Numerical Plans for the NIMROD Plasma Simulation Code

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Theme: the numerical algorithm presently used in the NIMROD code has allowed us to investigate important plasma behavior, but further significant developments are needed to reach the goal of simulating realistic plasma conditions.

Fluid Model

The electromagnetic activity of the system can be modeled with a set of fluid and Maxwell's equations:

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

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

$$\frac{n_\alpha}{\gamma - 1}\left(\frac{\partial}{\partial t} + \mathbf{V}_\alpha\cdot\nabla\right)T_\alpha = -p_\alpha\nabla\cdot\mathbf{V}_\alpha - \nabla\cdot\mathbf{q}_\alpha + Q_\alpha - \Pi_\alpha : \mathbf{V}_\alpha$$

$$p_\alpha = n_\alpha k T_\alpha$$

$$\mathbf{E} = -\mathbf{V}\times\mathbf{B} + \eta\mathbf{J} + \frac{1}{en}\mathbf{J}\times\mathbf{B} + \frac{1}{\varepsilon_0\omega_p^2}\left[\frac{\partial\mathbf{J}}{\partial t} + \nabla\cdot(\mathbf{JV} + \mathbf{VJ}) + \sum_\alpha \frac{q_\alpha}{m_\alpha}(\nabla p_\alpha + \nabla\cdot\Pi_\alpha)\right]$$

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

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

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.

- Accurate modeling of many important phenomena requires extending the fluid model to include kinetic effects.

Numerical Challenges

Conditions in magnetic confinement plasmas lead to extreme stiffness and anisotropy.

- Considering resistive MHD behavior alone, characteristic times for different effects may differ by 4-10 orders of magnitude in experiments. [Explicit algorithms are not viable, and there is sensitivity to numerical dissipation. Implicit matrices are ill-conditioned.]

- Strong anisotropy results from the magnetic field.

  - Shearing and compressive motions along and perpendicular to the magnetic field result in physically different responses from the system. [We need to avoid truncation errors that artificially couple different responses.]

  - Helical disturbances resonate with the magnetic distribution along closed surfaces and show radically different behavior in narrow layers about the surfaces. [Like boundary layers but internal to the domain.] [Nonuniform meshing and parallel decomposition of large grids are required.]

- Comparison with experiment requires an accurate representation of the geometry in some cases. [Geometric flexibility is important.]

- Two-fluid and kinetic effects introduce further spatial and temporal stiffness.

NIMROD Algorithm

The NIMROD algorithm uses a semi-implicit advance with a finite-element/Fourier series spatial representation to address the challenges of numerical fusion physics.

Equations are re-written for perturbations about a steady-state:

$$\left.\frac{\partial \mathbf{B}}{\partial t}\right|_{\mathrm{MHD}} = \nabla \times \left(\mathbf{V} \times \mathbf{B} - \eta \mathbf{J} \right)$$

$$\Downarrow$$

$$\left.\frac{\partial \mathbf{b}}{\partial t}\right|_{\mathrm{MHD}} = \nabla \times \left(\mathbf{V}_{\mathrm{ss}} \times \mathbf{b} + \mathbf{v} \times \mathbf{B}_{\mathrm{ss}} + \mathbf{v} \times \mathbf{b} - \eta \mathbf{j} \right)$$

Semi-implicit time-advance:

- Stabilizes wave-propagation at large time-step.
- Accuracy depends on choice of differential operator.
- Cannot time-center entire plasma model directly.
- Synergistic wave/advection effects require additional consideration.

Finite element representation:

- Offers geometric and numerical flexibility.
- Preserves self-adjoint property where appropriate.
- Consistency between 1st and 2nd order differencing is nontrivial.
- Divergence constraint is not automatically satisfied with most representations.

Semi-implicit methods extend the domain of convergence for leap-frog algorithms while preserving symplectic integration.

- A 1D linear sound wave serves as an example.

$$p^{n+1/2} - p^{n-1/2} = -\Delta t \gamma P_0 \frac{\partial v^n}{\partial x}$$

$$\left(1 - C \frac{\partial^2}{\partial x^2}\right)\left(v^{n+1} - v^n\right) = -\frac{\Delta t}{\rho} \frac{\partial p^{n+1/2}}{\partial x}$$

- With an e^{ikx} spatial dependence,

$$\begin{pmatrix} p \\ v \end{pmatrix}^{new} = \begin{pmatrix} 1 & 0 \\ -\dfrac{ik\Delta t}{\rho\left(1 + Ck^2\right)} & 1 \end{pmatrix} \begin{pmatrix} 1 & -ik\Delta t \gamma P_0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} p \\ v \end{pmatrix}^{old}$$

- Determinant of time-advance matrix is unity (area preserving).
- Can choose C to have complex conjugate eigenvalues→stable advance.

Successes with Present Algorithm

- Simulations of Current-driven activity in alternates
  - Electrostatic formation and sustainment of spheromaks
  - Toroidal geometry effects in reversed-field pinches

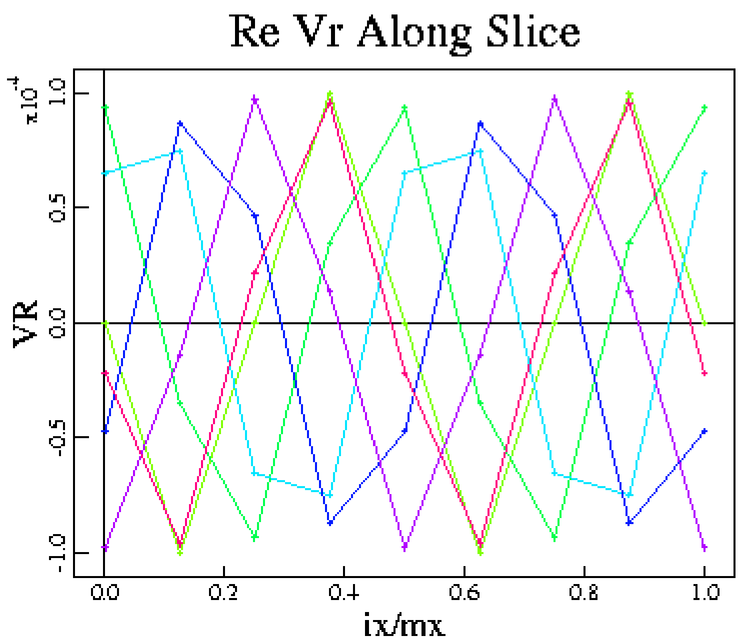
- Numerical accuracy in extremely anisotropic conditions
  - Thermal conduction
  - Tokamak physics strongly dependent on anisotropy

Difficulties with Present Algorithm
(Numerical Opportunities)

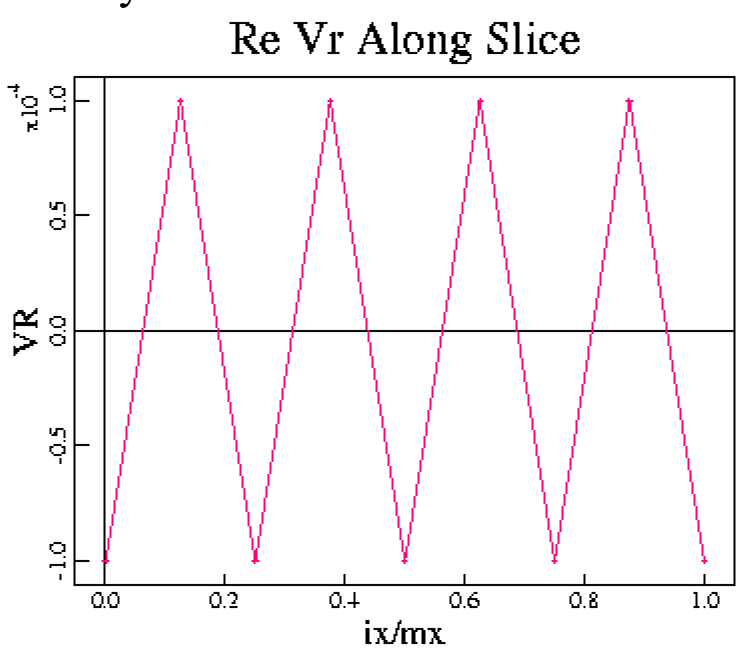
- Overall computational performance is disappointing.
  - Parallel scaling is reasonable, however
  - Matrix solution is demanding, and
  - The efficiency of our finite element computations is questionable.
- Accuracy with electron-fluid physics requires severe limits time-step.
  - Relatively little numerical work has been done on the general problem.
- Strong advection in conditions with weak physical dissipation is problematic.
- Nonlinear activity when physical dissipation is not introduced in all equations is also problematic.

Advection Demonstration

Uniform advection of passive scalar sign wave.



Case A. Eight cells, $k = \pi/2\Delta x$, 25 time-steps (green to red), final overlays initial in exact solution.



Case B. Same except $k = \pi/\Delta x$--nothing happens.

This characteristic can lead to undamped oscillations.

Advection Analysis

Advection in NIMROD is based on a predictor/corrector approach to avoid explicit upwinding, which is complicated in finite element representations.

Predictor/corrector advection:

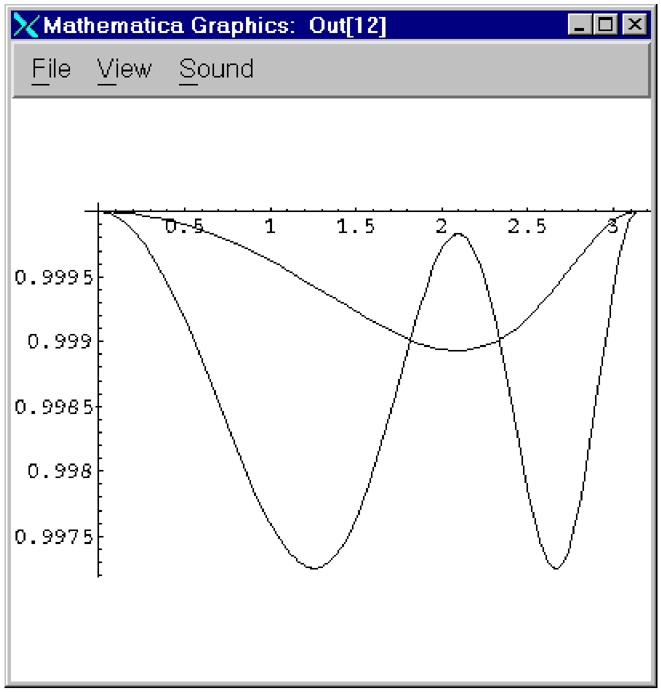
$$p^* - p^n = -\Delta t \mathbf{C} \cdot \nabla p^n$$
$$p^{n+1} - p^n = -\Delta t \mathbf{C} \cdot \nabla \left[f p^* + (1-f) p^n \right]$$

Analyze for 1D $p_k e^{ikx}$ dependence, linear finite elements with distributed mass matrix, and separate mass matrix solves for predictor and corrector:

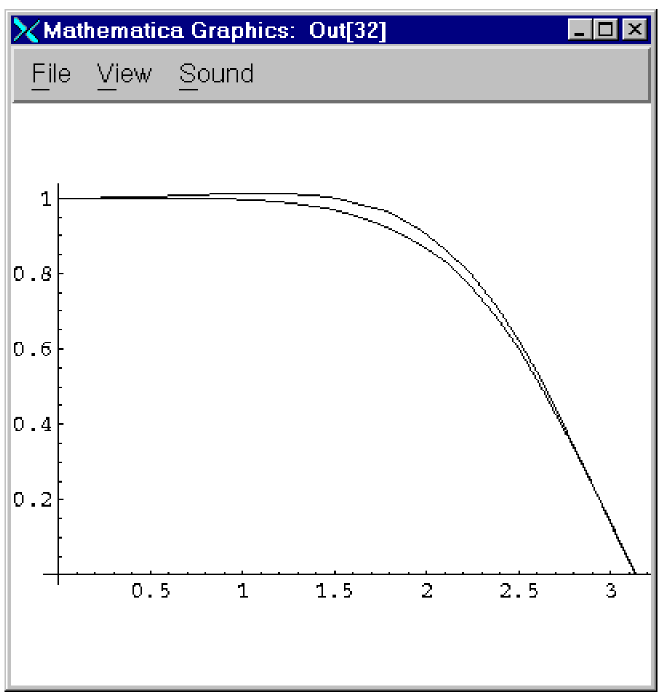
The numerical eigenvalue, $p_k^{n+1} = \lambda \, p_k^n$ is

$$\lambda = 1 - \frac{i\sigma\eta + \frac{f\sigma^2\eta^2}{m}}{m}$$

where $\eta = c\Delta t / \Delta x$, $\sigma = Sin(k\Delta x)$, and $m = 1 - \mathrm{K}/6$ with $K = 2\left(1 - Cos(k\Delta x)\right)$.

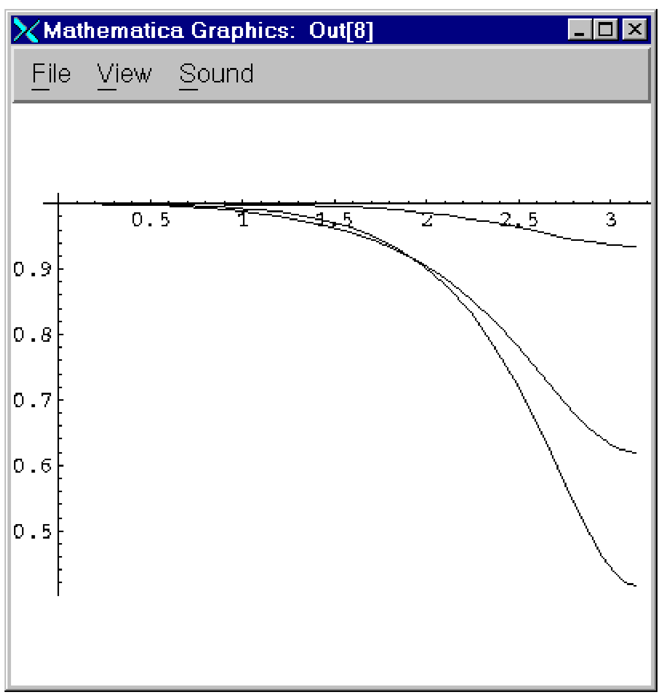


Dissipation error is slight, as indicated by $|\lambda|$ plotted vs. $k\Delta x$ at η=0.1 and η=0.3. Here f=0.54.



Dispersion error is significant at f=0.54, as indicated by $\mathrm{Arg}(\lambda)/(-\eta k\Delta x)$ plotted vs. $k\Delta x$ at η=0.1 and η=0.3.

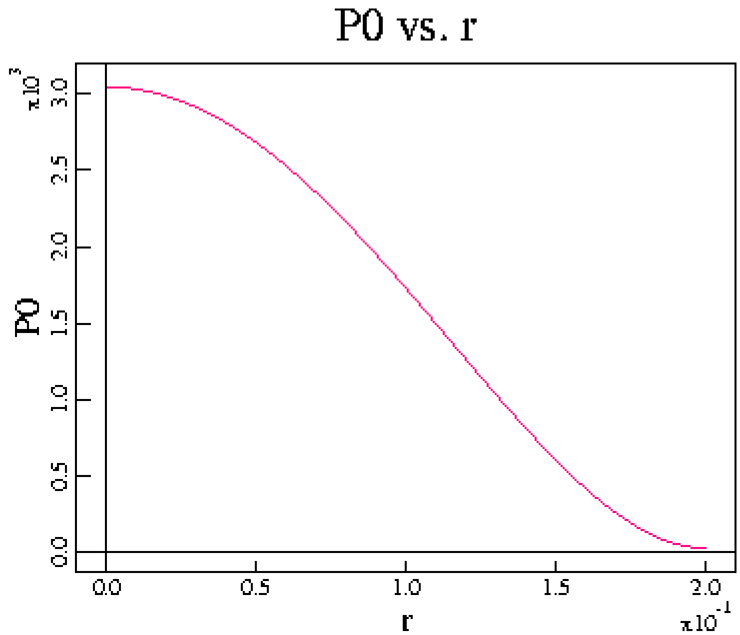
- Effective ‘central differencing’ of 1st order derivatives loses $k = \pi/\Delta x$ oscillations.
  - Must be damped everywhere by local dissipation if other truncation error provide a source.
  - A continuous system may propagate large k oscillations to be damped nonlocally.
- Using a discontinuous representation for the predicted fields gives an effective 2nd order operator that is sensitive to $k = \pi/\Delta x$ oscillations.
  - New eigenvalue is $\lambda = 1 - \dfrac{i\sigma\eta + f\mathrm{K}\eta^2}{m}$.

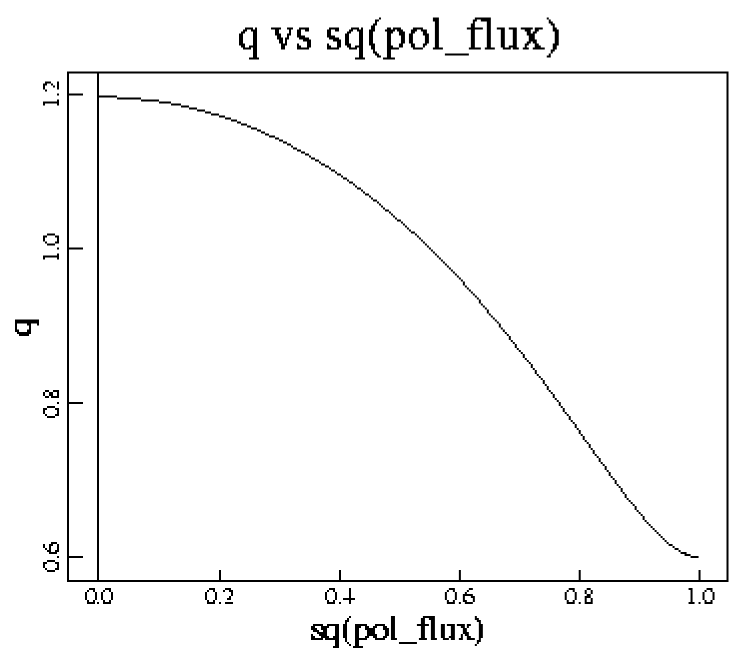


Dissipation error is much more significant, as indicated by $|\lambda|$ plotted vs. $k\Delta x$ at η=0.1, η=0.3, and η=0.5. Here f=0.54. Dispersion error is comparable to original form; though, unphysically fast propagation occurs at large η.

Nonlinear Issue

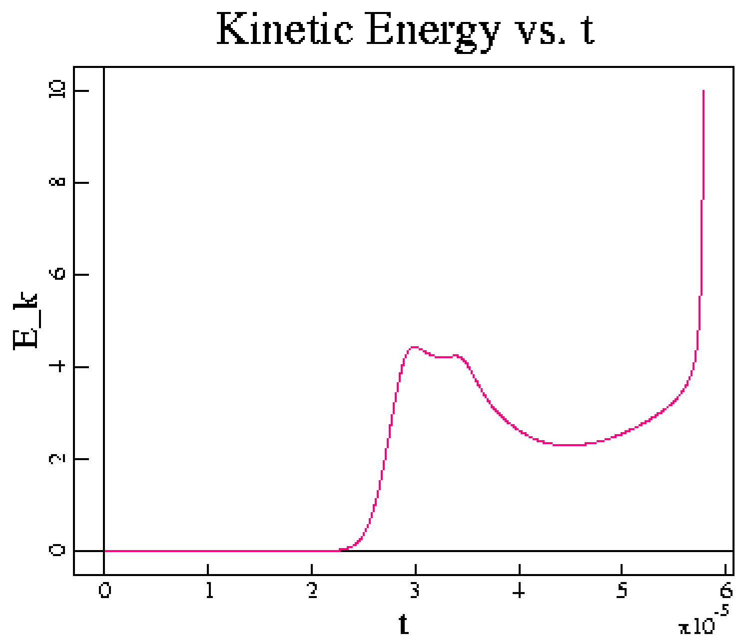
A resistive interchange (?) mode in a periodic cylinder run to saturation on a 30x4 mesh of quadratic elements illustrates the problem.

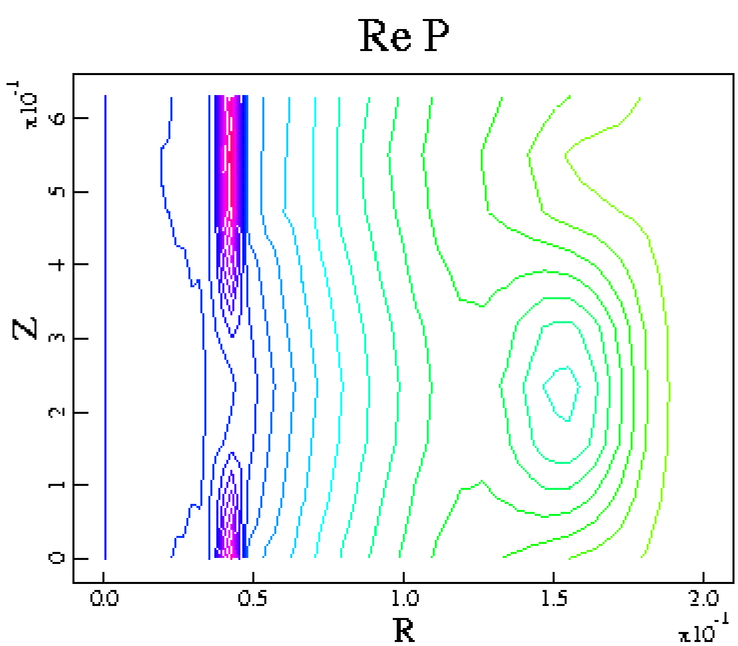




- $S \equiv \tau_r / \tau_A = 5000, \quad Pm \equiv \nu\mu_0/\eta = 1, \quad \beta = 3\%$

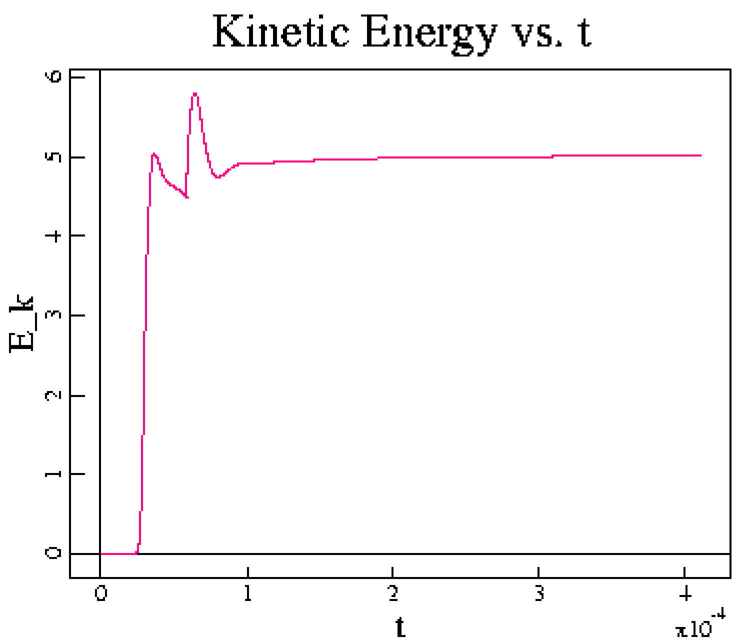
An adiabatic simulation runs through the saturation phase, but crashes very suddenly due to a localized excursion at the rational surface.

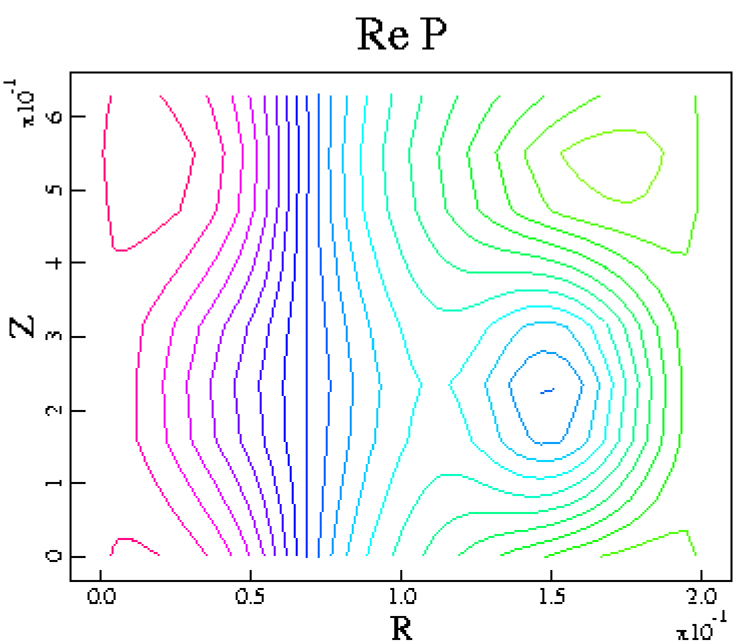




- Increasing spatial resolution does not correct the problem.

Adding a small amount of isotropic diffusion to the pressure equation ($\kappa = \mu_0 / \eta$) prevents the error.





- Lack of high-k propagation with the continuous representation is again suspect.
  - Here, sound waves should propagate the disturbance, and dissipation can occur via viscosity.

- Using discontinuous bases for some fields will allow wave propagation for all k.
  - Analogous to staggered grids in finite differences/volumes.
  - Dissipative terms in the equations for the discontinuous fields will require mixed methods.
  - Adds further complexity to the code.