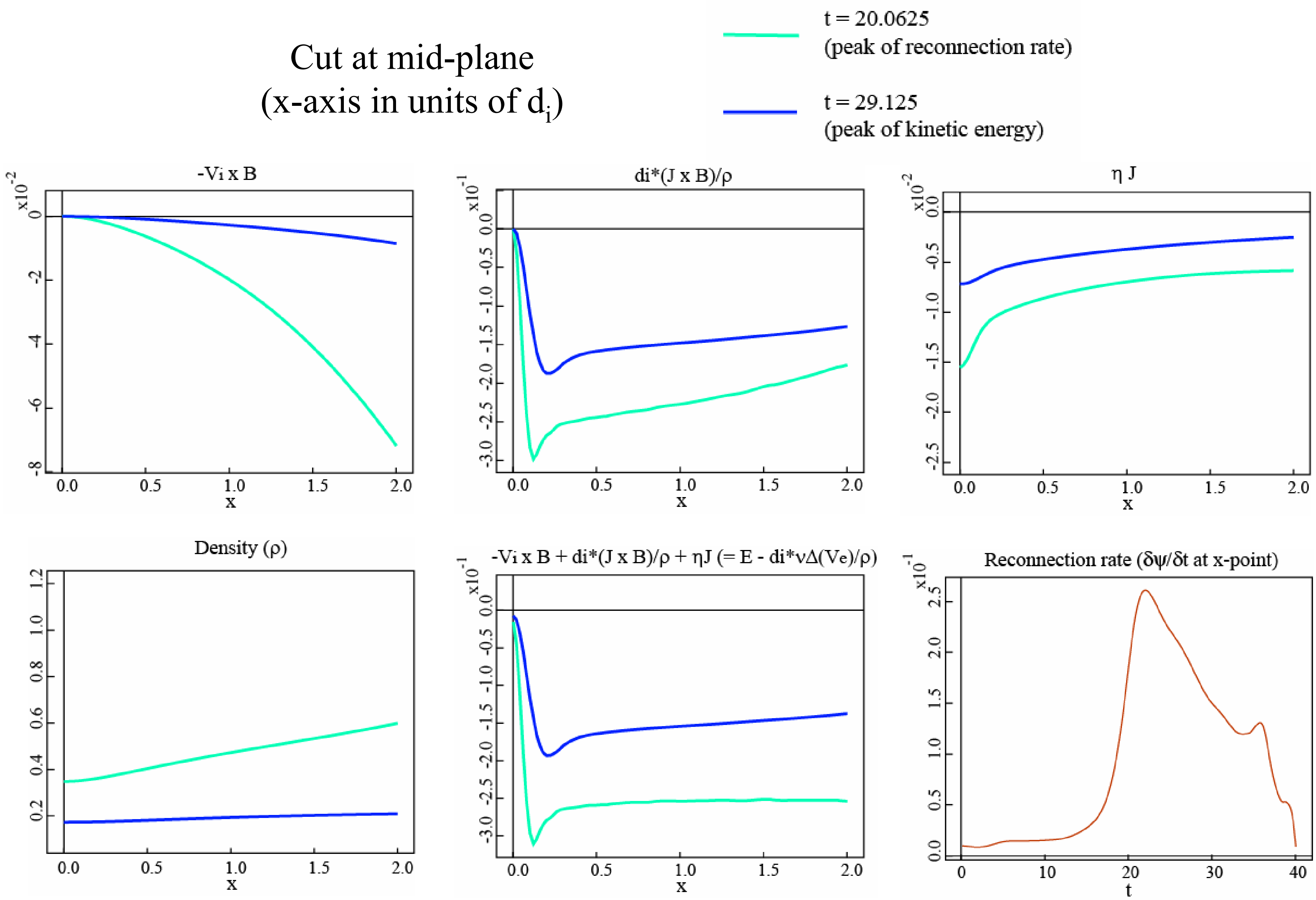
GEM Hall MHD Benchmark





GEM Hall MHD Benchmark

Cut at mid-plane
(x-axis in units of d_i)



Measure of Merit for Static Regrid
(magnetic reconnection in reduced MHD)

Compare several identical simulation runs while varying only the polynomial order **np** of the grid [nx,ny]=[6,16].

np	cpu time	griderr	efficacy	# of regrids	fraction of time for regrid
12	$8.784*10^{4}$ sec	$4.11*10^{-3}$	$2.77*10^{-3}$	0	0
11	$8.774*10^{4}$ sec	$4.69*10^{-4}$	$2.43*10^{-2}$	3	7.4 %
10	$3.544*10^{4}$ sec	$9.26*10^{-4}$	$3.04*10^{-2}$	3	7.8 %
9	$2.49*10^{4}$ sec	$1.01*10^{-3}$	$3.97*10^{-2}$	4	11.3 %
8	$1.696*10^{4}$ sec	$1.53*10^{-3}$	$3.85*10^{-2}$	5	14.7 %

griderr ≡ MAXVAL(C_ξ, C_η); efficacy (“merit”) ≡ 1 / (runtime * griderr)