Grad-Shafranov Refinement Using High-Order Spectral Elements

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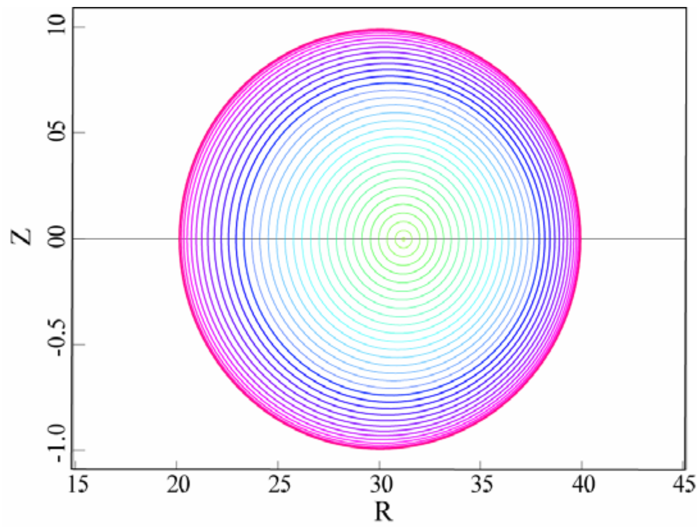
Grad-Shafranov Refinement

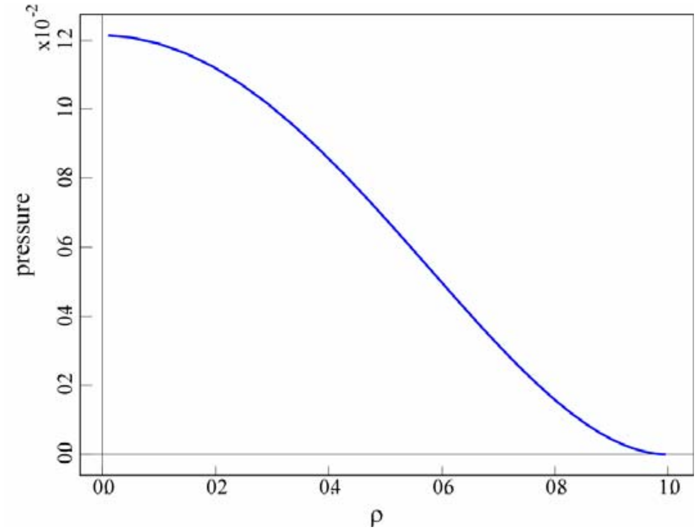
- DCON reads equilibria from 20 different Grad-Shafranov solvers, both direct and inverse.
- It processes all equilibria into internal inverse form.
- Almost all equilibria are accurate enough for ideal stability analysis.
- Resistive stability analysis is much more sensitive to imperfections. Most equilibria are not accurate enough.
- Goal: Develop a fast, accurate iterative Grad-Shafranov solver to refine a pretty good equilibrium into a very accurate one.
- Application of spectral element code: high accuracy, advanced numerical methods.

Resistive DCON: Simple Test Case

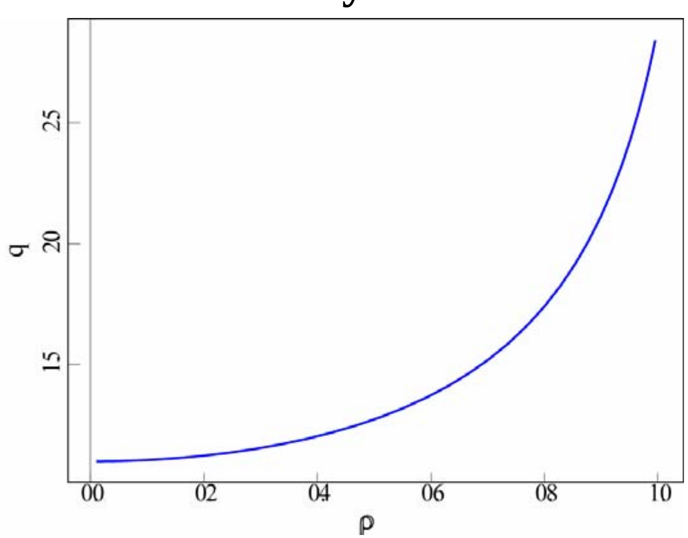
Flux Surfaces



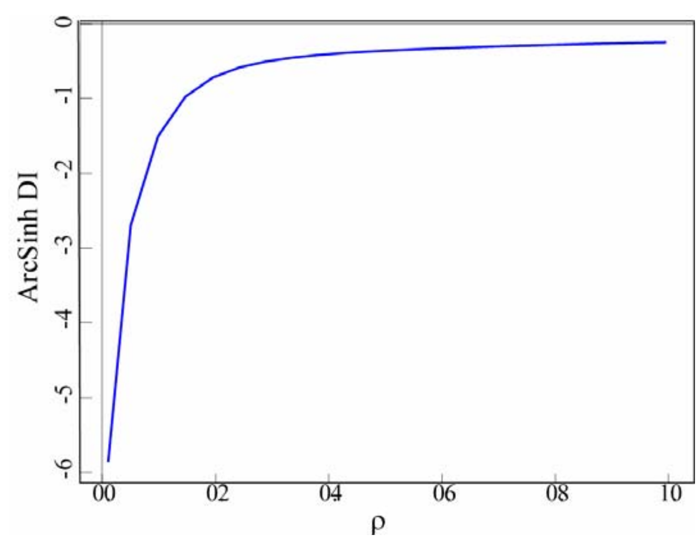
Pressure Profile



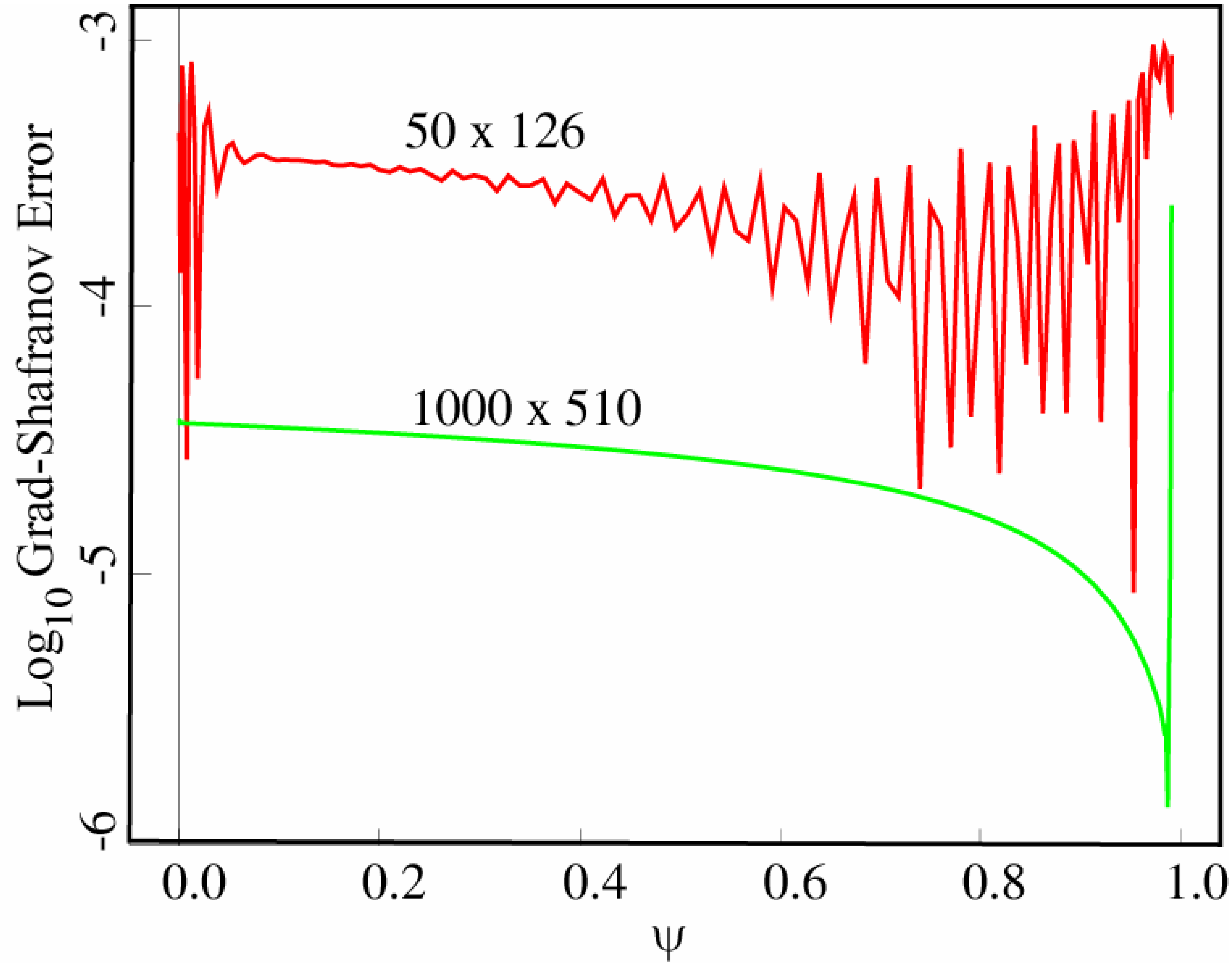
Safety Factor



Mercier Criterion

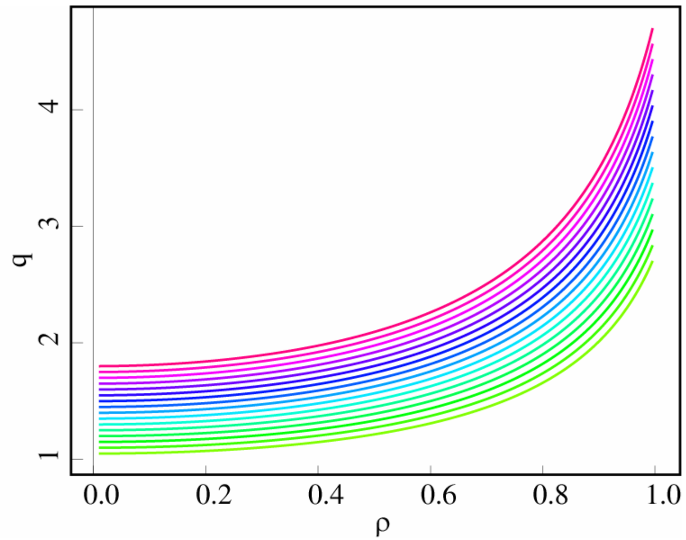


Coarse and Fine Equilibria

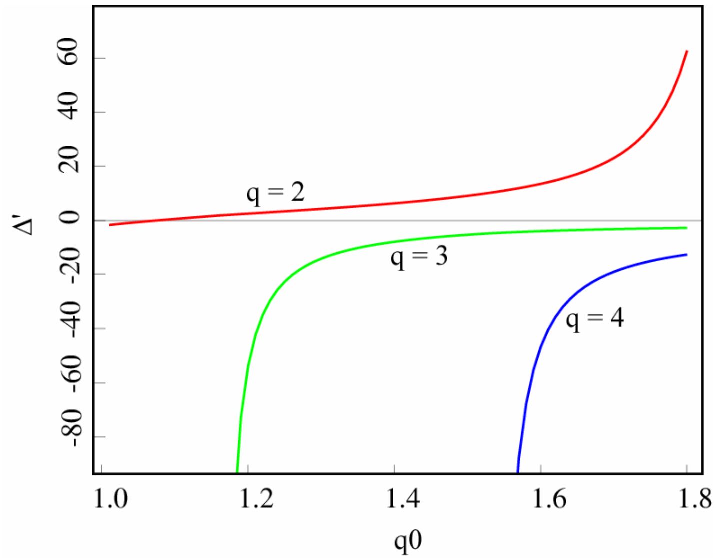


Sensitivity to Numerical Equilibrium Quality

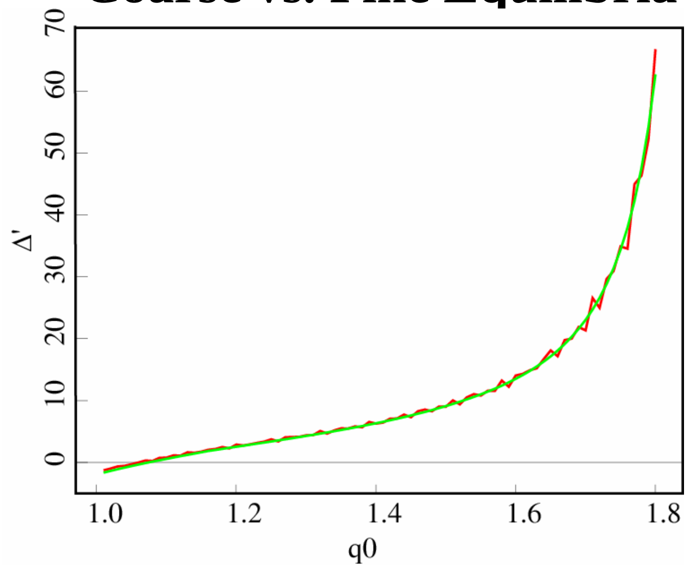
Safety Factor Profiles



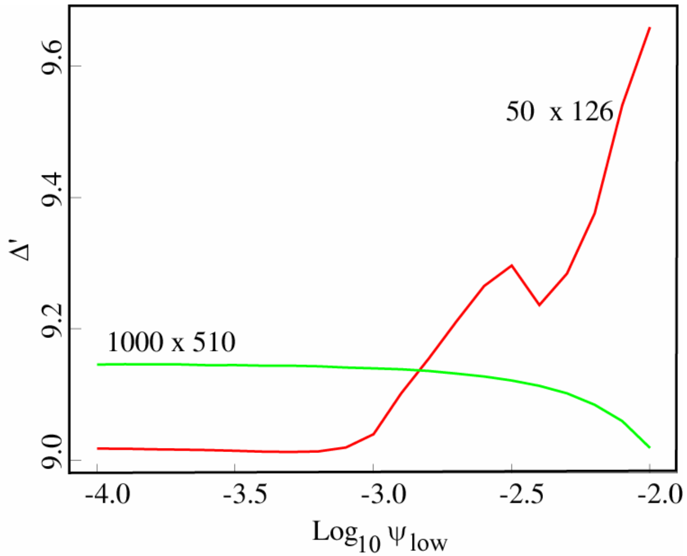
Resistive Stability Results



Coarse vs. Fine Equilibria



Coarse vs. Fine Equilibria



SEL Code Features

- Spectral elements: exponential convergence of spatial truncation error + adaptive grid + parallelization.
  - George Em Karniadakis and Spencer J. Sherwin, "Spectral/*hp* Element Methods for CFD," Oxford, 1999.
  - Ronald D. Henderson, "Adaptive spectral element methods for turbulence and transition," in *High-Order Methods for Computational Physics*, T.J. Barth & H. Deconinck (Eds.), Springer, 1999.
- Grid alignment with evolving magnetic field + adaptation to regions of sharp gradients
- Time step: fully implicit, 2^{nd}-order accurate, static condensation preconditioning, Newton-Krylov iteration or parallel direct.
- Highly efficient massively parallel operation with MPI and PETSc.
- Flux-source form: simple, general problem setup.

Spatial Discretization

Flux-Source Form of Equations

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

$$\mathbf{F}^i = \mathbf{F}^i(t, \mathbf{x}, u^j, \nabla u^j)$$

$$S^i = S^i(t, \mathbf{x}, u^j, \nabla u^j)$$

Galerkin Expansion

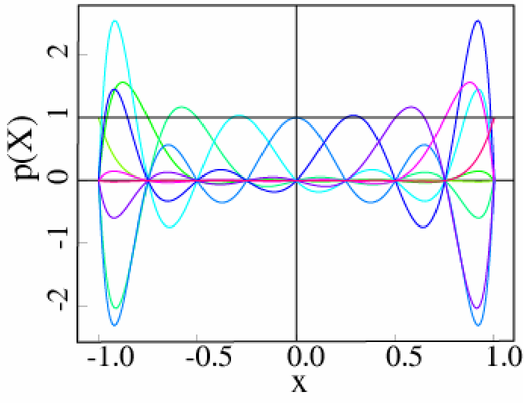
$$u^i(t, \mathbf{x}) \approx \sum_{j=0}^{n} u^i_j(t)\alpha_j(\mathbf{x})$$

Weak Form of Equations

$$(\alpha_i, \alpha_j)\dot{u}^k_j = \int_\Omega d\mathbf{x} \left(S^k \alpha_i + \mathbf{F}^k \cdot \nabla \alpha_i \right) - \int_{\partial\Omega} d\mathbf{x} \alpha_i \mathbf{F}^k \cdot \hat{\mathbf{n}}$$

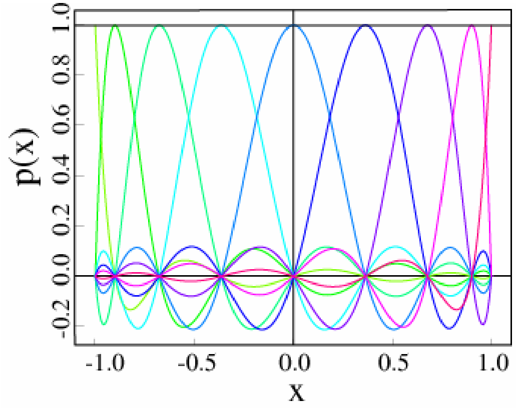
Alternative Polynomial Bases

Uniform Nodal Basis



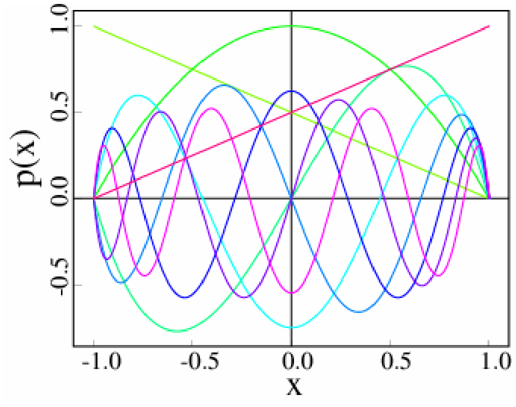
- Lagrange interpolatory polynomials
- Uniformly-spaced nodes
- Diagonally subdominant

Jacobi Nodal Basis



- Lagrange interpolatory polynomials
- Nodes at roots of $(1-x^2)\, P_n^{(0,0)}(x)$
- Diagonally dominant

Spectral (Modal) Basis



- Jacobi polynomials $(1+x)/2$, $(1-x)/2$, $(1-x^2)\, P_n^{(1,1)}(x)$
- Nearly orthogonal
- Manifest exponential convergence

Fully Implicit Time Step: Theta Scheme

$$\mathbf{M}\dot{\mathbf{u}} = \mathbf{r}$$

$$\mathbf{M}\left(\frac{\mathbf{u}^{+} - \mathbf{u}^{-}}{h}\right) = \theta\mathbf{r}^{+} + (1-\theta)\mathbf{r}^{-}$$

$$\mathbf{R}\left(\mathbf{u}^{+}\right) \equiv \mathbf{M}\left(\mathbf{u}^{+} - \mathbf{u}^{-}\right) - h\left[\theta\mathbf{r}^{+} + (1-\theta)\mathbf{r}^{-}\right] = 0$$

$$\mathbf{J} \equiv \mathbf{M} - h\theta\left\{\frac{\partial r_i^{+}}{\partial u_j^{+}}\right\}$$

$$\mathbf{R} + \mathbf{J}\delta\mathbf{u}^{+} = 0, \quad \delta\mathbf{u}^{+} = -\mathbf{J}^{-1}\mathbf{R}\left(\mathbf{u}^{+}\right), \quad \mathbf{u}^{+} \rightarrow \mathbf{u}^{+} + \delta\mathbf{u}^{+}$$

- Nonlinear Newton iteration.
- Elliptic equations: **M** = 0.
- Static condensation, fully parallel.
- PETSc: Krylov (GMRES) with Schwarz ILU, overlap of 3, fill-in of 5; or parallel LU.

Static Condensation

$$\mathbf{L}\mathbf{u} = \mathbf{r} \tag{1}$$

Partition: (1) element edges: (2) element interiors

$$\mathbf{u} = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix}, \quad \mathbf{r} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{pmatrix}, \quad \mathbf{L} = \begin{pmatrix} \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{pmatrix} \tag{2}$$

$$\begin{aligned} \mathbf{L}_{11}\mathbf{u}_1 + \mathbf{L}_{12}\mathbf{u}_2 &= \mathbf{r}_1 \\ \mathbf{L}_{21}\mathbf{u}_1 + \mathbf{L}_{22}\mathbf{u}_2 &= \mathbf{r}_2 \end{aligned} \tag{3}$$

$$\mathbf{L}_{22}\mathbf{u}_2 = \mathbf{r}_2 - \mathbf{L}_{21}\mathbf{u}_1 \tag{4}$$

$$\begin{aligned} \bar{\mathbf{L}}_{11} &\equiv \mathbf{L}_{11} - \mathbf{L}_{12}\mathbf{L}_{22}^{-1}\mathbf{L}_{21} \\ \bar{\mathbf{r}}_1 &\equiv \mathbf{r}_1 - \mathbf{L}_{12}\mathbf{L}_{22}^{-1}\mathbf{r}_2 \end{aligned} \tag{5}$$

$$\bar{\mathbf{L}}_{11}\mathbf{u}_1 = \bar{\mathbf{r}}_1 \tag{6}$$

- Equation (4) solved by local LU factorization and back substitution.
- Equation (6), substantially reduced, solved by global Newton-Krylov.

Inverse Grad-Shafranov Equation

$$\psi = \psi_0 \rho^2, \quad \psi_\rho = 2\psi_0 \rho, \quad \mathcal{J} \equiv \left(\nabla\rho \times \nabla\theta \cdot \nabla\phi\right)^{-1}$$

$$\Delta^* \psi = -f \frac{df}{d\psi} - R^2 \frac{dp}{d\psi}$$

$$\begin{aligned}
\Delta^* \psi \equiv & \nabla \cdot \left(\frac{1}{R^2} \nabla \psi \right) \\
= & \frac{1}{\mathcal{J}} \left\{ \frac{\partial}{\partial \rho} \left[\frac{\psi_\rho}{\mathcal{J}} \left(\frac{\partial R}{\partial \theta} \frac{\partial R}{\partial \theta} + \frac{\partial Z}{\partial \theta} \frac{\partial Z}{\partial \theta} \right) \right] \right. \\
& \left. - \frac{\partial}{\partial \theta} \left[\frac{\psi_\rho}{\mathcal{J}} \left(\frac{\partial R}{\partial \theta} \frac{\partial R}{\partial \rho} + \frac{\partial Z}{\partial \theta} \frac{\partial Z}{\partial \rho} \right) \right] \right\}
\end{aligned}$$

$$\frac{f}{R^2} \frac{df}{d\psi} + \frac{dp}{d\psi} = \frac{1}{\psi_\rho} \left(\frac{f}{R^2} \frac{df}{d\rho} + \frac{dp}{d\rho} \right)$$

Jacobian Specification

$$\begin{aligned}
v \equiv & \nabla \cdot \left(\frac{R^2}{2} \nabla Z \times \nabla \phi \right) \\
= & \frac{1}{\mathcal{J}} \frac{\partial}{\partial \rho} \left(\frac{R^2}{2} \frac{\partial Z}{\partial \theta} \right) - \frac{1}{\mathcal{J}} \frac{\partial}{\partial \theta} \left(\frac{R^2}{2} \frac{\partial Z}{\partial \rho} \right) \\
= & \frac{R}{\mathcal{J}(\rho, \theta)} \left(\frac{\partial R}{\partial \rho} \frac{\partial Z}{\partial \theta} - \frac{\partial R}{\partial \theta} \frac{\partial Z}{\partial \rho} \right) = 1
\end{aligned}$$

Parabolic Equations, Pseudo-Time

$$\frac{\partial \psi}{\partial t} = \nabla \cdot \left(\frac{1}{R^2} \nabla \psi \right) + \frac{f}{R^2} \frac{df}{d\psi} + \frac{dp}{d\psi}$$

$$\frac{\partial v}{\partial t} = -(v - 1)$$

Integral Relations, Relaxation

$$\frac{d}{dt} \int_\Omega \frac{1}{2} \psi^2 d\mathbf{x} = \int_\Omega \left[-\frac{|\nabla \psi|^2}{R^2} + \psi \left(\frac{f}{R^2} \frac{df}{d\psi} + \frac{dp}{d\psi} \right) \right] d\mathbf{x} + \int_{\partial\Omega} \frac{\psi}{R^2} \hat{\mathbf{n}} \cdot \nabla \psi d\mathbf{x}$$

$$\frac{d}{dt} \int_\Omega \frac{1}{2} (v-1)^2 d\mathbf{x} = -\int_\Omega (v-1)^2 d\mathbf{x}$$

Time Derivatives

$$\frac{\partial \psi}{\partial t} = \frac{\psi_\rho R}{\mathcal{J}} \left(\frac{\partial R}{\partial t} \frac{\partial Z}{\partial \theta} - \frac{\partial Z}{\partial t} \frac{\partial R}{\partial \theta} \right)$$

$$\begin{aligned} \frac{\partial v}{\partial t} = & \frac{1}{\mathcal{J}(\rho,\theta)} \left[\frac{\partial R}{\partial t} \left(\frac{\partial R}{\partial \rho} \frac{\partial Z}{\partial \theta} - \frac{\partial R}{\partial \theta} \frac{\partial Z}{\partial \rho} \right) \right. \\ & \left. + R \left(\frac{\partial^2 R}{\partial \rho \partial t} \frac{\partial Z}{\partial \theta} + \frac{\partial R}{\partial \rho} \frac{\partial^2 Z}{\partial \theta \partial t} - \frac{\partial^2 R}{\partial \theta \partial t} \frac{\partial Z}{\partial \rho} - \frac{\partial R}{\partial \theta} \frac{\partial^2 Z}{\partial \rho \partial t} \right) \right] \end{aligned}$$

Flux-Source Form

$$u^j \equiv (R, Z), \quad \xi^k \equiv (\rho, \theta), \quad u^j(\xi^k, t) = u_i^j(t)\alpha^i(\xi^k)$$

$$(u, v) \equiv \int uv \; d\mathbf{x} = \int uv \; \mathcal{J} \; d\rho \; d\theta \; d\phi = 2\pi \int uv \; \mathcal{J} \; d\rho \; d\theta$$

$$j = 1: \quad \left(\alpha^i, \frac{\partial \psi}{\partial t} - \nabla \cdot \left(\frac{1}{R^2}\nabla\psi\right) - \frac{f}{R^2}\frac{df}{d\psi} - \frac{dp}{d\psi}\right) = 0$$

$$j = 2: \quad \left(\alpha^i, \frac{\partial v}{\partial t} + (v-1)\right) = 0$$

$$M_{jk}^{il}\dot{u}_l^k + \frac{\partial F_j^{il}}{\partial \xi^l} = S_j^i$$

Mass Matrix

$$M_{11}^{il} = \int \psi_\rho R Z_\theta \alpha^i \alpha^l \; d\rho \; d\theta$$

$$M_{12}^{il} = -\int \psi_\rho R R_\theta \alpha^i \alpha^l \; d\rho \; d\theta$$

$$M_{21}^{il} = \int \alpha_i \left[\left(R_\rho Z_\theta - R_\theta Z_\rho\right)\alpha_j + R Z_\theta \alpha_{j,\rho} - R Z_\rho \alpha_{j,\theta}\right] \; d\rho \; d\theta$$

$$M_{22}^{il} = -\int \alpha_i \left[R R_\theta \alpha_{j,\rho} - R R_\rho \alpha_{j,\theta}\right] \; d\rho \; d\theta$$

Fluxes

$$F_1^{i1} = -\int \left(R_\theta^2 + Z_\theta^2\right) \frac{\partial \alpha^i}{\partial \rho} \frac{\psi_\rho}{\mathcal{J}} \; d\rho \; d\theta$$

$$F_1^{i2} = \int \left(R_\rho R_\theta + Z_\rho Z_\theta\right) \frac{\partial \alpha^i}{\partial \theta} \frac{\psi_\rho}{\mathcal{J}} \; d\rho \; d\theta$$

$$F_2^{i1} = \int \frac{R^2}{2} \frac{\partial Z}{\partial \theta} \frac{\partial \alpha^i}{\partial \rho} \; d\rho \; d\theta$$

$$F_2^{i2} = -\int \frac{R^2}{2} \frac{\partial Z}{\partial \rho} \frac{\partial \alpha^i}{\partial \theta} \; d\rho \; d\theta$$

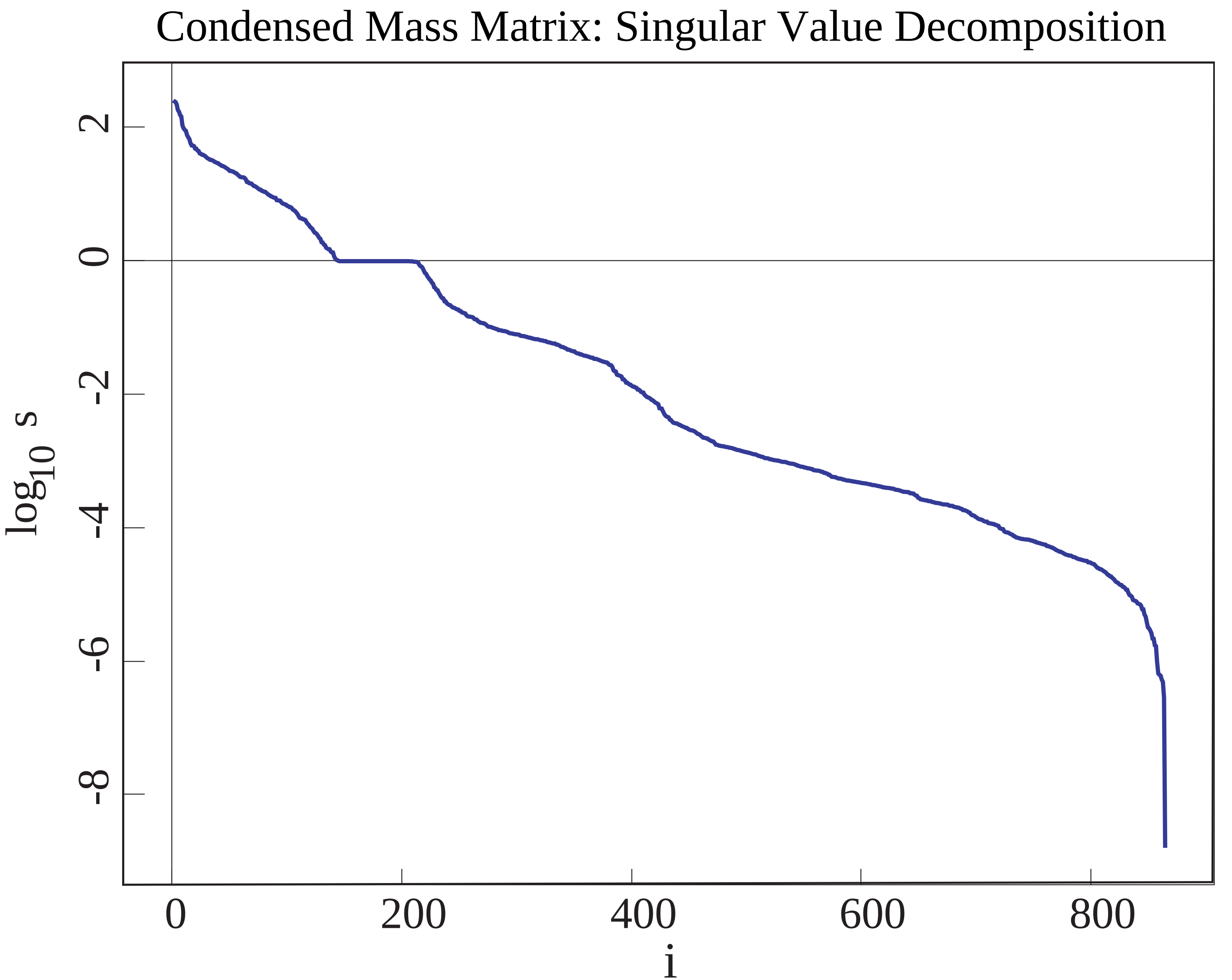
Sources

$$S_1^i = \int \left(\frac{f}{R^2} \frac{df}{d\rho} + \frac{dp}{d\rho}\right) \alpha^i \frac{\mathcal{J}}{\psi_\rho} \; d\rho \; d\theta$$

$$S_2^i = \int \alpha^i \; \mathcal{J} \; d\rho \; d\theta$$

Problem: Mass Matrix Has Huge Condition Number

C = 1.6×10^{11}, Amplifies Errors, Inhibits Convergence



Other Attempted Treatments

- **Newton Iteration**
  - Drop mass matrix, solve as static root finding
  - Noise in initial conditions inhibits convergence
- **Line Search with Backtracking**
  - Globally convergent Newton iteration
  - Reduces length of Newton correction while keeping direction.
  - Converges from poor initial conditions, far from root
  - Doesn’t help with noisy initial conditions
- **Filter Initial Conditions**
  - Suppress high-order spectral elements in initial conditions.
  - Has little effect on SVD spectrum of mass matrix.
  - Increases initial Grad-Shafranov error, inhibits convergence.

Conclusions and Status

- Resistive DCON works correctly but requires highly accurate Grad-Shafranov solution.
- Spectral element code seems like a natural method.
- Parabolic formulation of GSEQ, relaxation, flux-source form.
- Unforeseen numerical problems caused by unavoidable noise in initial conditions, inhibit convergence.
- Direct solve?
- Advice welcome.