A Scalable Parallel Extended MHD Solver: Application of Physics-Based Preconditioning to High-Order Spectral Elements

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Scalability of Extended MHD Simulation

- 3D extended MHD modeling of magnetically confined fusion plasmas requires petascale computing: 1 petaflop = 10^{15} flops ~10^5 procs.
- Scalability: doubling problem size and number of processors causes little or no change in cpu time to solution.
- Advanced extended MHD codes use high-order methods of spatial discretization. NIMROD, M3D, HiFi.
- Known scalable methods for elliptic and parabolic systems:
  - Geometric multigrid: Applicable to low-order spatial discretization.
  - Algebraic multigrid: Applicable to high-order spectral elements?
  - FETI-DP: Applicable to SPD problems.
- Extended MHD is dominated by hyperbolic waves, multiple time scales. Physics-based preconditioning. Luis Chacon. Reduces matrix order, increases diagonal dominance.
- Formulation in general flux-source form: solver library, application code.

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Organization of Presentation

- The HiFi spectral element code.
- Physics-based preconditioning; parabolization.
- Approximate Schur complement for visco-resistive MHD.
- Solution procedures for reduced equations.
- Test problem: GEM challenge.
- Scaling results and conclusions.
- Future plans.

HiFi 2D/3D Spectral Element Code

- Flux-source form: simple, general problem setup.
- Spatial discretization:
  - High-order C^0 spectral elements, modal basis
  - Harmonic grid generation, adaptation, alignment
- Time step: fully implicit, 2^{nd}-order accurate,
  - θ-scheme
  - BDF2
- Static condensation, Schur complement.
  - Small local direct solves for grid cell interiors.
  - Preconditioned GMRES for Schur complement.
- Distributed parallel operation with MPI and PETSc.

Spatial Discretization

Flux-Source Form of Equations

$$\frac{\partial u^i}{\partial t} + \nabla \cdot \mathbf{F}^i = S^i$$

$$\mathbf{F}^i = \mathbf{F}^i(t, \mathbf{x}, u^j, \nabla u^j)$$

$$S^i = S^i(t, \mathbf{x}, u^j, \nabla u^j)$$

Galerkin Expansion

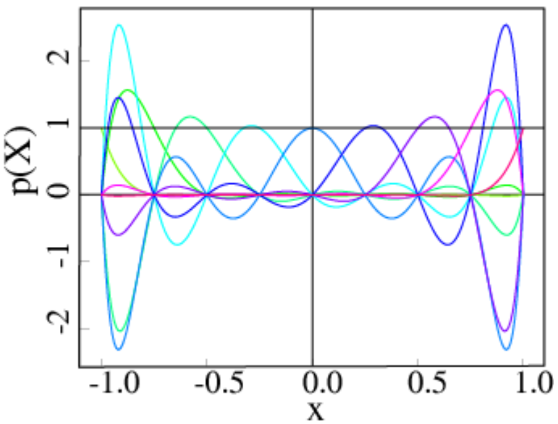
$$u^i(t, \mathbf{x}) \approx \sum_{j=0}^{n} u^i_j(t)\alpha_j(\mathbf{x})$$

Weak Form of Equations

$$(\alpha_i, \alpha_j)\dot{u}^k_j = \int_\Omega d\mathbf{x} \left(S^k \alpha_i + \mathbf{F}^k \cdot \nabla \alpha_i \right) - \int_{\partial\Omega} d\mathbf{x} \alpha_i \mathbf{F}^k \cdot \hat{\mathbf{n}}$$

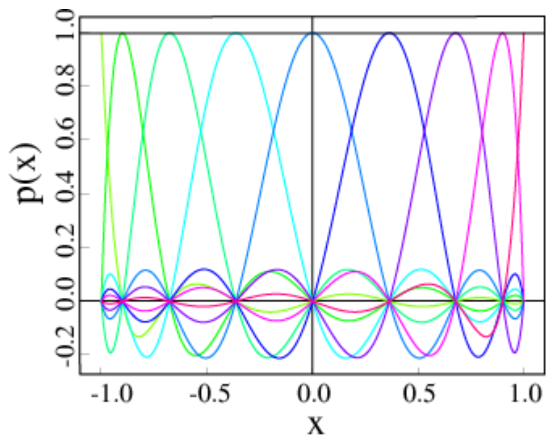
Alternative Polynomial Bases

Uniform Nodal Basis



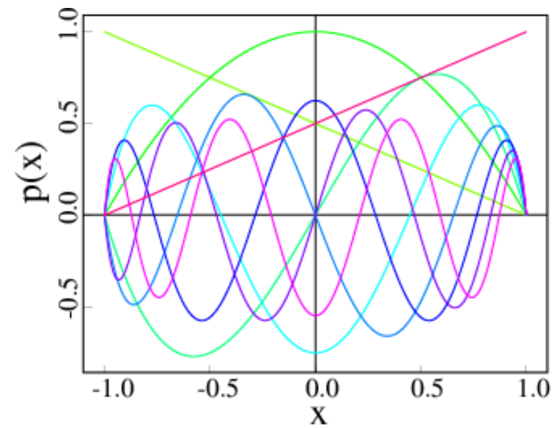
- Lagrange interpolatory polynomials
- Uniformly-spaced nodes
- Diagonally subdominant

Jacobi Nodal Basis



- Lagrange interpolatory polynomials
- Nodes at roots of $(1-x^2)\,P_n^{(0,0)}(x)$
- Diagonally dominant

Spectral (Modal) Basis



- Jacobi polynomials $(1+x)/2$, $(1-x)/2$, $(1-x^2)\,P_n^{(1,1)}(x)$
- Nearly orthogonal
- Manifest exponential convergence

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Implicit Time Discretization: θ-Scheme

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

$$\mathbf{M}\left(\frac{\mathbf{u}^{+} - \mathbf{u}^{-}}{h}\right) = \theta\mathbf{r}^{+} + (1-\theta)\mathbf{r}^{-}$$

$$\mathbf{R}\left(\mathbf{u}^{+}\right) \equiv \mathbf{M}\left(\mathbf{u}^{+} - \mathbf{u}^{-}\right) - h\left[\theta\mathbf{r}^{+} + (1-\theta)\mathbf{r}^{-}\right] \to 0$$

$$\mathbf{J} \equiv \mathbf{M} - h\theta\left\{\frac{\partial r_i^{+}}{\partial u_j^{+}}\right\}$$

$$\mathbf{R}\left(\mathbf{u}^{+}\right) + \mathbf{J}\delta\mathbf{u}^{+} = \mathbf{0}, \quad \delta\mathbf{u}^{+} = -\mathbf{J}^{-1}\mathbf{R}\left(\mathbf{u}^{+}\right), \quad \mathbf{u}^{+} \to \mathbf{u}^{+} + \delta\mathbf{u}^{+}$$

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Physics-Based Preconditioning

Factorization and Schur Complement

Linear System

$$\mathbf{L}\mathbf{u} = \mathbf{r}, \quad \mathbf{L} \equiv \begin{pmatrix} \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix}, \quad \mathbf{r} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{pmatrix}$$

Factorization

$$\mathbf{L} \equiv \begin{pmatrix} \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{L}_{21}\mathbf{L}_{11}^{-1} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{L}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{S} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{L}_{11}^{-1}\mathbf{L}_{12} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}$$

Schur Complement

$$\mathbf{S} \equiv \mathbf{L}_{22} - \mathbf{L}_{21}\mathbf{L}_{11}^{-1}\mathbf{L}_{12}$$

Exact and Approximate Inverse

Preconditioned Krylov Iteration

Inverse

$$\mathbf{L}^{-1} = \begin{pmatrix} \mathbf{I} & -\mathbf{L}_{11}^{-1}\mathbf{L}_{12} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{L}_{11}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{L}_{21}\mathbf{L}_{11}^{-1} & \mathbf{I} \end{pmatrix}$$

Exact Solution

$$\mathbf{s}_1 = \mathbf{L}_{11}^{-1}\mathbf{r}_1, \quad \mathbf{s}_2 = \mathbf{r}_2 - \mathbf{L}_{21}\mathbf{s}_1$$

$$\mathbf{u}_2 = \mathbf{S}^{-1}\mathbf{s}_2, \quad \mathbf{u}_1 = \mathbf{s}_1 - \mathbf{L}_{11}^{-1}\mathbf{L}_{12}\mathbf{u}_2$$

Preconditioned Krylov Iteration

$$\mathbf{P} \approx \mathbf{L}^{-1}, \quad (\mathbf{LP})\left(\mathbf{P}^{-1}\mathbf{u}\right) = \mathbf{r}$$

Outer iteration preserves full nonlinear accuracy.
Need approximate Schur complement **S**
and scalable solution procedure for $\mathbf{L}_{11}$ and **S**.

Visco-Resistive MHD Schur Complement

Visco-Resistive MHD Equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \quad \frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B} - \eta \mathbf{J})$$

$$\frac{\partial p}{\partial t} + \mathbf{v} \cdot \nabla p + \gamma p \nabla \cdot \mathbf{v} = \frac{2}{3} \left(\eta J^2 + \pi : \mathbf{vv} \right) - \frac{2}{3} \nabla \cdot \mathbf{q}$$

$$\frac{\partial}{\partial t} (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{vv} + \pi + \mathsf{T}) = 0$$

$$\mathsf{T} = \left(p + \frac{B^2}{2} \right) \mathsf{I} - \mathbf{BB}, \quad \nabla \cdot \mathsf{T} = \nabla p - \mathbf{J} \times \mathbf{B}$$

Schur Complement

$$\frac{\partial^2}{\partial t^2} (\rho \mathbf{v}) + \nabla \cdot \dot{\mathsf{T}} = \mathbf{s}_2$$

$$\dot{\mathsf{T}} = \dot{\mathsf{T}}^{\dagger} = \left(\mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial t} + \frac{\partial p}{\partial t} \right) \mathsf{I} - \mathbf{B} \frac{\partial \mathbf{B}}{\partial t} - \frac{\partial \mathbf{B}}{\partial t} \mathbf{B}$$
$$= \left[\mathbf{B} \cdot \nabla \times (\mathbf{v} \times \mathbf{B}) - \gamma p \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \nabla p \right] \mathsf{I} - \mathbf{B} \nabla \times (\mathbf{v} \times \mathbf{B}) - \nabla \times (\mathbf{v} \times \mathbf{B}) \mathbf{B}$$

$$\mathsf{S} = \mathsf{M} - h^2 \theta^2 \left\langle \nabla \cdot \dot{\mathsf{T}} \right\rangle, \quad \mathsf{M} = \text{mass matrix}$$

Interchanges order of substitution and discretization
Flux-source form, restores sparseness of matrix.

Scalar Components, General Form

Schur Complement Equation, General Coordinates

$$\frac{\partial^2}{\partial t^2}(\rho \mathbf{v}) + \nabla \cdot \dot{\mathsf{T}} = \mathrm{s}_2$$

$$\frac{\partial^2}{\partial t^2}(\mathcal{J}\rho\mathbf{v}\cdot\nabla x_i) + \frac{\partial}{\partial x_j}\left(\mathcal{J}\dot{\mathsf{T}} : \nabla x_i \nabla x_j\right) = \mathcal{J}\dot{\mathsf{T}} : \nabla\nabla x_i + \mathcal{J}\mathrm{s}_2\cdot\nabla x_i$$

Scalar Components of Stress Tensor

$$\begin{aligned}
\dot{T}_{ij} =& \dot{T}_{ji} \equiv \mathcal{J}\dot{\mathsf{T}} : \nabla x_i \nabla x_j \\
=& \left\{ \frac{1}{2}\epsilon_{klm}\left(\mathcal{J}\mathbf{B}\cdot\nabla x_k \times \nabla x_l\right)\frac{\partial}{\partial x_n} \right. \\
& \quad \left[\left(\mathcal{J}\mathbf{v}\cdot\nabla x_m\right)\left(\mathbf{B}\cdot\nabla x_n\right) - \left(\mathcal{J}\mathbf{v}\cdot\nabla x_n\right)\left(\mathbf{B}\cdot\nabla x_m\right)\right] \\
& \quad \left. -\gamma p\frac{\partial}{\partial x_k}\left(\mathcal{J}\mathbf{v}\cdot\nabla x_k\right) - \left(\mathcal{J}\mathbf{v}\cdot\nabla x_i\right)\frac{\partial p}{\partial x_i}\right\}\left(\nabla x_i\cdot\nabla x_j\right) \\
& - \left(\mathbf{B}\cdot\nabla x_i\right)\frac{\partial}{\partial x_k}\left[\left(\mathcal{J}\mathbf{v}\cdot\nabla x_j\right)\left(\mathbf{B}\cdot\nabla x_k\right) - \left(\mathcal{J}\mathbf{v}\cdot\nabla x_k\right)\left(\mathbf{B}\cdot\nabla x_j\right)\right] \\
& - \left(\mathbf{B}\cdot\nabla x_j\right)\frac{\partial}{\partial x_k}\left[\left(\mathcal{J}\mathbf{v}\cdot\nabla x_i\right)\left(\mathbf{B}\cdot\nabla x_k\right) - \left(\mathcal{J}\mathbf{v}\cdot\nabla x_k\right)\left(\mathbf{B}\cdot\nabla x_i\right)\right]
\end{aligned}$$

General Form of $\dot{T}_{ij}$

$$\dot{T}_{ij} = S_{ijkl}\partial_k\left(\mathcal{J}\mathbf{v}\cdot\nabla x_l\right) + R_{ijk}\left(\mathcal{J}\mathbf{v}\cdot\nabla x_k\right)$$

$$S_{ijkl} \equiv \frac{\partial \dot{T}_{ij}}{\partial\left[\partial_k\left(\mathcal{J}\mathbf{v}\cdot\nabla x_l\right)\right]}, \quad R_{ijk} \equiv \frac{\partial \dot{T}_{ij}}{\partial\left(\mathcal{J}\mathbf{v}\cdot\nabla x_k\right)}$$

Representative Scalar Components

Representative Components of S

$$S_{1111} = (\mathbf{B}\cdot\nabla x_1)(\mathcal{J}\mathbf{B}\cdot\nabla x_2\times\nabla x_3) - \left(B^2+\gamma p\right)$$

$$S_{1122} = 2(\mathbf{B}\cdot\nabla x_1)^2 + (\mathbf{B}\cdot\nabla x_2)(\mathcal{J}\mathbf{B}\cdot\nabla x_3\times\nabla x_1) - \left(B^2+\gamma p\right)$$

$$S_{1121} = (\mathbf{B}\cdot\nabla x_2)\left[(\mathcal{J}\mathbf{B}\cdot\nabla x_2\times\nabla x_3) - 2(\mathbf{B}\cdot\nabla x_1)\right]$$

$$S_{1112} = (\mathbf{B}\cdot\nabla x_1)(\mathcal{J}\mathbf{B}\cdot\nabla x_3\times\nabla x_1), \quad S_{1123} = (\mathbf{B}\cdot\nabla x_2)(\mathcal{J}\mathbf{B}\cdot\nabla x_1\times\nabla x_2)$$

$$S_{1211} = (\mathbf{B}\cdot\nabla x_1)(\mathbf{B}\cdot\nabla x_2), \quad S_{1212} = -(\mathbf{B}\cdot\nabla x_1)^2, \quad S_{1221} = -(\mathbf{B}\cdot\nabla x_2)^2$$

$$S_{1231} = -(\mathbf{B}\cdot\nabla x_2)(\mathbf{B}\cdot\nabla x_3), \quad S_{1213} = 0, \quad S_{1233} = 2(\mathbf{B}\cdot\nabla x_1)(\mathbf{B}\cdot\nabla x_2)$$

Representative Components of R

$$\begin{aligned} R_{111} =& \left[(\mathcal{J}\mathbf{B}\cdot\nabla x_2\times\nabla x_3) - 2(\mathbf{B}\cdot\nabla x_1)\right]\left[\frac{\partial}{\partial x_2}(\mathbf{B}\cdot\nabla x_2) + \frac{\partial}{\partial x_3}(\mathbf{B}\cdot\nabla x_3)\right] \\ & - (\mathcal{J}\mathbf{B}\cdot\nabla x_3\times\nabla x_1)\frac{\partial}{\partial x_1}(\mathbf{B}\cdot\nabla x_2) - (\mathcal{J}\mathbf{B}\cdot\nabla x_1\times\nabla x_2)\frac{\partial}{\partial x_1}(\mathbf{B}\cdot\nabla x_3) - \frac{\partial p}{\partial x_1} \end{aligned}$$

$$\begin{aligned} R_{112} =& (\mathcal{J}\mathbf{B}\cdot\nabla x_3\times\nabla x_1)\left[\frac{\partial}{\partial x_1}(\mathbf{B}\cdot\nabla x_1) + \frac{\partial}{\partial x_3}(\mathbf{B}\cdot\nabla x_3)\right] \\ & - \left[(\mathcal{J}\mathbf{B}\cdot\nabla x_2\times\nabla x_3) - 2(\mathbf{B}\cdot\nabla x_1)\right]\frac{\partial}{\partial x_2}(\mathbf{B}\cdot\nabla x_1) \\ & - (\mathcal{J}\mathbf{B}\cdot\nabla x_1\times\nabla x_2)\frac{\partial}{\partial x_2}(\mathbf{B}\cdot\nabla x_3) - \frac{\partial p}{\partial x_2} \end{aligned}$$

$$R_{121} = -(\mathbf{B}\cdot\nabla x_2)\left[\frac{\partial}{\partial x_2}(\mathbf{B}\cdot\nabla x_2) + \frac{\partial}{\partial x_3}(\mathbf{B}\cdot\nabla x_3)\right] + (\mathbf{B}\cdot\nabla x_1)\frac{\partial}{\partial x_1}(\mathbf{B}\cdot\nabla x_2)$$

$$R_{123} = (\mathbf{B}\cdot\nabla x_1)\frac{\partial}{\partial x_3}(\mathbf{B}\cdot\nabla x_2) + (\mathbf{B}\cdot\nabla x_2)\frac{\partial}{\partial x_3}(\mathbf{B}\cdot\nabla x_1)$$

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Newton-Krylov Solution Procedure

- The full Jacobian **L** is formed, stored, partitioned, and reused until it needs re-evaluation, as indicated by increasing Newton iterations. The approximate Schur complement is formed at this time.
- The residual vector **r** is formed, stored, and partitioned on each NK iteration.
- Physics-based preconditioning requires solving $\mathbf{L}_{11}$, **S**, and $\mathbf{L}_{11}$ again. We solve $\mathbf{L}_{11}$ numerically rather than approximately and analytically.
- Each matrix is reduced by static condensation, eliminating the interior (higher-order) elements in each grid cell in terms of the boundary (linear) elements, using a small, local, direct LAPACK method, leaving a latticework grid to be solved by global distributed parallel methods.
- The latticework matrices are preconditioned with an LU factorization on each processor with additive Schwarz across processors. This is followed by FGMRES on the global matrix.
- The full, nonlinear system is solved with PETSc SNES methods, using matrix-free FGMRES.
- Approximations introduced into the Schur complement affect the number of NK iterations but not the accuracy of the final solution.

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Test Problem: GEM Challenge

Initial Conditions: Harris Sheet + Perturbation

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

Periodic in x, conducting wall in y

$$\psi = -\lambda \ln \cosh\left(\frac{y}{\lambda}\right) - \delta \cos\left(\frac{2\pi x}{l_x}\right) \cos\left(\frac{\pi y}{l_x}\right)$$

$$\mathbf{B} = \hat{\mathbf{e}}_z \times \nabla\psi = \tanh\left(\frac{y}{\lambda}\right) + \delta\mathbf{B}, \quad j_z = \hat{\mathbf{e}}_z \cdot \nabla \times \mathbf{B} = \nabla^2\psi$$

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

Parameters

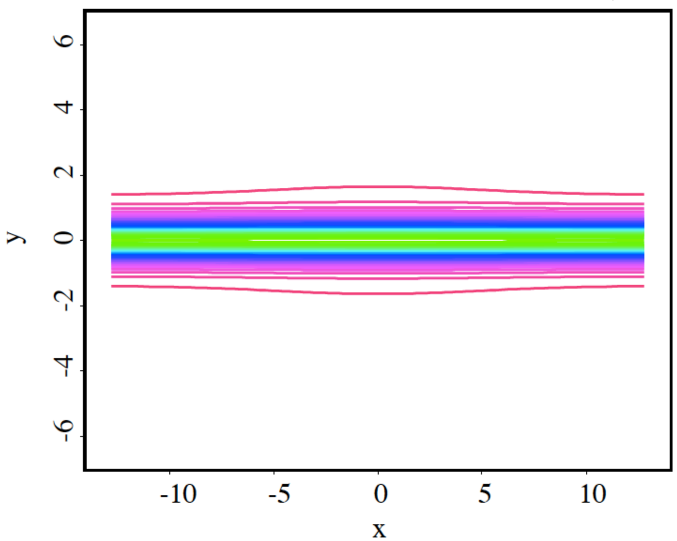
$$l_x = 25.6, \quad l_y = 12.8, \quad ,\lambda = \frac{1}{2}, \quad p_0 = .2, \quad \delta = .1$$

$$\eta = 5 \times 10^{-3}, \quad \mu = 5 \times 10^{-2} \quad \kappa = 2 \times 10^{-2}$$

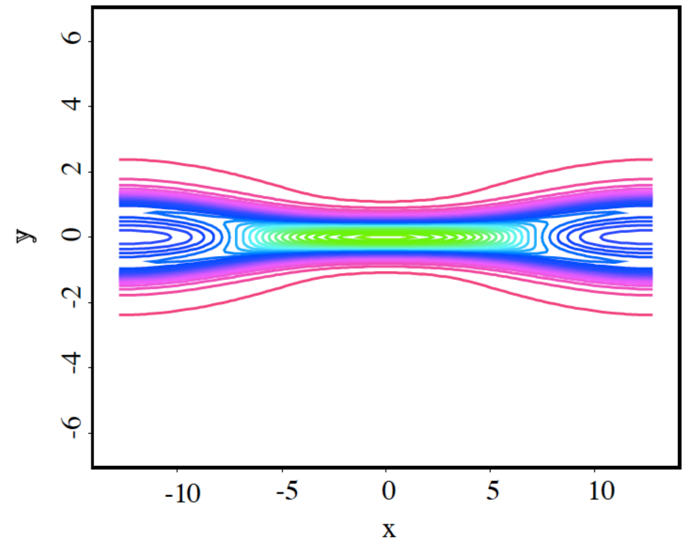
J. Birn *et al*, JGR **106**, A3, 3715-3719 (2001).

Test Problem: GEM Challenge

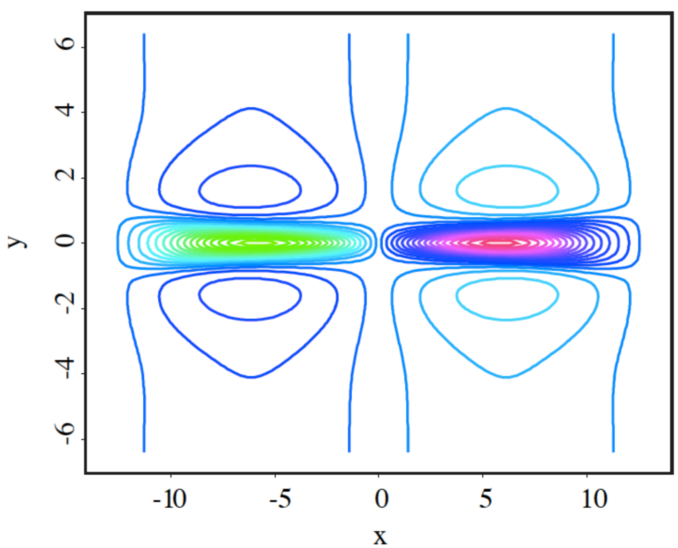
Initial Current Density



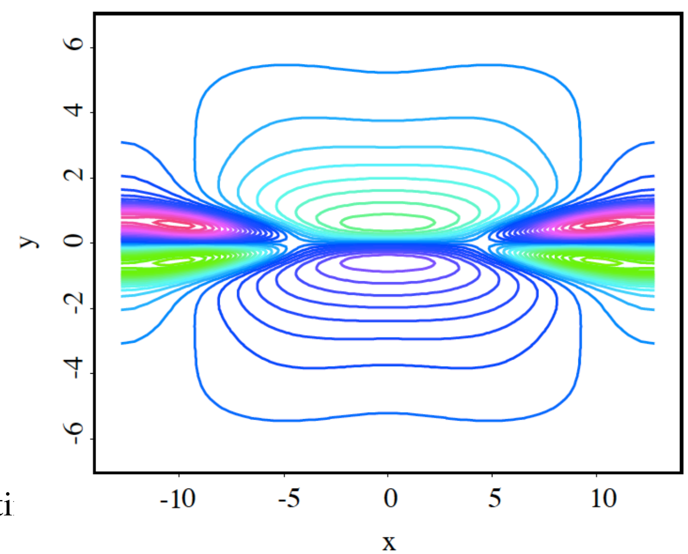
Reconnecting Current Density



X Momentum



Y Momentum



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Weak Scaling Test Results

Size				Physics Based Preconditioning							Full Static Condensation						
				Performance			Ratios				Performance			Ratios			
nx	ny	nproc	cfl	ksp	it	cpu	ksp/it	it/step	cpu/step	cpu/t	ksp	it	cpu	ksp/it	it/step	cpu/step	cpu/t
8	16	16	4	1,508	754	143	2.0	3.8	0.715	3.58	1,478	739	142	2.0	3.7	0.708	3.54
8	32	32	8	3,210	849	160	3.8	4.2	0.799	3.99	2,395	818	190	2.9	4.1	0.952	4.76
16	32	64	8	3,226	853	183	3.8	4.3	0.915	4.58	2,367	813	357	2.9	4.1	1.785	8.93
16	64	128	16	6,106	985	225	6.2	4.9	1.126	5.63	3,367	783	475	4.3	3.9	2.376	11.88
32	64	256	16	6,361	1,024	241	6.2	5.1	1.204	6.02	3,738	860	439	4.3	4.3	2.195	10.98
32	128	512	32	20,060	1,670	457	12.0	8.4	2.285	11.42	6,084	757	670	8.0	3.8	3.350	16.75
64	128	1,024	32	21,563	1,864	508	11.6	9.3	2.538	12.69	8,606	1,084	941	7.9	5.4	4.704	23.52
64	256	2,048	64	50,153	2,377	1,014	21.1	11.9	5.070	25.35	18,667	1,223	1,890	15.3	6.1	9.450	47.25

- All runs performed with 400 fixed time steps to t = 40.0, one Jacobian evaluation, on franklin.nersc.gov Cray XT-4.
- Physics-based preconditioning runs faster than full static condensation because of reduced matrix orders, indicating accuracy of approximate Schur complement.
- CPU time increases because of increasing Krylov iterations with increasing CFL, showing need for improved underlying solution procedure, *e.g.* Algebraic MultiGrid.
- Parabolization of Schur complement makes it diagonally dominant, as required by AMG, unlike full static condensation.
- Preliminary tests with Hypre/BoomerAMG scale well up to nproc = 32, then fail, for reasons not yet understood.

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Future Plans

- Algebraic multigrid will be further investigated to enable true parallel scalability for reduced, diagonally dominant matrices $\mathbf{L}_{11}$ and **S**,
  - BoomerAMG, Hypre, and PETSc libraries.
  - Spectral element multigrid
- Approximate Schur complement matrix will be developed for two-fluid effects, e.g. Hall term, gyroviscosity.
- 3D: HiFi and other codes. Since physics-based preconditioning involves physical rather than geometric decomposition, and doesn't require large memory, extension to 3D should be straightforward. Scalable memory usage makes direct extension to 3D feasible.
- Application to other extended MHD codes, e.g. M3D-C^1.