Adaptive Grid Generation for Magnetically Confined Plasmas

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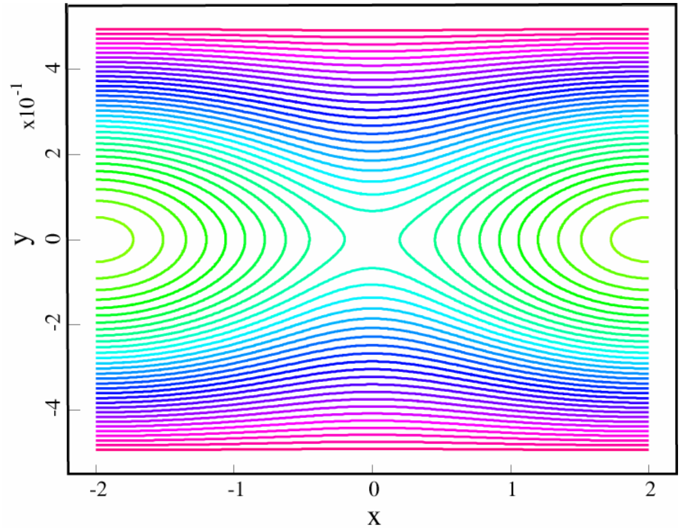
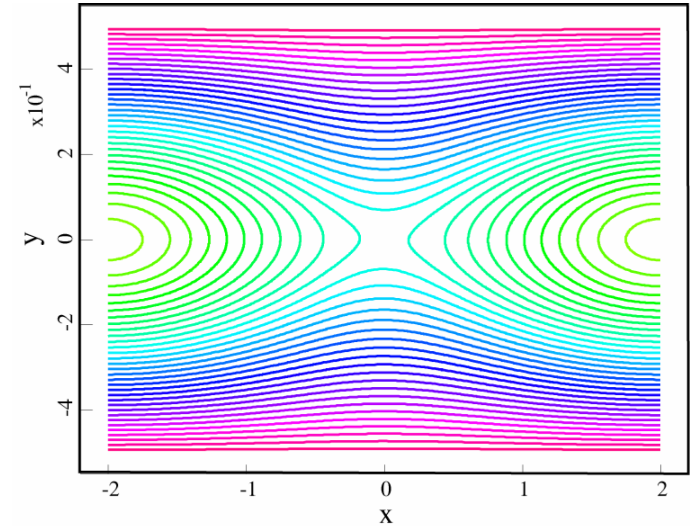
Presented at the
American Physical Society, Division of Plasma Physics Meeting
Savannah, Georgia, November 15-19, 2004

Magnetic Reconnection, Final State

Magnetic Flux



Stream Function



$A = 1$

$M = 1/2$

$\eta = 10^{-4}$

$\mu = 10^{-4}$

$\varepsilon = 10^{-4}$

$dt = 20$

$nx = 6$

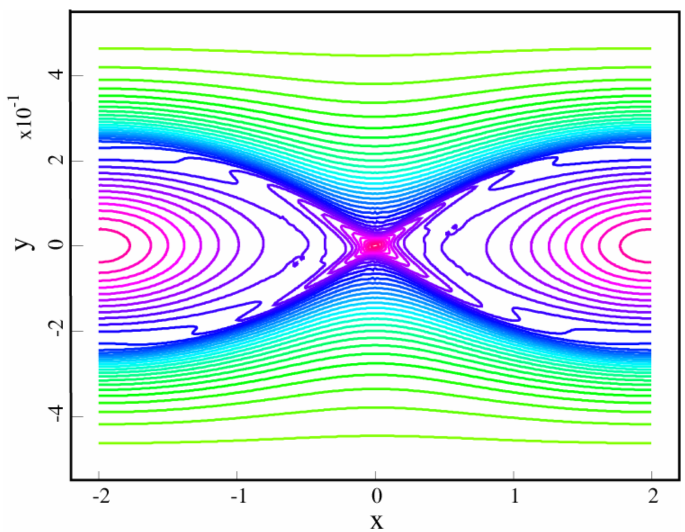
$ny = 16$

$np = 12$

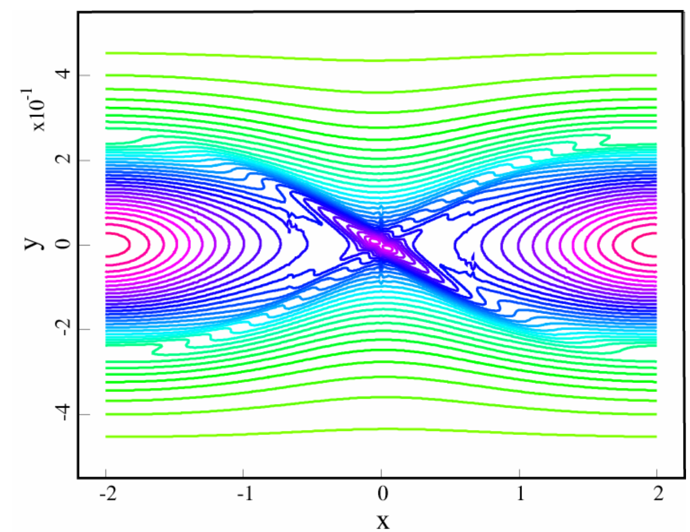
$nproc = 16$

$cpu = 3.5$ hr

Current Density



Vorticity



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 larger than necessary 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.

Adaptive Mesh Refinement
vs.
Harmonic Grid Generation

Adaptive Mesh Refinement

1. Coarse and fine patches of rectangular grid.
2. Complex data structures.
3. Oblique to magnetic field.
4. Static regrid.
5. Explicit time step; implicit a research problem.
6. Berger, Collela, Samtaney, Jardin

Harmonic Grid Generation

1. Harmonic mapping of rectangular grid onto curvilinear grid.
2. Logically rectangular
3. Aligned with magnetic field.
4. Static or dynamic regrid.
5. Explicit or implicit time step.
6. Liseikin, Winslow, Dvinsky, Brackbill

SEL Code Features

- Spectral elements: exponential convergence of spatial truncation error + adaptable 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.
- Time step: fully implicit, 2nd-order accurate, Newton-Krylov iteration, static condensation preconditioning.
- 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

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

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: **M** = 0.
- Static condensation, fully parallel.
- PETSc: GMRES with Schwarz ILU, overlap of 3, fill-in of 5.

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.

Adaptive Grid Kinematics:
How to Use Logical Coordinates.

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

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

$$\frac{\partial u^k}{\partial t} + \nabla \cdot \mathbf{F}^k = S^k, \quad \frac{\partial u^k}{\partial t} + \frac{1}{\mathcal{J}}\frac{\partial}{\partial \xi^j}\left(\mathcal{J}\mathbf{F}^k \cdot \nabla\xi^j\right) = S^k$$

$$u^k(t,\mathbf{x}) \approx \sum_{j=0}^{n} u_j^k(t)\alpha_j(\xi), \quad (u,v) \equiv \int_\Omega uv d\mathbf{x} = \int_\Omega uv\mathcal{J} d\xi$$

$$(\alpha_i, \alpha_j)\dot{u}_j^k = \int_\Omega \left(S^k\alpha_i + \mathbf{F}^k \cdot \nabla\xi^j \frac{\partial \alpha_i}{\partial \xi^j}\right)\mathcal{J} d\xi - \int_{\partial\Omega} \alpha_i \mathbf{F}^k \cdot \hat{\mathbf{n}}\mathcal{J} d\xi$$

Adaptive Grid Dynamics: How to Choose Logical coordinates.

$$\mathcal{L} \equiv \frac{1}{2} \int \left[\left(\mathbf{B} \cdot \nabla \xi^j \right)^2 + \epsilon |\nabla \xi^j|^2 \right] d\mathbf{x}$$

$$\frac{\delta \mathcal{L}}{\delta \xi^j} = 0 \Rightarrow \nabla \cdot \left(\mathbf{g} \cdot \nabla \xi^j \right) = 0, \quad \mathbf{g} \equiv \mathbf{B}\mathbf{B} + \epsilon \mathbf{I}$$

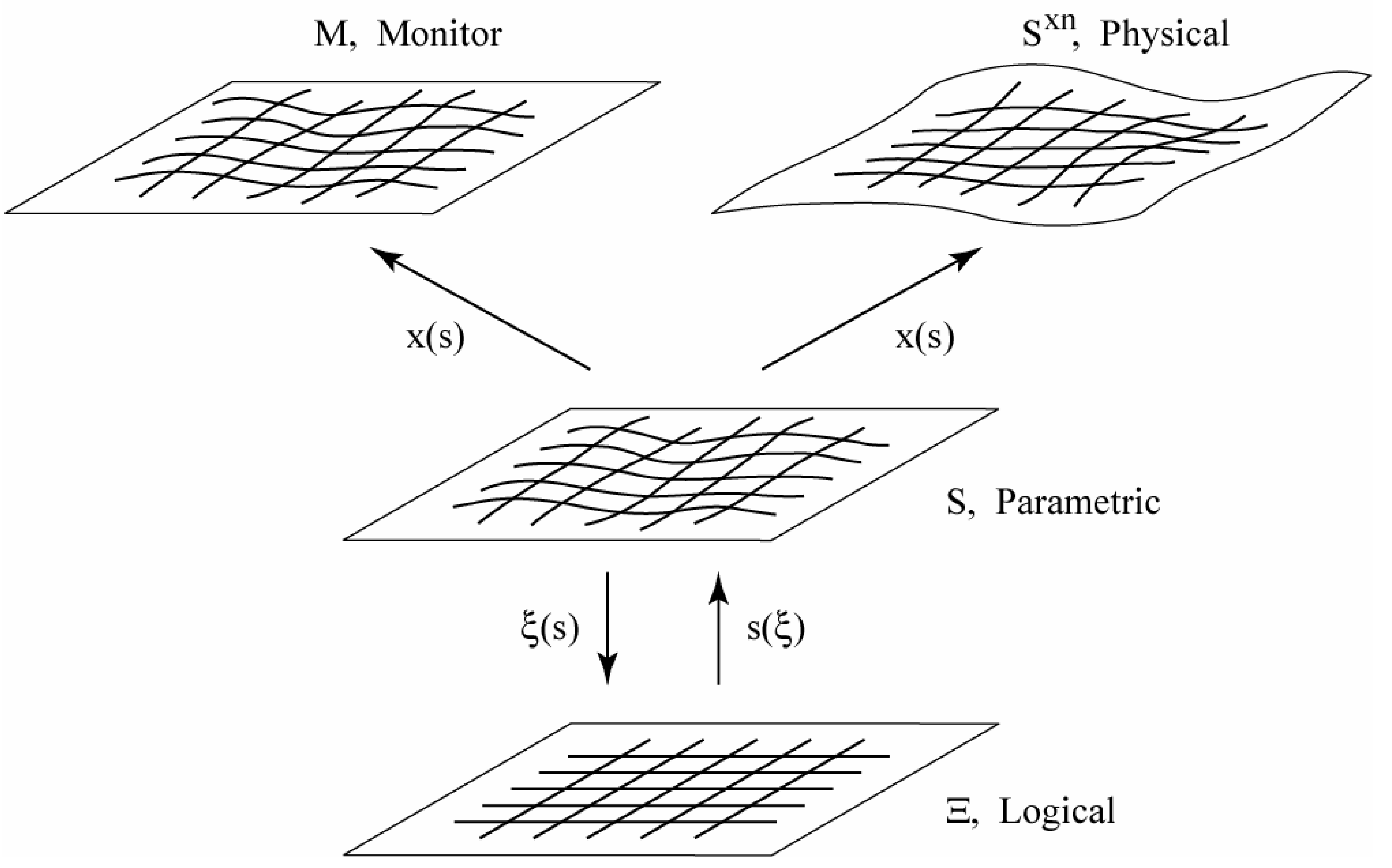
Beltrami equation + boundary conditions $\Rightarrow$ logical coordinates.
Alignment with magnetic field except where $\mathbf{B} \rightarrow 0$, isotropic term dominates.

Vladimir D. Liseikin
A Computational Differential Geometry Approach to Grid Generation
Springer Series in Synergetics, 2003

Domains and Transformations

Used in Harmonic Grid Generation

Figure by Andrei Simakov



Modified Beltrami Equation

Variational Principle

$$\mathcal{L} = \frac{1}{2}\int_\Omega \frac{1}{w\sqrt{g}}\mathbf{g} : \nabla\xi^i \nabla\xi^i d\mathbf{x}$$

Euler-Lagrange Equation

$$\nabla \cdot \left(\frac{1}{w\sqrt{g}}\mathbf{g} \cdot \nabla\xi^i\right) = 0$$

Expressed in Logical Coordinates (Chacon)

$$\frac{1}{\mathcal{J}}\frac{\partial}{\partial\xi^j}\left(\frac{\mathcal{J}}{w\sqrt{g}}g^{kl}\frac{\partial\xi^i}{\partial x^k}\frac{\partial\xi^j}{\partial x^l}\right) = 0, \quad \frac{\partial\xi^i}{\partial x^j} \rightarrow \frac{\partial x^i}{\partial\xi^j}$$

Metric Tensor Used for Alignment

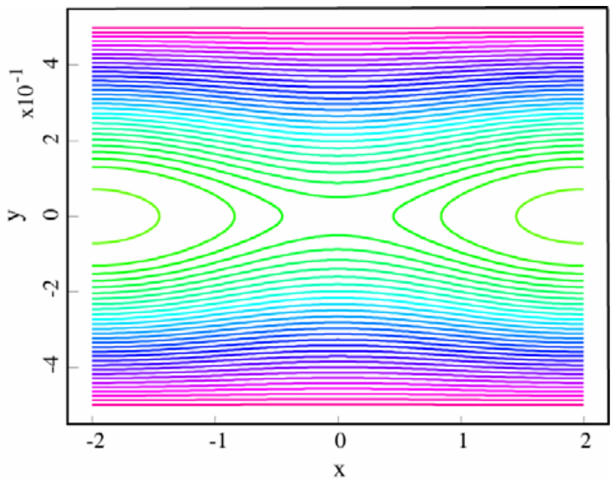
$$\mathbf{g} = \mathbf{B}_1\mathbf{B}_1 + \mathbf{B}_2\mathbf{B}_2 + \epsilon\mathbf{I}, \quad \mathbf{B}_1 \equiv \hat{\mathbf{z}} \times \nabla\psi, \quad \mathbf{B}_2 = k\hat{\mathbf{z}} \times \mathbf{B}^1$$

Boundary Conditions

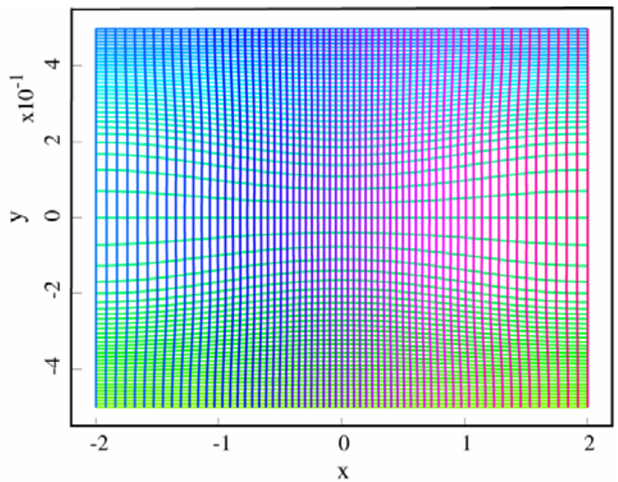
At each boundary, one of the x^i is held fixed
at the edge of the domain and $\nabla x^i \cdot \nabla x^j = 0$ for $i \neq j$.

Pure Alignment, w = 1

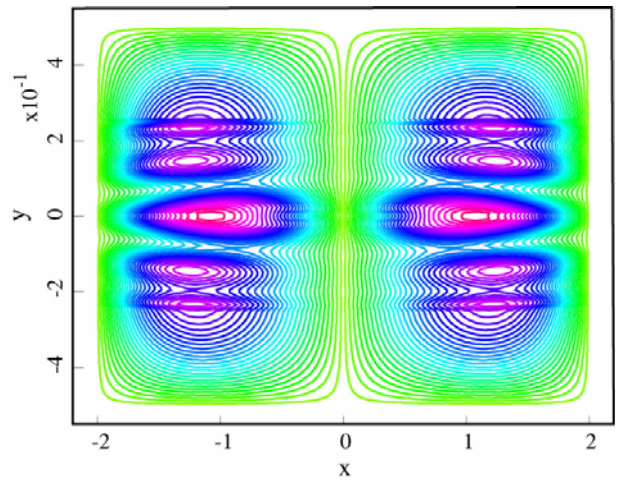
Magnetic Flux Function ψ



Grid Lines

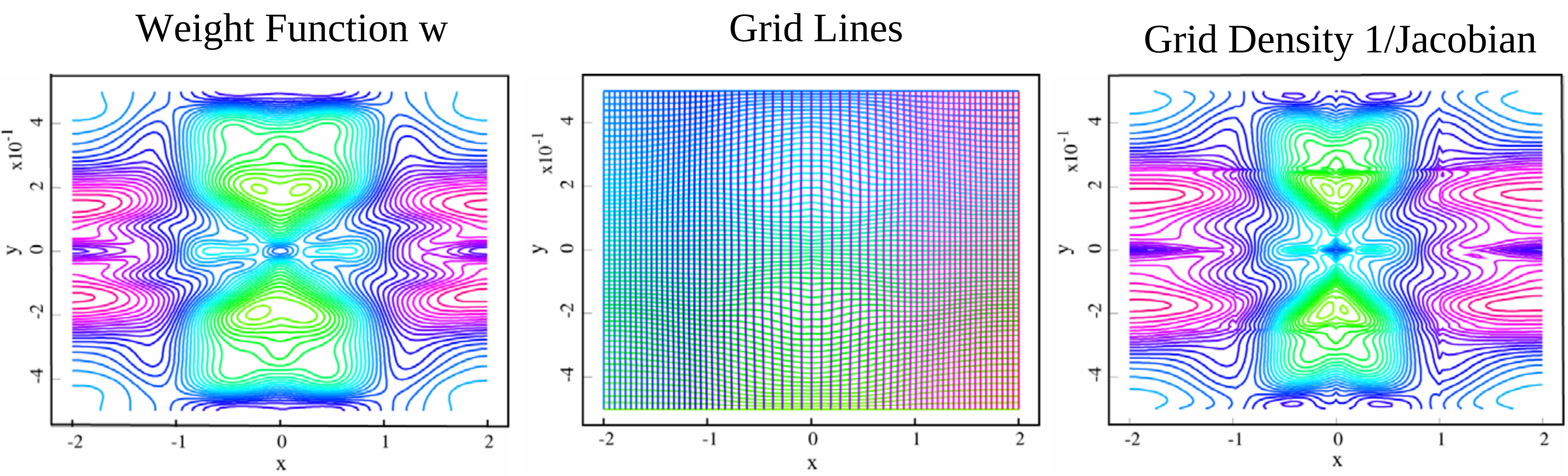


Alignment Error |**B**·∇w|



Magnetic flux is multiply connected; grid is simply connected.
Crossings occur where **B = z** ⑨ ∇ ψ is small.
Alignment Error: 0.012 max, 0.0055 RMS.

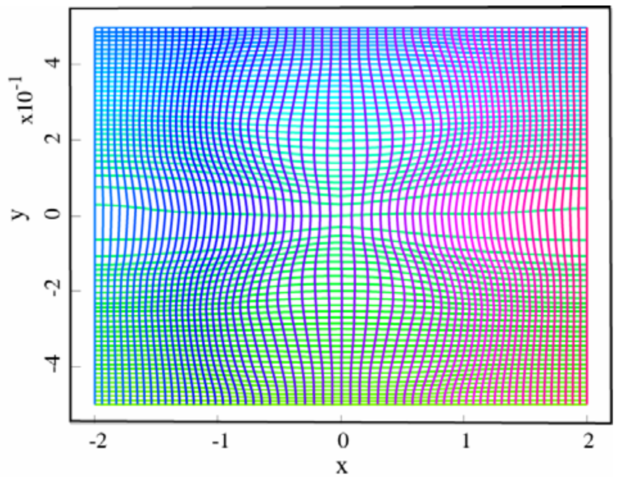
Pure Adaptation, g = I



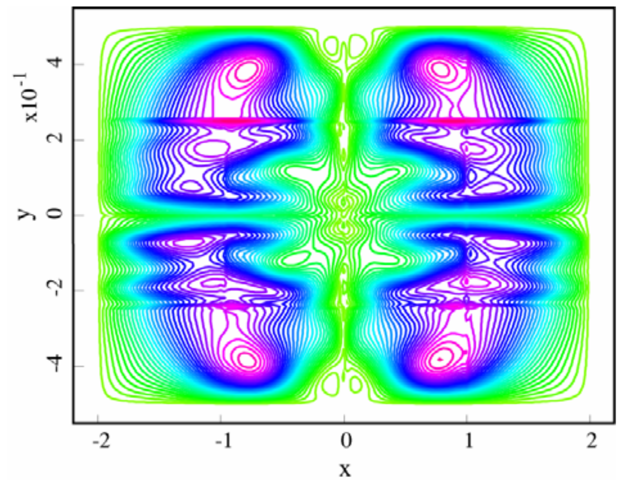
Weight function derived from log of spatial truncation error.
Grid density almost perfectly reproduces weight function,
including absolute magnitudes.

Alignment + Adaptation

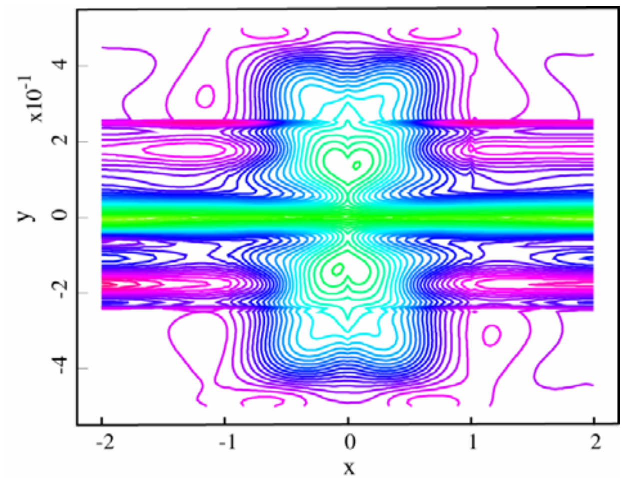
Grid Lines



Alignment Error |**B**·∇w|



Grid Density 1/Jacobian



This is a compromise. Neither the alignment nor the adaptation is quite as good as for the pure cases. Alignment Error: 0.036 max, 0.018 RMS.

Conclusions

- Pure alignment works very well, giving a simply-connected grid which is well-aligned except where **B** is small.

- Pure adaptation works very well, concentrating the grid in regions of large spatial truncation error.

- Alignment + adaptation works reasonably well, a good compromise.

- Imperfections are compensated by high-order spectral elements.

Next

- Use adapted grid for computations.

Vladimir D. Liseikin
Esteemed Colleague and Good Friend