

# Harmonic Grid Generation for the Tokamak Edge Region

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Collaborators:

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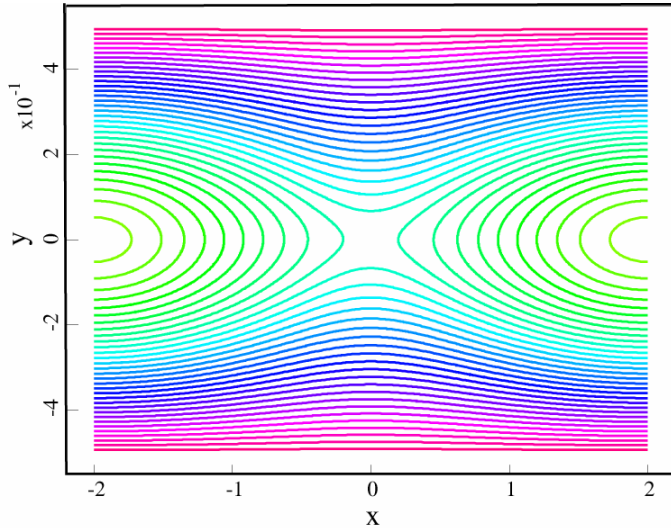
V. S. Lukin, A. N. Simakov



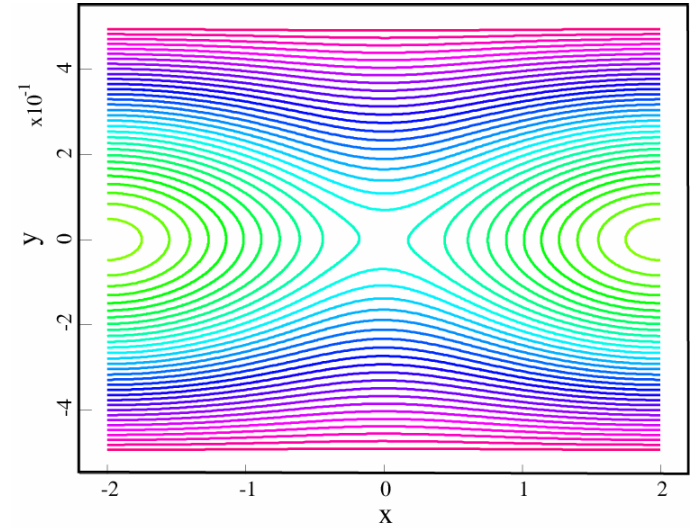
Presented at the  
2005 International Sherwood Theory Meeting  
Stateline, Nevada, April 11, 2005

# Magnetic Reconnection, Final State

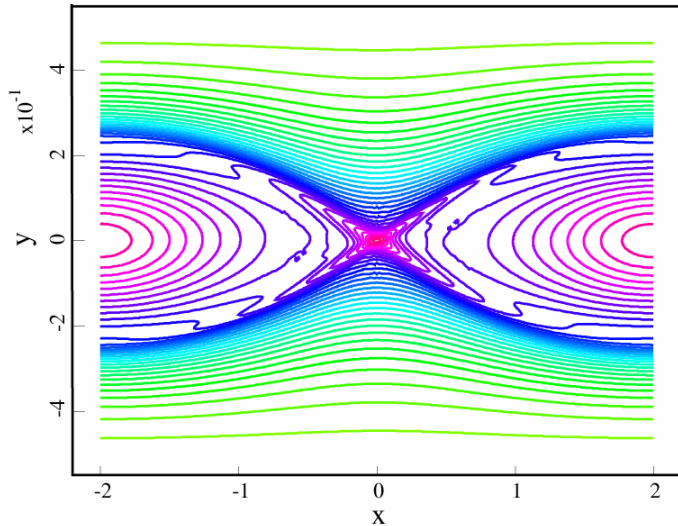
## Magnetic Flux



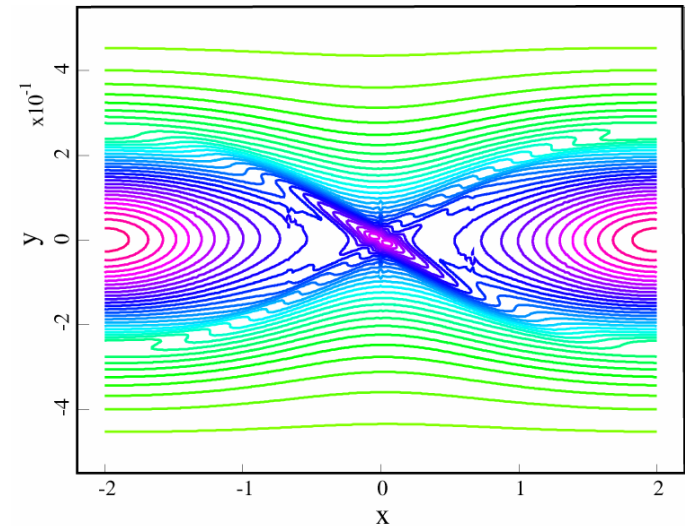
## Stream Function



## Current Density



## Vorticity



$A = 1$   
 $M = 1/2$   
 $\eta = 10^{-4}$   
 $\mu = 10^{-4}$   
 $\varepsilon = 10^{-4}$   
 $dt = 20$   
 $n_x = 6$   
 $n_y = 16$   
 $n_p = 12$   
 $n_{proc} = 16$   
 $cpu = 3.5 \text{ hr}$

# The Need for a 3D Adaptive Field-Aligned Grid

- An essential feature of magnetic confinement is very strong anisotropy,  $\chi_{\parallel} \gg \chi_{\perp}$ .
- The most unstable modes are those with  $k_{\parallel} \approx 1/R < 1/a \approx k_{\perp}$ .
- 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, Gombosi, Colella, 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, Knupp

## Adaptive Grid Kinematics: How to Use Logical Coordinates.

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

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

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

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

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

# Adaptive Grid Dynamics: How to Choose Logical coordinates.

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

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

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

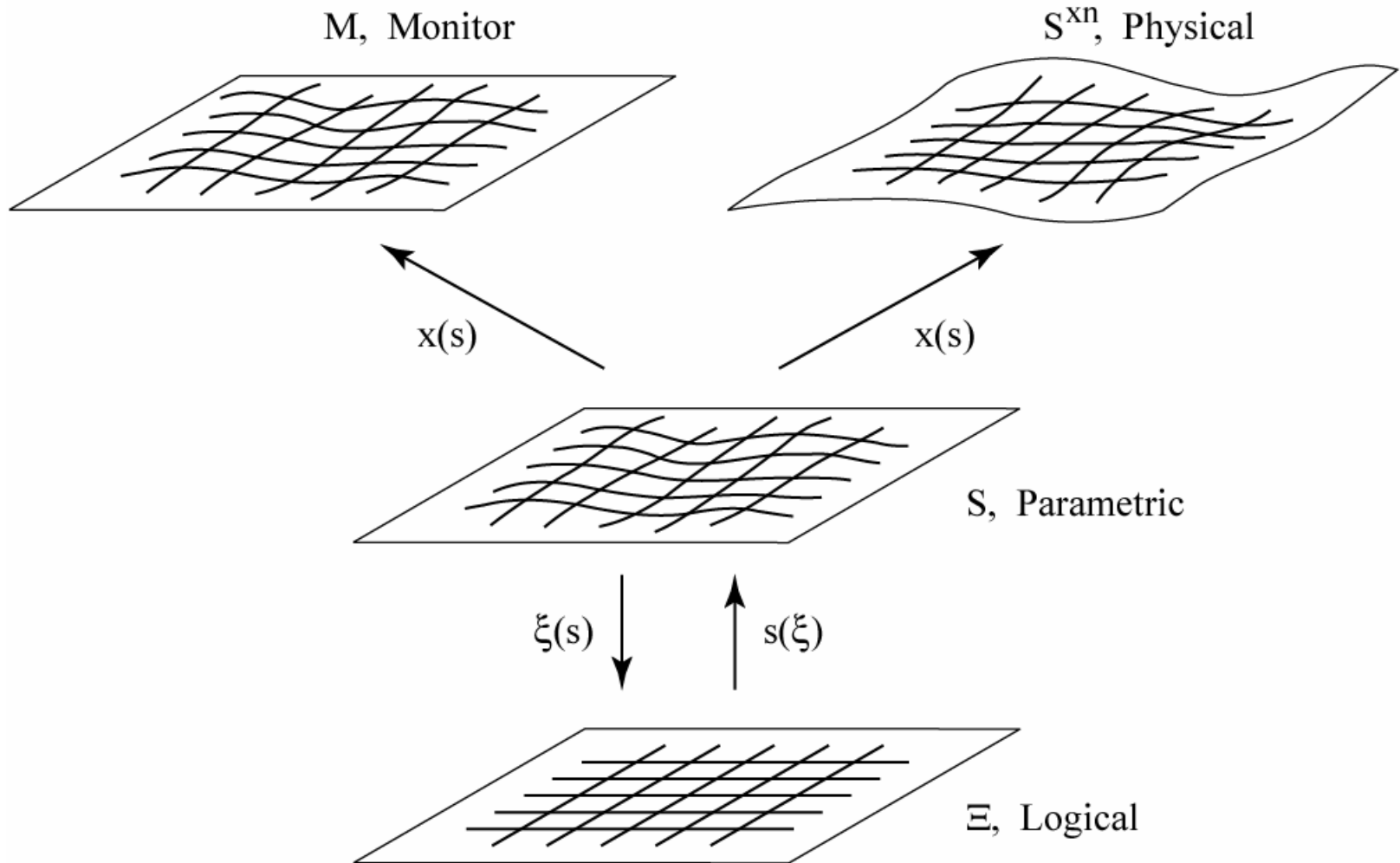
Vladimir D. Liseikin

*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



# Harmonic Grid Generation

Variational Principle

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

Beltrami's Equation

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

Expressed in Logical Coordinates

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

Metric Tensor Used for Alignment

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

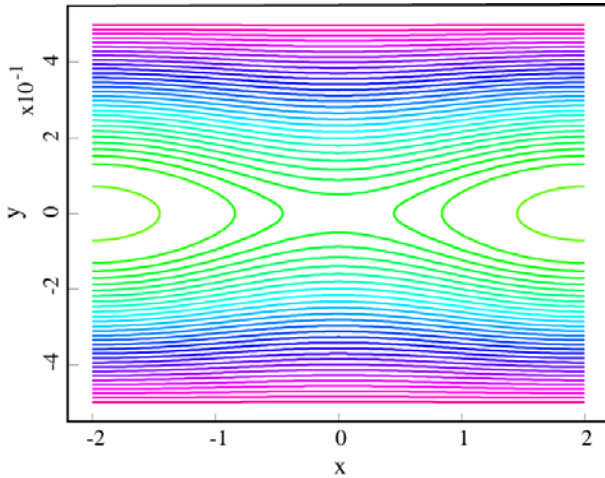
## Boundary Conditions

- At the flux surface boundaries, normal grid displacement vanishes while tangential motion slides freely. The coordinates are orthogonal at the boundary but not in the interior.
- At the plate boundaries, the grid vertices are held fixed with equal-arc-length spacing.

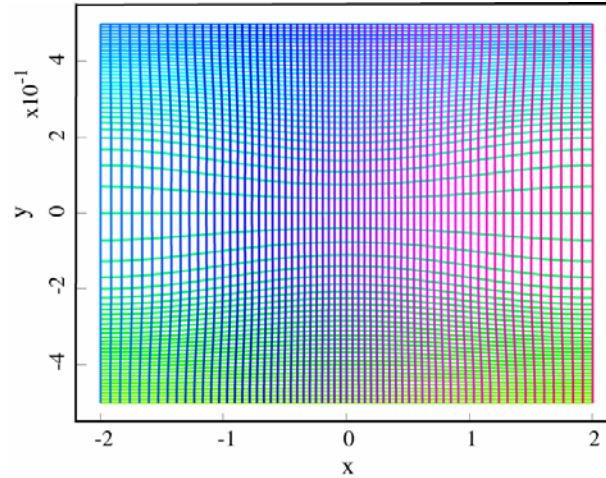


# Field-Aligned Grid, Simple Topology

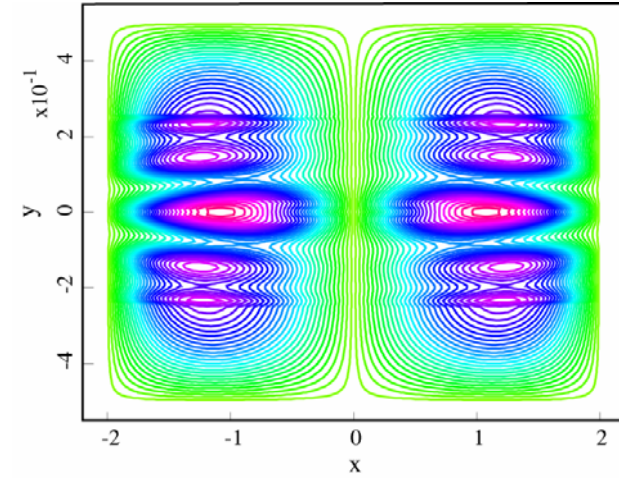
Magnetic Flux Function  $\psi$



Grid Lines



Alignment Error  $|\mathbf{B} \cdot \nabla w|$



Magnetic flux is multiply connected; grid is simply connected.

Crossings occur where  $\mathbf{B} = \mathbf{z} \odot \nabla \psi$  is small.

Alignment Error: 0.012 max, 0.0055 RMS.

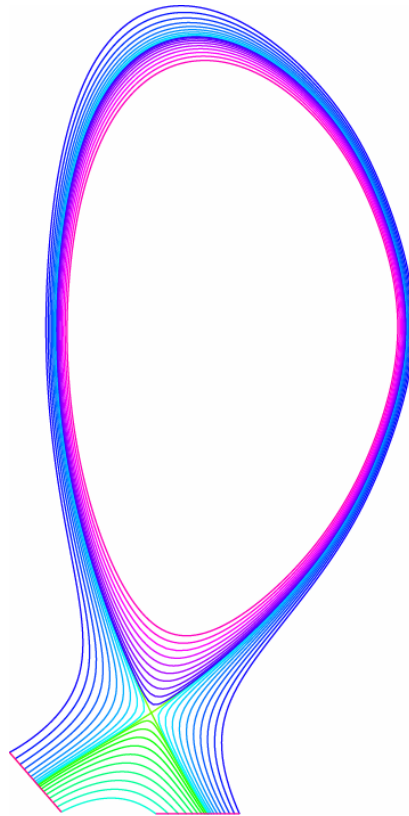
Topology of initial conditions constrains final grid.

# Field-Aligned Grids for the Tokamak Edge Region

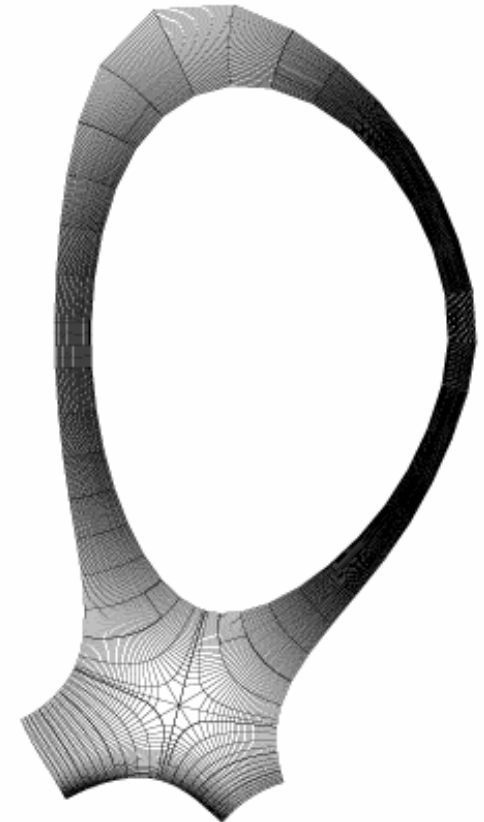
**Flux Contour Plot**



**Edge Flux Surfaces**



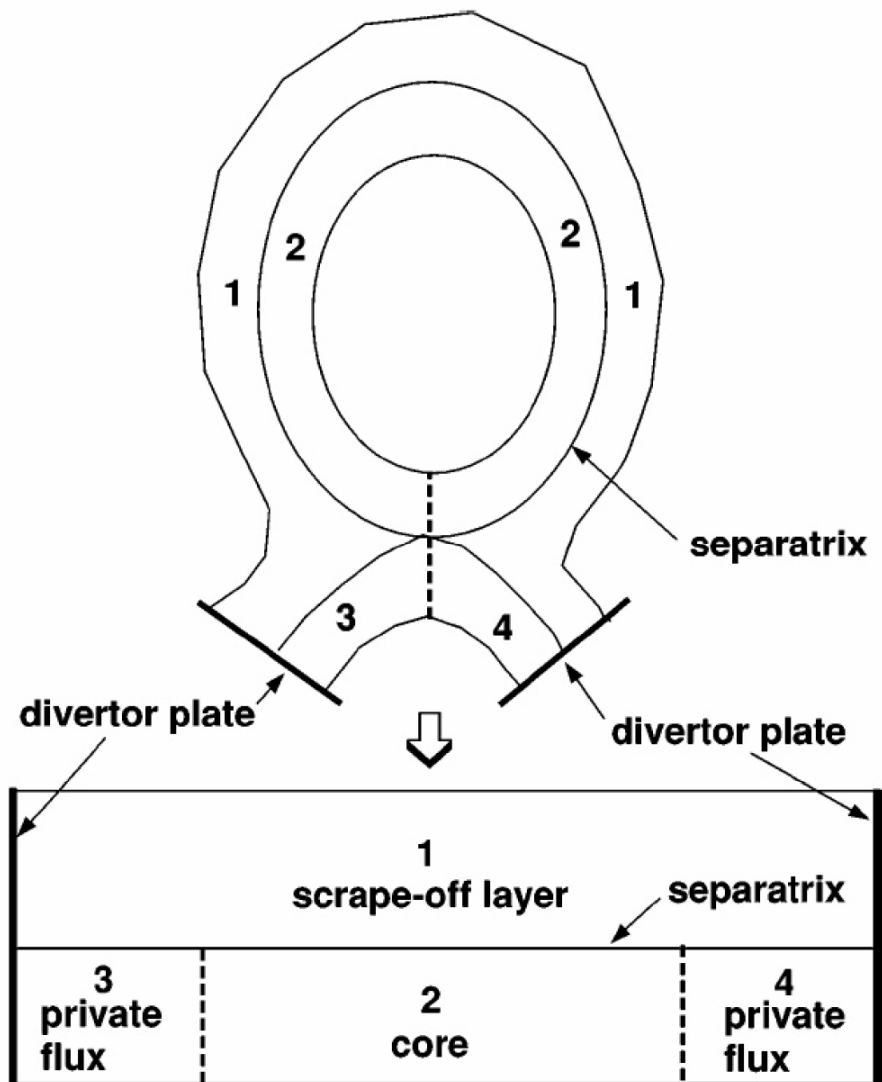
**LLNL Grid**



LLNL grid: orthogonal construction, non-optimal spacing.  
Can we do better?

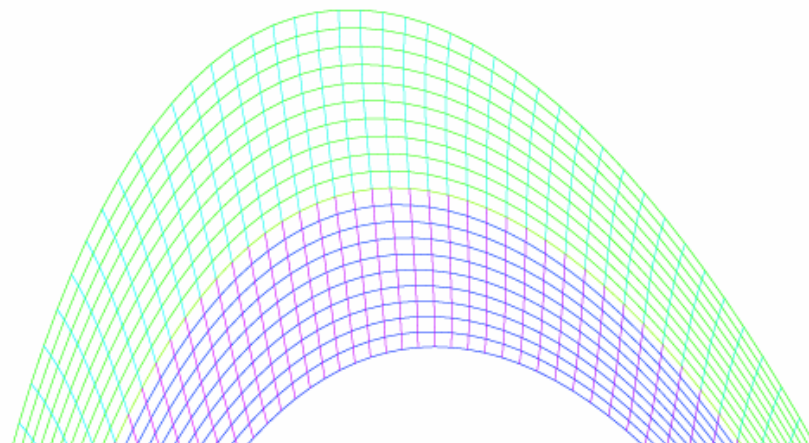
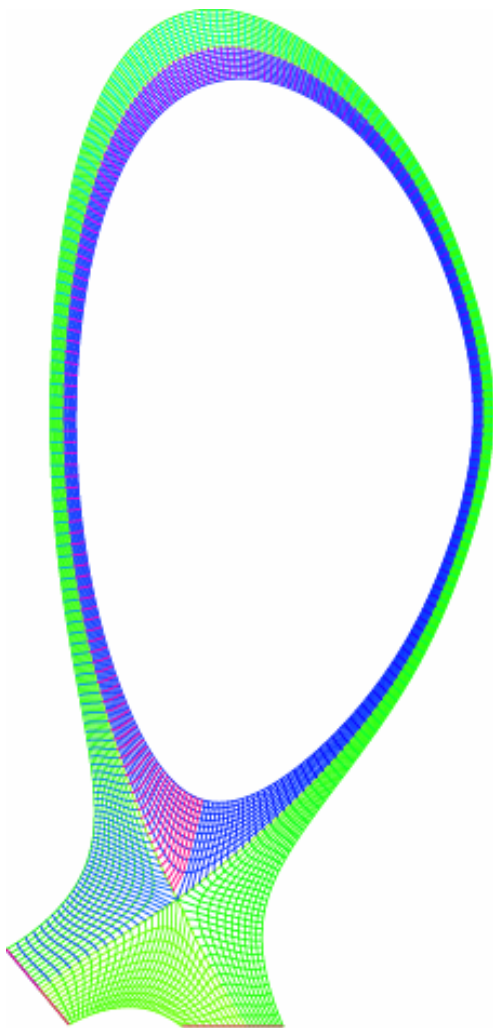
# Edge Subdomains for Parallelization

T. D. Rognlien, X. Q. Xu, and A. C. Hindmarsh, JCP **175**, 249–268 (2002)

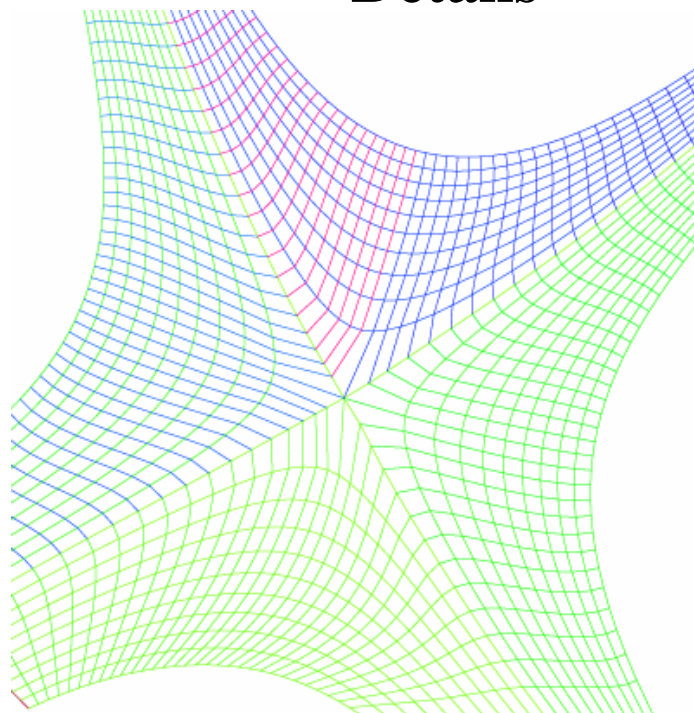


# Field-Aligned Grid for the Tokamak Edge Region

## Full Domain



## Details



# Present Status

- **Harmonic grid generation, alignment with 2D flux surface, has been successfully applied to the Tokamak edge region.**
- **C++ code: Kitaeva & Liseikin**
  - Classic numerical methods, single processor, slow.
  - Uses Microsoft class libraries; non-portable.
  - Proof of principle.
- **Fortran 95 code: Glasser, Lukin, & Simakov**
  - Advanced numerical methods, parallel operation, Unix/Linux, portable
  - Petsc leader Barry Smith: help with complex connectivity
  - Functional on simple rectangular domains, not yet Tokamak edge region.

# Future Plans

- **Finish Fortran 95 code, tune numerical parameters.**
- **Alignment + adaptation to regions of strong transverse gradients.**
- **Transformation to new grid and computation on it.**
- **3D grid: align with field lines.**
- **SciDAC/FSP: “Proposal for a Fusion Simulation Prototype Center For Edge Plasmas”**

# Vladimir Liseikin and Irina Kitaeva

