Numerical Analysis of The NIMROD Formulation

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KEY FEATURES OF NIMROD

- Designed to study mode-locking and disruptions; low-n, global, separatrix, resistive wall; nonlinear, time-dependent, realistic geometry and dynamics.
- Nation-wide collaboration, using **I**ntegrated **P**roduct **D**evelopment (IPD) and **Q**uality **F**unction **D**eployment (QFD).
- Graphic pre-processor, solver, and graphic post-processor all controlled by **G**raphical **U**ser **I**nterface (GUI).
- **O**bject-**O**riented **P**rogramming (OOP) using Fortran 90 for solver.
- Physics based on Quiet Implicit Pic (QIP) model: 2-fluid + δf particles + Maxwell. Braginskii++
- Spatial discretization uses multiple grid blocks, both logically rectangular and unstructured triangular. Finite elements, flux coordinates, domain decomposition. Designed for parallelization.
- Implicit time step, preconditioned congjugate gradients. Direct solution within blocks, CG over blocks.
- Web page: http:/www.nersc.gov/research/Nimrod
  User Name: mhd, Password: www4mhd.

NUMERICAL DANGERS

- **Large Truncation Error**
  Anisotropy can amplify error, as in the problem of spectral pollution found in eigenvalue codes.

- **The Red-Black Problem**
  Decoupling of adjacent grid nodes can introduce jitter.

- **Indefinite Matrices**
  Causes Conjugate Gradient Method to be unreliable.

- **Many Variables Per Node**
  Requires excessive run time and storage space.

- **Spurious Numerical Modes**
  Introduces noise and uncertainty.

- $\nabla \cdot \mathbf{B} \neq 0$

Two-Fluid Equations

$$\frac{\partial n_j}{\partial t} + \nabla \cdot (n_j \mathbf{v}_j) = 0$$

$$\rho_j \left(\frac{\partial \mathbf{v}_j}{\partial t} + \mathbf{v}_j \cdot \nabla \mathbf{v}_j \right) + \nabla P_j + \nabla \cdot \Pi_j = n_j q_j \left(\mathbf{E} + \frac{1}{c} \mathbf{v}_j \times \mathbf{B} \right) + \mathbf{R}_j$$

$$\frac{3}{2} \left(\frac{\partial P_j}{\partial t} + \mathbf{v}_j \cdot \nabla P_j \right) + \frac{5}{2} P_j \nabla \cdot \mathbf{v}_j + \nabla \cdot \mathbf{q}_j + \Pi_j : \nabla \mathbf{v}_j = Q_j$$

Maxwell's Equations

$$\nabla \cdot \mathbf{B} = \nabla \times \mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{B}}{\partial t} = 0$$

$$\mathbf{B} = \nabla \times \mathbf{A} \quad \mathbf{E} = -\nabla \varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}$$

$$\nabla^2 \mathbf{A} = -\frac{4\pi}{c} \mathbf{J}$$

$$\nabla \cdot \mathbf{A} = \nabla \cdot \mathbf{J} = 0$$

Constitutive Equations

$$\mathbf{J} = \sum_j \mathbf{J}_j = \sum_j n_j q_j \mathbf{v}_j$$

$\mathbf{q}$ and Π derived from particle moments

Finite Element Discretization

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

$$u(t, \mathbf{x}) = u_i(t)\alpha_i(\xi(\mathbf{x}), \eta(\mathbf{x}))$$

$$\mathcal{L} \equiv \int d\mathbf{x} \left[\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F} - S\right]^2, \quad \frac{\delta \mathcal{L}}{\delta(\partial u/\partial t)} = 0$$

$$(f, g) \equiv \int f(\mathbf{x})g(\mathbf{x})d\mathbf{x} = \int f(\xi, \eta)g(\xi, \eta)\mathcal{J}(\xi, \eta)d\xi d\eta$$

$$\mathcal{J} \equiv \frac{\partial x}{\partial \xi}\frac{\partial y}{\partial \eta} - \frac{\partial x}{\partial \eta}\frac{\partial y}{\partial \xi}$$

$$-(\alpha_i, \nabla \cdot \mathbf{F}) = \int d\mathbf{x}\mathbf{F} \cdot \nabla \alpha_i = \int d\xi d\eta \mathcal{J} \left(\mathbf{F} \cdot \nabla \xi \frac{\partial \alpha_i}{\partial \xi} + \mathbf{F} \cdot \nabla \eta \frac{\partial \alpha_i}{\partial \eta}\right)$$

$$(\alpha_i, \alpha_j)\dot{u}_j = \int d\xi d\eta \mathcal{J} \left(S\alpha_i + \mathbf{F} \cdot \nabla \xi \frac{\partial \alpha_i}{\partial \xi} + \mathbf{F} \cdot \nabla \eta \frac{\partial \alpha_i}{\partial \eta}\right)$$

Use Gaussian Quadrature Over Rblocks and Tblocks

EXACT CONSERVATION LAW

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{F} = 0$$

$$U(\Omega, t) \equiv \int_\Omega u(\mathbf{x}, t)\; d\mathbf{x}$$

$$\frac{dU(\Omega, t)}{dt} = -\int_{\partial\Omega} \mathbf{F} \cdot \hat{\mathbf{n}}\; d\mathbf{x}$$

FINITE ELEMENT CONSERVATION LAW

$$u(\mathbf{x}, t) = u_i(t)\alpha_i(\mathbf{x}), \quad (f, g) \equiv \int_V f(\mathbf{x})g(\mathbf{x})\; d\mathbf{x}$$

$$(\alpha_i, \alpha_j)\frac{du_j}{dt} = -(\alpha_i, \nabla \cdot \mathbf{F}) = \int_V \mathbf{F} \cdot \nabla\alpha_i\; d\mathbf{x}$$

$$U(\Omega, t) \equiv \int_\Omega u(\mathbf{x}, t)\varphi(\Omega, \mathbf{x})\; d\mathbf{x}$$

Ω bounded by grid lines, $\varphi(\Omega, \mathbf{x}) = \sum_i \alpha_i(\mathbf{x}) \to 0$ on $\partial\Omega$

$$\frac{dU(\Omega, t)}{dt} = \int_{\partial\Omega} \mathbf{F} \cdot \nabla\varphi(\Omega, \mathbf{x})\; d\mathbf{x}$$

Equation of Motion

$$\frac{\partial \mathbf{J}_j}{\partial t} + \Omega_j \hat{\mathbf{b}} \times \mathbf{J}_j = \frac{\omega_j^2}{4\pi}\mathbf{E}, \quad \Omega_j \equiv \frac{e_j B}{m_j c}, \quad \omega_j^2 \equiv \frac{4\pi n_j e_j^2}{m_j}$$

$$\frac{\mathbf{J}_j^{n+1} - \mathbf{J}_j^n}{\Delta t} + \Omega_j \hat{\mathbf{b}} \times \left[\mathbf{J}^n + f_\Omega(\mathbf{J}_j^{n+1} - \mathbf{J}_j^n)\right] = \frac{\omega_j^2}{4\pi}\mathbf{E}$$

$$\left\{(\lambda - 1)\mathsf{I} + \left[1 + f_\Omega(\lambda - 1)\right](\Omega_j \Delta t)\hat{\mathbf{b}} \times \mathsf{I}\right\} \cdot \mathbf{J}_j = \frac{\omega_j^2 \Delta t}{4\pi}\mathbf{E}$$

$$\mathbf{J}_j = \frac{c^2 \Delta t}{4\pi}\mathsf{L}_j \cdot \mathbf{E}$$

The L Matrix

$$\mathbf{J} = \frac{c^2 \Delta t}{4\pi} \mathsf{L} \cdot \mathbf{E}, \quad \mathsf{L} \equiv \sum_j \mathsf{L}_j$$

$$\mathsf{L}_j = L_{j,\parallel} \hat{\mathbf{b}}\hat{\mathbf{b}} + L_{j,\perp} (\mathsf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) - L_{j,\times} \hat{\mathbf{b}} \times \mathsf{I}$$

$$L_{j,\parallel} = \frac{(\omega_j/c)^2}{\lambda - 1}$$

$$L_{j,\perp} = \frac{(\omega_j/c)^2 (\lambda - 1)}{(\lambda - 1)^2 + \left[1 + f_\Omega(\lambda - 1)\right]^2 (\Omega_j \Delta t)^2}$$

$$L_{j,\times} = \frac{(\omega_j/c)^2 \left[1 + f_\Omega(\lambda - 1)\right] (\Omega_j \Delta t)}{(\lambda - 1)^2 + \left[1 + f_\Omega(\lambda - 1)\right]^2 (\Omega_j \Delta t)^2}$$

$$\text{For } (\Omega_j \Delta t)^2 \gg 1, \quad L_\parallel \approx \frac{\omega_p^2/c^2}{\lambda - 1}, \quad L_\perp \approx \frac{\lambda - 1}{\left[1 + f_\Omega(\lambda - 1)\right]^2 (c_A \Delta t)^2}$$

$$L_\parallel \gg L_\perp \gg L_\times, \quad \omega_p^2 \equiv \sum_j \omega_j^2, \quad \frac{c^2}{c_A^2} \equiv \sum_j \frac{\omega_j^2}{\Omega_j^2}$$

Curl-Curl Formulation

$$\nabla \times \mathbf{E} + \frac{1}{c}\frac{\partial \mathbf{B}}{\partial t} = 0, \quad \nabla \times \mathbf{B} = \frac{4\pi}{c}\mathbf{J}$$

$$\nabla \times \nabla \times \mathbf{E} + \frac{4\pi}{c}\frac{\partial \mathbf{J}}{\partial t} = \nabla\nabla \cdot \mathbf{E} - \nabla^2 \mathbf{E} + (\lambda - 1)\mathsf{L} \cdot \mathbf{E} = 0$$

$$\mathbf{E} = \mathbf{E}_0 e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \mathsf{D} \cdot \mathbf{E}_0 = \left[k^2 \mathsf{I} - \mathbf{k}\mathbf{k} + (\lambda - 1)\mathsf{L}\right] \cdot \mathbf{E}_0 = 0$$

$$\begin{aligned} D =& (\lambda - 1)\Big\{(\lambda - 1)^2 L_{\|}(L_{\perp}^2 + L_{\times}^2) + (\lambda - 1)\left[k_{\perp}^2(L_{\perp}^2 + L_{\times}^2) + (k^2 + k_{\|}^2)L_{\|}L_{\perp}\right] \\ & + k^2(k_{\|}^2 L_{\|} + k_{\perp}^2 L_{\perp})\Big\} \\ \approx& (\lambda - 1)L_{\|}\left[(\lambda - 1)L_{\perp} + k^2\right]\left[(\lambda - 1)L_{\perp} + k_{\|}^2\right] = 0 \end{aligned}$$

Factors into 3 waves:
Compressional Alfvén; Shear Alfvén;
Zero Frequency Electrostatic, $\nabla \times \mathbf{E} = 0$

Basic Implicit Dispersion Relation

$$(\lambda - 1)L_\perp + k_\parallel^2 \approx \frac{(\lambda-1)^2}{\left[1 + f(\lambda - 1)\right]^2 (c_A \Delta t)^2} + k_\parallel^2 = 0$$

$$x \equiv \lambda - 1 \approx i\omega\Delta t, \quad x_0 \equiv \omega_0 \Delta t, \quad \omega_0 \equiv c_A k_\parallel$$

$$x^2 + (1 + fx)^2 x_0^2 = 0$$

$$x = \frac{\pm i x_0 - f x_0^2}{1 + f^2 x_0^2}$$

For $f x_0 \ll 1, \quad x = \pm i x_0 (1 + i f x_0)(1 - f^2 x_0^2 + \cdots)$

For $f x_0 \gg 1, \quad x \approx -1/f$

$$\lambda = 1 + x = \frac{1 + f(f-1)x_0^2 \pm i x_0}{1 + f^2 x_0^2}$$

$$\Im \omega_0 = 0, \quad |\lambda|^2 \le 1 \quad \Leftrightarrow \quad f \ge 1/2$$

Finite Element Discretization

$$\nabla\nabla\cdot\mathbf{E}-\nabla^2\mathbf{E}+(\lambda-1)\mathsf{\mathbf{L}}\cdot\mathbf{E}=0$$

$$\mathbf{E}(\mathbf{x},t)=\sum_i\mathbf{E}_i(t)\alpha_i(\mathbf{x})$$

$$\mathbf{E}_i=\mathbf{E}_0\exp[i(\mathbf{k}\cdot\mathbf{x}_i-\omega t)]$$

$$\kappa\equiv\frac{\sum_j\exp[i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_i)]\int\alpha_i\nabla\alpha_j\mathbf{dx}}{i\sum_j\exp[i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_i)]\int\alpha_i\alpha_j\mathbf{dx}}$$

$$\mathsf{\mathbf{K}}\equiv-\frac{\sum_j\exp[i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_i)]\int\nabla\alpha_i\nabla\alpha_j\mathbf{dx}}{\sum_j\exp[i\mathbf{k}\cdot(\mathbf{x}_j-\mathbf{x}_i)]\int\alpha_i\alpha_j\mathbf{dx}}$$

$$\mathsf{\mathbf{D}}\cdot\mathbf{E}_0=[(\mathrm{tr}\ \mathsf{\mathbf{K}})\mathsf{\mathbf{I}}-\mathsf{\mathbf{K}}+(\lambda-1)\mathsf{\mathbf{L}}]\cdot\mathbf{E}_0=0$$

$$D\equiv\det\mathsf{\mathbf{D}}=0$$

Evaluation of κ and K

Uniform Grid in x-y Plane, Fourier in z, $\quad \kappa = \mathcal{I}_1/\mathcal{I}_0, \quad \mathsf{K} = \mathcal{I}_2/\mathcal{I}_0$

$$\mathcal{I}_0 \equiv \sum_j \exp[i\mathbf{k}\cdot(\mathbf{x}_j - \mathbf{x}_i)] \int \alpha_i \alpha_j d\mathbf{x}$$
$$= (4 + 2\cos k_x h_x + 2\cos k_y h_y + \cos k_x h_x \cos k_y h_y) h_x h_y / 9$$

$$\mathcal{I}_1 \equiv -i \sum_j \exp[i\mathbf{k}\cdot(\mathbf{x}_j - \mathbf{x}_i)] \int \alpha_i \nabla \alpha_j d\mathbf{x}$$
$$= [\hat{\mathbf{x}}(6 + 3\cos k_y h_y)\sin k_x h_x / h_x + \hat{\mathbf{y}}(6 + 3\cos k_x h_x)\sin k_y h_y / h_y$$
$$+ \hat{\mathbf{z}}(4 + 2\cos k_x h_x + 2\cos k_y h_y + \cos k_x h_x \cos k_y h_y) k_z] h_x h_y / 9$$

$$\mathcal{I}_2 \equiv -\sum_j \exp[i\mathbf{k}\cdot(\mathbf{x}_j - \mathbf{x}_i)] \int \nabla \alpha_i \nabla \alpha_j d\mathbf{x}$$
$$= [\hat{\mathbf{x}}\hat{\mathbf{x}}(12 + 6\cos k_y h_y)(1 - \cos k_x h_x)/h_x^2 + \hat{\mathbf{y}}\hat{\mathbf{y}}(12 + 6\cos k_x h_x)(1 - \cos k_y h_y)/h_y^2$$
$$+ \hat{\mathbf{z}}\hat{\mathbf{z}} k_z^2 (4 + 2\cos k_x h_x + 2\cos k_y h_y + \cos k_x h_x \cos k_y h_y)$$
$$+ (\hat{\mathbf{x}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{x}})(6 + 3\cos k_y h_y)(\sin k_x h_x / h_x) k_z + (\hat{\mathbf{y}}\hat{\mathbf{z}} + \hat{\mathbf{z}}\hat{\mathbf{y}})(6 + 3\cos k_x h_x)(\sin k_y h_y / h_y) k_z$$
$$+ 9(\hat{\mathbf{x}}\hat{\mathbf{y}} + \hat{\mathbf{y}}\hat{\mathbf{x}})(\sin k_x h_x / h_x)(\sin k_y h_y / h_y)] h_x h_y / 9$$

For $k_x h_x, \; k_y h_y \ll 1, \quad \kappa = \mathbf{k} - \frac{1}{180}\left[(k_x h_x)^4 k_x \hat{\mathbf{x}} + (k_y h_y)^4 k_y \hat{\mathbf{y}}\right] + \cdots,$

$$\mathsf{K} = \mathbf{k}\mathbf{k} + \frac{1}{12}\left[\hat{\mathbf{x}}\hat{\mathbf{x}} k_x^2 (k_x h_x)^2 + \hat{\mathbf{y}}\hat{\mathbf{y}} k_y^2 (k_y h_y)^2\right] + \cdots$$

Discretized Dispersion Relation, Curl-Curl Formulation

$$
\begin{aligned}
D \equiv{}& \det \mathsf{D} \\
={}&(\lambda-1)^3 L_{\|}(L_\perp^2 + L_\times^2) \\
&+ (\lambda-1)^2\Big\{L_{\|}L_\perp(\mathsf{I}+\hat{\mathbf{b}}\hat{\mathbf{b}}):\mathsf{K} + (L_\perp^2+L_\times^2)(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}}):\mathsf{K}\Big\} \\
&+ (\lambda-1)\Big\{L_{\|}\Big[(\mathsf{K}:\mathsf{I})(\hat{\mathbf{b}}\hat{\mathbf{b}}:\mathsf{K}) + \Big|\hat{\mathbf{b}}\hat{\mathbf{b}} + (\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}})\cdot\mathsf{K}\cdot(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}})\Big|\Big] \\
&\quad + L_\perp\Big[\mathsf{K}:(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}})(\mathsf{I}+\hat{\mathbf{b}}\hat{\mathbf{b}}):\mathsf{K} \\
&\qquad + \Big|(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}}) + (\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}})\cdot\mathsf{K}\cdot\hat{\mathbf{b}}\hat{\mathbf{b}} + \hat{\mathbf{b}}\hat{\mathbf{b}}\cdot\mathsf{K}\cdot(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}})\Big|\Big]\Big\} \\
&- \Big|\mathsf{K} - (\mathrm{tr}\ \mathsf{K})\mathsf{I}\Big| \\
\approx{}&(\lambda-1)L_{\|}\Big\{\Big[(\lambda-1)L_\perp + \mathrm{tr}\ \mathsf{K}\Big]\Big[(\lambda-1)L_\perp + \hat{\mathbf{b}}\cdot\mathsf{K}\cdot\hat{\mathbf{b}}\Big] \\
&\quad + \det\Big[\hat{\mathbf{b}}\hat{\mathbf{b}} + (\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}})\cdot\mathsf{K}\cdot(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}})\Big]\Big\} = 0
\end{aligned}
$$

The last line is a truncation error which vanishes in the continuous limit $\mathsf{K} \to \mathbf{kk}$. It couples the fast and slow waves and prevents accurate representation of low-frequency shear Alfvén modes with $\hat{\mathbf{b}}\cdot\mathsf{K}\cdot\hat{\mathbf{b}} \to 0$. Related to spectral pollution in spectral codes.

Coulomb Gauge Formulation

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \quad \nabla \cdot \mathbf{A} = 0$$

$$\nabla^2 \mathbf{A} = -\frac{4\pi}{c}\mathbf{J}, \quad \nabla \cdot \mathbf{J} = 0, \quad \mathbf{J} = \frac{c^2 \Delta t}{4\pi}\mathsf{L} \cdot \mathbf{E}$$

$$\mathsf{L} \cdot [(\lambda - 1)\mathbf{A} + (c\Delta t)\nabla\varphi] - \nabla^2 \mathbf{A} = 0,$$
$$\nabla \cdot \{\mathsf{L} \cdot [(\lambda - 1)\mathbf{A} + (c\Delta t)\nabla\varphi]\} = 0$$

$$(\mathbf{A}, \varphi) = (\mathbf{A}_0, \varphi_0)e^{i\mathbf{k}\cdot\mathbf{x}}$$

$$\mathsf{L} \cdot [(\lambda - 1)\mathbf{A} + (c\Delta t)i\mathbf{k}\varphi] + k^2 \mathbf{A} = 0$$
$$\mathbf{k} \cdot \mathsf{L} \cdot [(\lambda - 1)\mathbf{A} + (c\Delta t)i\mathbf{k}\varphi] = 0$$

$$\mathbf{u} \equiv (\mathbf{A}_0, ic\Delta t\ \varphi_0), \quad \mathsf{D} \cdot \mathbf{u} = 0$$

$$\begin{aligned} D \equiv \det \mathsf{D} = 0 = k^4 \Big\{ & L_\parallel \left(L_\perp^2 + L_\times^2\right)(\lambda - 1)^2 \\ & + \left[k_\perp^2 \left(L_\perp^2 + L_\times^2\right) + (k^2 + k_\parallel^2) L_\parallel L_\perp\right](\lambda - 1) + k^2 \left(k_\parallel^2 L_\parallel + k_\perp^2 L_\perp\right)\Big\} \\ \approx & k^4 L_\parallel \left[L_\perp(\lambda - 1) + k^2\right]\left[L_\perp(\lambda - 1) + k_\parallel^2\right] \end{aligned}$$

First Discretized Coulomb Gauge Formulation

$$(\mathbf{A},\varphi)(\mathbf{x},t)=\sum_i(\mathbf{A}_i,\varphi_i)(t)\alpha_i(\mathbf{x}),\quad (\mathbf{A}_i,\varphi_i)=(\mathbf{A}_0,\varphi_0)e^{i\mathbf{k}\cdot\mathbf{x}_i}$$

$$[(\lambda-1)\mathsf{L}+(\mathrm{tr}\ \mathsf{K})\mathsf{I}]\cdot\mathbf{A}_0+\kappa(ic\Delta t)\varphi_0=0,$$

$$(\lambda-1)\kappa\cdot\mathsf{L}\cdot\mathbf{A}_0+(\mathsf{L}:\mathsf{K})(ic\Delta t)\varphi_0=0$$

$$\mathbf{u}\equiv[\mathbf{A}_0,(ic\Delta t)\varphi_0],\quad \mathsf{D}\cdot\mathbf{u}=0$$

$$\begin{aligned}
D\equiv\det\mathsf{D}&=(\lambda-1)^3L_{\|}(L_\perp^2+L_\times^2)\mathsf{L}:(\mathsf{K}-\kappa\kappa)\\
&+(\lambda-1)^2(\mathrm{tr}\ \mathsf{K})\Big\{(\mathrm{tr}\ \mathsf{K})L_{\|}(L_\perp^2+L_\times^2)+2\hat{\mathbf{b}}\hat{\mathbf{b}}:(\mathsf{K}-\kappa\kappa)L_{\|}^2L_\perp\\
&\quad+(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}}):(\mathsf{K}-\kappa\kappa)\left[L_\perp^2(L_\perp+L_{\|})+L_\times^2(L_\perp-L_{\|})\right]\\
&\quad-[\mathrm{tr}\ (\hat{\mathbf{b}}\times\mathsf{K})]L_\times(L_\perp^2+L_\times^2+2L_\perp L_{\|})\Big\}\\
&+(\lambda-1)(\mathrm{tr}\ \mathsf{K})^2\Big\{(L_\perp^2+L_\times^2)(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}}):\mathsf{K}\\
&\quad+L_{\|}\left[2L_\perp\hat{\mathbf{b}}\hat{\mathbf{b}}:\mathsf{K}+(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}}):(\mathsf{L}\cdot\mathsf{K})\right]+\mathrm{tr}\ (\mathsf{L}\cdot\mathsf{K}\cdot\mathsf{L})\Big\}+(\mathrm{tr}\ \mathsf{K})^3\mathsf{L}:\mathsf{K}=0
\end{aligned}$$

Truncation errors are amplified by higher powers of $L_{\|}$, producing large errors.
Cause: Ampére's Law and Quasineutrality contain inconsistent expressions for $E_{\|}$.

Second Discretized Coulomb Gauge Formulation

$$(\mathbf{A},\varphi,\mathbf{J})(\mathbf{x},t)=\sum_i(\mathbf{A}_i,\varphi_i,\mathbf{J}_i)(t)\alpha_i(\mathbf{x}),\quad(\mathbf{A}_i,\varphi_i,\mathbf{J}_i)=(\mathbf{A}_0,\varphi_0,\mathbf{J}_0)e^{i\mathbf{k}\cdot\mathbf{x}_i}$$

$$\frac{4\pi}{c}\mathbf{J}_0=-\mathsf{L}\cdot\left[(\lambda-1)\mathbf{A}_0+\kappa(ic\Delta t)\varphi_0\right],\quad\frac{4\pi}{c}\mathbf{J}_0-(\mathrm{tr}\ \mathsf{K})\mathbf{A}_0=0,\quad\kappa\cdot\mathbf{J}_0=0$$

$$\mathsf{L}\cdot[(\lambda-1)\mathbf{A}_0+\kappa(ic\Delta t)\varphi_0]+(\mathrm{tr}\ \mathsf{K})\mathbf{A}_0=0,$$
$$\kappa\cdot\mathsf{L}\cdot[(\lambda-1)\mathbf{A}_0+\kappa(ic\Delta t)\varphi_0]=0$$

$$\mathbf{u}\equiv[\mathbf{A}_0,(ic\Delta t)\varphi_0],\quad\mathsf{D}\cdot\mathbf{u}=0$$

$$D\equiv\det\mathsf{D}=(\mathrm{tr}\ \mathsf{K})\Big\{(\lambda-1)^2\kappa^2L_\parallel\left(L_\perp^2+L_\times^2\right)+(\lambda-1)(\mathrm{tr}\ \mathsf{K})$$
$$\times\left[\kappa_\perp^2\left(L_\perp^2+L_\times^2\right)+(\kappa^2+\kappa_\parallel^2)L_\parallel L_\perp\right]+(\mathrm{tr}\ \mathsf{K})^2\left(\kappa_\parallel^2L_\parallel+\kappa_\perp^2L_\perp\right)\Big\}$$
$$\approx(\mathrm{tr}\ \mathsf{K})\kappa^2L_\parallel\left[L_\perp(\lambda-1)+(\mathrm{tr}\ \mathsf{K})\right]\left[L_\perp(\lambda-1)+(\mathrm{tr}\ \mathsf{K})\kappa_\parallel^2/\kappa^2\right]=0$$

Discretization of **J** eliminates inconsistency and amplification of truncation error.
But $\kappa=0$ for $k_xh_x=k_yh_y=\pi$, Red-Black Problem.

Third Discretized Coulomb Gauge Formulation

$$(\mathbf{A}, \varphi, J_{\|})(\mathbf{x}, t) = \sum_i (\mathbf{A}, \varphi, J)_i(t)\alpha_i(\mathbf{x}), \quad (\mathbf{A}, \varphi, J)_i(t) = (\mathbf{A}, \varphi, J)_0(t)e^{i\mathbf{k}\cdot\mathbf{x}_i}$$

$$\frac{4\pi}{c} J_0 = -L_{\|}\left[(\lambda - 1)A_{\|,0} + \kappa_{\|}(ic\Delta t)\varphi_0\right]$$

$$(\mathrm{tr}\ \mathsf{K})\mathbf{A}_0 + \mathsf{L} \cdot (\mathsf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) \cdot [(\lambda - 1)\mathbf{A}_0 + \kappa(ic\Delta t)\varphi_0] = 0$$
$$+ \hat{\mathbf{b}}L_{\|}\left[(\lambda - 1)A_{\|,0} + \kappa_{\|}(ic\Delta t)\varphi_0\right] = 0,$$
$$\kappa \cdot \mathsf{L} \cdot (\mathsf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) \cdot (\lambda - 1)\mathbf{A}_0 + \mathrm{tr}\ [\mathsf{K} \cdot (\mathsf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) \cdot \mathsf{L}](ic\Delta t)\varphi_0$$
$$+ \kappa_{\|}L_{\|}\left[(\lambda - 1)A_{\|,0} + \kappa_{\|}(ic\Delta t)\varphi_0\right] = 0$$

$$\mathbf{u} \equiv [\mathbf{A}_0, (ic\Delta t)\varphi_0], \quad \mathsf{D} \cdot \mathbf{u} = 0$$

$$D \equiv \det \mathsf{D} \approx L_{\|}\Big\{(\lambda - 1)^3 L_{\perp}^3 \left(\mathrm{tr}\ \mathsf{K}_{\perp} - \kappa_{\perp}^2\right)$$
$$+ (\lambda - 1)^2 L_{\perp}^2 (\mathrm{tr}\ \mathsf{K}) \left[\kappa^2 + 2\left(\mathrm{tr}\ \mathsf{K}_{\perp} - \kappa_{\perp}^2\right)\right]$$
$$+ (\lambda - 1)L_{\perp}(\mathrm{tr}\ \mathsf{K})^2 \left(2\kappa_{\|}^2 + \mathrm{tr}\ \mathsf{K}_{\perp}\right) + (\mathrm{tr}\ \mathsf{K})^3\kappa_{\|}^2\Big\} = 0$$

No amplification of error, no Red-Black Problem.
But spurious high-frequency mode, 5 variables per node, and non-SPD matrix.

Magnetic Formulation

$$\frac{4\pi}{c}\mathbf{J} = \nabla\times\mathbf{B} = (c\Delta t)\mathsf{L}\cdot\mathbf{E}, \quad (c\Delta t)\mathbf{E} = \mathsf{L}^{-1}\cdot\nabla\times\mathbf{B}$$

$$\mathsf{M} \equiv \mathsf{L}^{-1} = \frac{\hat{\mathbf{b}}\hat{\mathbf{b}}}{L_{||}} + \frac{L_\perp(\mathsf{I}-\hat{\mathbf{b}}\hat{\mathbf{b}}) + L_\times\hat{\mathbf{b}}\times\mathsf{I}}{L_\perp^2 + L_\times^2}$$

$$\frac{\partial\mathbf{B}}{\partial t} + c\nabla\times\mathbf{E} = 0, \quad (\lambda-1)\mathbf{B} + (c\Delta t)\nabla\times\mathbf{E} = 0$$

$$(\lambda-1)\mathbf{B} + \nabla\times(\mathsf{M}\cdot\nabla\times\mathbf{B}) = 0$$

$$\mathbf{B} = \mathbf{B}_0 e^{i\mathbf{k}\cdot\mathbf{x}}, \quad \mathsf{D}\cdot\mathbf{B}_0 = 0, \quad \mathsf{D} = (\lambda-1)\mathsf{I} - \mathbf{k}\times(\mathsf{M}\cdot\mathbf{k}\times\mathsf{I})$$

$$\begin{aligned} D \equiv \det\mathsf{D} = (\lambda-1)\Big\{&(\lambda-1)^2 + (\lambda-1)\left[M_\perp(k^2+k_{||}^2) + M_{||}k_\perp^2\right] \\ &+ k^2\left[(M_\perp^2+M_\times^2)k_{||}^2 + M_\perp M_{||}k_\perp^2\right]\Big\} \\ \approx&(\lambda-1)\left[(\lambda-1)+M_\perp k_{||}^2\right]\left[(\lambda-1)+M_\perp k^2\right] = 0 \end{aligned}$$

Magnetic Formulation, Discretized Dispersion Relation

$$D \approx \left[(\lambda - 1) + M_\perp(\hat{\mathbf{b}}\hat{\mathbf{b}} : \mathsf{K})\right] \left\{(\lambda - 1)\left[(\lambda - 1) + M_\perp((\mathrm{tr}\ \mathsf{K}))\right] + M_\perp^2 \left[(\hat{\mathbf{b}}\hat{\mathbf{b}} : \mathsf{K})\mathsf{K} : (\mathsf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) - \hat{\mathbf{b}} \cdot \mathsf{K} \cdot (\mathsf{I} - \hat{\mathbf{b}}\hat{\mathbf{b}}) \cdot \mathsf{K} \cdot \hat{\mathbf{b}}\right]\right\}$$

- The use of $\mathsf{M} = \mathsf{L}^{-1}$ rather than L in the magnetic formulation implies that truncation errors associated with the parallel direction are suppressed rather than amplified.

- The slow, shear Alfvén wave factors out and is therefore unaffected by truncation error.

- The fast and zero-frequency waves are coupled. The effect on the fast wave is negligible. The effect on the zero-frequency wave is neglible if large gradients are aligned with the grid.

- $\nabla \cdot \mathbf{B}$ does not vanish exactly, but is acceptably small if large gradients are aligned with the grid.

Divergence of B

$$\mathbf{B} = \sum_i \mathbf{B}_i \alpha_i(\mathbf{x}), \quad \mathbf{B}_i = \mathbf{B}_0 e^{i\mathbf{k}\cdot\mathbf{x}_i}, \quad \hat{\mathbf{b}} \equiv \mathbf{B}_0/B_0$$

$$\hat{\mathbf{e}}_1 \equiv \frac{\mathbf{k}}{k}, \quad \hat{\mathbf{e}}_2 \equiv \frac{\hat{\mathbf{z}} \times \mathbf{k}}{|\hat{\mathbf{z}} \times \mathbf{k}|}, \quad \hat{\mathbf{e}}_3 \equiv \hat{\mathbf{e}}_1 \times \hat{\mathbf{e}}_2, \quad \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = \delta_{i,j}$$

$$\hat{\mathbf{b}} = \hat{\mathbf{e}}_2 \cos\phi + \hat{\mathbf{e}}_3 \sin\phi, \quad \mathbf{k} \cdot \hat{\mathbf{b}} = 0$$

$$\epsilon \equiv \frac{\int d\mathbf{x}\, |\nabla \cdot \mathbf{B}|^2}{\int d\mathbf{x} |\mathbf{B}|^2} = \hat{\mathbf{b}} \cdot \mathsf{K} \cdot \hat{\mathbf{b}}$$

$$\epsilon \approx \Big[k_x^2 k_y^2 (k_x^2 h_x^2 + k_y^2 h_y^2) \cos^2\phi + 2 k_x k_y \frac{k_z}{k} (k_x^4 h_x^2 - k_y^4 h_y^2) \sin\phi \cos\phi$$
$$+ \frac{k_z^2}{k^2} \left(k_x^6 h_x^2 + k_y^6 h_y^2 \right) \sin^2\phi \Big] / 12 (k_x^2 + k_y^2)$$

$$k_x \gg k_y, k_z \quad \Rightarrow \quad \epsilon \sim k_y^2 (k_x^2 h_x^2 + k_y^2 h_y^2)$$

Conclusions

- The NIMROD finite element formulation rests is on a solid analytical footing, confirmed by numerical experience.

- The flux coordinate grid plays a major role in avoiding numerical difficulties.

- The triangular core block avoids problems associated with a coordinate system pole at the o-point. A similar solution can be used for x-point.

- The magnetic formulation avoids all known numerical problems.