Nonlinear Fusion Magneto-Hydrodynamics with Finite Elements

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OBJECTIVE

The objective of this presentation is to discuss the advantages and pitfalls of using finite elements for time-dependent magnetohydrodynamic simulations. Computations of resistive tearing with the NIMROD code show convergence rates that are near theoretical predictions.

OUTLINE

- Introduction
  - Project summary
  - Code features
- Finite element discretization
  - Relation to incompressible Navier-Stokes
  - Review of INS Analysis
    - Formulation
    - Divergence-stability
    - Convergence
  - Time-dependent problems
    - Error diffusion
    - Test results
- Semi-implicit advance
- Summary

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EQUATIONS

NIMROD solves Maxwell's equations plus a set of fluid-moment relations:

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}\,, \qquad \nabla \cdot \mathbf{B} = 0$$

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

$$\rho\left(\frac{\partial}{\partial t} + \mathbf{V}\cdot\nabla\right)\mathbf{V} = \mathbf{J}\times\mathbf{B} - \nabla p' - \nabla\cdot\Pi'$$

$$\mathbf{E} = -\mathbf{V}\times\mathbf{B} + \frac{1}{en}\frac{\left(1 - Z_e m_e/m_i\right)}{\left(1 + Z_e m_e/m_i\right)}\mathbf{J}\times\mathbf{B} + \eta\mathbf{J}$$
$$+ \frac{1}{\varepsilon_0 \omega_p^2}\left[\frac{\partial \mathbf{J}}{\partial t} + \nabla\cdot\left(\mathbf{JV} + \mathbf{VJ}\right) + \sum_\alpha \frac{q_\alpha}{m_\alpha}\left(\nabla p'_\alpha + \nabla\cdot\Pi'_\alpha\right)\right]$$

$$\frac{3}{2}\left(\frac{\partial}{\partial t} + \mathbf{V}_\alpha\cdot\nabla\right)p_\alpha = -\frac{5}{2}p_\alpha\nabla\cdot\mathbf{V}_\alpha - \nabla\cdot\mathbf{q}_\alpha + Q_\alpha$$

where quasineutrality, $n_e \cong Zn_i \equiv n$, $Z \equiv -q_i/q_e$, is assumed, ω_p is the plasma frequency, and ρ is the mass density.

- Density evolution will be added.
- T. Gianakon has implemented neoclassical closures (1D33).
- C. Kim is implementing particle-based closures (1D07).

FINITE ELEMENT DISCRETIZATION

- The finite element approach starts with the solution space and not the differential operators.

- After choosing a family of discrete spaces, a field is represented by a sum over basis functions:

  $$\mathbf{V}(\mathbf{x}) \Rightarrow \sum_{\mathrm{jk}} V_{\mathrm{jk}} \alpha_{\mathrm{j}}(\mathbf{x}) \hat{\mathbf{e}}_{\mathrm{k}}(\mathbf{x}) \ ,$$

  where $\alpha_{\mathrm{j}}(\mathbf{x})$ is a local basis of the piecewise polynomial representation.

- Substituting the discrete representation for each field into a weak form of the set of partial differential equations, or into its variational form, leads to either a linear or a nonlinear matrix equations for the set of all coefficients.

- A finite element representation is said to be *conforming* if the chosen discrete space is a subset of the admissible space for the variational form of the original set of PDEs.

We note that our time-advance for **B** has a lot in common with the time-independent incompressible Navier-Stokes equations.

Magnetic field equation: [Simplifying to resistive MHD]

$$\frac{\mathbf{B}^{n+1}}{\Delta t} - \theta \nabla \times (\mathbf{V} \times \mathbf{B})^{n+1} [+\nabla \phi] + \theta \nabla \times (\eta \nabla \times \mathbf{B})^{n+1}$$

$$= \frac{\mathbf{B}^{n}}{\Delta t} + (1-\theta) \nabla \times (\mathbf{V} \times \mathbf{B})^{n} - (1-\theta) \nabla \times (\eta \nabla \times \mathbf{B})^{n}$$

$$\nabla \cdot \mathbf{B} = 0$$

Incompressible Navier-Stokes

$$\mathbf{U} \cdot \nabla \mathbf{U} + \nabla p - \nu \nabla^{2} \mathbf{U} = \mathbf{f}$$

$$\nabla \cdot \mathbf{U} = 0$$

The application of finite element methods to incompressible Navier-Stokes equations has received considerable mathematical analysis over the last three decades. And, we can take advantage of that work!

See, for example:

M. D. Gunzburger, "Mathematical aspects of finite element methods for incompressible viscous flows," in *Finite Element Theory and Application,* D. L. Dwoyer, M. Y. Hussaini, and R. G. Voigt, eds., (Springer-Verlag, 1988).

C. Cuvelier, A. Segal, and A. A. van Steenhoven, *Finite Element Methods and Navier Stokes Equations,* (D. Reidel Publishing Co., 1986).

Incompressible Navier-Stokes Analysis

PDE

$$\mathbf{U} \cdot \nabla \mathbf{U} + \nabla p - \nu \nabla^2 \mathbf{U} = \mathbf{f}$$

$$\nabla \cdot \mathbf{U} = 0 , \qquad \text{in } \Omega$$

$$\mathbf{U} = \mathbf{0} , \qquad \text{on } \partial\Omega$$

Weak Form

$$\int_\Omega \mathbf{U} \cdot \nabla \mathbf{U} \cdot \mathbf{V} - \int_\Omega p \nabla \cdot \mathbf{V} + \int_\Omega \nu \nabla \mathbf{U} : \nabla \mathbf{V} = \int_\Omega \mathbf{f} \cdot \mathbf{V}$$

for all $\mathbf{V} \in \mathbf{H}_0^1(\Omega)$ [Subscript implies b. c. satisfied.]

$$-\int_\Omega q \nabla \cdot \mathbf{U} = 0$$

for all $q \in \mathrm{L}_0^2(\Omega)$ [Subscript implies 0 mean.]

Beside the nonlinear term, the divergence-free condition makes INS a much more challenging application than ordinary structural mechanics problems.

- Using discrete spaces for the primitive variables is the most common and flexible approach, but the divergence issue must be dealt-with directly.
  - The "integrated method" solves the weak finite element form with the divergence constraint equation.
  - The "penalty method" modifies the continuity equation to

    $$\varepsilon p + \nabla \cdot \mathbf{U} = 0 \quad .$$

    This introduces finite compressibility, and solutions should be checked in the limit of $\varepsilon \to 0$.
  - Divergence-free elements are also possible (see R. Gruber and J. Rappaz, *Finite Element Methods in Linear Ideal Magnetohydrodynamics* (Springer-Verlag, 1985) but they may be the most restrictive.

- A potential representation may be used to satisfy the divergence condition analytically. [The unstructured M3D code does this--see H. R. Strauss, et. al., "MHD Simulations on an Unstructured Mesh," in Proceedings of the Workshop on Nonlinear MHD and Extended MHD, March 25-26, 1998, UW-CPTC 98-1.]
  - In general, this leads to lower-order spatial convergence on the physical fields, however.
  - Applying boundary conditions may be more complicated than a primitive-variable formulation.

A necessary condition for convergence with the integrated and penalty function methods is that the solution space satisfies the Ladyzhenskaya - Babuska - Brezzi or *divergence - stability* condition:

There exists a $\gamma > 0$, independent of the mesh spacing, h, such that

$$\inf_{0 \neq q^h \in S^h} \; \sup_{\mathbf{0} \neq \mathbf{v}^h \in \mathbf{V}^h} \left\{ \frac{-\int_\Omega q^h \nabla \cdot \mathbf{v}^h}{\left\|\mathbf{v}^h\right\|_1 \left\|q^h\right\|_0} \right\} \geq \gamma$$

for the chosen family of solution spaces, $\mathbf{Z}^h = \left\{\mathbf{V}^h, S^h\right\}$.

This condition ensures that the discrete divergence-free vector field approaches a continuous divergence-free field in the limit as $h \rightarrow 0$.

- $\Theta(h) \equiv \sup_{\mathbf{z}^h \in \mathbf{Z}^h, \left\|\mathbf{z}^h\right\|_q = 1} \; \inf_{\mathbf{z} \in \mathbf{Z}} \left\|\mathbf{z} - \mathbf{z}^h\right\|_1$
- $\lim_{h \rightarrow 0} \Theta(h) = 0$
- $\mathbf{Z}$ is defined as the set of subspaces satisfying $-\int_\Omega q \nabla \cdot \mathbf{v} = 0$.

The end result is a limit on the acceptable sets of $\{\mathbf{V}^h, S^h\}$.

- Acceptable 2D element pairs include:
  - continuous, 6-pt quadratic $\mathbf{V}^h$ and continuous, linear S^h on triangles (Taylor-Hood)
  - continuous, 9-pt biquadratic $\mathbf{V}^h$ and continuous, bilinear S^h on quadrilaterals (Taylor-Hood)
  - continuous, 6-pt quadratic $\mathbf{V}^h$ and piecewise constant S^h on triangles (Crouzeix-Raviart)
  - continuous, 7-pt quadratic $\mathbf{V}^h$ and piecewise linear S^h on triangles (Crouzeix-Raviart)
  - continuous, 9-pt biquadratic $\mathbf{V}^h$ and piecewise linear S^h on quadrilaterals (Crouzeix-Raviart)

- Unfortunately, simpler element pairs are not acceptable:
  - continuous, linear $\mathbf{V}^h$ and piecewise-constant S^h on triangles [This gives an over-determined system.]
  - continuous, bilinear $\mathbf{V}^h$ and piecewise-constant S^h on quadrilaterals [A checkerboard pressure mode allows any velocity field to satisfy the divergence constraint.]
  - Other element pairs fail in a more subtle way; see the Gunzburger reference.

If *divergence-stability* is satisfied and a unique solution exists (conditions are not turbulent), then convergence is assured.

$$\left\|\mathbf{u}-\mathbf{u}^h\right\|_1 \le C_1 \inf_{\mathbf{v}^h \in \mathbf{V}^h} \left\|\mathbf{u}-\mathbf{v}^h\right\|_1 + C_2\Theta(h) \inf_{q^h \in \mathrm{S}^h} \left\|p-q^h\right\|_0$$

$$\left\|p-p^h\right\|_0 \le C_3 \inf_{\mathbf{v}^h \in \mathbf{V}^h} \left\|\mathbf{u}-\mathbf{v}^h\right\|_1 + C_4 \inf_{q^h \in \mathrm{S}^h} \left\|p-q^h\right\|_0$$

- The difference between the finite element solution and the best piecewise polynomial approximation for the solution is independent of mesh spacing. The rate of spatial convergence is then tied to the polynomial degree used for the basis functions.

- This applies to regular or irregular meshes, hence the attractiveness of the finite element method for domains with complicated borders.

- If the solution is sufficiently smooth,

$$\left\|\mathbf{u}-\mathbf{u}^h\right\|_0 \le C_5\, h \left\|\mathbf{u}-\mathbf{u}^h\right\|_1 \quad .$$

Time-dependent Problems

A discrete time advance allows alternative implementations of the divergence constraint. On a fundamental level, all share characteristics with the steady-state treatments.

- NIMROD uses an error-diffusion technique[*] for controlling $\nabla \cdot \mathbf{B}$. Faraday's law is modified to:

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} + \kappa_b \nabla\nabla \cdot \mathbf{B}\,, \quad \frac{\partial \mathbf{B}}{\partial t} \cdot \hat{\mathbf{n}} = 0 \ \text{ on } \ \partial\Omega$$

$$\rightarrow \frac{\partial(\nabla \cdot \mathbf{B})}{\partial t} = \nabla \cdot \kappa_b \nabla(\nabla \cdot \mathbf{B})$$

  This is related to the "projection method" of Brackbill and Barnes.[♣]

  - Advance to $\mathbf{B}^*$ with physical terms.
  - Solve $\nabla^2 \phi = \nabla \cdot \mathbf{B}^*$
  - $\mathbf{B}^{n+1} = \mathbf{B}^* - \nabla\phi$

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[*] B. Marder, "A Method for Incorporating Gauss' Law into Electromagnetic PIC Codes," J. Comput. Phys. **68**, 48 (1987).

[♣] J. U. Brackbill and D. C. Barnes, "The Effect of a Nonzero $\nabla \cdot \mathbf{B}$ on the Numerical Solution of Magnetohydrodynamic Equations," J. Comput. Phys. **35**, 426 (1980).

Error diffusion is also closely related to the penalty method for incompressible Navier-Stokes.

$$\frac{1}{\kappa_b}\phi + \nabla\cdot\mathbf{B}^{n+1} = 0 \qquad \leftrightarrow \qquad \varepsilon p + \nabla\cdot\mathbf{U} = 0$$

$$\frac{\mathbf{B}^{n+1}}{\Delta t} + \nabla\phi = \frac{\mathbf{B}^{n}}{\Delta t} - \nabla\times\mathbf{E} \qquad \leftrightarrow \qquad \mathbf{U}\cdot\nabla\mathbf{U} + \nabla p - \nu\nabla^2\mathbf{U} = \mathbf{f}$$

The penalty method needs to satisfy *divergence-stability*.

- If p^h is eliminated numerically after choosing an acceptable $\{\mathbf{V}^h, S^h\}$ pair, the condition is still satisfied.

- If p is eliminated analytically, acceptability depends on the form of $\nabla \cdot \mathbf{v}^h$.

  $$\int_\Omega \nabla \cdot \mathbf{v}^h \nabla \cdot \mathbf{u}^h \sim \int_\Omega r^h \nabla \cdot \mathbf{u}^h$$

  Is the space represented by $\{\mathbf{V}^h, \mathrm{R}^h\}$ acceptable?

- This condition is not satisfied for linear $\mathbf{V}^h$ on triangles, or for bilinear $\mathbf{V}^h$ on quadrilaterals.

- For 7-pt. quadratic $\mathbf{V}^h$ on triangles and 9-pt. biquadratic $\mathbf{V}^h$ on quadrilaterals, the piecewise linear scalar field is a subset of all possible $\nabla \cdot \mathbf{v}^h$, so the analytic elimination penalty method or error diffusion method are acceptable. (Effectively producing Crouzeix-Raviart elements)

The NIMROD finite element representation has been generalized to allow arbitrary degree polynomial bases of the Lagrange type (H^1).

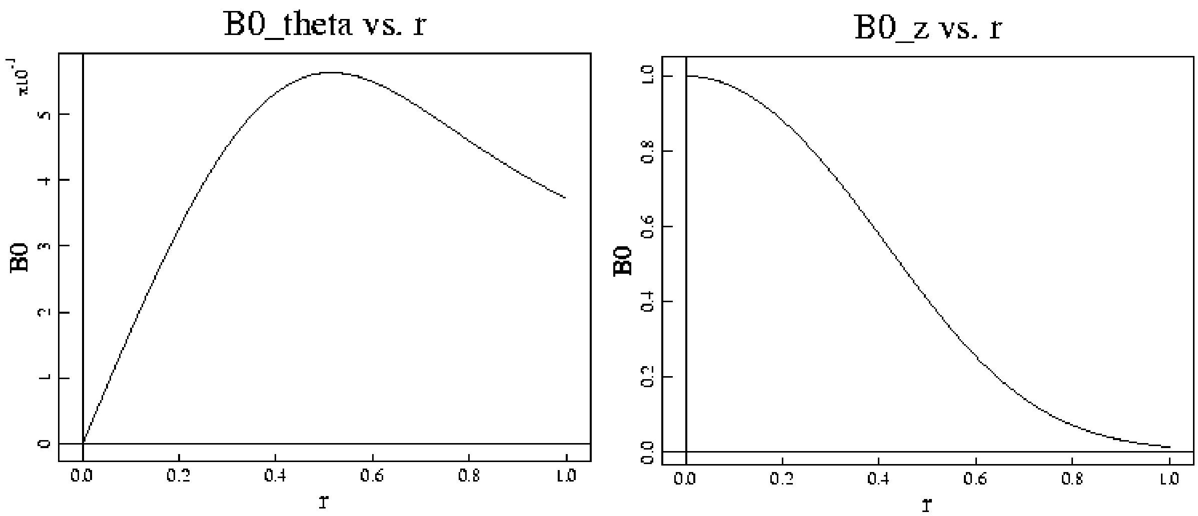
- By selecting second order (and higher?) degree polynomials, error diffusion is divergence-stable with arbitrarily large values of κ_b.
  - This statement does **not** imply that every computation with an acceptable solution space has zero magnetic divergence,
  - nor does it imply that magnetic divergence has no effect on the rest of the solution.
  - It implies that spatial convergence with an acceptable solution space removes magnetic divergence and its effects.
- We have not yet verified that the Fourier representation of the periodic direction does not change acceptability for toroidal components where $n \neq 0$.

- We have successfully used bilinear and linear elements for **B** in many computations. However, some cases fail catastrophically. Why does it work with unacceptable elements in some cases?

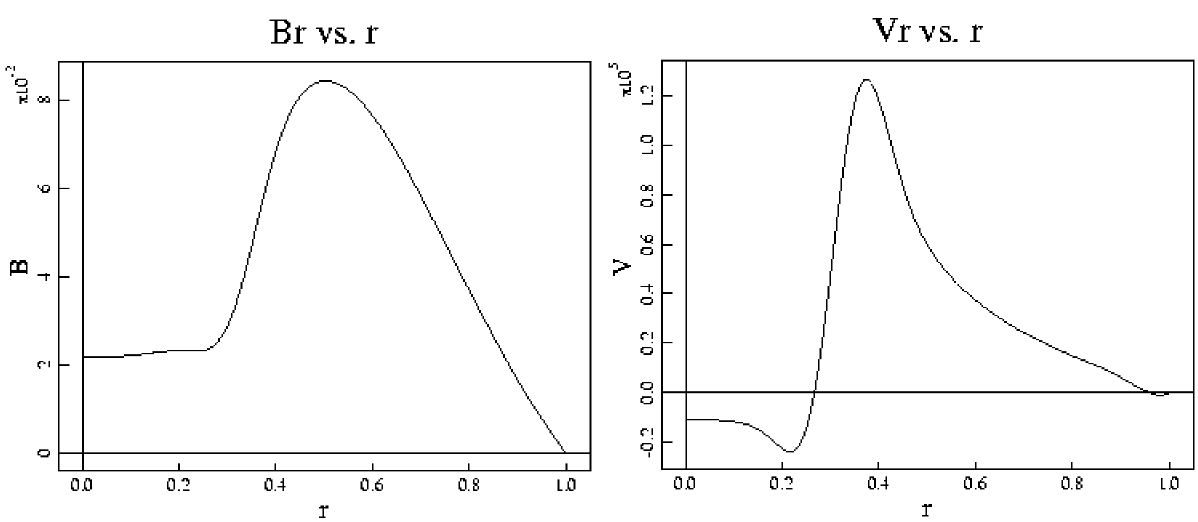
  - A clue is that κ_b must be $\sim \eta$.

A linear tearing mode serves as a test for divergence error and convergence.

The geometry is a circular cross section, periodic cylinder. The polar grid is composed of quadrilaterals. $S=10^4$ and $P_m=1$.

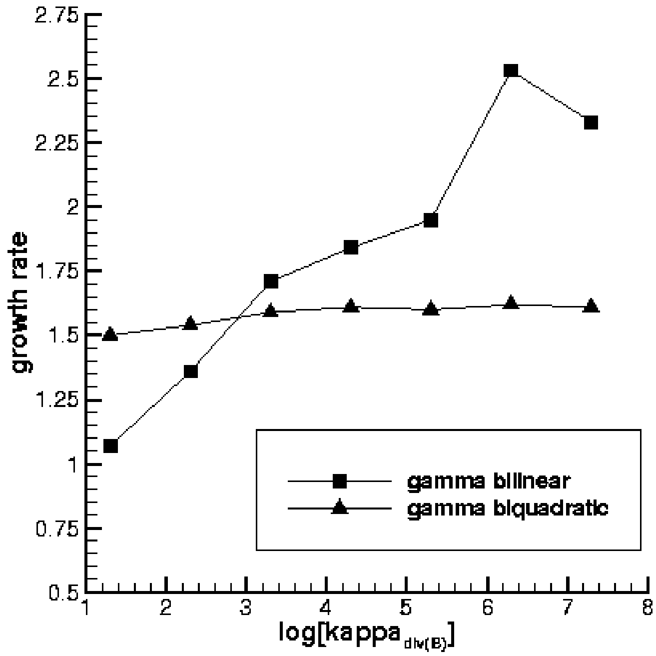


Equilibrium **B**

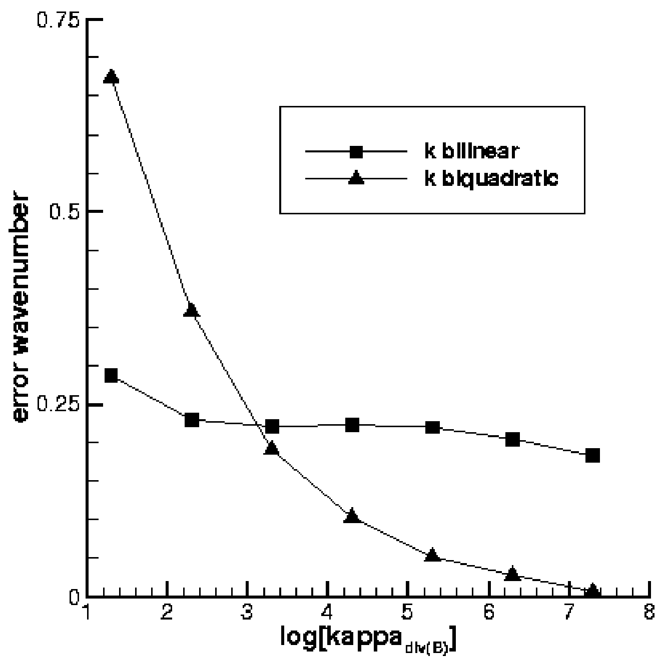


Linear Eigenfunction $\sim \exp\left[i\theta + i\frac{2\pi z}{L}\right]$

We have varied κ_b over orders of magnitude to compare bilinear (32x32 mesh) and biquadratic solutions (16x16 mesh).

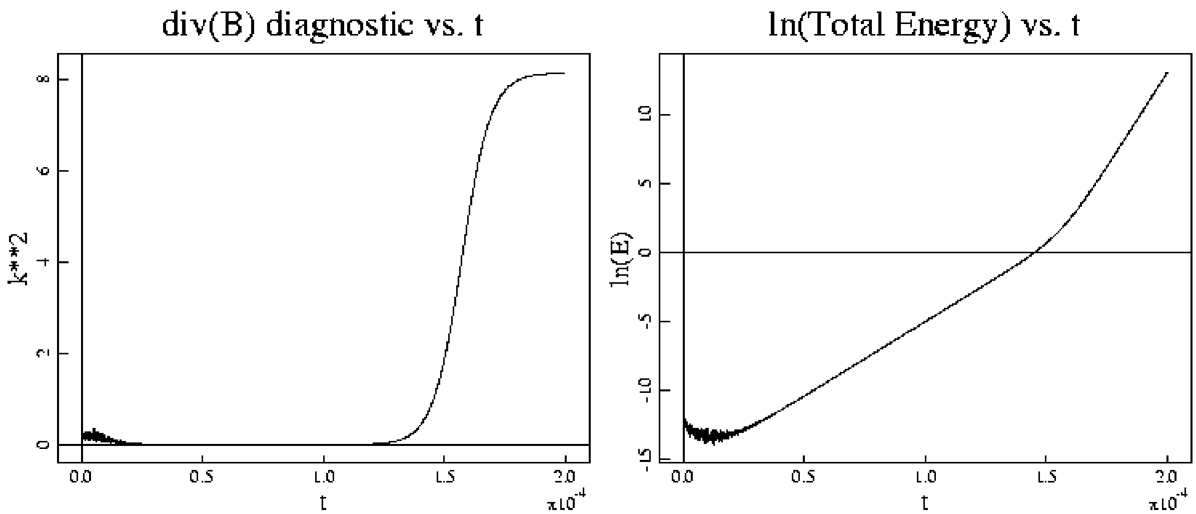


Linear Growth Rate vs. log(κ_b)

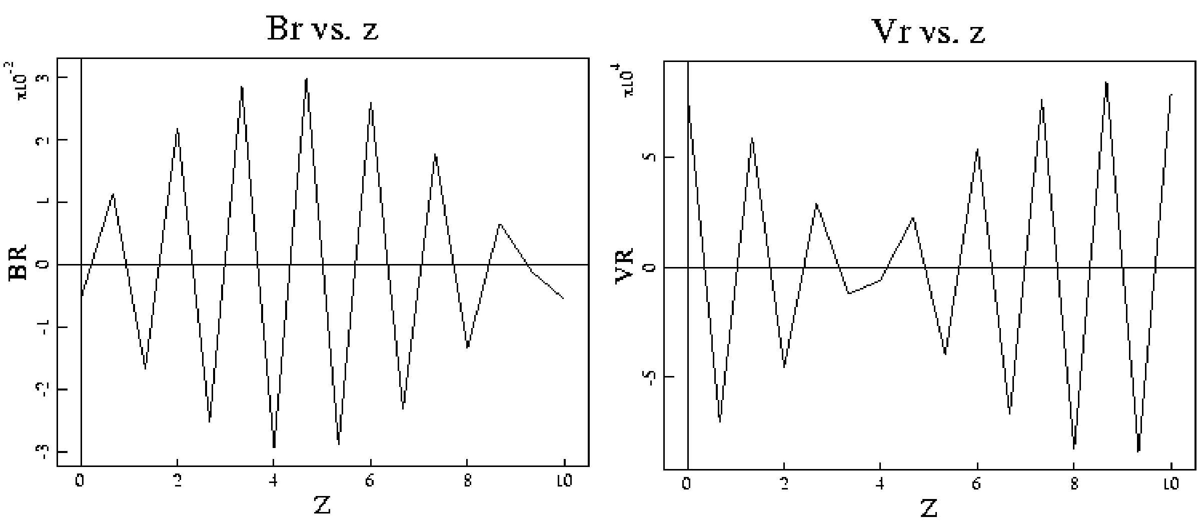


Divergence Error, $\|\nabla \cdot \mathbf{b}\| / \|\mathbf{b}\|$, vs. log($\kappa_b$)

In a similar, but doubly-periodic slab, using κ_b=50η was catastrophic for bilinear elements:



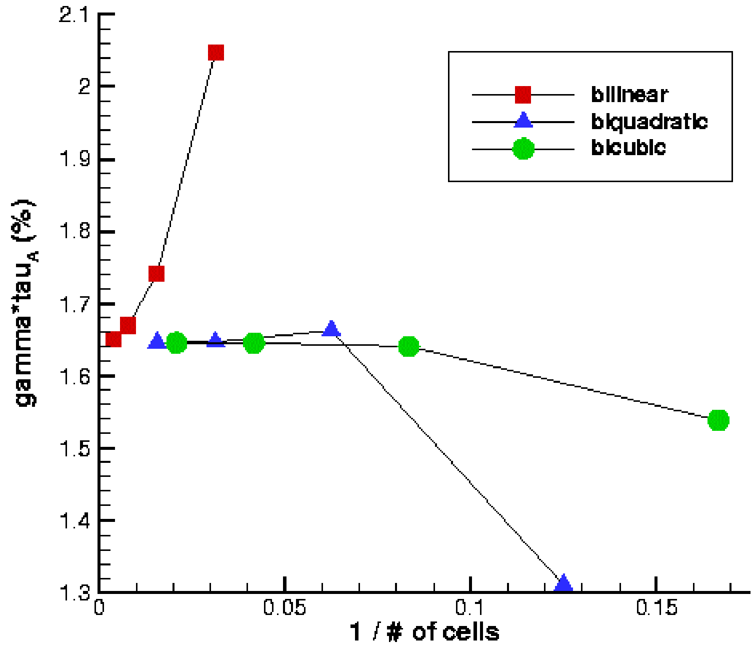
- A slow numerical mode arose after 0.15 diffusion times.



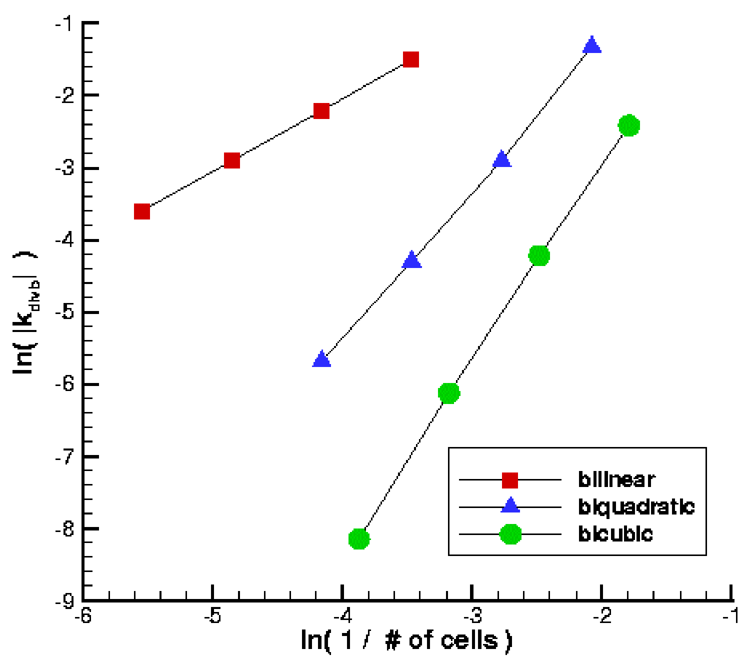
- There is a $k = \pi/L$ mode in the envelope of the eigenfunction.

Repeating the computation either with κ_b=η and bilinear elements or with κ_b=50η and biquadratic elements avoided the vertex-to-vertex oscillations.

Convergence of the solution and $\nabla \cdot \mathbf{B}$ error improve with polynomial degree in the cylindrical problem, as predicted.



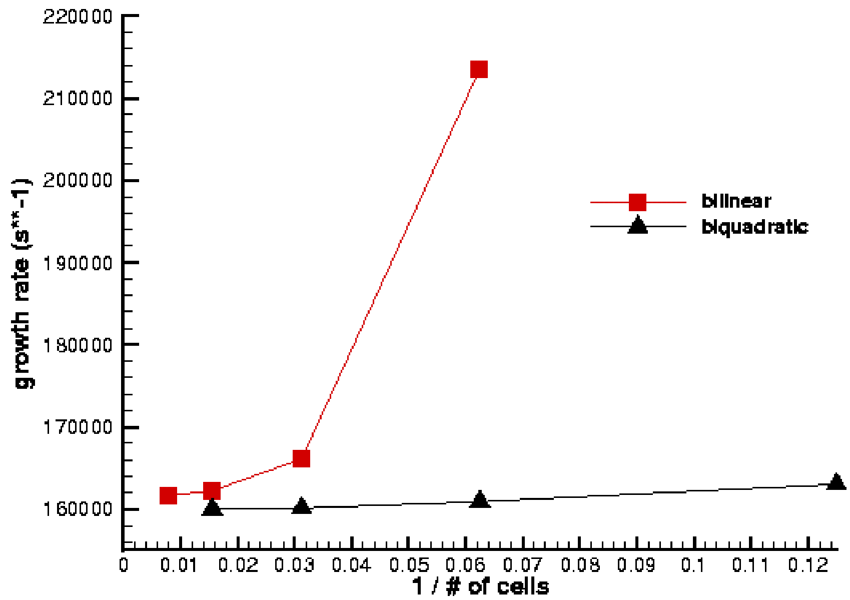
Linear Growth Rate vs. Mesh Spacing



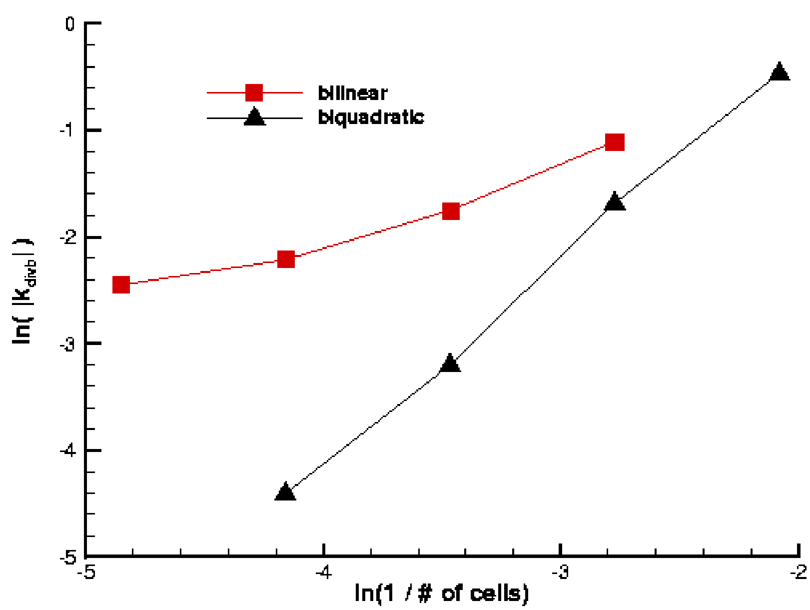
ln(Divergence Error) vs. ln(Mesh Spacing)

Radial and azimuthal resolution are varied together. [κ_b=2000η]

Convergence of the solution and error are compared for the cylindrical problem, varying only the number of cells in the azimuthal direction. $[\kappa_b=2\eta]$



Linear Growth Rate vs. Mesh Spacing



ln(Divergence Error) vs. ln(Mesh Spacing)

SEMI-IMPLICIT ADVANCE

A semi-implicit algorithm [Schnack, J. Comput. Phys. **70**, 330, for example] is used to advance the solution from initial conditions.

A simple example with a 1D linear sound wave provides a review:

$$\frac{\partial p}{\partial t} = -\gamma P_0 \frac{\partial v}{\partial x}$$

$$\rho \frac{\partial v}{\partial t} = -\frac{\partial p}{\partial x}$$

A semi-implicit scheme replaces mass density in the momentum equation with a new spatial operator

$$\rho\left(1 - f c^2 \Delta t^2 \frac{\partial^2}{\partial x^2}\right)$$

After normalizing pressure by P_0 , velocity by the sound speed, and assuming an e^{ikx} dependence, the modified leap-frog advance has the form,

$$p^{n+1} - p^{n} = -i\gamma\zeta v^{n} , \qquad \zeta \equiv kc\Delta t$$

$$\left(1+f\zeta^2\right)\left(v^{n+1} - v^{n}\right) = -\frac{i\zeta}{\gamma} p^{n+1}$$

The complex eigenvalue representing the linear operations of the time step,

$$\begin{pmatrix} p \\ v \end{pmatrix}^{n+1} = \lambda \begin{pmatrix} p \\ v \end{pmatrix}^{n}$$

satisfies

$$\lambda^2 - b\lambda + 1 = 0$$

where $b = -2 + \dfrac{\zeta^2}{1 + f\zeta^2}$

The magnitude of λ is unity (advance is numerically stable without dissipation) if

$$|b| \leq 2$$

Setting the coefficient

$$f \geq \frac{1}{4}$$

ensures stability for all Δt.

A coefficient exceeding the linear numerical stability requirement stabilizes nonlinear terms, which may then appear in explicit form.

The choice of semi-implicit operator has a strong influence on accuracy at large Δt (large compared with propagation times of normal modes).

The NIMROD semi-implicit scheme for the MHD advance includes the following equation for velocity:

$$\rho \frac{\Delta \mathbf{V}}{\Delta t} + \frac{f_a \Delta t^2}{\mu_0} \nabla \times \nabla \times \left(\mathbf{B}_0 \times \frac{\Delta \mathbf{V}}{\Delta t} \right) \times \mathbf{B}_0 + f_a \Delta t^2 \mathbf{J}_0 \times \nabla \times \left(\mathbf{B}_0 \times \frac{\Delta \mathbf{V}}{\Delta t} \right)$$
$$- f_a \Delta t^2 \gamma \nabla P_0 \nabla \cdot \frac{\Delta \mathbf{V}}{\Delta t} - f_a \Delta t^2 \nabla \left(\frac{\Delta \mathbf{V}}{\Delta t} \cdot \nabla P_0 \right) - f_i \Delta t^2 \nabla \cdot \left(\delta c^2 \right) \nabla \frac{\Delta \mathbf{V}}{\Delta t}$$
$$= -\rho \mathbf{V} \cdot \nabla \mathbf{V} + \mathbf{J} \times \mathbf{B} - \nabla p$$

- After integration by parts in the finite element procedure, the linear part of the operator has the form of the linear potential energy of the ideal MHD system.

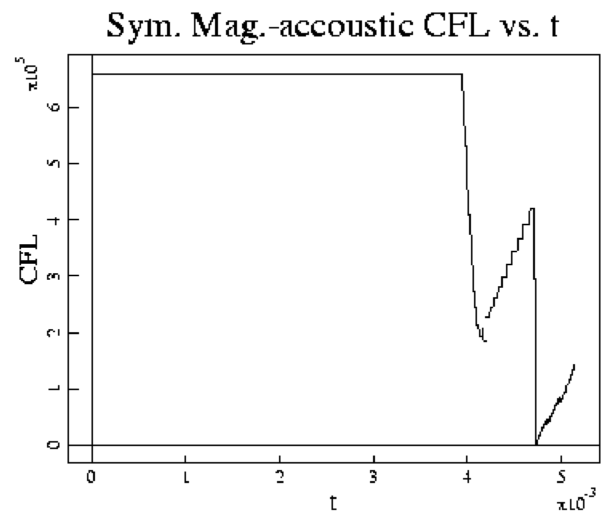
- This is very similar to the scheme by K. Lerbinger and J. F. Luciani, J. Comput. Phys. **97**, 444 (1991), but the 0-subscripted fields here contain the n=0 part of the solution, in addition to the equilibrium, and the coefficient for the isotropic operator is updated with the magnitude of nonsymmetric perturbations to avoid CFL constraints imposed by nonlinear waves.

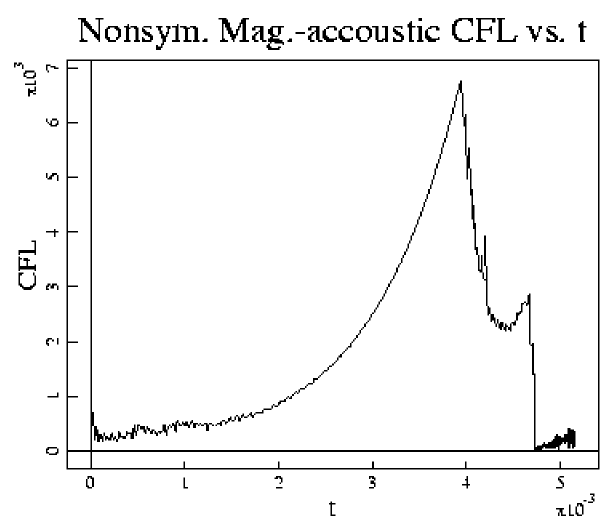
- This is computationally efficient for fusion problems where the magnetic field is dominantly symmetric. There is no toroidal coupling in the matrices, permitting parallel decomposition over n.

- Hall terms, when used, are time-split from the MHD advance of **B**, and require a separate semi-implicit operator. [Harned, J. Comput. Phys. **83**, 1]

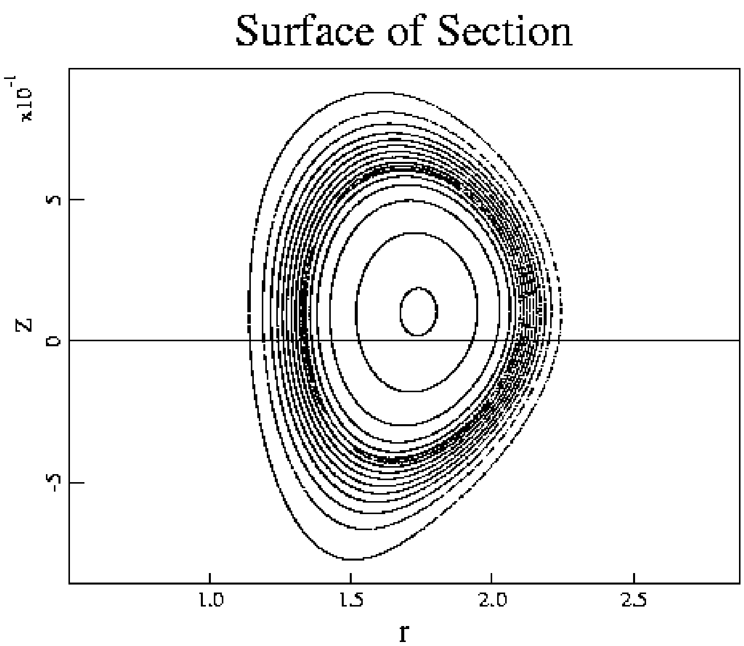
For nonlinear tokamak simulations, the coefficient for the isotropic part of the operator may be much smaller than that for the anisotropic part.

- A simulation of a (3,2) tearing mode in DIII-D serves as an example.
- Coefficients are proportional to the square of the respective CFL number.





- See the presentation by Schnack, et al. (1C24) for more details on this computation.



SUMMARY

- Numerical analysis of finite elements applied to the incompressible Navier-Stokes equations has proven extremely valuable for understanding and improving the treatment of magnetic field in the NIMROD code.

- Our original formulation with linear and bilinear elements did not satisfy the *divergence-stability* condition.

- The error diffusion technique with $\kappa_b \sim \eta$ works with low-order elements in cases where the generation of $\nabla \cdot \mathbf{B}$ is easily controllable.

- The *divergence-stability* condition is satisfied with quadratic elements (and higher order elements?) and the error diffusion technique.

- **The rate of convergence increases with polynomial degree, and results are less sensitive to the value of κ_b.**

- A semi-implicit advance is computationally efficient for fusion applications.

This poster will be available from http://nimrodteam.org , along with many other presentations on the NIMROD code development project.