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The Computational Physics Program of the National MFE Computer Center

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I. INTRODUCTION

Since June 1974, the MFE Computer Center has been engaged in a significant computational physics effort. The principal objective of the Computational Physics Group is to develop advanced numerical models for the investigation of plasma phenomena and the simulation of present and future magnetic confinement devices. In addition, the group interacts with the systems programming staff to improve services; it fills the roles of internal critic and advisor by representing a user viewpoint.

The group currently consists of six Ph.D. physicist/mathematicians - D.V. Anderson, G.D. Kerbel, A.E. Koniges, M.G. McCoy, A.A. Mirin and D.E. Shumaker. In addition, students in the Department of Applied Science (U.C. Davis) are engaged in fusion research under the guidance of senior group members.

The computational physics group is involved in several areas of fusion research. One main area is the application of multidimensional Fokker-Planck, transport and combined Fokker-Planck/transport codes to both toroidal and mirror devices. Another major area is the investigation of linear and nonlinear resistive magnetohydrodynamics in two and three dimensions, with applications to all types of fusion devices. The MHD work is often coupled with the task of numerically generating equilibria which model experimental devices. In addition to these computational physics studies, investigations of more efficient numerical algorithms are being carried out. In particular, the group is making a major effort at ascertaining how to efficiently utilize multiprocessor computers.

One of the principal objectives of the computational physics group is to provide support for experimental and theoretical work within the MFE community. At present, this support falls into the following areas:

RF heating and current drive in tokamaks	GA, PPPL
Fokker-Planck and transport analyses of tandem mirror systems	LLNL, SAI
Tandem mirror equilibria	LLNL, MIT
Resistive stability of RFP	LANL, SAI
Compact torus transport/equilibrium	LANL, U. Wash.
MHD evolution of Spheromak	LANL

A summary of our program follows.

II. COMPUTATIONAL STUDIES

A. MHD EQUILIBRIA AND STABILITY

1. TIME INDEPENDENT MAGNETOHYDRODYNAMICS

In simple 1-D configurations the calculation of plasma equilibrium profiles is rather trivial. For more realistic two and three dimensional plasmas the determination of the equilibrium magnetic fields and the plasma pressure is a complicated non-linear problem involving the solution of elliptic partial differential equations. One of the goals of this work is to obtain configurations like those seen in experiments; accordingly some of our calculations use boundaries and external coil sets which accurately represent the devices under study. A secondary goal is to compute equilibria of sufficient accuracy so that the results can be used by stability codes with some confidence. In this connection high order finite element or finite difference representations have been used. These equilibria are also used to explore single particle effects in equilibirium magnetic fields.

Most of our codes solve Ampere's law given some non-linear dependence of the currents on the fields. Other codes use a dynamic evolutionary approach with artificial damping to obtain steady flow equilibria. Still others merely numerically evaluate known analytical equilibrium profiles. Several of these codes are briefly described in Table 1.

Our research has been in the following areas:

•A code has been developed to solve the 2D equilibrium problem for compact toroids. The algorithm is applicable to elongated plasmas. Finite elements are used to solve the Grad-Shafranov equation. The region in which the equilibrium is computed may contain a separatrix, and plasma may be present both inside and outside of the separatrix. The equilibrium is determined from adiabatic quantities, magnetic fluxes and entropy; hence, the solver is suitable for insertion in a transport code.

•Tandem mirror equilibrium calculations have been undertaken in 3D, with the goal of making the simulations as realistic as possible. A multispecies plasma is modeled in a multi-region configuration to account for the various types of trapped and passing components known to exist in these devices. Ambipolar effects are included. High beta and finite curvature effects are modeled without making low beta or long-thin approximations. A finite element representation is used on a rectangular grid. The effect of sheath formation has been shown to be in agreement with other theory and experiments. Some species, such as sloshing ions, are poorly represented by adhoc pressure functions, so these are being supplemented by models using correct moments of microscopic distribution functions.

•A code which computes the vacuum magnetic field inside a toroidal vessel of arbitrary cross-section has been developed and applied to HELIAC. General curvilinear coordinates conforming to the shape of the vessel are used. The magnetic scalar potential is expanded as a double Fourier series in the poloidal and toroidal angles. The resulting magnetic fields have been evaluated for their minimum-average-B and shear stability properties using the field line tracing code TUBE. The aim has been to find optimum vessel configurations by calculating the resulting surface currents and later discretizing these skin currents with closed current loops.

Our time-independent MHD publications are summarized in Appendix A1.

2. TIME DEPENDENT MAGNETOHYDRODYNAMICS

A principal technique for determining macroscopic plasma behavior is through the solution of the time dependent MHD equations. Of particular interest is the nonlinear evolution and saturation of fluid instabilities. Accurate simulation of such phenomena requires the solution of the full set of MHD equations, which comprises a coupled system of eight nonlinear partial differential equations. This is a formidable task for any computer system. In order to make these computations tractable, approximations have often been made, including reduction in dimensionality, linearization, restriction to a particular geometry and the assumptions of infinite conductivity and/or low "beta" ("beta" is the ratio of plasma pressure to magnetic pressure). The infinite conductivity assumption (called ideal MHD) greatly simplifies the numerics, since the MHD equations are then hyperbolic rather than parabolic. Moreover, resistive MHD instabilities tend to grow more slowly than ideal MHD instabilities, thereby requiring longer running times. The low beta assumption allows an ordering in which the problem is reduced to the solution of two scalar equations.

At the MFECC, the emphasis has been on constructing resistive MHD codes which are applicable to all plasmas, independent of beta. Both linear and nonlinear codes have been written which solve the full set of resistive, "finite-beta" MHD equations in two and three dimensions (see Table 2). Moreover, most of these codes use an implicit time discretization, so that there is no restrictive non-physical upper bound on the size of the timestep.

Our MHD research is in the following areas:

- Linear and 3D nonlinear studies of resistive interchange modes in the Reversed Field Pinch are being carried out. The effects of including the Hall terms in Ohm's law are being modeled. Tensor thermal conductivity and viscosity are included.

- Our nonlinear 3D code is being applied to the behavior of resistive modes in compact toroids. Whether or not a general equilibrium relaxes to a force free state, and if it does, how long it takes and how the relaxation is affected by MHD modes, is under investigation.

- A study of the stability of long, thin theta-pinch equilibria to the n = 1 tilt mode has been completed. Earlier numerical work predicting a fast growing tilt instability was in contradiction to the long quiescent times of the experiments. The hypothesis that the computations were based on incorrect models of the theta pinch equilibrium is now refuted. Usage of a resistive MHD stability code has shown that stretching of the closed elliptical flux surfaces (making them more racetrack as in the experiments) is destabilizing. The stability of these devices to this mode is due to effects beyond the MHD model. In particular, kinetic effects must be taken into consideration.

- A study of rippling modes in tokamaks is about to begin.

Our time-dependent MHD publications are summarized in Appendix A2.

B. PLASMA TRANSPORT

Transport codes are used to evaluate macroscopic plasma parameters (e.g. density, temperature) on a timescale comparable to the lifetime of the plasma. They differ from other fluid codes in that the fast timescale physics is integrated out of the problem.

At the MFECC, transport codes are being applied to tandem mirrors, tokamaks and compact toroids. A list of our transport codes and their applications appears in Table 3.

Over the past few years we have made a great deal of progress in the following areas:

- Radial transport in tandem mirrors
- Fokker-Planck/transport studies of tokamaks
- Transport in compact toroids
- Anomalous electron transport in tokamaks

A brief summary follows.

- Radial Transport in Tandem Mirrors

A tandem mirror machine consists of a long, solenoidal cell with minimum-B mirrors (plugs) at either end which act to electrostatically confine the central cell ions. The rate at which charged particles and heat diffuse in radius is of crucial importance. Of special significance is the expected enhanced transport of ions due to resonance between their azimuthal drift and axial bounce motions, which results from the presence of a non-axisymmetric magnetic field in the transition regions between the end plugs and the solenoid. A radial transport code, TMT, has been written in order to investigate this and other related phenomena. This multispecies code computes radial profiles of densities and temperatures in both the central solenoid and the end plugs along with a self-consistent electric field. Classical and neoclassical effects on transport are taken into account. This code has been used to study the Tandem Mirror Experiment and to help design larger tandem mirror devices.

- Fokker-Planck/Transport Studies of Neutral Beam-Heated Tokamaks

Neutral beam-heated tokamaks are characterized by the presence of one or more energetic ion species which are quite non-Maxwellian along with a warm Maxwellian bulk plasma. For scenarios in which there is a large energetic ion population, it is very important to represent these energetic species by means of velocity space distribution functions and to follow their evolution in time by integrating the Fokker-Planck equations. It is essential to utilize the full nonlinear Fokker-Planck operator to assure that the slowing down and scattering of these energetic species is computed accurately and realistically.

Our Fokker-Planck/transport code (FPT), in addition to solving radial transport equations for the bulk plasma densities and temperatures, solves nonlinear Fokker-Planck equations in 2D velocity space for the energetic ion distribution functions. The FPT code is unique in that it is the only tokamak transport code which does not either linearize the Fokker-Planck operator or ignore it altogether. Also, neutral beam deposition and neutral transport are computed using appended Monte Carlo codes developed at Princeton.

During the past few years, FPT has been applied principally to PLT, TFTR and DITE.

- Transport in Compact Toroids

The compact torus experiments (field reversed theta pinch and spheromaks) differ from the tokamak in that the plasma extends to the axis of rotational symmetry. Interest in the compact torus is due to the fact that it is likely to attain high beta and the fact that there is an engineering advantage of not having any structure through the center of the torus.

A transport code, CTT, has been written to describe the evolution of the plasma and magnetic field in a compact torus. This code differs from the tokamak transport codes in that the plasma extends to the axis of rotational symmetry and the 2-D equilibrium calculation contains a separatrix. The system evolves by alternating between the solution of four 1-D transport equations and the calculation of a 2-D equilibrium. The independent variable is the poloidal magnetic flux. Classical diffusion, Pfirsch-Schluter diffusion, radiation, Joule heating, lower hybrid drift diffusion and open field line loss are modeled.

The code has been used to model the FRX experiment at LANL. Simulation of other compact toroids is under way.

●Anomalous Electron Transport in Tokamaks

Recently, there has been considerable interest in the effects of anomalous electron transport due in part to magnetic surface destruction. Since this heat loss represents a major problem in toroidal confinement, there has been a need for a program which would simulate this loss and allow for credible estimates of the effects of electron transport on lower hybrid heating, D.C. conductivity and soft x-ray spectra.

The computer program (LDL) which has consequently been developed is 2-D with independent variables velocity magnitude and radial position. It combines a velocity and radially dependent heat source and a 1-D Fokker-Planck treatment of electron collisions with a loss operator simulating diffusion in velocity-radius. This program has been applied to the Doublet experiments at GA Technolgoies, Inc.

Our transport publications are summarized in Appendix B.

C. FOKKER-PLANCK

The Fokker-Planck equation is needed to treat plasmas in which the charged particle velocity space distribution functions are non-Maxwellian. In a magnetic mirror device, charged particles will tend to leak out the ends of the device, resulting in a "loss cone" in velocity space. In tokamaks or mirrors where there is neutral beam injection, the ion distribution functions will be characterized by an energetic component (in addition to the maxwellian background). These are two situations which require the use of Fokker-Planck codes.

The MFECC has led the nation in the development and implementation of multispecies Fokker-Planck codes employing the complete nonlinear two-dimensional Fokker-Planck operator. Since our codes have been generalized to deal with toroidal and open-ended configurations, many physical effects have been incorporated in them and a variety of physical problems have been studied. A summary of our Fokker-Planck codes appears in Table 4.

Progress has been made in the following areas:

●We have developed a user-oriented package, FPPAC, which computes the coefficients of the complete nonlinear 2D velocity-space Fokker-Planck collision operator and time-integrates the corresponding finite difference equations. This package runs from 10 to 14 times as fast on the CRAY-1 as on the CDC 7600. The tremendous gain in speed is due not only to the vectorization efficiency of the CFT compiler, but also to the the fact that on the CRAY, one does not have to constantly move data between small and large core. FPPAC has been made available to the MFE community.

•Tandem Mirror Applications

A study of electrostatically trapped electrons in a tandem mirror thermal barrier has recently been completed. This has required solving Fokker-Planck equations for trapped electrons in the presence of passing electrons and under the influence of electron cyclotron resonant heating.

Calculations of fusion performance in D-D tandem mirrors have also been completed. Fokker-Planck equations for deuterons and the four reaction products have been solved. Radiation losses, recycling and drift pumping for ash removal have been included. Some p-based calculations have also been carried out.

A 2D nonlinear multispecies code is being used to assess trapping rates of passing ions in tandem mirror end cells in an attempt to develop scaling laws for single species and multispecies scenarios.

•A nonlinear multispecies Fokker-Planck code (CQL) which bounce-averages the differential operators of Coulomb collisions, quasilinear resonant diffusion induced by wave-particle interaction and an Ohmic electric field has been recently developed. A zero banana width is assumed. CQL is designed primarily to simulate toroidal devices, although it can be utilized for mirror applications. Salient properties of the rf wave field are modeled using the Appleton-Hartree cold plasma dispersion relation. Finite plasma effects, nonlinear effects and effects dependent on the locally non-Maxwellian character of the distribution functions are computed self-consistently. The code will be put in package form and made available to the MFE community. Inclusion of a relativistic electrons model is under study.

•To obtain a global view of tokamak operation, the two dimensional code (v,θ) CQL described above is being incorporated into a three dimensional driver, CQL3D, which will allow the calculation to proceed at several radial mesh points simultaneously. Due to the bounce averages, the resulting picture will in most cases be actually four dimensional, if one considers the poloidal perspective. To provide linkage between radial mesh points, a wave damping calculation to compute electric fields and other relevant wave parameters as a function of position (radial and poloidal) is being carried out. These updated quantities are then employed to obtain the quasi-linear operator. This program is well-suited to implementation in a multitasking environment. Distribution functions at the various radial mesh points can be advanced independently. The program is being written with both the CRAY-1 and the CRAY-2 in mind.

Our Fokker-Planck publications are summarized in Appendix C.

D. EFFICIENT NUMERICAL AND PROGRAMMING ALGORITHMS

•Solution of Implicit Systems

A general study of the Incomplete Cholesky Conjugate Gradient Method (ICCG) for solving sparse linear systems is being carried out. This technique has been shown to be considerably faster than other traditional linear solvers such as SOR and ADI. ICCG solvers applicable to scalar nine point two-dimensional difference operators and to 7, 15, 19 and 27 point 3D operators have been written and are available to the MFE community. Extensions to coupled implicit systems are under way.

•Multitasking

The CRAY-XMP and CRAY-2 computers possess more than one CPU and hence have the capability of parallel computation. Computer codes that require large fractions of the central memory or that need fast real time performance can benefit if they are written such that parallel computation is feasible. This mode of calculation is referred to as multitasking in the CRAY environment. The computational physics group is investigating the efficient utilization of the CRAY-2 and CRAY-XMP devices in this direction.

The group is expected to develop/convert codes of the following types: (a) multidimensional Fokker-Planck/transport, (b) time dependent 3D resistive MHD, (c) 3D MHD equilibria and (d) multidimensional electromagnetic particle, to make efficient use of the enhanced capabilities of a multiprocessor environment. The group could then act in an advisory capacity to the MFECC community of over 2000 users.

Publications in efficient algorithms are summarized in Appendix D.

E. OTHER AREAS

Although most of our research has dealt with equilibria, MHD stability, transport, and Fokker-Planck equations, we have undertaken some projects in other areas -- in particular Vlasov and particle simulations, and convergent neutral beam studies.

A self-consistent guiding center particle model coupled with a fluid equlibrium code has been used to study ion beam motion in a toroidal geometry. Applications include the study of collisionless beam behavior including strong counterstreaming beams and the steady state modeling of a CIT reactor, in which steady state beam currents and energy reinjection rates are computed.

A fully three-dimensional electromagnetic particle code is being written to study kinetic effects in Field Reversed Configurations. The code will take advantage of multiprocessing and is expected to run principally on the CRAY-2.

A single particle orbit following code allows us to make detailed studies of the confinement properties of equilibrium fields in two and three dimensions. Studies of adiabaticity as well as resonant orbital effects have been made. Experimentalists have used the code to design ion probe diagnostics.

A study has been made involving the creation of a very dense plasma by injecting convergent neutral beams into spherical or cylindrical chambers. Calculations of particle distribution functions, densities, ionization rate parameters and ionization probabilties have been carried out for both geometries.

A one-dimensional Vlasov finite difference code for ions and electrons has been written to study the formation of a plasma sheath and to compute steady state distribution functions along with a plasma potential.

A code has been developed to solve nonlinear elliptic equations on domains of very general shape.

Publications in these areas are summarized in Appendices E, F and G.

TABLE 1. MFECC EQUILIBRIA CODES

CODE	CONTACT	CHARACTERISTICS AND APPLICATIONS
CYLEQ	D.V. ANDERSON	2D (R,Z), Bicubic Splines, Finite Element, Tensor Pressure; Tandem Mirrors, Compact Toroids
VEPEC	D.V. ANDERSON	3D (X,Y,Z), Tricubic Splines, Finite Element, Vector Potential, Tensor Pressure, Ambipolar Effects, Vlasov Species; Tandem Mirrors
ABCXYZ, TPSIC	D.V. ANDERSON	Auxiliary codes for VEPEC
HILLSV	D.V. ANDERSON	Auxiliary code for CYLEQ
EIV	D.E. SHUMAKER	2D, Flux Coordinates, Finite Elements, Open and Closed Field Lines; Compact Toroids
VAFIS	A.I. SHESTAKOV*	3D, Double Fourier Series, General Coordinates; Stellarators, HELIAC
TUBE	A.A. MIRIN	Field Line Tracing Code; General Magnetic Fields

*Currently in X-Division (LLNL)

TABLE 2. MFECC TIME DEPENDENT MHD CODES

CODE	CONTACT	CHARACTERISTICS AND APPLICATIONS
TEMCO	A.A. MIRIN	3D (R,ϕ,Z), Nonlinear, Explicit, Resistive, Fourier Expansion in ϕ, Viscous, Hall terms; Compact Toroids, RFP
RIPPLE VI	A.I. SHESTAKOV*	2D (R,Z), Linear, Nonaxisymmetric Perturbations, Implicit, Resistive; Compact Toroids
ALIMO	A.I. SHESTAKOV*	2D (R,Z), Linear, Axisymmetric Perturbations, Implicit, Resistive; Compact Toroids
RIPPLE V	A.I. SHESTAKOV*	1D (y), Linear, Implicit, Equilibrium Flow
RIPPLE IV	A.I. SHESTAKOV*	1D (r), Linear, Implicit, Resistive; Tokamaks, RFP
ODRIC	A.A. MIRIN	1D (r), Linear, Implicit, Resistive, Compressible, Viscous, Thermal Conductivity, Hall terms; Tokamaks, RFP
STABCRIT	D.V. ANDERSON	2D (R,Z), Ballooning Modes, Energy Principle

*Currently in X-Division (LLNL)

TABLE 3. MFECC TRANSPORT CODES

CODE	CONTACT	CHARACTERISTICS AND APPLICATIONS
TMT	A.A. MIRIN	1D (R); Tandem Mirrors
FPT	A.A. MIRIN	Combined Fokker-Planck/Transport, 1D (R) plus 2D (V,θ); Tokamaks
CTT	D.E. SHUMAKER	1D (Poloidal Flux)/2D Equilibrium; Compact Toroids
TRANSPORT	A.A MIRIN	1D (R); Tokamaks
LDL	M.G. McCOY	2D (R,V); Electron Transport; Tokamaks

TABLE 4. MFECC FOKKER-PLANCK CODES

CODE	CONTACT	CHARACTERISTICS AND APPLICATIONS
HYBRID II	A.A. MIRIN	2D (V,θ), Nonlinear, Multispecies Ions; Mirrors and Tokamaks
TDMFP	A.A. MIRIN	2D (V,θ), Nonlinear, Multispecies Ions and Electrons; Mirrors
TDMSZ	A.A. MIRIN	3D (V,θ,Z), Nonlinear, Multispecies Ions and Electrons
FPPAC	M.G. McCOY	2D (V,θ), Nonlinear, Multispecies Ions; General Package
ISOTIONS	A.A. MIRIN	1D (V), Nonlinear, Multispecies Ions and Electrons; Mirrors and Tokamaks
CQL	M.G. McCOY	2D (V,θ), Nonlinear, Bounce Average, Multispecies Ions; Tokamaks
CQL3D	M.G. McCoy	3D (r,V,θ), Nonlinear, Bounce Average, Multispecies Ions and Electrons, RF with Wave Damping; Tokamaks

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