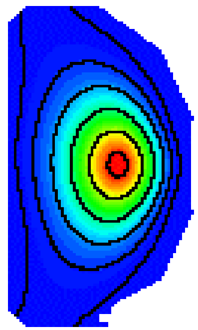
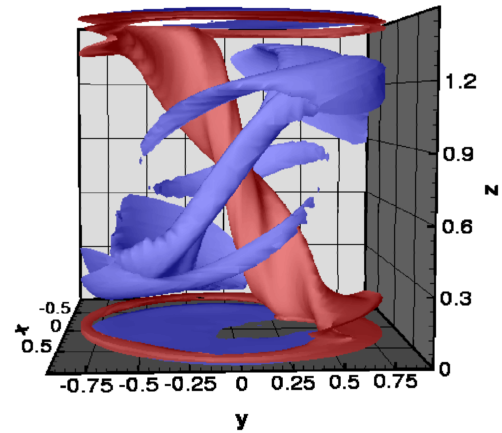
NIMROD and the Application of Conforming Finite Elements to Nonlinear MFE Simulations





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Theme: The finite element approach provides accuracy and flexibility to nonlinear magnetofluid modeling, as shown by NIMROD computations, but it also introduces a few significant numerical considerations.

I. Introduction: equations, targeted physics, and geometric flexibility

II. Numerical ingredients: variational spatial discretization and a semi-implicit advance

III. Resulting convergence properties

IV. Issues for MHD: magnetic divergence control, compressional flow, and matrix condition numbers

V. Conclusions and Directions for NIMROD

While the goal of NIMROD is two-fluid modeling with kinetic closure effects, nonideal MHD forms a basis for the algorithm.

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \kappa_{divb} \nabla\nabla \cdot \mathbf{B}$$

$$\mathbf{E} = -\mathbf{V} \times \mathbf{B} + \eta \mathbf{J}$$

$$\mu_0 \mathbf{J} = \nabla \times \mathbf{B}$$

$$\frac{\partial n}{\partial t} + \nabla \cdot \left(n\mathbf{V} \right) = \nabla \cdot D \nabla n$$

$$\rho \left(\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) = \mathbf{J} \times \mathbf{B} - \nabla p + \nabla \cdot \nu \rho \nabla \mathbf{V}$$

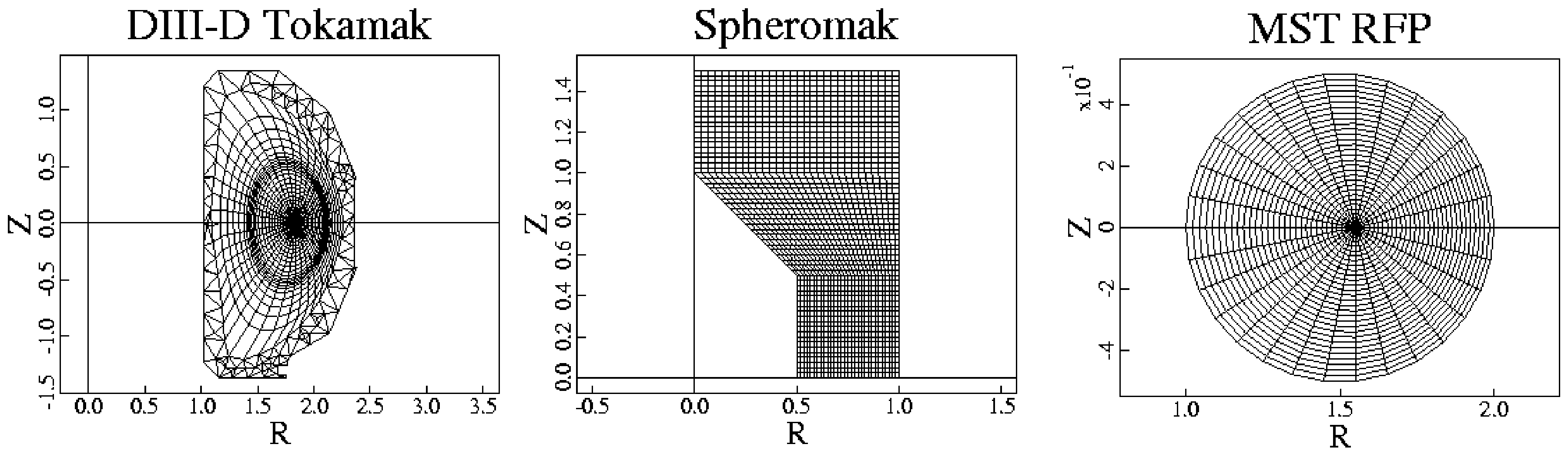
$$\frac{n}{\gamma - 1} \left(\frac{\partial T}{\partial t} + \mathbf{V} \cdot \nabla T \right) = -p \nabla \cdot \mathbf{V} + \nabla \cdot n \left[\left(\chi_{||} - \chi_{\perp} \right) \hat{\mathbf{b}}\hat{\mathbf{b}} + \chi_{\perp} \mathbf{I} \right] \cdot \nabla T + Q$$

- System is of higher-order than ideal MHD.
- Density and magnetic-divergence diffusion are for numerical purposes.

- Physics simulation objectives of the NIMROD project focus on the nonlinear evolution of global electromagnetic modes in realistic geometry.
  - Tearing behavior in tokamaks
  - Magnetic relaxation physics in alternates
  - Disruptive instabilities
- Conditions of interest possess two properties that pose great challenges to numerical approaches—anisotropy and stiffness.
  - Anisotropy produces subtle balances of large forces, nearly singular behavior at rational surfaces, and vastly different parallel and perpendicular transport properties.
  - Stiffness reflects the vast range of time-scales in the system, and targeted physics is slow (~transport scale).

The finite element method provides an approach to spatial discretization that has the needed flexibility and accuracy.

NIMROD uses 2D finite elements for the poloidal plane and finite Fourier series for the periodic direction, which may be toroidal, azimuthal, or a periodic linear coordinate.



If each step of a time-advance can be put into variational form, we can use standard finite element analysis to understand spatial convergence rates. [a la Strang and Fix:]

- The 'strain energy' norm for each equation satisfies:

$$a\left(u-u^h, u-u^h\right) \le C^2 h^{2(k-1)} |u|_k^2$$

The inner product $a(u,v)$ is defined by implicit terms in each equation, h is a measure of (possibly nonuniform) mesh spacing, u^h is the finite element solution for basis functions of degree k-1.

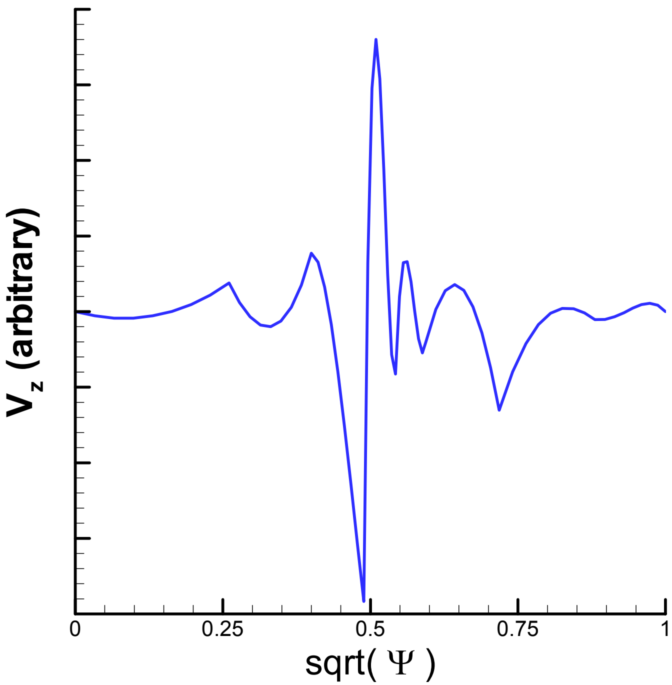
- Relating norms leads to convergence estimates based on Taylor expansion; convergence properties then result from the selection of the space.

$$\left|u-u^h\right|_0 \le C_0 h^k |u|_k \qquad \left|u-u^h\right|_1 \le C_1 h^{k-1} |u|_k$$

The dissipation terms in nonideal MHD require more continuity in the solution space than does ideal MHD in order for a solution space to be admissible in variational problems resulting from the time-advance.

- Admissible means all terms in the weak form are integrable.
- We have not considered nonconforming approximations.

- NIMROD uses a general implementation where the possible solution spaces have function-value continuity at element boundaries, but derivatives may be discontinuous.



The semi-implicit method provides a time-advance that works well for our applications. [Schnack JCP, 1987]

- When resolving resistive nonlinear behavior in time, the stiffness results primarily from the linear terms.

- The treatment of the linear stiffness is the most important aspect for temporal convergence at large time-step.

The semi-implicit algorithm leads to a set of self-adjoint elliptic PDEs for the time advance. [Positive eigenvalues are also assured for all reasonable time-steps.]

- These characteristics allow the variational approach to spatial discretization for each advance.

- The finite element formulation maintains symmetry by construction—matrices are Hermitian positive definite.

Detail The differential approximation for an implicit time advance for ideal linear MHD with arbitrary time centering θ is:

$$\rho\frac{\partial \mathbf{V}}{\partial t}-\theta\,\Delta t\left[\frac{1}{\mu_0}\left(\nabla\times\frac{\partial \mathbf{B}}{\partial t}\right)\times\mathbf{B}_0+\mathbf{J}_0\times\frac{\partial \mathbf{B}}{\partial t}-\nabla\frac{\partial p}{\partial t}\right]=\frac{1}{\mu_0}(\nabla\times\mathbf{B})\times\mathbf{B}_0+\mathbf{J}_0\times\mathbf{B}-\nabla p$$

$$\frac{\partial \mathbf{B}}{\partial t}-\theta\,\Delta t\nabla\times\left(\frac{\partial \mathbf{V}}{\partial t}\times\mathbf{B}_0\right)=\nabla\times(\mathbf{V}\times\mathbf{B}_0)$$

$$\frac{\partial p}{\partial t}+\theta\,\Delta t\left(\frac{\partial \mathbf{V}}{\partial t}\cdot\nabla p_0+\gamma p_0\nabla\cdot\frac{\partial \mathbf{V}}{\partial t}\right)=-(\mathbf{V}\cdot\nabla p_0+\gamma p_0\nabla\cdot\mathbf{V})$$

Using the alternative differential approximation to the resulting wave equation leads to

$$\rho\frac{\partial \mathbf{V}}{\partial t}-\theta^2\Delta t^2\mathbf{L}(\partial\mathbf{V}/\partial t)=\frac{1}{\mu_0}(\nabla\times\mathbf{B})\times\mathbf{B}_0+\mathbf{J}_0\times\mathbf{B}-\nabla p+2\theta\Delta t\mathbf{L}(\mathbf{V})$$

$$\frac{\partial \mathbf{B}}{\partial t}=\nabla\times(\mathbf{V}\times\mathbf{B}_0)$$

$$\frac{\partial p}{\partial t}=-(\mathbf{V}\cdot\nabla p_0+\gamma p_0\nabla\cdot\mathbf{V})$$

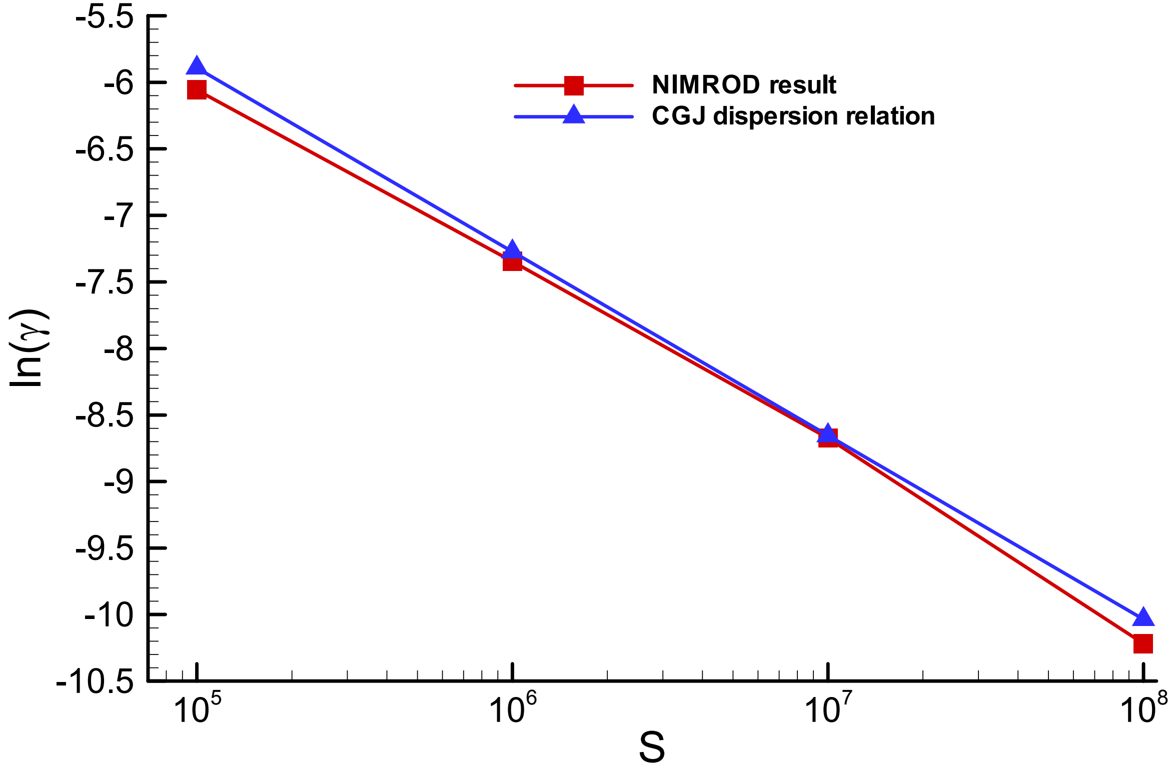
where $\mathbf{L}$ is the ideal MHD force operator. We may drop the Δt term on the rhs to avoid numerical dissipation and arrive at a semi-implicit advance stable for all Δt where $\mathbf{V}$ is leap-frogged with $\mathbf{B}$ and p.

The NIMROD semi-implicit operator is based on the (self-adjoint) linear ideal MHD force operator plus a Laplacian with a small coefficient, like what is in XTOR [Lerbinger and Luciani, JCP '91]. However, performance on nonlinear problems is improved by

- Relaxing the definition of the 'equilibrium' fields to include the time-evolving, toroidally symmetric solution. [The finite element construction allows explicit symmetrization.]

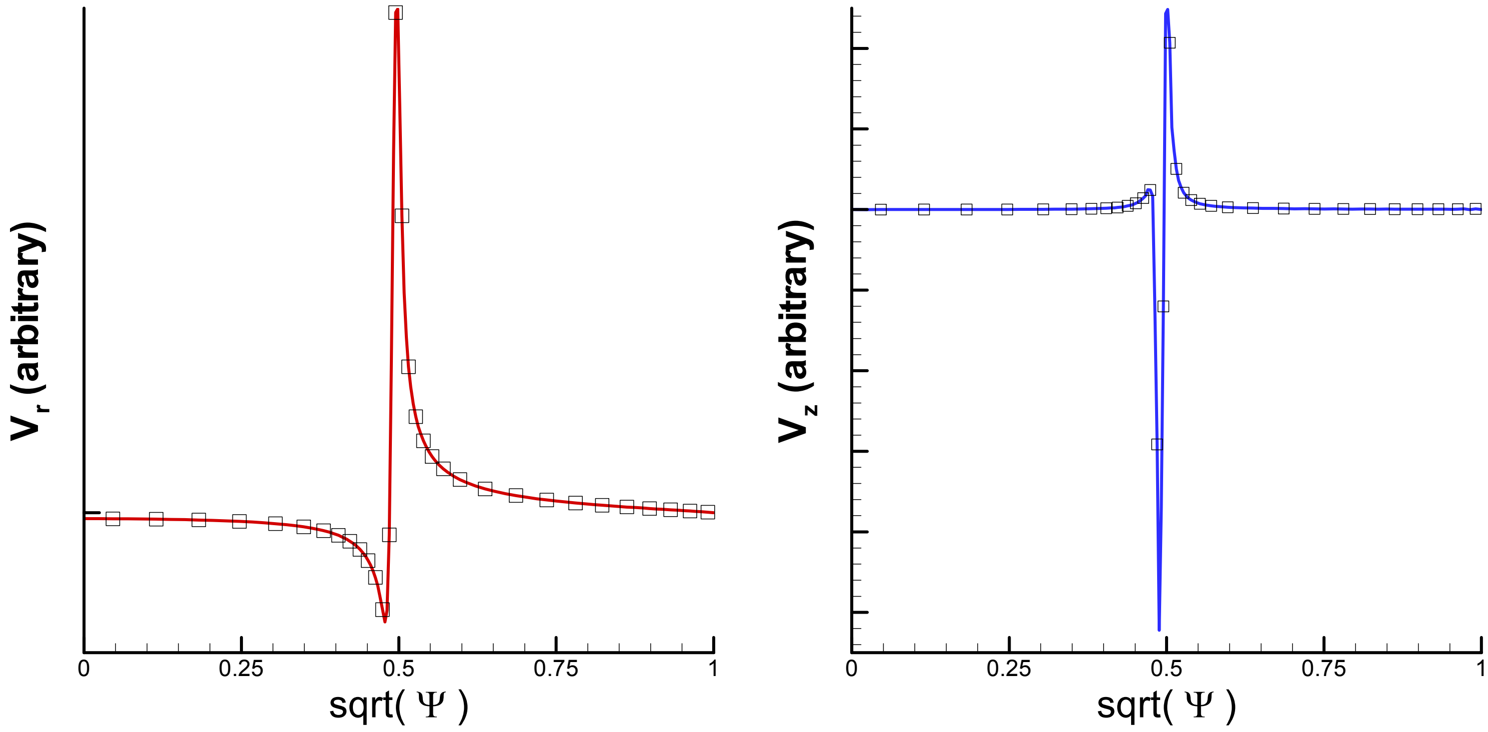
- The coefficient for the Laplacian is updated dynamically to ensure stability in evolving nonlinear states.

A linear resistive tearing study in a periodic cylinder shows that asymptotic growth rate scaling and nearly singular behavior can be reproduced with packed finite elements and a large time-step.



The equilibrium is a paramagnetic pinch, Pm=10^{-3}. S=10^8 is not resolved.

The computed eigenfunctions illustrate how strong mesh packing can be used to represent a tearing layer efficiently.



• This $S=10^6$ computation has a 32x32 mesh of bicubic elements and $\Delta t=100\tau_A$ (1.8×10^5 times explicit). γ is within 2%.

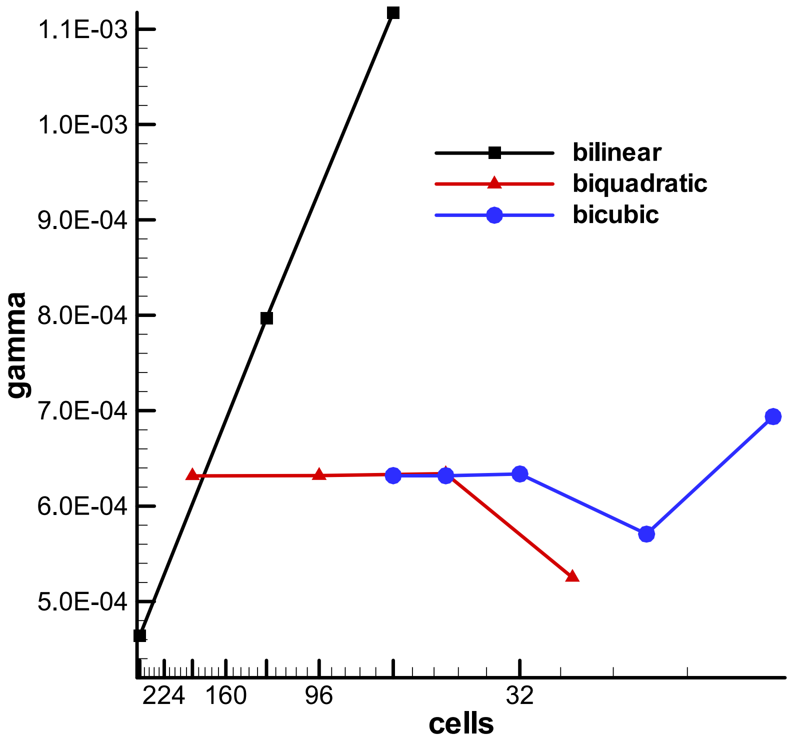
Detail Mesh packing for circular tearing modes:

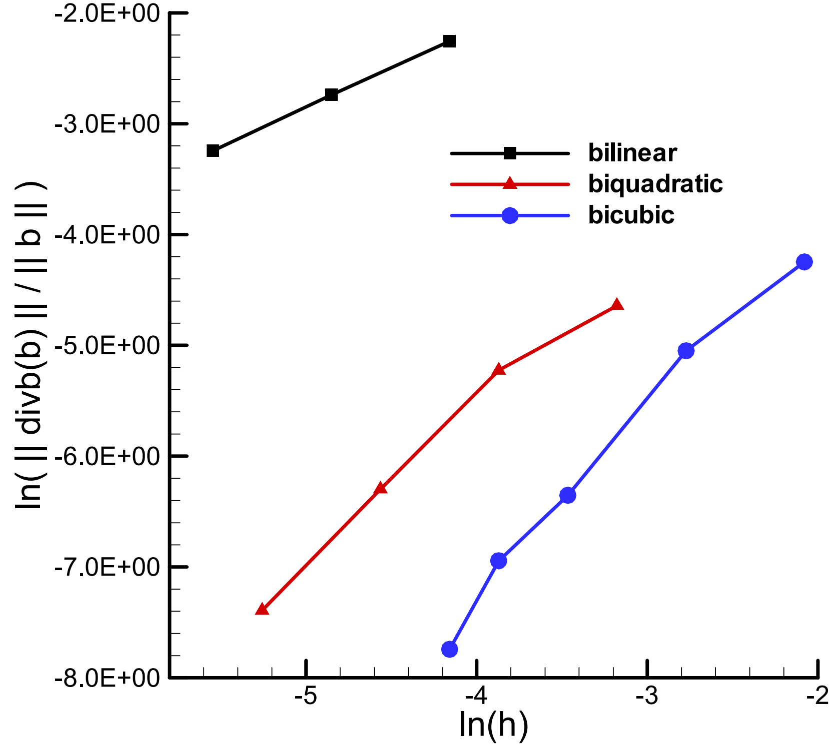
- Determine equilibrium on a uniform mesh.
- Find a cumulative distribution function with density weighting near rational surfaces.

$$f_{\mathrm{i}} = \sum_{\mathrm{j}=1}^{\mathrm{j}=\mathrm{i}} 1 + A_p \exp\left\{ -\frac{\left[q(r_{\mathrm{j}}) - q(r_s)\right]^2}{W_p^2\left[q(0) - q(a)\right]^2} \right\}$$

- Partition distribution function equally.
- Find new mesh locations by interpolating uniform partitioning back to radii associated with initial grid.

Accuracy while varying the mesh and degree of polynomial basis functions meets expectations for biquadratic and bicubic elements.





- Divergence errors are too large with bilinear elements for these $S=10^6$ conditions and the numerical parameters.

Thermal conduction also exercises spatial accuracy for realistic ratios of thermal conductivity coefficients (~10^9).

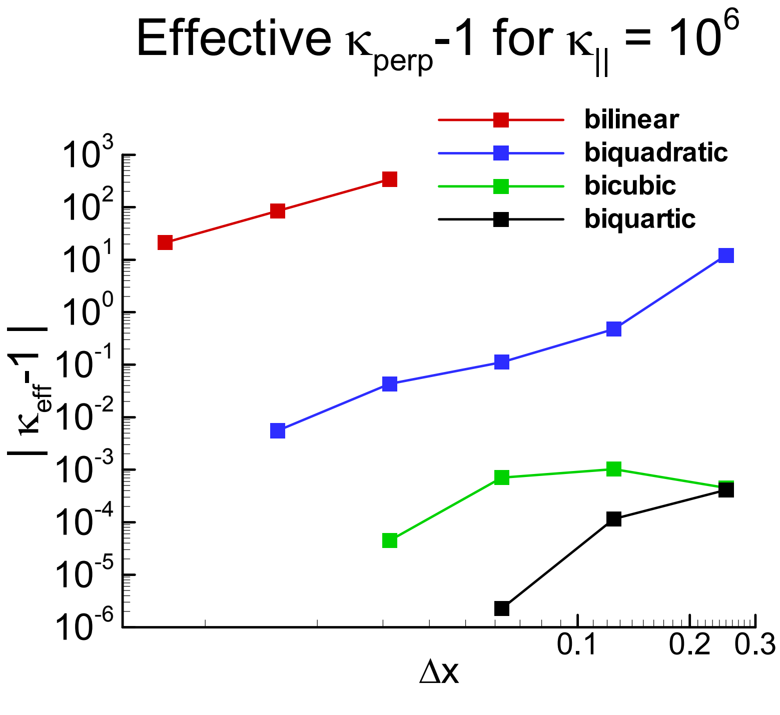
- Adaptive meshing alone cannot provide the needed accuracy in nonlinear 3D simulations; magnetic topology changes across islands and stochastic regions.

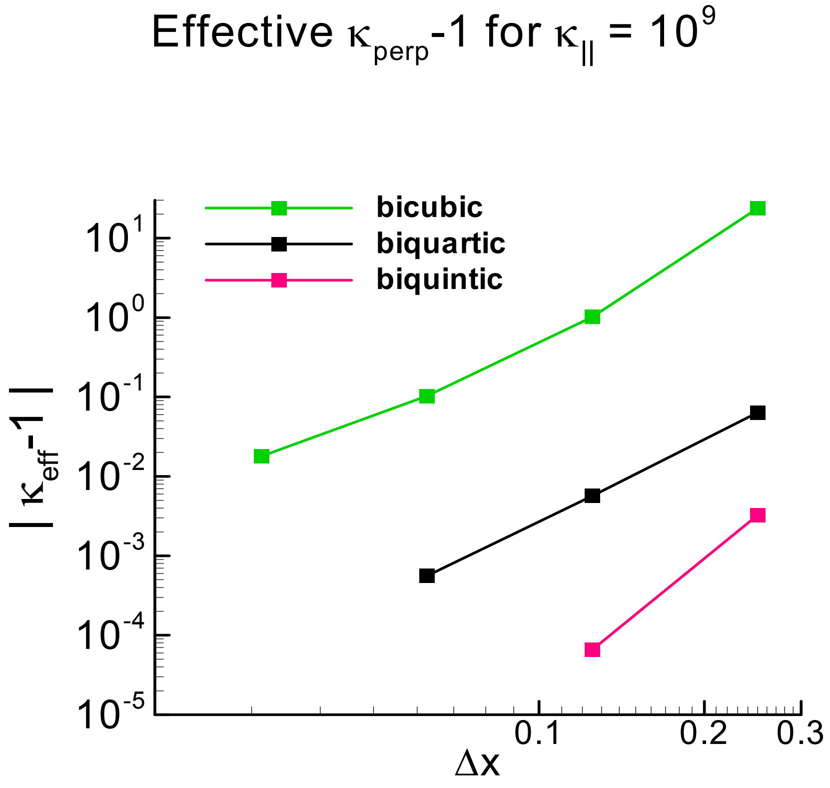
- High-order finite elements provide a solution.

A simple but revealing quantitative test is a box, 1m on a side, with source functions to drive the lowest eigenmode, $\cos(\pi x)\cos(\pi y)$, in $T(x,y)$ and $J_z(x,y)$. Mass density is large to keep **V** negligible.

- Analytic solution is independent of $\chi_{\|}$, $T(x,y) = \chi_{\perp}^{-1}\cos(\pi x)\cos(\pi y)$
- Computed $T^{-1}(0,0)$ measure effective cross-field conductivity.
- Any simple rectangular mesh has poor alignment.

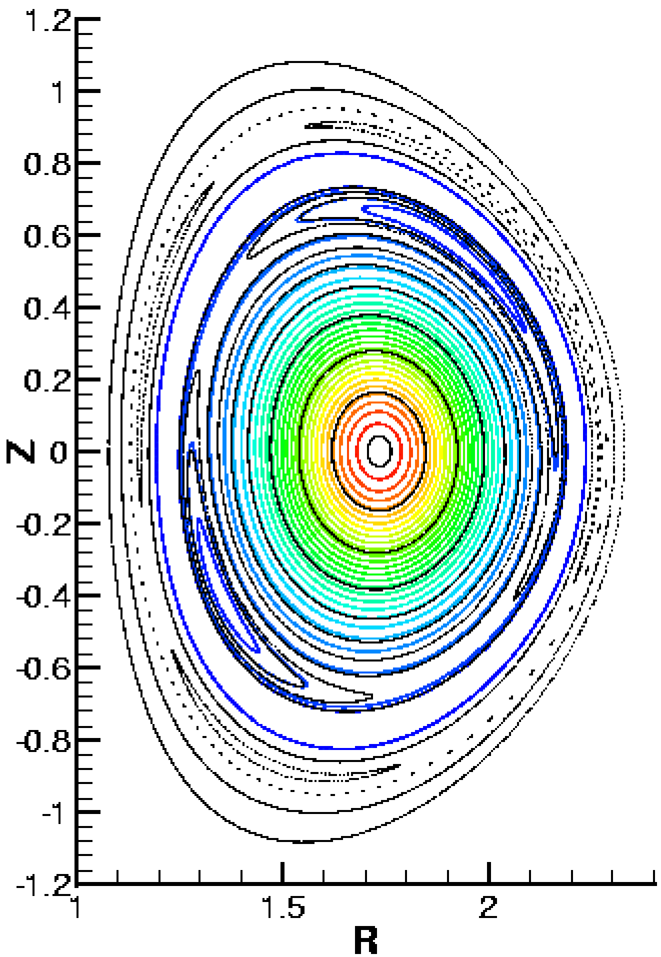
Convergence of the steady state solution shows that even bicubic elements are sufficiently accurate for realistic parameters.

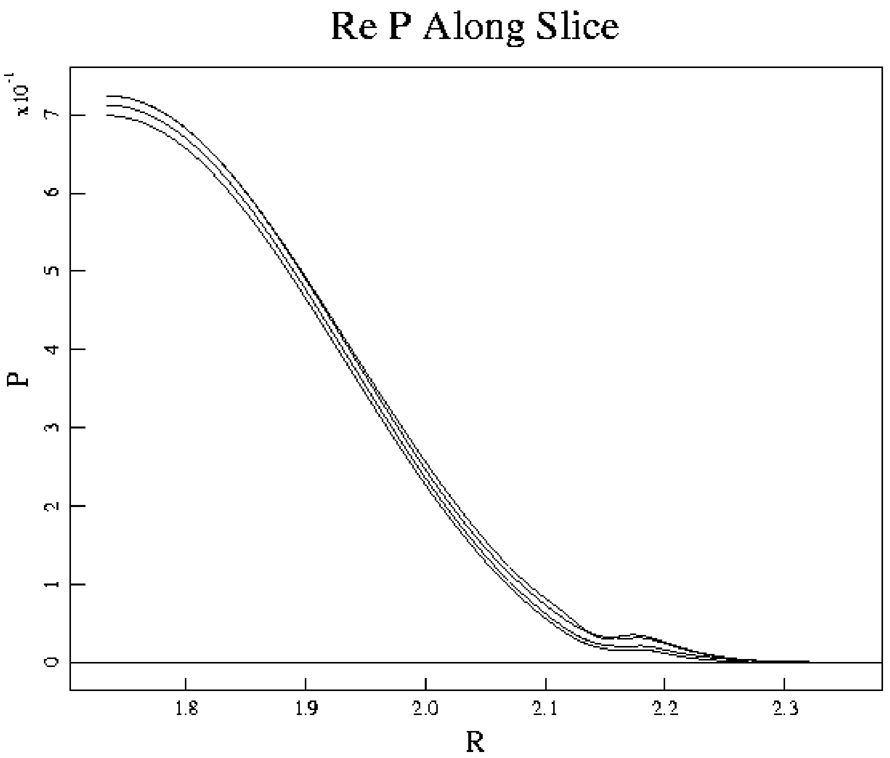




- Bilinear elements have severe difficulties with the test by conductivity-ratio values of 10^6.

Simulations of realistic configurations bring together the MHD influence on magnetic topology and rapid transport along field lines to show the net effect on confinement.





SWINDLE: these plots were handy but the computation ran the MHD first, then thermal conduction.

As evident by the tests, magnetic divergence error can be controlled with continuous basis functions, but basis functions of degree 2 or larger are essential for reliability.

• Our approach adds an error diffusion term [~Marder, JCP '87] to Faraday's law:

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \kappa_{divb} \nabla \nabla \cdot \mathbf{B}$$

• In the weak form of the time-advanced equation, $\Delta t \kappa_{divb}$ has the role of a Lagrange multiplier:

$$\int d\mathbf{x} \left\{ \mathbf{c}^* \cdot \mathbf{b}^{\mathrm{j+3/2}} + \Delta t \frac{\eta}{\mu_0} (\nabla \times \mathbf{c}^*) \cdot \left(\nabla \times \mathbf{b}^{\mathrm{j+3/2}} \right) + \Delta t \, \kappa_{divb} (\nabla \cdot \mathbf{c}^*) \left(\nabla \cdot \mathbf{b}^{\mathrm{j+3/2}} \right) \right\}$$

$$= \Delta t \int d\mathbf{x} (\nabla \times \mathbf{c}^*) \cdot \left(\mathbf{v}^{\mathrm{j+1}} \times \overline{\mathbf{b}} \right) - \Delta t \oint d\mathbf{s} \times \mathbf{E} \cdot \mathbf{c}^*$$

Divergence continued:

- For large values of $\Delta t \kappa_{divb}$, the system is over-constrained by test functions represented in div(**c***) with Lagrange elements.

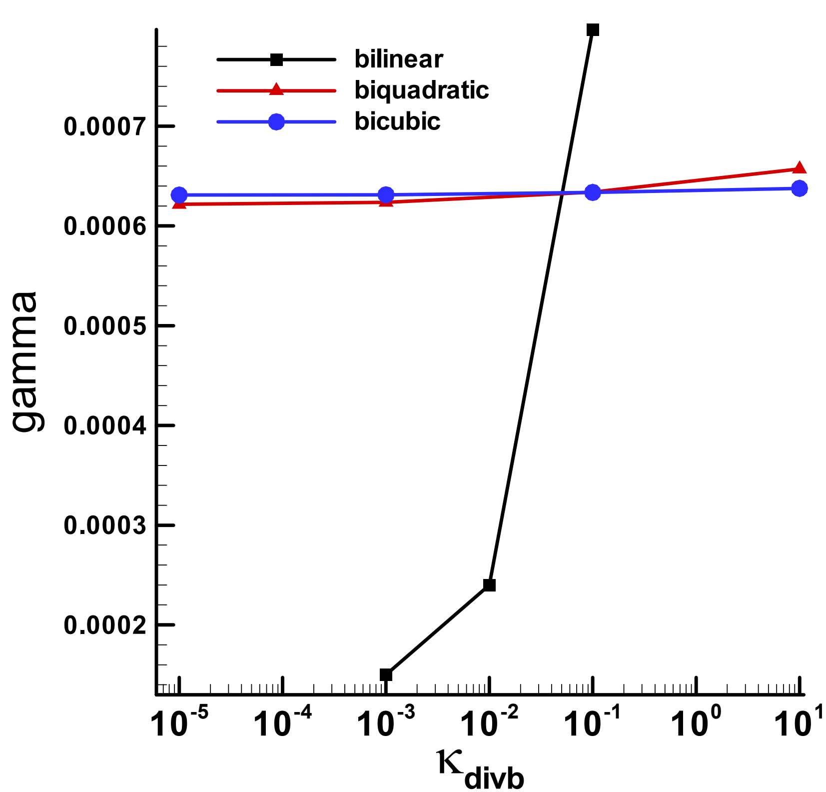
- Special basis functions satisfying the constraint exactly do not have the continuity required for resistive diffusion.

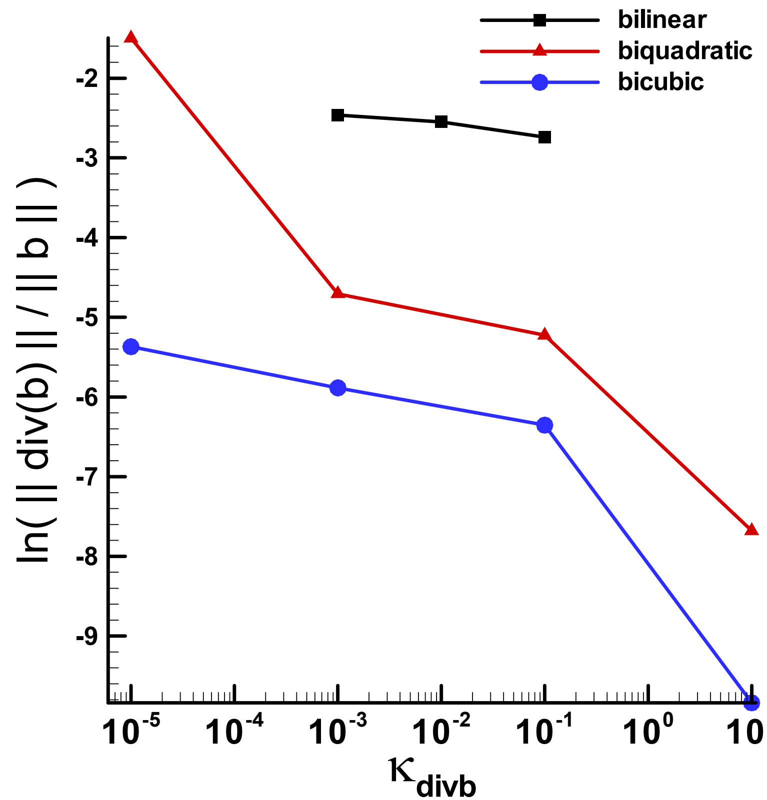
- Finite element modeling of steady incompressible fluid flow provided motivation for a decade of mathematical analysis.

- Present common practice for fluids is to use *divergence-stable* spaces for $\{\mathbf{V}, p\}$ or reduced integration.

- Time-dependent problems allow more flexibility, where only the **rate** of error generation needs to be controlled.

• Independence of physical results with respect to κ_{divb} measures success.





• Growth rate is nearly independent for biquadratic and bicubic elements. Performance of linear elements is application-dependent.

There are related issues with respect to the semi-implicit operator. It contains the large compressive responses:

$$C_0\,\Delta t^2\left[\frac{B_0^2}{\mu_0}(\nabla\cdot\mathbf{w}_\perp *)(\nabla\cdot\Delta\mathbf{v}_\perp)+\gamma p_0(\nabla\cdot\mathbf{w}*)(\nabla\cdot\Delta\mathbf{v})\right]$$

• Poor representation of divergence in an MHD eigenvalue code would lead to unphysical coupling of discrete and continuous parts of the spectrum, 'spectral pollution.' [Gruber & Rappaz, Springer]

• This is somewhat less important for time-dependent codes, where $\Delta t < \gamma^{-1}$ for the fastest ideal MHD instability. Accuracy is realized with Δt-convergence, but improvements will help stiffness issue.

Solving ill-conditioned matrices is often the most performance-limiting aspect of the algorithm.

- The condition number of the velocity-advance matrix can be estimated as

  $$v_A^2 k_{\max}^2 \Delta t^2$$

  which can be > 10^{11} in some computations.

- We have been using a home-grown conjugate gradient method solver with a parallel line-Jacobi preconditioner.
  - It has been running out of wind on some of the more recent applications, forcing a reduction of time-step.
  - We are presently implementing calls to Sandia's AZTEC library, but we are interested in other possibilities, too.

Conclusions

- Test results and past and present physics applications show the effectiveness of combining the semi-implicit method with a variational approach to spatial representation.
- Improved performance is expected from algorithm *refinements*.
    - Iterative solution methods
    - Adaptive meshing
    - Advection (not discussed here)

Directions for the Project

- Hall and other two-fluid terms are in the NIMROD code, but the implementation requires small time-steps for accuracy.
    - We are working on improved formulations.
    - The ability to solve nonsymmetric matrices is important for this.
- Kinetic physics:
    - Parallel electron streaming effects [E. Held, USU]
    - Gyrokinetic hot ion effects [C. Kim and S. Parker, CU]
- Resistive wall and external vacuum fields [T. Gianakon, S. Kruger, and D. Schnack]