Progress in the Development of the SEL Macroscopic Modeling Code

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SEL Code Features

- Spectral elements: exponential convergence of spatial truncation error.
- Adaptive grid: alignment with evolving magnetic field + adaptive grid packing normal to field
- Fully implicit, 2nd-order time step, Newton-Krylov iteration, static condensation preconditioning.
- Highly efficient massively parallel operation with MPI and PETSc.
- Flux-source form: simple, general problem setup.
- AVS and XDRAW visualization

New Developments

- Static condensation highly successful.
- Speed increased by a factor of 1000.
- Significant improvements made in 1D adaptive gridding. Slava Lukin.
- Major progress made in formulating grid alignment with the evolving magnetic field.

Spatial Discretization

Flux-Source Form of Equations

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

$$\mathbf{F}^i = \mathbf{C}^i(t, \mathbf{x}, u^j) - \mathbf{D}^{i,k}(t, \mathbf{x}, u^j) \cdot \nabla u^k$$

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

Galerkin Expansion

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

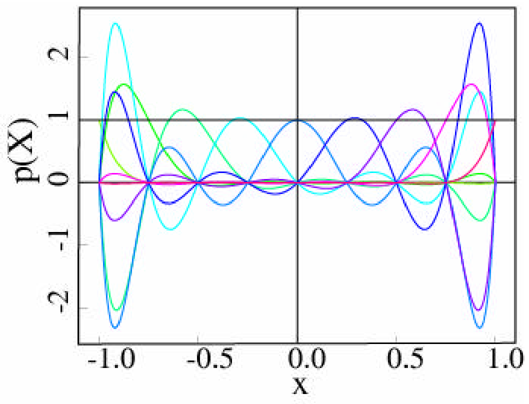
Weak Form of Equations

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

Alternative Polynomial Bases

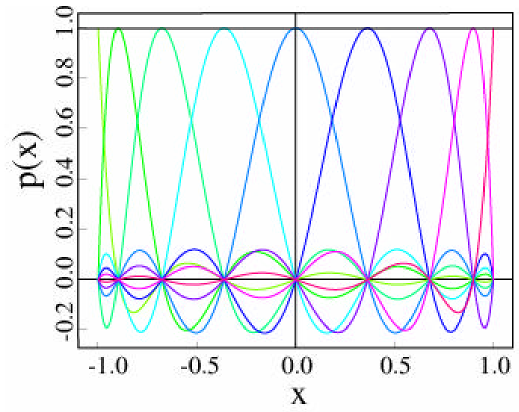
Ronald D. Henderson, "Adaptive spectral element methods for turbulence and transition," in *High-Order Methods for Computational Physics*, T.J. Barth & H. Deconinck (Eds.), Springer, 1999.

Uniform Nodal Basis



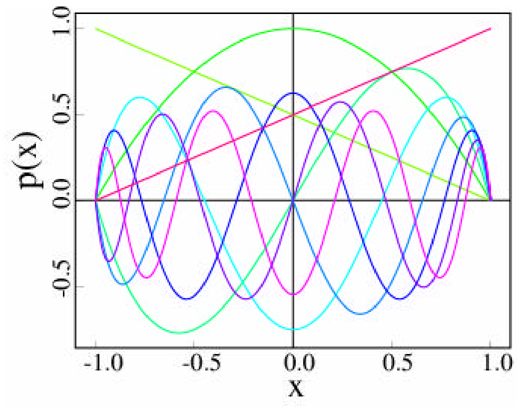
- Lagrange interpolatory polynomials
- Uniformly-spaced nodes
- Diagonally subdominant

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 Newton-Krylov Time Step

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

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

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

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

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

- Nonlinear Newton-Krylov iteration.
- Elliptic equations: $\mathbf{M} = 0$.
- Static condensation, fully parallel.
- PETSc: GMRES with Schwarz ILU, overlap of 3, fill-in of 5.

Preconditioning with 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.

Incompressible Magnetic Reconnection

$$\mathbf{B} = B_0\hat{\mathbf{z}} + \hat{\mathbf{z}} \times \nabla\psi, \quad j \equiv \hat{\mathbf{z}} \cdot \nabla \times \mathbf{B} = \nabla^2\psi$$

$$\mathbf{v} = \hat{\mathbf{z}} \times \nabla\varphi, \quad \omega \equiv \hat{\mathbf{z}} \cdot \nabla \times \mathbf{v} = \nabla^2\varphi$$

$$\frac{\partial\psi}{\partial t} + \mathbf{v} \cdot \nabla\psi = \eta\nabla^2\psi + S_\psi$$

$$\frac{\partial\omega}{\partial t} + \mathbf{v} \cdot \nabla\omega = \mu\nabla^2\omega + \mathbf{B} \cdot \nabla j + S_\omega$$

Flux-Source Form

$$\frac{\partial\psi}{\partial t} + \nabla \cdot [(\psi\hat{\mathbf{z}} \times \nabla\varphi - \psi_0\hat{\mathbf{z}} \times \nabla\varphi_0) - \eta\nabla(\psi - \psi_0)] = 0$$

$$\begin{aligned} \frac{\partial\omega}{\partial t} &+ \nabla \cdot [(\omega\hat{\mathbf{z}} \times \nabla\varphi - \omega_0\hat{\mathbf{z}} \times \nabla\varphi_0) \\ &- (j\hat{\mathbf{z}} \times \nabla\psi - j_0\hat{\mathbf{z}} \times \nabla\psi_0) - \mu\nabla(\omega - \omega_0)] = 0 \end{aligned}$$

$$j = \nabla^2\psi, \quad \nabla^2\varphi = \omega$$

Initial Conditions

$$-L_x/2 \le x \le L_x/2, \quad -1/2 \le y \le 1/2$$
$$k_x = 2\pi/L_x, \quad k_y = \pi, \quad k^2 \equiv k_x^2 + k_y^2$$

$$\psi(x,y,0) = A\left[\psi_0(y) + \epsilon\psi_1(x,y)\right]$$
$$\psi_0(y) \equiv \lambda_\psi \ln\cosh(y/\lambda_\psi)$$
$$\psi_1(x,y) \equiv -\cos(k_x x)\cos(k_y y)/k^2$$
$$j(x,y,0) = \nabla^2\psi(x,y,0)$$

$$\varphi(x,y,0) = M\left[\varphi_0(y) + \epsilon\varphi_1(x,y)\right]$$
$$\varphi_0(y) \equiv \lambda_\varphi \ln\cosh(y/\lambda_\varphi)$$
$$\varphi_1(x,y) \equiv -\cos(k_x x)\cos(k_y y)/k^2$$
$$\omega(x,y,0) = \nabla^2\varphi(x,y,0)$$

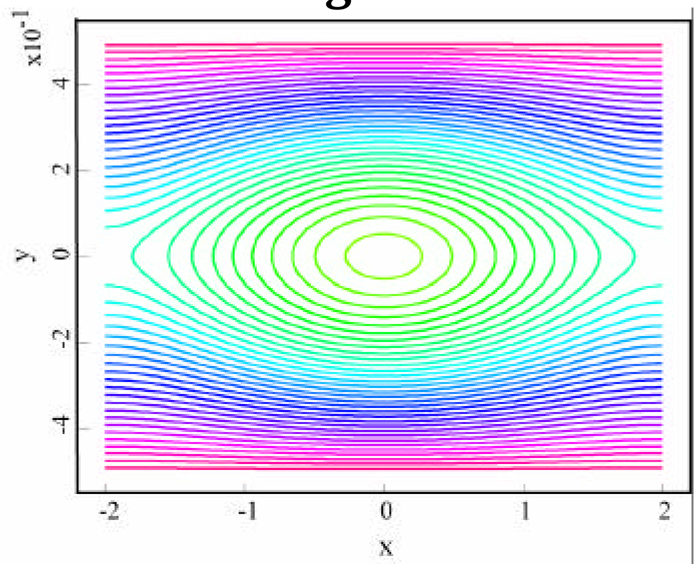
Boundary Conditions

Periodic in x

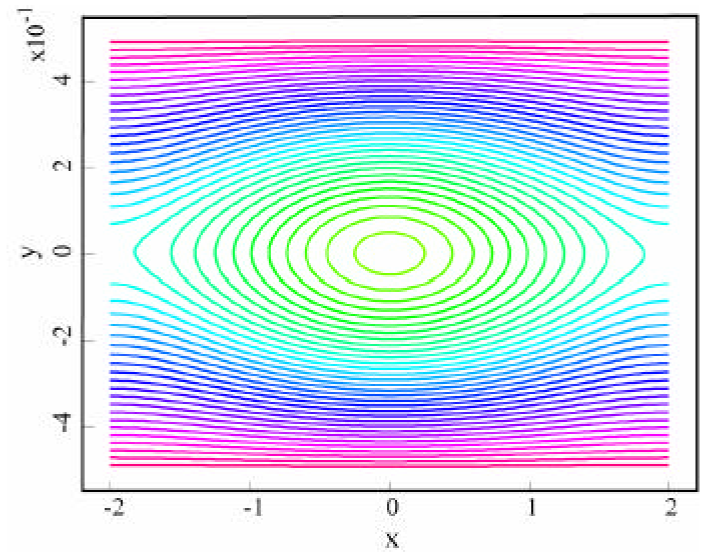
$$\psi(x,\pm 1/2,t) = \psi_0(x,\pm 1/2)$$
$$j(x,\pm 1/2,t) = \nabla^2\psi(x,y,t)|_{y=\pm 1/2}$$
$$\varphi(x,\pm 1/2,t) = \varphi_0(x,\pm 1/2)$$
$$\omega(x,\pm 1/2,t) = \nabla^2\varphi(x,y,t)|_{y=\pm 1/2}$$

Magnetic Reconnection, Final State

Magnetic Flux



Stream Function



$A = 1$

$M = 1/2$

$\eta = 10^{-4}$

$\mu = 10^{-4}$

$\varepsilon = 10^{-4}$

$dt = 20$

$nx = 6$

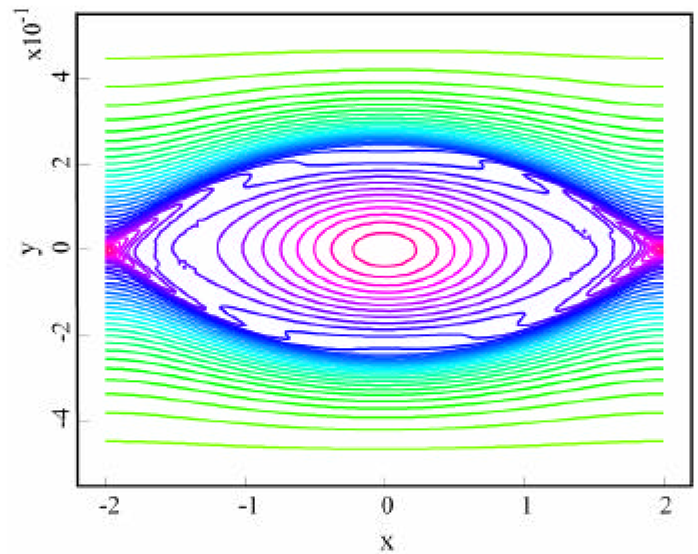
$ny = 16$

$np = 12$

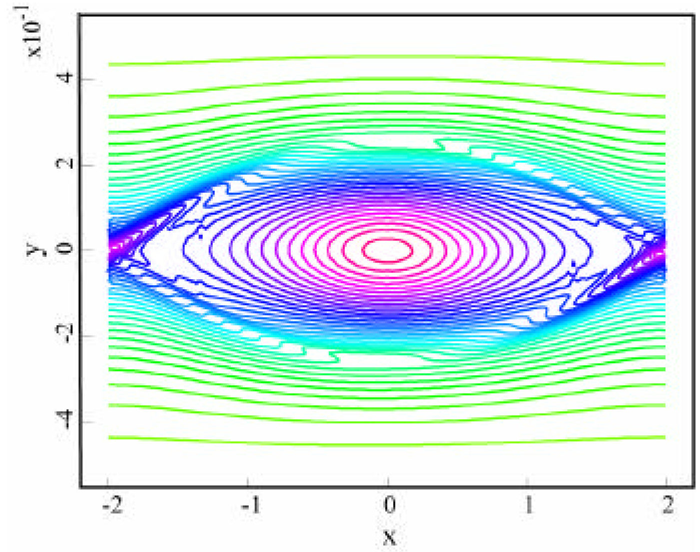
$nproc = 16$

$cpu = 3.5$ hr

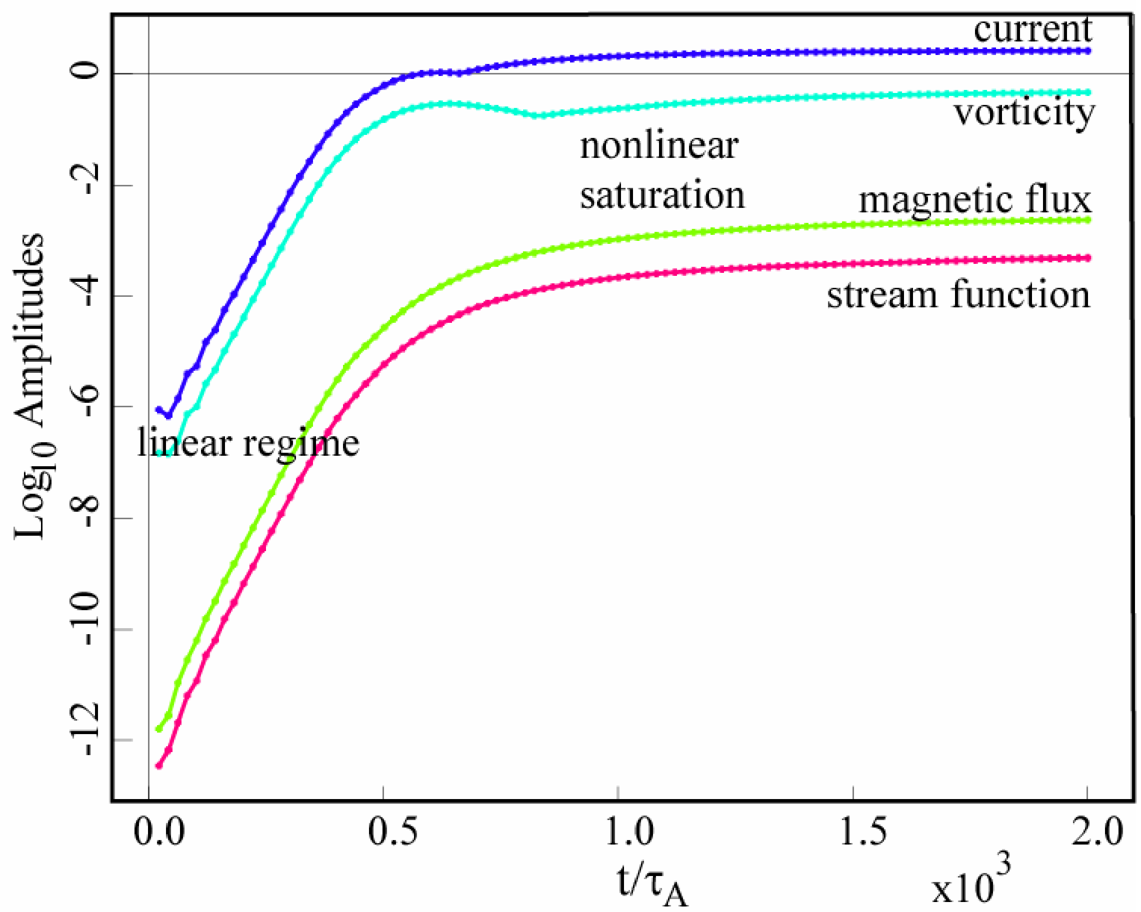
Current Density



Vorticity



Magnetic Reconnection, Time Dependence



$\gamma = 0.015$, $dt = 20$, $\gamma\,dt = 0.3$

Second-order-accurate time step

Excellent agreement with linear analysis and code

Linearized Equations

$$\eta j = \frac{\partial \psi}{\partial t} + \nabla \cdot [\psi_0 \hat{\mathbf{z}} \times \nabla \varphi + \psi \hat{\mathbf{z}} \times \nabla \varphi_0]$$

$$\begin{aligned}\mu \nabla^2 \omega = \frac{\partial \omega}{\partial t} + \nabla \cdot [&(\omega_0 \hat{\mathbf{z}} \times \nabla \varphi + \omega \hat{\mathbf{z}} \times \nabla \varphi_0) \\ &- (j_0 \hat{\mathbf{z}} \times \nabla \psi + j \hat{\mathbf{z}} \times \nabla \psi_0)]\end{aligned}$$

$$\nabla^2 \psi = j, \quad \nabla^2 \varphi = \omega$$

Ordinary Differential Equations

$$\mathbf{u}(x, y, t) = \mathbf{v}(y) e^{ikx + st}, \quad f' \equiv df/dy$$

$$\eta j = (s - ik\varphi_0')\psi + (ik\psi_0')\varphi$$

$$\mathbf{v} = \begin{pmatrix} \psi \\ \varphi \\ \omega \end{pmatrix}, \quad \mathbf{v}'' = \mathbf{L}\mathbf{v}$$

$$\mathbf{L} = \begin{pmatrix} k^2 + (s - ik\varphi_0')/\eta & ik\psi_0'/\eta & 0 \\ 0 & k^2 & 1 \\ \alpha & \beta & k^2 + (s - ik\varphi_0')/\mu \end{pmatrix}$$

$$\begin{aligned}\alpha =& [\psi_0'(s - ik\varphi_0')/\eta - j_0']ik/\mu \\ \beta =& (\psi_0'^2 ik/\eta + \omega_0')ik/\mu\end{aligned}$$

$$\psi = \varphi = \omega = 0 \text{ at } y = \pm 1/2$$

The Need for a 3D Adaptive Field-Aligned Grid

- An essential feature of magnetic confinement is very strong anisotropy, $\chi_{||} >> \chi_{\perp}$.
- The most unstable modes are those with $k_{||} << 1/R < 1/a << k_{\perp}$.
- The most effective numerical approach to these problems is a field-aligned grid packed in the neighborhood of singular surfaces and magnetic islands. NIMROD.
- Long-time evolution of helical instabilities requires that the packed grid follow the moving perturbations into 3D.
- Multidimensional oblique rectangular AMR grid is too large and does not resolve anisotropy.
- Novel algorithms must be developed to allow alignment of the grid with the dominant magnetic field and automatic grid packing normal to this field.
- Such methods must allow for regions of magnetic islands and stochasticity.

Grid Alignment Kinematics: Logical Coordinates

$$x^j(\xi^k) = \sum_i x_i^j \alpha_i(\xi^k), \quad j,k = 1,2$$

$$\mathcal{J} \equiv (\hat{\mathbf{z}} \cdot \nabla\xi^1 \times \nabla\xi^2)^{-1} = \frac{\partial x^1}{\partial \xi^1}\frac{\partial x^2}{\partial \xi^2} - \frac{\partial x^1}{\partial \xi^2}\frac{\partial x^2}{\partial \xi^1}$$

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

$$\frac{\partial}{\partial t}(\mathcal{J}u) + \frac{\partial}{\partial \xi^j}\left(\mathcal{J}\mathbf{F} \cdot \nabla\xi^j\right) = \mathcal{J}S$$

Grid Alignment Dynamics: Variational Principle

$$\xi \to \xi'(\xi), \quad \xi^{j\prime}(\xi^k) = \sum_i \xi_i^{j\prime} \alpha_i(\xi^k)$$

$$\mathcal{L} \equiv \frac{1}{2}\int \left(\mathbf{B} \cdot \nabla\xi^{2\prime}\right)^2 d\mathbf{x}$$

$$L_{i,j} \equiv \int (\mathbf{B} \cdot \nabla\alpha_i)(\mathbf{B} \cdot \nabla\alpha_j)\mathcal{J}\, d\xi^1 d\xi^2$$

$$L_{i,j}\xi_j^{2\prime} = 0$$

Grid Alignment Matrix

$$\psi = \sum_i \psi_i \alpha_i(x,y), \quad \Psi = \sum_i \Psi_i \alpha_i(x,y), \quad \mathbf{B} = \hat{\mathbf{z}} \times \nabla\Psi$$

$$\begin{aligned}
L_{i,j} &\equiv \int dx dy \mathcal{J} (\mathbf{B}\cdot\nabla\alpha_i)(\mathbf{B}\cdot\nabla\alpha_j) \\
&= \int dx dy \mathcal{J}^{-1} \left(\frac{\partial\Psi}{\partial x}\frac{\partial\alpha_i}{\partial y} - \frac{\partial\Psi}{\partial y}\frac{\partial\alpha_i}{\partial x} \right) \left(\frac{\partial\Psi}{\partial x}\frac{\partial\alpha_j}{\partial y} - \frac{\partial\Psi}{\partial y}\frac{\partial\alpha_j}{\partial x} \right) \\
&= \sum_{k,l} \Psi_k \Psi_l \int dx dy \mathcal{J}^{-1} \\
&\quad \times \left(\frac{\partial\alpha_k}{\partial x}\frac{\partial\alpha_i}{\partial y} - \frac{\partial\alpha_k}{\partial y}\frac{\partial\alpha_i}{\partial x} \right) \left(\frac{\partial\alpha_l}{\partial x}\frac{\partial\alpha_j}{\partial y} - \frac{\partial\alpha_l}{\partial y}\frac{\partial\alpha_j}{\partial x} \right)
\end{aligned}$$

$$\begin{aligned}
\sum_j L_{i,j}\psi_j &= \sum_{k,l,j} \Psi_k \Psi_l \psi_j \int dx dy \mathcal{J}^{-1} \\
&\quad \times \left(\frac{\partial\alpha_k}{\partial x}\frac{\partial\alpha_i}{\partial y} - \frac{\partial\alpha_k}{\partial y}\frac{\partial\alpha_i}{\partial x} \right) \left(\frac{\partial\alpha_l}{\partial x}\frac{\partial\alpha_j}{\partial y} - \frac{\partial\alpha_l}{\partial y}\frac{\partial\alpha_j}{\partial x} \right)
\end{aligned}$$

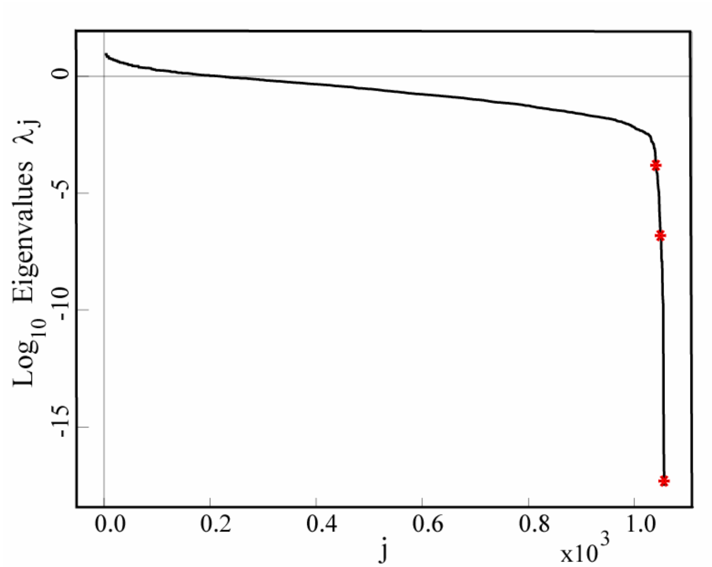
$$\sum_j L_{i,j}\Psi_j = 0$$

2D: Poloidal flux function is exact solution.

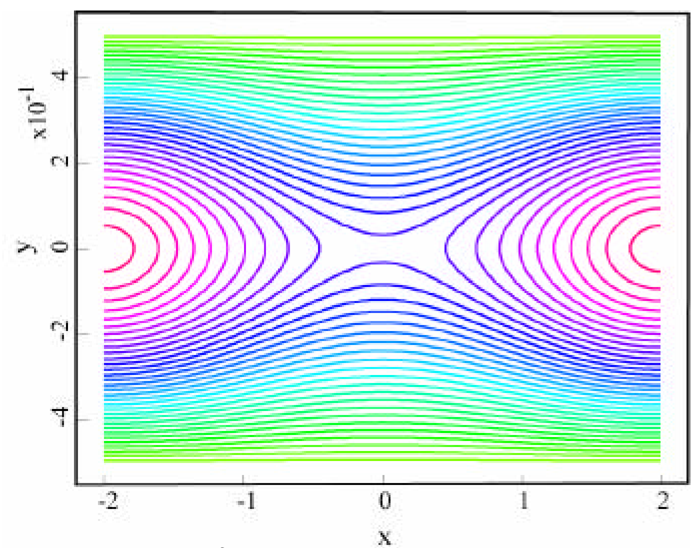
3D: No exact solution, but should provide useful approximate solution.

Singular Value Decomposition with LAPACK Routine DGESVD

Eigenvalues λ

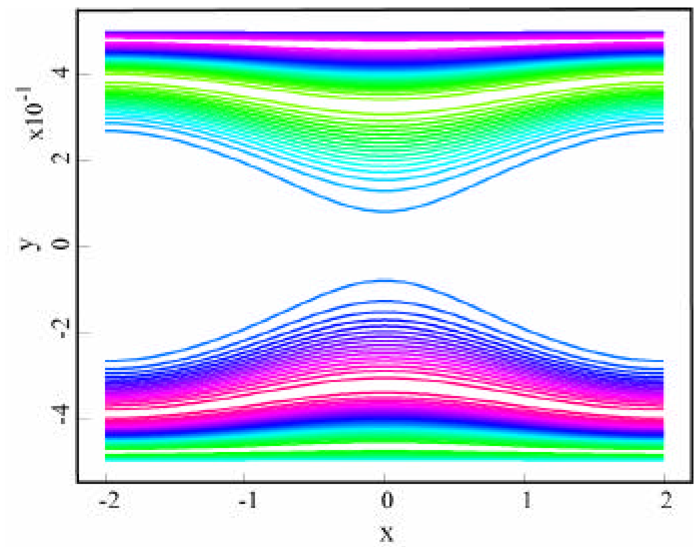


$\lambda = 3.241 \times 10^{-18}$

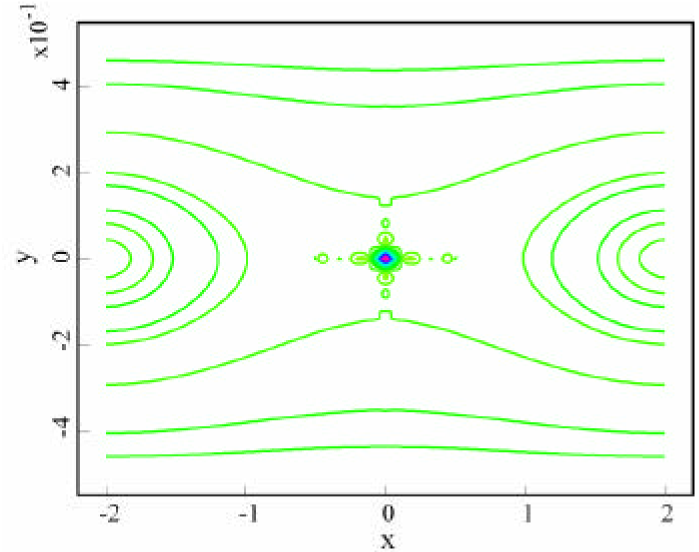


$Lu_\lambda = \lambda u_\lambda$

$\lambda = 1.538 \times 10^{-7}$



$\lambda = 1.019 \times 10^{-4}$



Lanczos Method for Singular Value Decomposition

- LAPACK direct method gives all the simple eigenpairs, $Lu_\lambda = \lambda u_\lambda$, of a full matrix L of order n, work scales as n^3.
- We need a few generalized eigenpairs of a sparse matrix, $Lu_\lambda = \lambda M u_\lambda$, mass matrix M determines orthogonality properties.
- Lanczos method, Krylov subspaces, *cf*. conjugate gradients.
- Golub & Van Loan, *Matrix Computations*, 3rd Edition, Johns Hopkins,1996; Cullum & Willoughby, *Lanczos Algorithms for Large Symmetric Eigenvalue Computations*, SIAM, 2002.
- Lowest few eigenpairs used for flux coordinate; highest few eigenpairs for angular coordinates.

Future Developments

- Curvilinear geometry using logical coordinates, metric tensor.
- 2D adaptive gridding.
- Multiple grid blocks.
- Plasma and fusion problems
  - Magetic reconnection
  - Scrape-off layer.
- 3D version
- Improved visualization
- Improved preconditioning as needed