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3D PLASMA FLUID SIMULATIONS IN DIVERTOR TOKAMAKS

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A. FEMHD UNSTRUCTURED MESH MHD CODE

The main accomplishment of this grant was the development of a finite element time dependent magnetofluid code, FEMHD. The code is nonlinear and three dimensional. In the poloidal plane, the elemental cells of the mesh are triangles, which offer both simplicity and adaptability. In the third, toroidal, direction, there is an option of a standard staggered finite difference mesh, or Fourier transforms.

The FEMHD code runs on several platforms, including Crays, UNIX workstations, and a parallel version runs on an IBM SP1.

The FEMHD mesh generation and discretization routines have been packaged as a C++ class library, MeshObject, which is callable from Fortran programs. Use of the C++ class library encapsulates and hides the finite element code from the calling Fortran, minimizing the chance of memory conflicts and interference. The MeshObject library has been integrated successfully with a version of the reduced MHD HIB code. Different makefile options can be chosen to produce a code that runs as a standard finite difference / Fourier code in circular geometry, or an unstructured mesh code in arbitrary geometry (including circular). The next step is to extend this to the PPPL MH3DK hybrid code, to produce a "supercode" with full MHD, hot particle species, and ability to run in a complex spatial domain.

Unstructured meshes offer two important advantages. They may be fitted to complicated boundaries. This is necessary for simulations of divertor tokamaks. A structured mesh based on flux coordinates encounters problems at the magnetic separatrix, such as poor resolution of the x point and the need for branch cuts. These problems are avoided with an unstructured mesh, which may nevertheless be aligned with the magnetic field.

The second advantage is the ability to introduce localized mesh refinement. For example, extra cells may be added at the magnetic x point. The mesh can be refined to adapt to the solution. Cells may be added to resolve current sheets, which have a fundamental role in MHD instability and fast magnetic reconnection.

Discretization of partial differential equations on the unstructured mesh is done by Galerkin expansion in basis functions. The most convenient basis functions are piecewise linear "tent" functions, which are non zero at a vertex common to several triangles, and which vanish at all other vertices. The resulting discrete matrix equations are very sparse, since the elements are non zero only on the triangles which include a particular vertex.

Figure 1: Computational mesh for tokamak edge region simulations.

Several problems have been considered with the unstructured mesh FEMHD code, and are described in Section B below.

B. MHD SIMULATIONS IN DIVERTOR TOKAMAKS

1. Poloidal flow spin up in a single null divertor geometry.

The up down asymmetry of a single null divertor tokamak causes poloidal shear flow in the closed flux surfaces near the separatrix. This is seen in numerical simulations and shown by theory [1]. The spin up occurs because the cross field diffusion terms, in particular $\kappa \nabla^2 p$, vary poloidally because of the magnetic field geometry. This result is relevant to the H mode in devices such as DIII-D.

The physics model consists of the dissipative MHD equations. The important dissipative terms are the compressional viscous stress, and the density or pressure cross field diffusion. It was convenient to use the CRMHD model, an aspect ratio expansion which retains the formally higher order coupling to sound waves.

A local analysis on a single flux surface shows that the equilibrium rotation speed is a root of a fifth order polynomial. In the theoretical model, the flux surfaces are assumed circular and the presence of the divertor introduces a $\sin \theta$ variation of the diffusive pressure flux. The equilibrium speed depends on the ratio of the poloidally varying part of the diffusion term to the sound wave transit frequency. When this ratio reaches a critical value of order unity, the rotation speed is attracted to a value $v_\theta > c_s/qR$, where c_s is the sound speed, R is the major radius, and q is the safety

Figure 2: Equilibrium magnetic flux function ψ in a single null divertor tokamak.

factor. Near the separatrix, q is large, and so spinup tends to occur in a thin layer, as in experiments.

Two dimensional, time dependent simulations with an unstructured mesh MHD code, FEMHD, described below, verify the essential features of the theory. The code solves the CRMHD equations, with the parallel viscous stress, in a realistic divertor tokamak geometry containing a magnetic separatrix inside the computational domain. A typical unstructured mesh is shown in Fig. 1. Equilibrium magnetic flux surfaces are shown in Fig. 2.

Poloidal rotation is observed at a speed comparable to the poloidal sound speed. The numerically computed poloidal flow is an $\mathbf{E} \times \mathbf{B}/B^2$ drift, with the radial electric field pointing inward, which agrees with experiment. Typical equilibrium electric potential contours are shown in Fig. 3.

2. Simulations of ELM - like Ballooning Modes in a Divertor Tokamak.

Edge ballooning modes are a likely cause of ELMs, edge disruptions which occur during H mode operation.

A numerical study is underway of low mode number pressure driven modes in the outer region of a tokamak, which includes the closed and open field lines adjacent to the magnetic separatrix.

Figure 3: Equilibrium electric potential ϕ caused by diffusion spinup.

The study is being done with a version of the FEMHD code, which has 2D, 3D linear, and 3D nonlinear options. The 2D option is used to prepare self consistent equilibria. Starting from a nonequilibrium initial state, the code is time advanced until a minimum potential energy state is reached, with kinetic energy removed by viscous dissipation. In the linear option, individual toroidal Fourier modes are evolved until they grow exponentially with a constant growth rate. In the 3D nonlinear option, the equilibrium and linear modes are used as initial conditions. The computational mesh is based on a B2 conformal mesh, with extra mesh refinement around the separatrix x point and in the outer half of the tokamak, where ballooning modes are concentrated.

The code has been compared with equilibrium and stability results obtained with the HIB code, for circular cross section high beta tokamaks. The codes show good agreement.

In divertor geometry, the FEMHD linear results give the growth rate of toroidal mode number $n = 1, 2$ instabilities as a function of β . The instability seems to behave like an external mode, in that there does not appear to be a second stable region in β . The plasma outside the separatrix was modelled as conducting, rather than vacuum.

Nonlinear runs are initialized with the $n = 1, 2$ linear eigenfunctions. The nonlinear growth of the mode saturates and no further growth is seen. An upwinded treatment of the pressure advection term was used. The nonlinear runs show advection similar to Rayleigh Taylor instabilities. An example of the nonlinearly saturated pressure in

Figure 4: 3D nonlinear pressure p in a ballooning unstable single null divertor tokamak.

a poloidal plane is shown in Fig. 4. The nonlinear flow pattern at the same time is shown in Fig. 5. The flow has two components. On the right (outboard) side of the tokamak are vortices of the ballooning modes. On the top, bottom, and left (inboard) side is a large scale flow aligned with the equilibrium magnetic surfaces. The large scale flow spins up when the modes saturate, and advects the pressure perturbations along the magnetic field in a counterclockwise direction.

The large scale flow might explain an experimental puzzle. If ELMs are caused by pressure driven instabilities localized to the outside of a tokamak, why is there a large flux to the *inboard* divertor? This flow, which convect material from the outboard to inboard side, could be the answer.

The spinup mechanism has yet to be analyzed. There are two possibilities: (1) Reynolds stress, which can be easily checked by turning off the nonlinear vorticity advection. (2) Stringer spinup, which is a 3D variation on the 2D spinup reported in the following. The ballooning modes provide an effective diffusion, which causes variation of pressure on magnetic surfaces. This causes a poloidal torque.

This work is being presented at the Fall 1995 APS meeting and is being prepared for publication.

3. Reconnection and Singular MHD Equilibria

Figure 5: 3D nonlinear electric potential ϕ during a model ELM.

In the last few years, we have studied three dimensional reconnection in line tied magnetic fields. The line tied boundary condition has an inhibiting effect on reconnection. Line tying is important in the solar corona, but may also be important on open field lines in a divertor geometry. The presence of a magnetic separatrix structure is an important feature associated with reconnection. We showed [2] that the presence of an x point largely offsets the effects of the boundary conditions, because of the exponential shrinking of scales near the x point. This may be important for understanding reconnection near the separatrix of a divertor tokamak.

C. COMPUTATIONAL ISSUES

1. Parallel Computation

The 3D FEMHD code has been parallelized and run on an RSM1 belonging to the NYU Academic Computing Facility. The IBM RSM1 is a cluster of 16 IBM RS6000 workstations connected by a fast network. Parallelization of FEM3D was achieved by using the PVM3 message passing library. The FEMHD code is well suited to coarse grain parallelization. The data divides naturally into sub arrays consisting of variables localized to a single poloidal plane. Each processor solves the RMHD equations on a few poloidal planes. Boundary data is be sent to neighboring processors at every time step.

The linear version of the code is even better suited to parallelization. Each processor solves the initial value problem for a single toroidal mode, independently of the other processors. There is only minimal message passing of kinetic energy per mode and other global data back to the host node.

The output shown in Figs. 4 and 5 was generated using the parallel version of the code.

2. Object Oriented Unstructured Mesh Package

I have made a C++ unstructured mesh MeshObject class library. A benefit of object oriented programming is that the objects are like black boxes whose inner workings are hidden from and protected from the user. They can be linked with other code in a simple way, without having to be concerned with details of their inner workings.

It's possible to coat Fortran code in a C++ wrapper. This approach allows existing Fortran code to be repackaged in a more modular and powerful way. I've found that this wrapping method is simple and straightforward. I've implemented it on the Cray machines as well as local Sun workstations. I expect to try it soon on an IBM RS6000. My mesh objects generate a FEMHD unstructured mesh create all necessary auxilliary arrays, and produce the sparse matrices needed for the calling code. The auxilliary arrays stay within the mesh objects. Also provided are a set of differential operators including gradient, curl, and divergence, as well as various Poisson solvers based on an ICCG solver.

The MeshObject package handles complex arithmetic, since it is intended to be used with semi spectral codes which use complex Fourier transforms. The package has already been integrated successfully with a version of the reduced MHD HIB code. Different makefile options can be chosen to produce a code that runs as a standard finited difference / Fourier code in circular geometry, or an unstructured mesh, arbitrary geometry (including circular). Equilibrium and stability calculations using the two versions have been compared and there is good agreement.

3. Adding Unstructured Mesh to PPPL MH3DK Code

The MeshObject approach will be tried in adding an unstructured mesh capability to the PPPL MH3DK code, a full MHD hybrid code. The basic subroutines needing replacement are already tested in a finite element code based on HIB, an ancestor of MH3DK. The idea is to divide the MH3DK code into two parts, one part which is mesh independent: the driver, the time advance of the variables, and the input / output. This part is compiled separately. The other part is mesh dependent and consists of subroutines for differential operations and plotting. There are two versions of these routines: the finite difference version, and the unstructured mesh version

which calls MeshObject functions. The user will have the option of loading from a structured mesh or unstructured mesh library.

(with Wunchull Park, PPPL)

4. Unstructured Mesh Edge Code

The unstructured mesh methods have been used to make a new edge plasma code. The initial work was done with Dmitry Rayevski. The code uses pieces of B2; the tables of ionization and other coefficients, and the initial mesh geometry.

The code solves continuity and parallel momentum equations for ions and neutrals. There is a single temperature equation. The transport coefficients, ionization, and charge exchange rates are functions of the densities and temperature as used in B2. An upwind method is used for advection terms. Reasonable progress was made with the code, but it needs more work on boundary conditions.

5. Workshop on Unstructured Mesh Methods

A Workshop on Adaptive Grid Methods for Fusion Plasmas, sponsored by SAIC, NERSC, and NYU, was held December 8-9, in Pleasanton, CA, to discuss adaptive grid methods and how to apply them to magnetic fusion problems. The organizers were H. Strauss, A. Koniges, and D. Schnack.

There is an urgent need to upgrade existing computing capability to include adaptive meshes. They are required for tokamak simulations involving divertors. High priority ITER relevant computations will not be done unless these methods are developed and applied.

Adaptive mesh methods have been used successfully in CFD (computational fluid dynamics) for a decade. Using adaptive mesh methods, it is possible to solve previously intractable problems involving complex boundary shapes and multiple spatial scales.

Similar kinds of difficult problems arise in magnetic fusion MHD. Divertor tokamaks have a complicated computational geometry, when both open and closed field lines are included in 3D MHD simulations. Conventional numerical approaches have been unsuccessful in allowing for the effects of a separatrix, which is critical for simulating ELMs and disruptions. The MHD theory working group has identified the need for such simulations as a high priority for ITER.

In the area of plasma edge modelling, fine scale structures can occur, such as ionization fronts. These fronts develop in detached radiative divertors. Existing codes cannot adequately resolve these fronts. The difficulty is even greater when these structures move around in the SOL (scrape off layer) in response to changing conditions. The edge theory working group has identified the need for adaptive grid detached plasma simulations as a high priority for ITER.

A reasonable starting point is with the numerical methods which work well in CFD. The workshop, summarized below, dealt with existing CFD approaches, as well as fusion implementations and applications.

There are two main approaches to adaptivity. The first approach is to use an unstructured grid, which can be readily refined where necessary to resolve features of the simulation. Review talks were given by David Bacon of SAIC, and Manoj Prasad of LLNL, which used this approach. The other approach to adaptivity was described in a talk by Phil Colella of Berkeley on the AMR code. This method makes use of structured, logically Cartesian grids, for which numerical hydrodynamics methods are well developed. Adaptivity is achieved by overlaying finer grids over coarser ones.

Several fusion researchers gave presentations, including H. Strauss, J. Wiley, A. Kuprat, D. Schnack, A. Koniges, and D. Hewitt. The workshop was successful in its objective of showing fusion researchers what has been done in CFD. At the same time, it was clear that fusion scientists have made great progress in introducing adaptive mesh methods into MHD and edge modelling. These methods are required in computational problems which include the presence of a divertor, such as MHD ELM simulations and radiative divertor modelling.

In addition to developing the adaptive mesh methods, there should also be an effort made to make adaptive mesh code packages which could be integrated into other codes. Use of object oriented languages such as C++ and Fortran 90 would be best for this.

(with Alice Koniges, NERSC and Dalton Schnack, SAIC)

PUBLICATIONS

1. H. R. Strauss, Poloidal Rotation Spinup in Divertor Tokamaks, *Physics of Plasmas* 2, 1229 (1995).
2. D. W. Longcope and H. R. Strauss, The form of ideal current layers in line-tied magnetic fields, *Ap. J.* 437: 851-859, (1994).

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