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A Moving Finite Element Model of the Tokamak Scrapeoff Layer

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Abstract

Most numerical simulations of the tokamak scrapeoff layer use a mapping to flux coordinates and a piecewise equidistributed grid in those coordinates to resolve the multiple length scales and anisotropy characteristic of this problem. We have developed an alternative numerical method using simple cylindrical coordinates with a complex adaptive grid scheme. It is based on an unstructured grid of triangles which move adaptively, aligning themselves with the magnetic field and concentrating in regions of sharp gradients.

1. Introduction

Numerical simulation of the scrapeoff layer of a tokamak is challenging because of high anisotropy and multiple length and time scales. Most approaches are based on mapping the physical domain to a flux coordinate system based on a fixed equilibrium magnetic field.¹ This approach suffers from some numerical difficulties. The flux coordinate system has a singularity at the x-point, it cannot naturally adapt to regions of sharp gradients near the plates, and it cannot treat time-dependent magnetic fields. Some methods use orthogonal coordinates, which cannot easily accommodate divertor plates at oblique angles to the magnetic field.

We have developed an alternative approach, using the adaptive grid method of Moving Finite Elements (MFE).² The computation is done in simple cylindrical coordinates (R, Z). Instead of mapping to a flux coordinate system, a nonuniform, adaptive, unstructured grid of triangles is used to discretize the nonlinear, time-dependent, partial differential equations of the fluid model with 2D linear finite elements. The vertices of the grid move smoothly and continuously, together with the time evolution of the solution, following the standard prescription of the method of MFE. The grid automatically adapts to the evolving solution, packing itself into regions of sharp gradients and aligning itself with the magnetic field in regions where

the poloidal field is strong. A stiffly-stable, second-order accurate time step is used to treat multiple time scales. A technique called Graph Massage is used to occasionally create and annihilate nodes, enabling our unstructured mesh to avoid tangling and to resolve the solution in a manner superior to that possible with a moving mesh of fixed topology. The data structures and techniques of Graph Massage have also made it straightforward to accomplish the related task of initially gridding the non-simply connected computational domain.

The rest of this paper is organized as follows. Section 2 presents our physical model; Section 3 describes our numerical methods; Section 4 presents results; and Section 5 discusses our conclusions.

2. Physical Models

Our physical model is determined by two goals. First, we want to verify the ability of our method to handle the numerical challenges presented by edge plasma modeling, including anisotropy, local regions of large gradients, and multiple time scales. Second, we want to develop a full, realistic edge code capable of competing with other numerical methods in this field. Our initial effort involved a simple model heat equation, with anisotropic and nonlinear thermal conductivity; this work has reached a satisfactory conclusion. Our present work treats the much more complete system of Braginskii's fluid equations for electrons and one species of ions.³ This code has been written and will be described here, but it has not yet been successfully run. Therefore, the results presented in Section 4, illustrating the method, are from the previous code. We discuss both of these models here. Future work will incorporate neutrals, impurities, and radiation.

Our simple model anisotropic tokamak heat equation is

$$\frac{\partial T}{\partial t} = \nabla \cdot (\chi \cdot \nabla T), \quad \chi = \chi_{\parallel} \hat{\mathbf{e}}_1 \hat{\mathbf{e}}_1 + \chi_{\perp} (\mathbf{I} - \hat{\mathbf{e}}_1 \hat{\mathbf{e}}_1), \quad \hat{\mathbf{e}}_1 \equiv \mathbf{B}/B. \quad (1)$$

The thermal conductivity tensor χ is defined in terms of the unit vector $\hat{\mathbf{e}}_1$ along a magnetic field $\mathbf{B}$ obtained from a numerical solution to the Grad-Shafranov equation. The parallel and transverse conductivities are taken to scale as

$$\chi_{\parallel} = \chi_0 (T/T_0)^{5/2}, \quad \chi_{\perp} = \chi_{\parallel} / [1 + (T/T_0)^3], \quad (2)$$

with $\chi_0 = 1$ and $T_0 = .4$ in the example discussed in Section 4. These scaling

assumptions mimic the behavior of the classical transport coefficients and test the ability of the code to treat nonlinearity and anisotropy.

Our more complete and realistic model is based on Braginskii's equations. These include particle conservation, with $n = n_e = n_i$,

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = 0, \quad (3)$$

conservation of momentum,

$$\rho \left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = \frac{1}{c} \mathbf{j} \times \mathbf{B} - \nabla p - \nabla \cdot \pi, \quad (4)$$

the heat equation for each species,

$$\frac{3}{2} n \left(\frac{\partial T_j}{\partial t} + \mathbf{v}_j \cdot \nabla T_j \right) + n T_j \nabla \cdot \mathbf{v}_j + \nabla \cdot \mathbf{q}_j + \pi_j : \nabla \mathbf{v}_j = \frac{1}{ne} \mathbf{j} \cdot \mathbf{R}, \quad (5)$$

Ohm's law,

$$ne \left(\mathbf{E} + \frac{1}{c} \mathbf{v} \times \mathbf{B} \right) = \mathbf{R} + \frac{1}{c} \mathbf{j} \times \mathbf{B} - \nabla p_e, \quad (6)$$

Maxwell's equations in the form

$$\mathbf{E} = -\nabla \varphi - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}, \quad \nabla^2 \mathbf{A} = -\frac{4\pi}{c} \mathbf{j}, \quad (7)$$

and the quasineutrality equation

$$\nabla \cdot \mathbf{j} = 0. \quad (8)$$

The momentum exchange term is given by

$$\mathbf{R} = \mathbf{R}_u + \mathbf{R}_T, \quad (9)$$

$$\mathbf{R}_u = \frac{1}{ne} \alpha \cdot \mathbf{j} = \frac{1}{ne} \left[\alpha_{\parallel} \hat{\mathbf{e}}_1 \hat{\mathbf{e}}_1 \cdot \mathbf{j} - \alpha_{\perp} \hat{\mathbf{e}}_1 \times \mathbf{j} + \alpha_{\perp} (\mathbf{I} - \hat{\mathbf{e}}_1 \hat{\mathbf{e}}_1) \cdot \mathbf{j} \right], \quad (10)$$

$$\mathbf{R}_T = -\beta \cdot \nabla T = -\left[\beta_{\parallel} \hat{\mathbf{e}}_1 \hat{\mathbf{e}}_1 \cdot \nabla T + \beta_{\perp} \hat{\mathbf{e}}_1 \times \nabla T + \beta_{\perp} (\mathbf{I} - \hat{\mathbf{e}}_1 \hat{\mathbf{e}}_1) \cdot \nabla T \right], \quad (11)$$

while the electron heat flux vector is given by

$$\mathbf{q} = \mathbf{q}_u + \mathbf{q}_T, \quad (12)$$

$$\mathbf{q}_u = -\frac{T}{ne}\beta \cdot \mathbf{j} = -\frac{T}{ne}\left[\beta_{\parallel}\hat{\mathbf{e}}_1\hat{\mathbf{e}}_1 \cdot \mathbf{j} + \beta_{\perp}\hat{\mathbf{e}}_1 \times \mathbf{j} + \beta_{\perp}\left(\mathbf{I} - \hat{\mathbf{e}}_1\hat{\mathbf{e}}_1\right) \cdot \mathbf{j}\right], \quad (13)$$

$$\mathbf{q}_T = -\chi \cdot \nabla T = -\left[\chi_{\parallel}\hat{\mathbf{e}}_1\hat{\mathbf{e}}_1 \cdot \nabla T + \chi_{\perp}\hat{\mathbf{e}}_1 \times \nabla T + \chi_{\perp}\left(\mathbf{I} - \hat{\mathbf{e}}_1\hat{\mathbf{e}}_1\right) \cdot \nabla T\right], \quad (14)$$

satisfying Onsager relations; the ion heat flux is given by Eq. (13) alone. For the viscous tensor, we retain only the terms arising from parallel and transverse gradients of the ion parallel velocity. All parallel transport coefficients are flux limited to treat local regions of long mean free path, and all transverse transport coefficients are enhanced by anomalous contributions.

Our final system of 5 equations is obtained from Eqs. (3) - (14) as follows. Equations (3) and (5) are used to determine n_e , T_e , and T_i ; the parallel component of Eq. (4) is used to determine the parallel momentum density $\pi_{\parallel}$; and Eq. (8) is used to determine the electrostatic potential φ . The transverse components of Eq. (6) are used to determine $\mathbf{v}_{\perp}$, while the transverse components of Eq. (4) are used to determine $\mathbf{j}_{\perp}$ and the parallel component of Eq. (7) is used to determine $j_{\parallel}$. Our boundary conditions are as follows:

<u>Core</u>	<u>Wall and Private</u>	<u>Plates</u>
$n = 3 \times 10^{19} \text{ m}^{-3}$	$\hat{\mathbf{n}} \cdot \nabla n _{\text{out}} = \hat{\mathbf{n}} \cdot \nabla n _{\text{in}}$	$\hat{\mathbf{n}} \cdot \nabla n _{\text{out}} = 0$
$T_e = 250 \text{ eV}$	$\hat{\mathbf{n}} \cdot \nabla T_e _{\text{out}} = \hat{\mathbf{n}} \cdot \nabla T_e _{\text{in}}$	$q_{e\parallel} = (\delta_e - 5/2)nT_e v_{e\parallel}$
$T_i = 250 \text{ eV}$	$\hat{\mathbf{n}} \cdot \nabla T_i _{\text{out}} = \hat{\mathbf{n}} \cdot \nabla T_i _{\text{in}}$	$q_{i\parallel} = (\delta_i - 5/2)n_i T_i v_{i\parallel}$
$p_{i\parallel} = 0$	$\hat{\mathbf{n}} \cdot \nabla p_{i\parallel} _{\text{out}} = \hat{\mathbf{n}} \cdot \nabla p_{i\parallel} _{\text{in}}$	$p_{i\parallel} = n[m_i(T_e + T_i)]^{1/2}$
$\hat{\mathbf{n}} \cdot \nabla \varphi _{\text{out}} = 0$	$\hat{\mathbf{n}} \cdot \nabla \varphi _{\text{out}} = \hat{\mathbf{n}} \cdot \nabla \varphi _{\text{in}}$	$\varphi = \kappa(T_e, T_i)T_e/c$

where $\hat{\mathbf{n}}$ denotes the unit vector normal to the boundary.

3. Moving Finite Elements

Both models describe in Section 2 can be expressed in the general form

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S}, \quad (15)$$

where t is the time, $\mathbf{x}$ is a vector of independent spatial variables, $\mathbf{u}$ is an n -vector of unknowns. For each component of $\mathbf{u}$ there is a flux $\mathbf{F}$ and a source $\mathbf{S}$ with the general form

$$\mathbf{F} = \mathbf{C}(t, \mathbf{x}, \mathbf{u}) - \mathbf{D}(t, \mathbf{x}, \mathbf{u}) \cdot \nabla \mathbf{u}, \quad \mathbf{S} = \mathbf{S}(t, \mathbf{x}, \mathbf{u}, \nabla \mathbf{u}), \quad (16)$$

where $\mathbf{C}$ represents convective flux and $\mathbf{D}$ is a diffusion tensor, and all functions may depend in an arbitrary nonlinear manner on their arguments. A variational for Eq. (15) is obtained by noting that

$$L = \frac{1}{2} \int \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{F} - \mathbf{S} \right]^2 w(t, \mathbf{x}, \mathbf{u}, \nabla \mathbf{u}) d\mathbf{x}, \quad (17)$$

with w an arbitrary weight function, is variational in the sense that

$$\frac{\delta L}{\delta(\partial \mathbf{u} / \partial t)} = 0 \quad (18)$$

recovers Eq. (15).

The general class of conventional Galerkin methods is obtained from Eqs. (17) and (18) by expanding $\mathbf{u}$ in a set of basis functions,

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_i(t) \alpha_i(\mathbf{x}), \quad (19)$$

where the $\mathbf{u}_i(t)$ are time-dependent amplitudes and the $\alpha_i(\mathbf{x})$ are the spatially-varying basis functions, which may, for example, be Fourier series, orthogonal polynomials, or conventional fixed finite elements. Since the time derivative of Eq. (19) contains only the amplitude variations,

$$\dot{\mathbf{u}}(\mathbf{x}, t) = \dot{\mathbf{u}}_i(t) \alpha_i(\mathbf{x}), \quad (20)$$

the discretized equations of the method are obtained from

$$\frac{\delta L}{\delta \dot{\mathbf{u}}_i} = 0, \quad (21)$$

which yields a coupled system of ordinary differential equations,

$$(\alpha_i, \alpha_j) \dot{\mathbf{u}}_j = (\alpha_i, \mathbf{g}), \quad (22)$$

where $\mathbf{g} = \mathbf{S} - \nabla \cdot \mathbf{F}$.

The key issue for any adaptive grid method is how to move the grid. In Moving Finite Elements, this issue is resolved by treating the grid positions in exactly the same manner as the amplitudes, *i.e.* as variational parameters. For basis functions

we choose linear finite elements on a grid of irregularly shaped and connected triangles in 2D, tetrahedra in 3D, and simplices in general. Because the grid is allowed to move, we replace Eqs. (19) and (20) by

$$\mathbf{u}(\mathbf{x}, t) = \mathbf{u}_i(t)\alpha_i[\mathbf{x}, \mathbf{s}_j(t)], \quad (23)$$

$$\dot{\mathbf{u}}(\mathbf{x}, t) = \dot{\mathbf{u}}_i(t)\alpha_i(\mathbf{x}, t) + \dot{\mathbf{s}}_i(t)\beta_i(\mathbf{x}, t), \quad (24)$$

where β_i is defined as the coefficient of $\dot{\mathbf{s}}_i$ obtained by differentiating Eq. (23). Then Eqs. (21) and (22) are generalized to

$$\frac{\delta L}{\delta \dot{\mathbf{u}}_i} = \frac{\delta L}{\delta \dot{\mathbf{s}}_i} = 0, \quad (25)$$

$$(\alpha_i, \alpha_j)\dot{\mathbf{u}}_j + (\alpha_i, \beta_j)\dot{\mathbf{s}}_j = (\alpha_i, \mathbf{g}), \quad (26)$$

$$(\beta_i, \alpha_j)\dot{\mathbf{u}}_j + (\beta_i, \beta_j)\dot{\mathbf{s}}_j = (\beta_i, \mathbf{g}). \quad (27)$$

Just as Eq. (22) determines the amplitudes by minimizing the positive-definite variational over the space of amplitudes, Eqs. (26) and (27) determine the amplitudes and node positions by minimizing over a larger space, and thus obtain a better minimum. This causes the nodes to move where they are needed to resolve the solution.

While the basic idea is simple, there are computational details which are essential to make the method work correctly. In regions where the solution is flat, the prescription for moving the nodes becomes indeterminate because a range of different node motions give equally “best” fits. This is manifested mathematically in the vanishing of the determinant of the mass matrix in Eqs. (26) and (27), and is resolved by adding regularization terms to L which can be interpreted as inter-nodal viscosity and grid tension. The weight function in Eq. (17) is chosen to be $w = [1 + (\nabla u)^2]^{-1/2}$, which converts the integral over the domain into an integral over the area of the solution manifold, resulting in much better node motion and in placing the independent spatial variables $\mathbf{x}$ and the dependent variables $\mathbf{u}$ on more of an equal basis. The time step must be implicit in order to exceed the Courant condition and use efficiently large step sizes. This requires the solution of large, sparse linear systems, which is currently done with a direct band solution but will

shortly be replaced with a more efficient iterative method using buffered relaxation as a preconditioner for a nonlinear Krylov subspace method.

In addition to the continuous node motion defined by the MFE method, we use a technique called Graph Massage (GM) to occasionally create and annihilate grid nodes, adding necessary topological flexibility to the continuous grid motion of MFE. Nodes are created when a triangular cell gets too elongated or when the graph gets too jagged (locally nonplanar). Nodes are deleted where they have overaccumulated, without significantly damaging the graph. For the scrapeoff layer problem, we have modified GM to use an anisotropic metric with principal axes aligned with the magnetic field.

GM has been adapted to the problem of initially triangulating the multiply connected domain of the scrapeoff layer. We start with a crude initial triangulation using only boundary nodes, and then use GM with the anisotropic metric to insert interior nodes. Additional smoothing procedures are used to improve the triangulation.

4. Code Results

A code has been written based on Braginskii's equations, Eqs. (3) - (14), but this code is not yet working. Our results so far are based on the model tokamak heat equation, Eqs. (1) and (2). Our principal diagnostic is a 3D color movie on an SGI Iris workstation. Our figures are stills from that movie. Figures 1 - 3 show the grid at various stages during the run. The magnetic field is obtained from numerical output from a numerical solution to the Grad-Shafranov equation, with parameters appropriate to ITER with a single null divertor.⁴ Our computational domain is bounded by flux surfaces for the core and private flux boundaries and by inboard and outboard divertor plates. Figure 1 shows the initial grid with only boundary nodes. Figure 2 shows the grid after Graph Massage has been used to generate interior nodes. Figure 3 shows the final grid, containing 1267 nodes, after it has been modified by Moving Finite Elements and additional applications of Graph Massage. Figure 4 shows the temperature distribution at the end of the run.

The status of the code is promising but not yet satisfactory. The behavior of Graph Massage is excellent; that of Moving Finite Elements is much less so. After each application of GM, the grid appears well distributed and the solution appears well resolved. MFE then moves the grid in such a way as to make it less well resolved in some regions, and the extent to which it aligns with the magnetic field is less than

expected. We believe this is due primarily to our treatment of gradient weighting. As discussed in Section 3, without gradient weighting the grid has a tendency to overemphasize regions of sharp gradients, leaving inadequate grid to resolve other regions. Gradient weighting reduces this effect when the gradients exceed some critical value determined by input scale factors. For the edge problem, the criterion for gradient weighting should be made anisotropic to properly treat the disparate length scales along and across the magnetic field. Such anisotropic scaling has been incorporated into GM but not MFE. Incorporating it into MFE is our next task.

The speed of the code is also not yet satisfactory, requiring several hours on an HP 735 workstation. We attribute this to two problems which we hope to solve. The time step depends critically on the success of MFE in moving the grid optimally, and as discussed above this has not yet been achieved. In addition, we use a direct method for large sparse matrix solution on an unstructured grid, and an iterative method could probably improve on this.

5. Conclusions

We have described an alternative numerical method for solving the equations of the tokamak scrapeoff layer, using an adaptive grid in a simple coordinate system rather than a piecewise uniform grid in a flux coordinate system. We have described a code with a fairly complete set of equations which has been written but not yet run. We have presented code results for a simpler model problem, showing promising but not yet perfect grid behavior, and we have indicated how this behavior can be perfected.

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Fig. 1. Initial grid with only boundary nodes.

Fig. 2. Initial grid after using Graph Message to generate internal nodes.

Fig. 3. Final grid after Moving Finite Elements and more Graph Messages.

Fig. 4. Final temperature distribution.

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