Nonlinear M3D-C^1 Plans

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Development history: 2D Nonlinear

- Initial formulation solved two-field reduced incompressible equations

$$\begin{cases} \dfrac{\partial}{\partial t}\nabla^2\phi = \left[\phi,\nabla^2\phi\right] - \left[\psi,\nabla^2\psi\right] + \mu\nabla^4\phi \\ \dfrac{\partial\psi}{\partial t} = \left[\phi,\psi\right] + \eta\nabla^2\psi \end{cases}$$

  on a 2D slab using reduced quintic (Q_{18}) basis functions on a regular triangular mesh. Verified with tilt mode.

- Next, out-of-plane velocity and B components were added, giving four-field reduced equations:

$$\begin{cases} \dfrac{\partial V_z}{\partial t} = \left[\phi,V_z\right] + \left[I,\psi\right] + \mu\nabla^2 V_z \\ \dfrac{\partial I}{\partial t} = \left[\phi,I\right] + \left[V_z,\psi\right] + \eta\nabla^2 I \end{cases}$$

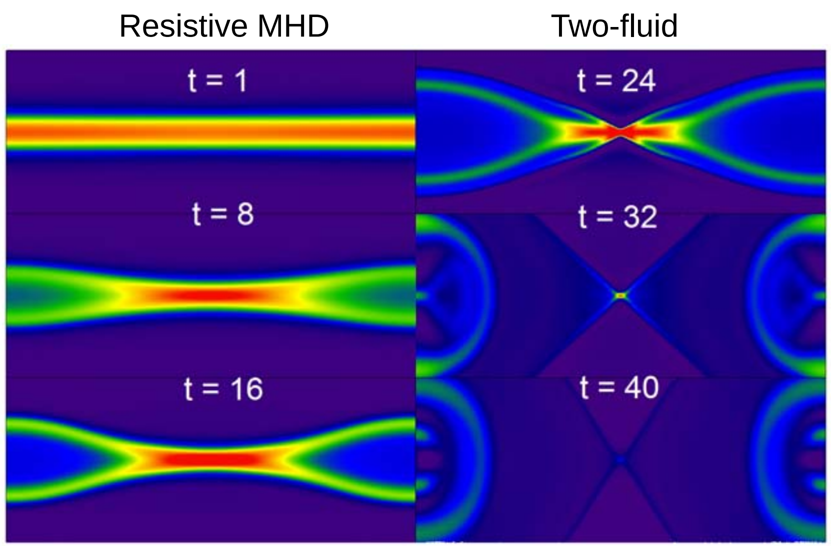
  This was verified with the GEM magnetic reconnection problem.

Reduced two-fluid

- Upgraded to two-fluid with addition of hall term, hyper-dissipation:

$$
\begin{cases}
\dfrac{\partial V_z}{\partial t} = [\phi, V_z] + [I, \psi] + \mu \nabla^2 V_z - \mu h \nabla^4 V_z \\
\dfrac{\partial \psi}{\partial t} = [\phi, \psi] + d_i [\psi, I] + \eta \nabla^2 \psi - \nu \nabla^4 \psi \\
\dfrac{\partial I}{\partial t} = [\phi, I] + d_i \left[\nabla^2 \psi, \psi\right] + [V_z, \psi] + \eta \nabla^2 I - \nu \nabla^4 I
\end{cases}
$$

Also verified with the GEM magnetic reconnection problem.



Full two-fluid equations

- Next, advanced to full two-fluid MHD by evolving density, energy. With

$$\mathbf{V} = \nabla U \times \hat{z} + \nabla \chi + V_z \hat{z},$$

the new equations are

$$\begin{cases} \dfrac{\partial n}{\partial t} + [n, U] + (n, \chi) + n\nabla^2 \chi = 0 \\ \dfrac{\partial p_\alpha}{\partial t} + [p_\alpha, U] + (p_\alpha, \chi) + \gamma p_\alpha \nabla^2 \chi = S_\alpha \end{cases}$$

- The pressure and density now appear in the momentum equation along with the Braginskii gyroviscous stress tensor:

$$n \frac{d\mathbf{V}}{dt} = -\nabla p - \nabla \cdot \Pi + \ldots$$

...which is then rewritten using the differential approximation

$$\left\{ n \frac{\partial}{\partial t} + (\Delta t)^2 \boldsymbol{\mathcal{L}} \right\} \mathbf{V} = -\nabla p - \nabla \cdot \Pi + \ldots$$

Implicit time advance

This enables a splitting of the eight-field equation time advance into separate operations with smaller block matrices:

velocity

$$\begin{bmatrix} S_{11}^v & S_{12}^v & S_{13}^v \\ S_{21}^v & S_{22}^v & S_{23}^v \\ S_{31}^v & S_{32}^v & S_{33}^v \end{bmatrix} \cdot \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n+1} = \begin{bmatrix} D_{11}^v & D_{12}^v & D_{13}^v \\ D_{21}^v & D_{22}^v & D_{23}^v \\ D_{31}^v & D_{32}^v & D_{33}^v \end{bmatrix} \cdot \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n} + \begin{bmatrix} R_{11}^v & R_{12}^v & R_{13}^v \\ R_{21}^v & R_{22}^v & R_{23}^v \\ R_{31}^v & R_{32}^v & R_{33}^v \end{bmatrix} \cdot \begin{bmatrix} \psi \\ I \\ p \end{bmatrix}^{n} + \begin{bmatrix} O_1^v \\ O_2^v \\ O_3^v \end{bmatrix}$$

followed by single-field updates of density and total pressure, and finally

$$\begin{bmatrix} S_{11}^b & S_{12}^b & S_{13}^b \\ S_{21}^b & S_{22}^b & S_{23}^b \\ S_{31}^b & S_{32}^b & S_{33}^b \end{bmatrix} \cdot \begin{bmatrix} \psi \\ I \\ p_e \end{bmatrix}^{n+1} = \begin{bmatrix} D_{11}^b & D_{12}^b & D_{13}^b \\ D_{21}^b & D_{22}^b & D_{23}^b \\ D_{31}^b & D_{32}^b & D_{33}^b \end{bmatrix} \cdot \begin{bmatrix} \psi \\ I \\ p_e \end{bmatrix}^{n} + \begin{bmatrix} R_{11}^b & R_{12}^b & R_{13}^b \\ R_{21}^b & R_{22}^b & R_{23}^b \\ R_{31}^b & R_{32}^b & R_{33}^b \end{bmatrix} \cdot \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n+1}$$

magnetic field,
electron pressure

$$+ \begin{bmatrix} Q_{11}^b & Q_{12}^b & Q_{13}^b \\ Q_{21}^b & Q_{22}^b & Q_{23}^b \\ Q_{31}^b & Q_{32}^b & Q_{33}^b \end{bmatrix} \cdot \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n} + \begin{bmatrix} O_1^b \\ O_2^b \\ O_3^b \end{bmatrix}$$

Also verified with the tilt mode and GEM magnetic reconnection problem.

2D Toroidal Option

- Now in (R, ϕ, z) coordinates, change variables using M3D-like formulation:

$$\mathbf{V} = R^2 \nabla U \times \nabla \varphi + \omega R^2 \nabla \varphi + R^{-2} \nabla_\perp \chi$$

$$\mathbf{B} = \nabla \times \mathbf{A} = \nabla \psi \times \nabla \varphi - \nabla_\perp f' + \left(F_0 + R^2 \nabla \cdot \nabla_\perp f \right) \nabla \varphi$$

and use projection operators to separate components:

incompressible component $\iint d^2 R \, \nu_i \nabla \varphi \cdot \nabla_\perp \times R^2 \quad \rightarrow \quad \iint d^2 R \, R^2 \nabla_\perp \nu_i \times \nabla \varphi \cdot$

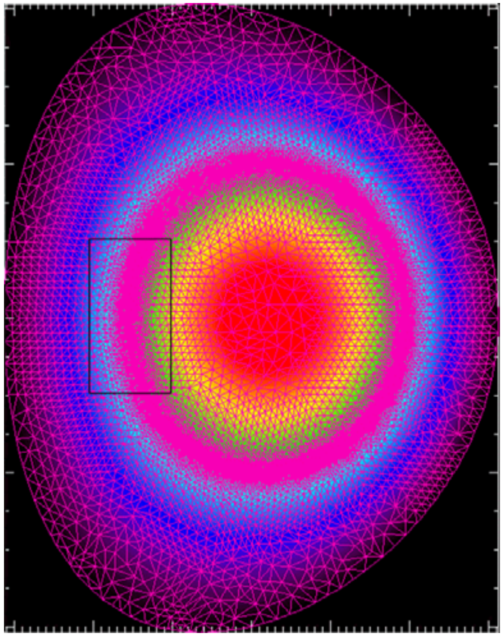
toroidal component $\iint d^2 R \, \nu_i R^2 \nabla \varphi \cdot \quad \rightarrow \quad \iint d^2 R \, \nu_i R^2 \nabla \varphi \cdot$

compressible component $-\iint d^2 R \, \nu_i \nabla_\perp \cdot R^{-2} \quad \rightarrow \quad \iint d^2 R \, R^{-2} \nabla_\perp \nu_i \cdot$

This version has been used to calculate tokamak equilibria with flow, including dissipative effects, parallel and gyroviscosity, and realistic heating, current drive, and particle sources.

Present Status: 3D Linear

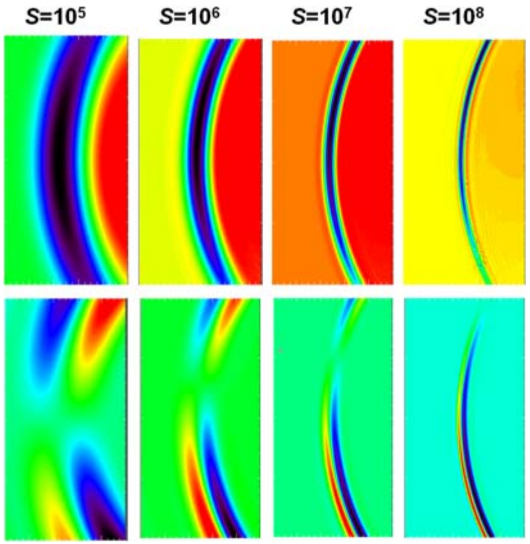
- Mesh has been generalized to fit triangles of arbitrary size and shape within arbitrary curved boundaries without impacting efficiency significantly.



- Complex perturbation with a single mode number is superimposed on a fixed real 2D equilibrium, advanced until convergence on eigenmode, e.g.

$$\dot{\tilde{\rho}} + \left[\rho_0, \tilde{U}\right] + \left(\rho_0, \tilde{\chi}\right) + \rho_0 \nabla^2 \tilde{\chi} + in\rho_0 \tilde{\omega} = 0$$

  - Matrix depends on equilibrium only; factored only once.
  - Validated against PEST, NOVA, ELITE, M3D.
  - Can access S up to 10^8.
  - Can use time steps up to 10 global Alfvén times, limited by accuracy.



Outline of Plans

- Extensions
  - Upgrade 3D linear option to eight-field equations with equilibrium flow.
    - Modify Grad-Shafranov solver to include flow
    - Linearize Hall terms, equilibrium flow terms
  - Add 3D elements to support 3D nonlinear option.
    - Reduced, two-field equations
    - Four-field
    - Eight-field
  - Optimize the 3D linear solvers.
  - Develop a hybrid option using gyrokinetic δf PIC routines adapted from M3D.

- Applications
  - Sawtooth
  - ELMs

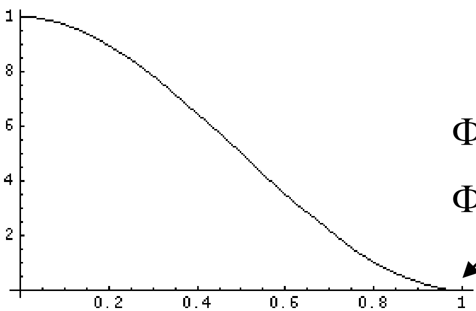
3D Basis Functions

Take tensor products of the Q_{18} 2D basis functions $Q_j(R, Z)$ on triangles with orthogonal Hermite cubic polynomial functions $\Phi_i(\phi)$, which have C^1 continuity:

$$\Phi_1(x) = \left(|x|-1\right)^2 \left(2|x|+1\right) \qquad \Phi_2(x) = x\left(|x|-1\right)^2$$

$\Phi_1(0) = 1$

$\Phi_1'(0) = 0$

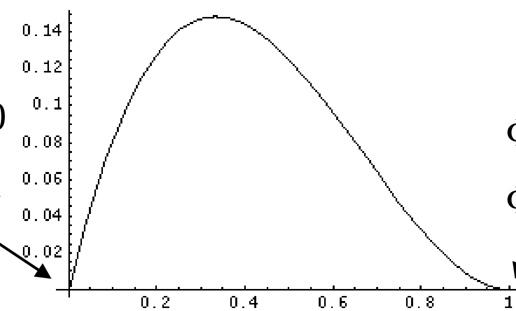


$\Phi_1(1) = 0$

$\Phi_1'(1) = 0$

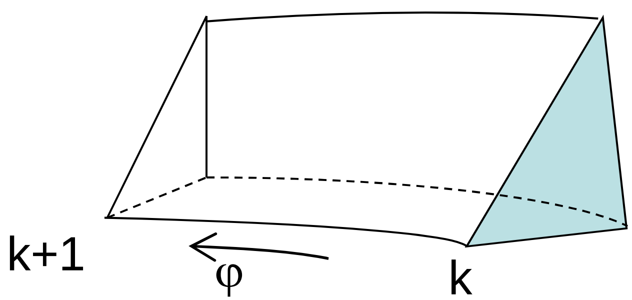
$\Phi_2(0) = 0$

$\Phi_2'(0) = 1$



$\Phi_2(1) = 0$

$\Phi_2'(1) = 0$



$$U(R,Z,\varphi) = \sum_{j=1}^{18} \nu_j(R,Z)\left[U_{j,k}^1 \Phi_1\left(\frac{\varphi}{h}\right) + U_{j,k}^2 \Phi_2\left(\frac{\varphi}{h}\right) + U_{j,k+1}^1 \Phi_1\left(1-\frac{\varphi}{h}\right) + U_{j,k+1}^2 \Phi_2\left(1-\frac{\varphi}{h}\right)\right]$$

Two-Field Version

- Beginning with the reduced system

$$[S]\cdot[U]^{n+1} = [D]\cdot[U]^{n} + [R]\cdot[\psi]^{n} + [O],$$

expand the vector U in terms of basis functions:

$$\dot{U} = \sum_{m=1}^{M}\sum_{q=1}^{2}\sum_{w=1}^{N}\sum_{j=1}^{18}\dot{U}_{w,j}^{m,q}\ \Phi_q^m(\varphi)\, Q_j^w(R,Z) = \sum_{m=1}^{M}\sum_{q=1}^{2}\left[\dot{\mathbf{U}}^{m,q}\right]\Phi_q^m(\varphi),$$

where $\left[\dot{\mathbf{U}}^{m,q}\right] = \sum_{w=1}^{N}\sum_{j=1}^{18}\dot{U}_{w,j}^{m,q} Q_j^w(R,Z)$ is the usual 2D function over plane m.

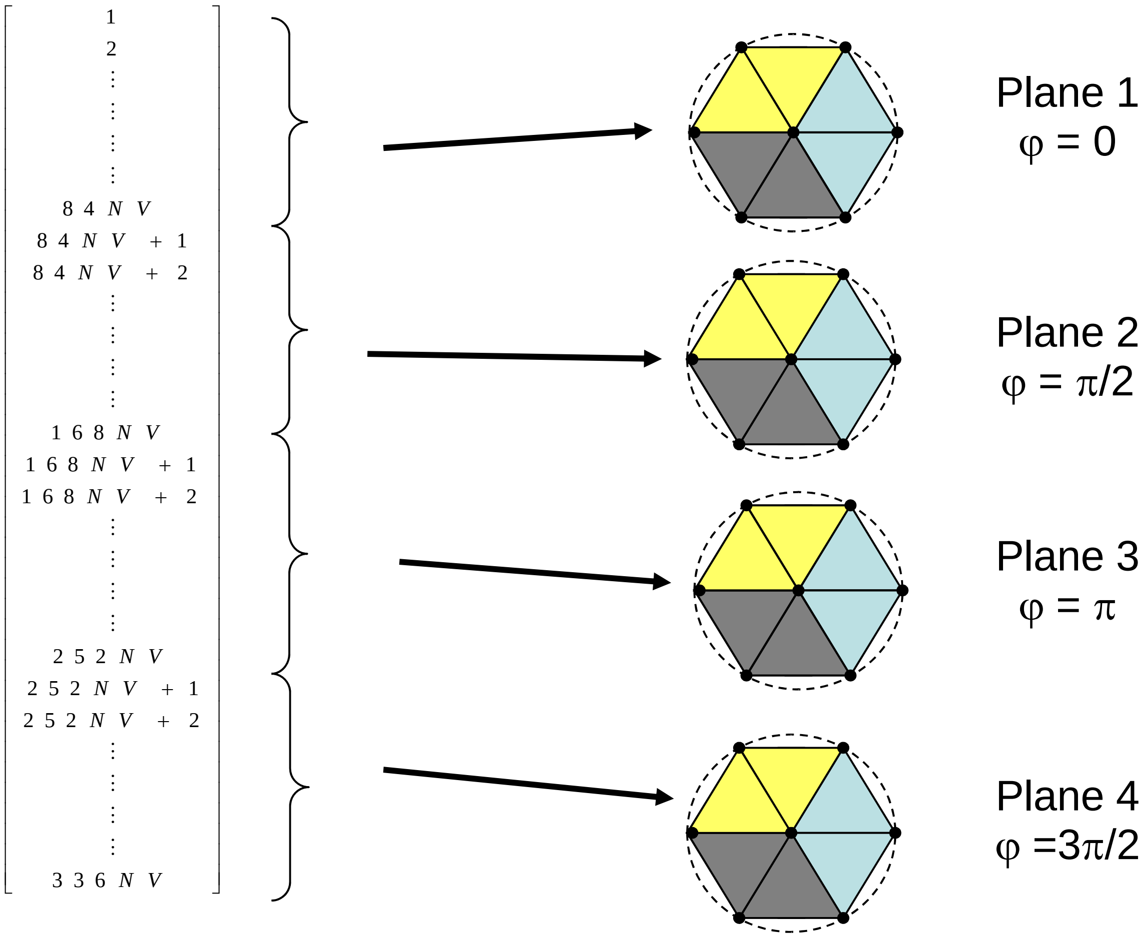
This results in a block stencil coupling neighboring planes:

$$\begin{bmatrix}
\bullet & \bullet & \bullet & \bullet & \mathbf{S}_{l-1,1}^{m,1} & \mathbf{S}_{l-1,1}^{m,2} & & & & \\
\bullet & \bullet & \bullet & \bullet & \mathbf{S}_{l-1,2}^{m,1} & \mathbf{S}_{l-1,2}^{m,2} & & & & \\
 & & \mathbf{S}_{l,1}^{m-1,1} & \mathbf{S}_{l,1}^{m-1,2} & \mathbf{S}_{l,1}^{m,1} & \mathbf{S}_{l,1}^{m,2} & \mathbf{S}_{l,1}^{m+1,1} & \mathbf{S}_{l,1}^{m+1,2} & & \\
 & & \mathbf{S}_{l,2}^{m-1,1} & \mathbf{S}_{l,2}^{m-1,2} & \mathbf{S}_{l,2}^{m,1} & \mathbf{S}_{l,2}^{m,2} & \mathbf{S}_{l,2}^{m+1,1} & \mathbf{S}_{l,2}^{m+1,2} & & \\
 & & & & \mathbf{S}_{l+1,1}^{m,1} & \mathbf{S}_{l+1,1}^{m,2} & \bullet & \bullet & \bullet & \bullet \\
 & & & & \mathbf{S}_{l+1,2}^{m,1} & \mathbf{S}_{l+1,2}^{m,2} & \bullet & \bullet & \bullet & \bullet
\end{bmatrix} \bullet \begin{bmatrix}
\bullet \\ \mathbf{U}^{m-1,1} \\ \mathbf{U}^{m-1,2} \\ \mathbf{U}^{m,1} \\ \mathbf{U}^{m,2} \\ \mathbf{U}^{m+1,1} \\ \mathbf{U}^{m+1,2} \\ \bullet
\end{bmatrix}$$

$$\mathbf{S}_{l,p}^{m,q} = \int_0^{2\pi} d\varphi\ \Phi_q^m(\varphi)\Phi_p^l(\varphi)\iint r\,dr\,dz\ Q_i^v(R,Z)Q_j^w(R,Z)$$

Domain Decomposition Example

NV=Number of Variables (1,2 or 3)



12 × NV DOF per node

Pictured here:

7 nodes per plane

4 planes

4 × 7 × 12 × NV = 336 NV DOF total

3 processors/plane × 4 = 12 processors total

Optimizing the 3D Solve

- Computing matrix elements is a local operation and should scale well with 3D domain decomposition.

- Solution of the linear equations is global and requires optimized solvers.
  - Using PETSc allows flexibility in choice of solver, options.
  - Precondition global solve with existing 2D solve in each plane?
  - ILU preconditioner based on near diagonal terms from 2D matrices?
  - Multigrid preconditioner in toroidal direction?

- Solicit advice from applied math collaborators in PETSc and TOPS.

A Hybrid Kinetic Option for M3D-C^1

- Adapt M3D's gyrokinetic δf PIC subroutines for hot particles.
  - Particle equations of motion are advanced on subcycles of the fluid time step using interpolated values of the magnetic field.
  - Particles couple back to fluid through kinetic stress tensor in momentum equation.
  - Consider energy-conserving symplectic integration technique to improve accuracy in particle push.

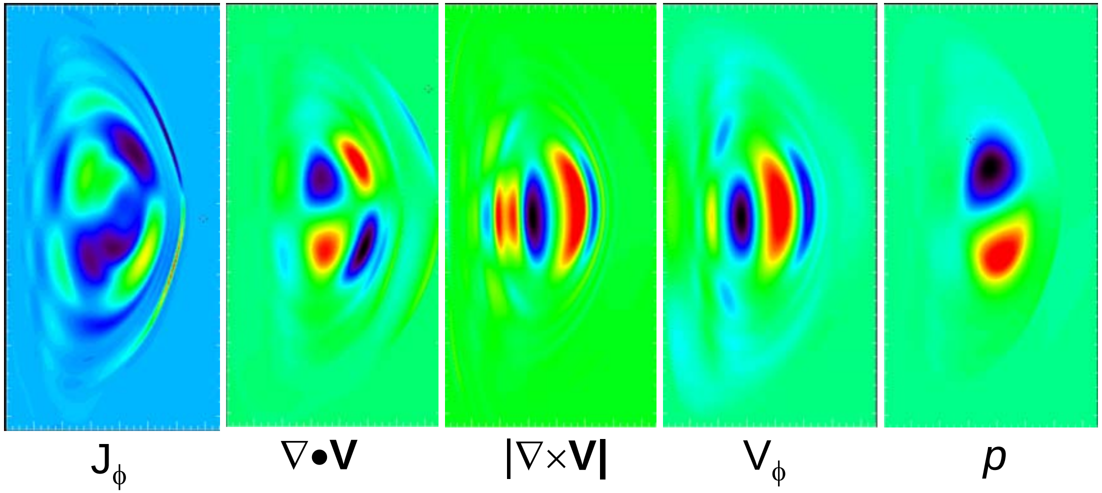
- A full f option may be considered for non-Maxwellian distributions.

- Optimize based on careful data organization and operation ordering.

- Benchmark with fishbone instability against NOVA-K and hybrid M3D.

Applications

- Linear version
  - Effects of two-fluid and flow terms on stability boundaries for ideal and non-ideal modes.



- Nonlinear version
  - Two-fluid sawtooth in high-*S* regime; giant sawteeth: kinetic effects
  - ELMs: mitigation strategies
  - Disruptions: vessel forces, currents
  - Tearing modes: destabilization by sawteeth