

COMPUTATIONAL PHYSICS AT THE NATIONAL ENERGY RESEARCH
SUPERCOMPUTER CENTER

Arthur A. Mirin

April, 1990

Lawrence
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COMPUTATIONAL PHYSICS AT THE NATIONAL ENERGY RESEARCH
SUPERCOMPUTER CENTER *

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The principal roles of the Computational Physics Group are (1) to develop efficient numerical algorithms, programming techniques and applications software for current and future generations of supercomputers, (2) to develop advanced numerical models for the investigation of plasma phenomena and the simulation of contemporary magnetic fusion devices, and (3) to serve as a liaison between the Center and the user community; in particular, to provide NERSC with an application-oriented viewpoint and to provide the user community with expertise on the effective usage of the computers. In addition, many of our computer codes employ state-of-the-art algorithms that test the prototypical hardware and software features of the various computers.

Our group currently consists of six physicist/mathematicians: Dave Anderson, Gary Kerbel, Alice Koniges, Art Mirin, Mike McCoy and Dan Shumaker. Three students in the Applied Science Department of the Univresity of California, Davis (Paul Amala, Dave Martin and Greg Tomaschke) are working with us while pursuing their graduate degrees.

This document describes the activities of the Computational Physics Group and was prepared with the assistance of the various Group members. The first part contains overviews on a number of our important projects. The second section lists our important computational models. The third part provides a comprehensive list of our publications.

I. Project Overviews

This section contains overviews of a number of our past and present research efforts.

PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Efficient Numerical Algorithms and Programming Techniques

D.V. Anderson, A.E. Koniges and A.A. Mirin
February 1990

In magnetic fusion plasma modeling with fluid or particle simulation techniques, it is often necessary to study phenomena over time scales long compared to the basic wave propagation times. Within the Computational Physics Group at the NERSC emphasis has been given to such long time scale phenomena, where for example, various resistive MHD problems, spatial diffusive transport, phase space transport (Fokker-Planck equation), as well as equilibrium and stability calculations have been studied [1-3]. The parabolic or elliptic PDE's that result share the common feature of being stiff and thus require implicit solution techniques.

To solve these matrix problems efficiently we have successfully combined powerful new methods of numerical analysis with the vectorization capabilities of the computers. The Preconditioned Conjugate Gradient (PCG) algorithms have been extended [4,5] and several publicly available code modules have been built [6-10,29] and optimized for the Cray-1, Cray X-MP, and Cray-2 computers.

For example, the modules ICCG2 and ILUGG2 solve the symmetric and asymmetric 9-banded matrix systems that frequently arise in 2-D problems. ICCG3 and ILUCG3 solve the corresponding 3-D problems for various band counts (7, 15, 19, or 27). These codes are largely vectorized except for the recursive loops, which have been coded for maximal scalar speed. An alternate method [11,12] of performing preconditioned conjugate gradient, based on cyclic reduction and which avoids tight recursions, has been used to develop the fully vectorized codes FVICCG and FVILUCG [13].

A variation of ILUCG called ILUBCG2, which uses the biconjugate gradient method, was introduced recently. In the solution of a coupled set of plasma stability equations, the ILUBCG method was shown to yield faster convergence than the ILUCG methods [14]. We therefore provided the BCG method as an alternative to the basic CG method in our solvers. Rather than use the BCG algorithm in the form used by Mikic [14], we developed a new form of the algorithm which naturally divides the work into two equal-sized parts [15]. This allowed us to multitask the BCG method, taking advantage of the bilateral symmetry. The multitasking algorithm gives a wall-clock-time speed-up of 40% over the unitasking BCG version which in turn is about 30% faster than the preconditioned CG solver; thus the overall speedup of the new solver was about

80%. We also recently built ILUBCG2-11, which is an eleven banded solver appropriate for 2D problems with singly periodic boundary conditions.

Recent plasma physics applications, including a field solver for the 3-D particle simulation code QN3D, have required routines suitable for coupled PDE systems. For this purpose new solvers that employ preconditioned conjugate gradient techniques were developed [16]. Both two and three dimensional problems are treated by the codes CPDES2 [17] and CPDES3 [18], respectively. In each of these the user may choose to use either the standard conjugate gradient method or the bi-conjugate gradient method. In the former convergence is guaranteed, while in the latter the rate of convergence is faster. These routines exploit the vector gather/scatter hardware available on the Cray-2 (and other recent computers) to produce a fully vectorized calculation. We identified four loops in the code where the indirect vectorization is implemented and where nearly all of the time is spent. Timings of these loops seemed to show that there was considerable room for optimization. We built a version of CPDES3 that used assembly code to optimize the execution of the loops employing indirect vectorization. The vectors encountered were not long enough for us to achieve a factor of four speedup that an asymptotic analysis (for long vectors) indicated. Instead we gained only a ~20% improvement in performance. Recently, we have learned of techniques employing "supernodes" that will allow us to use direct vectorization in future versions of CPDES2 and CPDES3.

In addition, we began investigating other iterative methods and various preconditioning techniques to determine which are the best methods both for our physics problems and for the multitasking environment. In a collaborative effort with the University of Texas Center for Numerical Analysis, we obtained the ITPACK 3 software [19] and used it for comparison tests of various methods.

We investigated the use of incomplete matrix inversion as a preconditioner. A special test code, PINK, was built to solve the same 9-banded systems that ILUBCG2 treats. It was determined that this form of preconditioning is effective but not nearly as good as incomplete factorization. However, PINK is fully vectorizable and parallelizable and thus may represent a viable approach for future sparse matrix solvers based on PCG techniques.

A survey of iterative solvers was conducted to determine what packages are being used and/or are available at the NERSC. It was found that apart from the ITPACK routines and the authors' own solvers, very few routines are available [20,21].

In addition to our work on iterative techniques, we have developed a direct matrix solver for block banded systems in which the blocks are dense [22]. Such a matrix form occurs in several 3-D applications where spectral representations are used in two coordinates and finite element or finite difference methods are used in the third. The code in question, PAMS (Parallelized Matrix Solver), exploits three levels of parallelism, namely: a) functional unit overlap, b) vectorization, and c) multitasking. This applications code is one of the fastest running on the Cray-2, where its average speed has been measured to be 1.25 Gflops in a timesharing environment

and 1.26 Gflops in a stand-alone environment, representing an improvement over the results presented in Ref. [23]. Sustained speeds, measured over intervals of several seconds, have exceeded 1.5 Gflops. We are in the process of replacing some of the basic Cal-2 subroutines with even faster ones to obtain further improvements in speed.

The matrix system solved by PAMS is also encountered in many other physics, engineering, and other technical disciplines. As such, it can be used as a benchmark calculation for purposes of comparing computers. Since most supercomputers will employ both multitasking and vectorization, it is important that the benchmark algorithms exploit both of these features efficiently. In collaboration with Ecole Polytechnique Federale de Lausanne, we have tested several supercomputers including the Cray X-MP, Cray-2, NEC SX-2, Fujitsu VP-200, CDC-205, and the Piper version of the ETA-10 [24]. Of these machines the NEC SX-2 has performed extremely well. For pure Fortran versions of PAMS, we've obtained 440 Mflops (compared to 140 Mflops multitasking on the Cray-2). Only when assembly code is used in PAMS does the Cray-2 outperform the SX-2.

Many applications in plasma physics use finite Fourier representations. When the equations are discretized, they often become large-scale matrix systems in which the form is block multi-diagonal with dense blocks. In a plasma stability application, each matrix element was found to be given by large integrals over the "angular" coordinates. It was discovered that many of these matrix elements could be computed one block at a time by recognizing that the angular integrals have the form of inner products, which allows their computation via matrix-matrix multiplication. Since many such matrix blocks are required, multitasking can be invoked. The concept has been tested in the MULFI (Multiple Flux Tube Integrals) routine and very high speeds on the Cray-2 (up to 1730 Mflops) have been obtained. We have incorporated this procedure into the 3D-MHD stability code TERPSICHORE [25,30] to make it the fastest scientific computer code running on a Cray Supercomputer (in the sense that it won first place in the 1989 Cray Research Gigaflop Performance Awards contest).

In a somewhat related effort we undertook a study of our major physics codes to learn where multitasking could be used to improve the performance of our multiprocessor computers - the Cray X-MP and the Cray-2. The VEPEC code (Vector Potential Equilibria Code) for tandem mirror calculations was one of our main test beds in this regard. Many different segments of the code, of varying granularities, were converted to multitasking and subsequently tested. The comparatively small memory of the X-MP tends to limit the granularities such that multitasking there is not often advantageous. In contrast, the Cray-2, with its larger memory and four processors, gives good multitasking performance over a wide range of granularity. The Douglas-Gunn algorithm (3-D ADI) which solves the implicit Ampere's equation was multitasked to give roughly a factor of 3 speedup. As such it represents the most difficult conversion within the VEPEC code, and by inference we believe that most of the remaining unitasking code segments could enjoy significant improvements in performance by straight forward conversions to multitasking.

Recent developments in automatic multitasking now allow us to implement these techniques with very few additional instructions beyond standard Fortran. Although the earlier form of multitasking, now dubbed macrotasking, is

obsolete, we still have learned a great deal from our experience with it because we became familiar with those algorithms that are amenable to parallel execution.

Our multitasked simulation code (SIMU) uses the concept of ensemble averaging to solve a prototypical three-wave interaction problem. The use of ensemble averaging, as opposed to time-averaging, turns the problem into an ideal candidate for multitasking. Since realizations of the dynamical equation can be grouped into arbitrary-sized packets, the multitasking nature of the code can be adapted for machines with arbitrary numbers of processors - from four to four thousand.

In order to run SIMU and guarantee reproducible results independent of the multitasking, we require a means of producing strings of random numbers for each process. This problem is very important in all Monte-Carlo calculations run on multiprocessor computers. We have devised a method for producing independent strings based on hopping through a random number sequence at large intervals and picking up a seed for each process [26]. This method is particularly useful for our application and shows promise for use in general Monte-Carlo codes.

Another important issue is the degree of multiprocessing efficiency one should expect to get under CTSS, which is an intense time-sharing environment. In this regard we have used our 3-D MHD code TEMCO to study multitasking performance as a function of task size and code field length. This has led to a theoretical model designed to predict the the multiprocessing performance under CTSS [27]. We have found in general that the CTSS scheduler allows good overlap provided the code is large and the task string (i.e., the set of tasks which are available to run consecutively on a processor) is of medium-to-large granularity.

In addition to our research into multitasking, we have been playing the roles of teacher, consultant, and collaborator in our interactions with our colleagues at other institutions. At many workshops and conferences we have presented the methods, strategies, and results of multitasking with the intention of convincing other workers of its viability. For example, we presented a review of parallel computing in plasma physics which concluded that most of the computational methods used therein can be straightforwardly modified to enjoy the performance advantages of multitasking [28]. With the advent of automatic multitasking, we expect many more computer users will be parallelizing their codes than was previously the case. We continue to explore what incentives, including modifications of the charging algorithm, could bring more people into the multitasking community.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Massively Parallel Computing

G.D. Kerbel, M.G. McCoy and A.A. Mirin
February 1990

Over the past several decades there has been a tremendous increase in computer power. Most of this increase has been due to improvements in hardware. Electrical components have now become so efficient, however, that more recently the concentration has been on improving the architecture of the computer. This has led to shared memory multiprocessor supercomputers such as the Cray-2 and the Cray-YMP. Although these multiprocessor devices have had a substantial impact on high speed computing, it has been recognized that a more cost effective approach might be to link together very large numbers of slower, cheaper processors, each with its own local memory. Such massively parallel computers, although not general purpose, have performed quite impressively in a number of problem areas, and the computing community is now beginning to think in terms of their use as production machines in the not-too-distant future.

The NERSC Computational Physics Group has begun an investigation into the suitability of the massively parallel technology for modeling plasma phenomena. Research has been carried out in two separate but related areas -- kinetics (using the Fokker-Planck approach) and turbulent transport.

PLASMA FOKKER-PLANCK. The Fokker-Planck equation, which is related to the Boltzmann equation of kinetic theory, can be used to model collisional relaxation in an ionized gas. In its full generality, the Fokker-Planck operator models time dependent phenomena in six dimensional phase space. However, certain common symmetry and ordering assumptions can often be made, allowing the dimensionality to be reduced to four -- two spatial and two velocity coordinates. When the magnetic field is uniform or when the particle bounce motion operates on a time scale sufficiently faster than other phenomena of interest, one spatial variable may be eliminated, reducing the dimensionality to three. And when diffusion across flux surfaces is small relative to velocity space dynamics, the other spatial coordinate may also be eliminated, leaving only two velocity coordinates.

A widely used code which invokes the assumptions discussed above is FPPAC [1], which solves the multispecies, uniform magnetic field, two-velocity-space-dimensional Fokker-Planck operator. During 1989 FPPAC was converted to run on the Connection Machine 2 (CM2), which is a massively parallel device manufactured by Thinking Machines Corp. The CM2 consists of up to 65536 single bit processors, each with 8 kbytes of random access memory.

Groups of 32 processors share Weitek floating point hardware. The CM2 is an SIMD device -- that is, all processors performing an operation must perform the same operation. This feature makes the device more restrictive but easier to program. Programs may be written in either assembly language or specialized extensions of Fortran, C or Common Lisp.

The conversion of FPPAC involved a number of steps. Variables had to be allocated either to the CM2 or its front end, and algorithms had to be arranged to minimize data flow, both between the CM2 and the front end and between the portions of local memory associated with the different processors. The Cray-optimized algorithms had to be replaced with ones minimizing the number of parallel steps. In particular, the procedure to compute the various moments of the distribution functions was recast so that it utilizes an algorithm to compute all partial sums of a sequence of numbers using a minimum number of parallel operations. The time integration procedure, which involves the solution of parallel tridiagonal systems, is carried out using a parallel form of cyclic reduction. This work was accomplished using the Fortran compiler.

Results on the Connection Machine have been found to be in good agreement with those of the Cray. The time required to solve the parallel tridiagonal systems is found to be comparable (if one were to extrapolate up to a 65536-processor CM2) [2]. The time required to compute the Fokker-Planck coefficients, however, is competitive only for very fine meshes and long Legendre expansions. That is because the CM2 matrix multiply routine is tuned for very large matrices. Moreover, such calculations have to be run using 64 bit arithmetic in order to be able to represent the wide range of exponents.

The next step is to convert FPPAC to the BBN Butterfly II and to compare performance between that machine, the CM2 and the Cray. Another related project which is just getting under way is that of a Monte Carlo Fokker-Planck calculation on the Butterfly II. Here massive parallelism might be harnessed to obtain more accurate statistical estimates of radial diffusion coefficients.

PLASMA TURBULENCE. One of the most challenging problems in plasma physics is to understand and perhaps control plasma transport in tokamaks. In principle, collisional transport processes can be described well by the Fokker-Planck approach above. In cases where the only significant cross field drift velocity is the magnetic or "grad-B" drift, neoclassical transport theory has used this approach. Yet there is a great deal of experimental evidence that transport in magnetic confinement devices is largely controlled by strongly turbulent convective processes which are the result of the nonlinear coupling of unstable modes of collective particle motion. The description of this type of process is computationally inaccessible by the Fokker-Planck approach at this time.

To resolve this difficulty, a fluid approach is taken [3]. After Fourier transformation of the simplified fluid equations, the nonlinear mode coupling takes the form of a convolution of the Fourier modes of the fields. In practice, the evaluation of this nonlinear coupling convolution takes the lion's share of the computer time in the Cray-2 version of the algorithm. As much as a factor of ten speedup could be gained simply by eliminating this

bottleneck. It has been the express purpose of this research to determine if and how this can be accomplished using the Connection Machine.

At the beginning of the project, the Cray-2 direct method routine for evaluating the convolution required 1.5 seconds to execute on our base case. This routine is exercised once per timestep for each field. Since the scheme is necessarily not fully implicit due to the nonlinearity, the timestep must be dynamically controlled to assure accuracy and stability. The comparatively small requisite timestep is the reason that optimization of the convolution computation is so important. Optimization performed on this routine in the early stages of the project resulted in a speedup on the Cray-2 so that the direct method now executes on the Cray-2 in .68 seconds on the base case.

Estimates based on CM2 floating point unit throughput suggested the possibility of speedup factors from ten to forty on the CM2. To realize this speedup, the numbers to be combined must be delivered to the floating point units as fast as they can be processed. What on the Cray-2 amounts to unrolling loops and generating common subexpressions to minimize the fetches from memory to the vector registers translates on the CM2 to requiring that communications be local (or nearest neighbor). Using this condition as a guide has led to the development of a local parallel vector-indirection CM2 direct convolution algorithm which has proven to be competitive with a single processor of the Cray-2 for the base case.

The scaling of this algorithm's performance with problem size is quite favorable for the CM2 and unfavorable for the Cray-2. The computation time scales roughly with the number of modes, N , on the CM2, but as "N squared" on the Cray. One quarter of the CM2 is utilized for this base case; using more of the CM2 is necessary to benefit from these economics of scale [4]. Increasing the problem size beyond the full CM machine size gains in computational efficiency due to the pipelining inherent in using virtual processor ratios greater than unity, but in that case scaling reverts to "N squared". Further substantial gains in performance (as much as a factor 5) can be realized by recoding the vector-indirection algorithm at the CM2 assembly language level.

Recognizing the advantages of pseudospectral techniques for problems larger than the base case, an optimized FFT convolution routine has been developed for the Cray-2 to compare with the direct method. It is further intended that a similar capability be developed using optimized CM2 FFT routines developed by Johnsson, et. al. [5] and the appropriate comparisons performed.

Beyond the SIMD CM2 approach to the problem, both of these algorithms can be directly implemented on the MIMD BBN TC-2000 currently planned for installation in March 1990 at LLNL. The technique involves a time advancement scheme executed on a per processor basis with the modes parcelled out among the processors in the cluster. Each processor retains all mode information for a subset of the total set of modes being followed by the computation in its local memory. This arrangement is different from the CM2 data decomposition in which each processor retains only a single radial datum for a given mode in its local memory. The mode coupling is then computed by copying the mode data to shared memory, performing the convolution with each processor doing a single radius

(flux surface) at a time. Returning the convolved fields to the appropriate local memories then completes the iteration.

What remains of the numerical algorithm necessary for the complete fluid turbulence calculation, putting the convolution algorithm aside, is the scheme for evolving an array of transport equations for the fields (pressure, parallel velocity, potential and vorticity), which are coupled linearly as well as nonlinearly. The algorithm developed for FPPAC using cyclic reduction could prove useful in this regard and needs to be compared with a parallel block SOR scheme for speed and accuracy on the CM2. It is likely that another scheme could prove more optimal on the BBN machine in this regard, and this is a topic of current study.

In addition to the above studies, we are presently in the process of forming an Office of Energy Research wide focus group in the area of massively parallel computing, with an eye toward the production environment. Toward this end we are looking into the possibility of using an intelligent data base to access appropriately catalogued information through the use of a network data retrieval system. Since the field of massively parallel computing is quite new, the ratio of neophyte to experienced users is quite high. It is our intention to provide a service that could, at a minimum, help accelerate the new user along the learning curve by pointing to critical basic information related to individualized interests. As a medium range goal, we are working towards the capability of providing network access to a distributed hypertext system for collaborative research in the area of massively parallel computing. Here the first level of data acquisition is represented by citations and text of published articles. Built on this foundation are articles and documents of a less formal nature supplied by individual or institutional subscribers, and at the top level, notes and personalized links to the cataloged data with access restricted by the respective individual owners. More experienced users could use the environment as a communication tool to increase the productivity of the collaborative activity in which they are involved.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Bounce Averaged Fokker-Planck Studies of Tokamaks with RF Excitation

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Non-uniform magnetic field effects (toroidicity) can play an essential role in determining plasma behavior. The electrical conductivity parallel to the magnetic field in a tokamak is strongly affected by the presence of a population of trapped electrons. Also, cyclotron resonance heating and the production or support of steady plasma currents to allow steady state operation of tokamaks are significantly affected by the magnetic field non-uniformity [1].

The bounce averaged Fokker-Planck code CQL (Collisional Quasi-Linear) was developed to allow the simulation and study of tokamak heating and current drive experiments [2,3]. The collision operator module can be relativistic (to order $\beta\beta'$), multispecies, and nonlinear. The fully relativistic quasilinear resonant diffusion operator module functions as an integral part of the Fokker-Planck time evolution model.

The consideration of these and other physical effects has required the analysis of a number of theoretical problems, the solutions to which provide the framework for the numerical methods utilized in CQL. Three illustrative examples follow: (1) Orbits which are nearly trapped but oppositely directed are topologically adjacent in velocity space and can populate each other through collisional or resonant wave/particle diffusion. Boundary layer jump conditions at the trapped/passing boundary are rigorously enforced by the numerical algorithm so as to maintain density conservation down to round-off; (2) The wave/particle interaction for a spectrum of waves including the effects of collisional gyrophase diffusion can be represented by a generalization of the method of integrating over unperturbed orbits. The generalization involves including a phase decorrelation factor which reduces contributions to the trajectory integral from the remote past due to intervening random events. The integrals occurring in a particular (numerical) experiment can be located in a precomputed database using certain dimensionless parameters relating wave/particle interaction autocorrelation, collisional diffusion, and bounce time scales. This technique reduces the associated cpu time at runtime from intractable levels to unnoticeable levels; (3) The plasma equilibrium used for the Fokker-Planck calculation can be generated independently by an equilibrium solver and read by CQL from a standardized format eqdsk file. Physical effects dependent on the plasma equilibrium, including the configuration of wave/particle resonances and the plasma trapping rate for neutral beams, are

computed consistently with the prior eqdsk equilibrium. Iteration through an external loop in which the equilibrium is adjusted quasistatically is thus prescribed.

The resonant diffusion (RF) module models the effects of Landau and cyclotron wave-particle interactions in tokamaks. Lower-hybrid and multiple harmonic cyclotron resonance heating and current drive scenarios are examples of problems of current interest which can be explored in this way. The evaluation of trajectory integrals for each gyro-orbit resonance through suitably scaling a universal function corresponds to bounce-averaging the wave/particle interaction operator. The collision operator is bounce-averaged directly by numerical integration. An auxiliary quasilinear module (VLF) is designed to study low frequency wave microstability. Here, high and low wave frequency are gauged relative to the bounce or transit frequency of guiding centers in the tokamak magnetic field.

Two numerical algorithms are available to compute solution distribution functions. If the time evolution of the plasma is of interest, the code employs an operator splitting technique, advancing in incremental time steps Δt whose magnitude is dictated by physical and numerical considerations. However, if the steady state alone is required, the differencing of the operators is fully implicit, and an extremely large (non-physical) time step is employed. The resulting sparse matrix is inverted with Gaussian elimination. For linear problems a solution is obtained with one matrix inversion. This inversion routine has been optimized for the Cray-2 within the physics group. It is capable of reaching speeds up to 400 MFLOPS on the F machine (the newer Cray-2 at NERSC). For example, the cpu time required to invert a problem with 100 theta mesh points and 100 speed (or momentum) mesh points is about .5 sec. To invert a system with 150 theta mesh points and 250 speed mesh points requires 4.2 sec of cpu time (with additional memory and system charges, of course). This code has been released to the community and to our knowledge is the fastest sparse matrix solver for matrices of order 1000 to 60000. For higher orders, iterative methods become more competitive. In one mode of operation, the implicit solver advances the system from one steady state to another, relaxing the wave spectrum to a state of balance where not only is the particle distribution steady, but so also are the wave amplitudes. This sort of computation can be done without monopolizing computing resources only because the matrix inversion engine is highly optimized.

The program CQL is currently being applied systematically to a number of problems and is undergoing further development as well. In collaboration with R. W. Harvey of GA Technologies, the code has been augmented by the addition of a radial coordinate, r [4]. The radial coordinate is introduced through a special module (TD) designed to manage profile data, disk I/O, and other information which exists in the extended 3-D domain. When this (TD) module is active we refer to the thus augmented code as CQL(3D). In this application the Fokker-Planck operator is time-advanced independently on a number of flux surfaces, and a 2-D wave transport equation is solved to determine the locally resolved wave energy density. This corresponds roughly to the calculation of a ray trajectory field. Wave polarizations and group velocities are represented on a 2-D mesh. The parallel wave number is taken to be a constant of the ray motion, a rather good approximation for ECH, which is less satisfactory for

lower hybrid wave propagation. The wave field information is then used to recompute the resonant diffusion coefficients in order to obtain a self-consistent picture of power absorption. The wave transport equation employs a fully relativistic dispersion relation routine, which has been benchmarked independently. The algorithm neglects reflections, assuming single pass absorption. For ECH this is usually adequate in large tokamaks. With this tool, we can examine global effects of inside and outside launch scenarios in DIII-D and in ITER. With modest modifications, a $k\parallel$ spectrum can be added (currently we assume a single $k\parallel$). Other researchers outside our group are using CQL (2-D) to estimate current drive efficiency for the proposed ITER experiment. With the global enhancement to CQL represented by CQL(3D), we can compare with and elucidate the explorative single flux surface CQL(2D) studies.

For less absorptive plasmas, a more elaborate ray tracing calculation involving multiple reflections is required. Efforts in this area have recently resulted in a new module (ULH), a lower hybrid and fast wave excitation module. The basic concepts are along the line of Bonoli, et al. [5] except that here the distribution function and the diffusion coefficients are 2D bounce averaged. The ULH routines interact dynamically with a Brambilla's ray tracing code [14], which provides the necessary wave characteristics and ray data to CQL(3D). The code utilizes the ULH routines to determine the RF diffusion coefficients, then it solves for the updated distribution functions on the flux surfaces. Finally, using the new distributions, the rays are individually damped to capture the local absorption data which is used to recompute the diffusion coefficients. If necessary, CQL(3D) calls the ray tracing code to extend rays which are not fully damped. This process is repeated to convergence.

As a benchmark calculation for CQL(2D) the effect of trapped electrons on electrical conductivity was examined. The enhanced resistivity was tabulated as a function of inverse aspect ratio, ϵ , and Z_{eff} . For the case $Z_{\text{eff}}=1$, where theoretical estimates exist [8], CQL agrees with theory for all values of ϵ to within 2 percent [2,3] (agreement is best where theory is most accurate). Runaway production rates as a function of ϵ have been calculated as well. CQL has been applied to study fusion reactivity enhancement by ICRF heating [6,7]. In the study heating was applied to one plasma species and the consequent reactivity enhancement was characterized by dividing the resulting bounce-averaged fusion rate by that obtained for an equivalent Maxwellian. Enhancement in high Q cases varied from 1.3 to 2.0. A more recent application of the code [9,10] examines the relative merits of inside vs. outside launch schemes for ECH current drive with particular attention to relativistic effects. This work appeared in Physical Review Letters [9].

Currently, code development is proceeding in a number of directions. First the zero banana width restriction has been relaxed to allow the calculation of non-Maxwellian corrections to neoclassical transport coefficients. This involves adding a finite banana width bounce-average and computing the (linearized) fluxes to neighboring flux surface velocity ensembles. The calculation takes place in two fully integrated modules developed by G. Tomaschke (WF and TR). This development can provide a useful tool for studying the effects on the transport matrix of a variety of non-classical mechanisms, including those depending on transfer of parallel

momentum between waves and particles. Enhanced transport due to neutral beam driven suprathermal tail distributions can also be studied with these modules. Some analytic work in this area has been done by Catto, et. al. [12]. Similar phenomena relating to tails driven by ICRF have been studied by Chang, et. al. [13].

Second, the code CQL(3D) has been augmented by the addition of an MHD equilibrium code and a neutral beam deposition code, NFREYA. CQL(3D) itself has been modified so that it can accept equilibrium code output and perform bounce-averages consistent with the non-circular plasma cross-sections. This allows the calculation of neutral beam heating current drive efficiencies in ITER where this measure of efficiency is of considerable importance in reactor design studies. Employing the wave transport calculation for ECH or the lower hybrid module (ULH) described above, CQL(3D) is capable of modeling ECH, LH and neutral beams simultaneously. This could prove useful in examining synergistic effects in dual heating/current drive schemes for ITER.

An international cooperative effort has begun in 1990 (NERSC, GA, Princeton and Varennes(Quebec)) to implement the combination of CQL(3D) with the Princeton transport code (TSC) developed by Steve Jardin [15]. This would allow global simulation of tokamak performance while retaining considerable kinetic detail. The Fokker-Planck calculation concentrates on the modeling of tail phenomena resulting from RF driven resonant diffusion or neutral beams, and the transport code describes the radial diffusion of thermal particles and energy transport. This approach, while not as complete as might result from a fully coupled 3-D calculation including finite banana width effects, does allow for more timely results. This code might first be applied to simulate the LHCD-PBX-M experiment at Princeton and the LH experiment at Garching, West Germany.

Third, efforts are proceeding to refine the ray optics calculations for ECRH, and the consequent quasilinear development of the underlying distributions. There exist several wave propagation codes in the community. Most of the codes are based on simpler models of the plasma supporting the waves, usually warm plasma, uniform field theory. The intent of the coordination is to provide a computational environment based on a kinetic model of the plasma in which to integrate wave propagation computations with Fokker-Planck/quasilinear computations. Whereas it might be argued that the propagation physics does not depend strongly on details of the non-Maxwellian underlying distributions, the wave damping physics does rely on the details of the quasilinear development of the distributions, especially for strongly driven systems. The mechanism by which this coordination is effected relies on the fact that the plasma absorbs (or emits) power from the wave field through resonant interaction between the particles and the waves. The constants of the motion of interacting particles determine where the resonant interaction occurs, thus providing a relationship between the phase space density and the local absorptivity of the plasma. Hence, coordination can be enforced between the time evolution of the local power spectrum and the local spectral absorptivity. Recent work by Carreras et. al. [11] make the linkage of these

two approaches for studying ion cyclotron tokamak excitation possible though no firm commitment for collaboration in this regard has yet materialized.

Fourth, we have developed the (VLF) facility in CQL to investigate properties of the marginally stable state, in which weak Alfvén turbulence persists in the presence of a driving reservoir of free energy due to the introduction of high energy neutral beams. This module has been used in production mode to study effects on current drive efficiency of weak turbulence including the significant influence of electron Landau damping [16].

Finally, a rather comprehensive effort has been undertaken to benchmark the entire code against a number of other codes in the community designed to perform in various limits accessible also to CQL. As part of this effort we generalized our mesh refinement scheme to operate in a mode which removes mesh dependence where it can obscure the direct comparison with independently obtained results. Additionally, we are preparing a comprehensive user manual for the code including case studies, theoretical bases and limitations, numerical algorithm descriptions, and complete cross reference indexing of internal and input variables. This project is quite time-consuming and is likely to proceed along with further code development during the future. It is our intention to maintain this documentation as we update the code as a set of texinfo directories for distribution with the sources.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center Computational Physics Group

Resistive MHD Studies

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The NERSC Computational Physics group, since its inception in 1974, has been engaged in studies of resistive magnetohydrodynamics. Even prior to the formation of the C.P. Group, linear incompressible time dependent codes for Cartesian and cylindrical geometries were developed by J. Killeen [1,2].

In the mid 1970's a compressible, linear, cylindrical, finite-beta code modeling the effects of isotropic viscosity and thermal conductivity was written [3]. Eigenmodes and their growth rates as functions of mode number, Lundquist number and wall radius, with respect to the force free (RFP-applicable) Bessel Function Model equilibrium, were computed. The effects of finite viscosity were modeled. Studies involving other equilibria were carried out.

A linear, incompressible Cartesian code allowing equilibrium flow was developed [4]. It was demonstrated that a finite equilibrium velocity, although having little effect on the eigenmodes themselves, would result in a lower growth rate and a smaller instability range in wave number space. Linear calculations (without equilibrium flow) for the double tearing mode were carried out. The resulting eigenfunctions, rather than having a spike at each singular surface, tended to be large over the region connecting the singular surfaces [5,6]. A study of rippling modes was also undertaken [7]. It was shown that these modes could indeed develop provided there was a gradient in the zeroth order resistivity. The transition from pure tearing to pure rippling was demonstrated.

A two-dimensional nonlinear code solving the compressible, primitive equations in orthogonal curvilinear coordinates was developed [8]. The nonlinear evolution of the tearing mode in a sheet pinch was demonstrated [6]. Nonlinear calculations of the double tearing mode were carried out. It was shown that the two islands would come closer and closer together, creating an extended region susceptible to cross-field transport [6]. Calculations of axisymmetric and helical tearing modes in a Reversed Field Pinch using the Bessel Function Model equilibrium were undertaken, showing that the $m=1$ mode was the most dangerous due to its larger growth rate and extended period of growth [9]. Simulations of resistive interchange modes in a RFP were also carried out using an equilibrium known to be stable to tearing modes [10]. It was demonstrated that the $m=0$ mode was the most dangerous.

Also in the 1970's a three-dimensional compressible, nonlinear code using orthogonal curvilinear coordinates was written [11]. It was shown that the $m=1, n=1$ resistive kink in a box evolved nonlinearly to a slow-growing $m=3, n=1$ mode, and that the $m=1, n=1$ mode in a square cross-sectional torus evolved to a steady axisymmetric state.

In the early 1980's a linear, incompressible 2-D code for toroidal geometry was developed [12]. This code would accept equilibria depending on r and z and solve for perturbations of the form $f(r, z)\exp(in\theta)$. Studies of the Field Reversed Theta Pinch were carried out, showing that equilibria ranging from elliptical to highly racetrack were unstable to internal tilting modes [13].

A compressible, linear, cylindrical finite-beta code, including tensor viscosity and thermal conductivity and the effects of Hall terms in Ohm's law, and solving for separate ion and electron temperature perturbations, was developed and released to the user community [14,15]. This code was used to simulate resistive interchange modes in a Reversed Field Pinch. Calculations were carried out for various values of poloidal and toroidal mode number, Lundquist number, Suydam parameter, Hall parameter, thermal conductivity and viscosity, with respect to equilibria known to be stable to tearing modes. It was shown that in the cold ion limit sufficiently large Hall terms would cause all modes tested to become stable, but that for warm ions ($T_i = T_e$) these modes were stable only when a classical tensor thermal conductivity was also included; inclusion of a classical tensor viscosity did not have that large an effect.

A 3-D compressible, finite beta, nonlinear code in cylindrical coordinates (r, ϕ, z) , using a spectral representation in ϕ and finite differences in r and z , and applicable to both toroidal and cylindrical geometry (in the latter case the z coordinate may be treated pseudospectrally), was developed [16,17]. In one application this code, along with four other 3-D codes (developed at other institutions), simulated the identical problem in RFP dynamics [18]. Of these five codes, three are compressible and two are incompressible. It was demonstrated that the three compressible codes agree with each other and the two incompressible codes agree with each other, but that the compressible and incompressible models show qualitatively different behavior. Most importantly, for a certain set of initial and boundary conditions the compressible codes predicted field reversal maintenance while the incompressible codes did not. In a related application this code was used to show that erroneous results could occur from an inconsistency between the constant current boundary condition in an RFP and other commonly used boundary conditions, especially when Hall terms were included in Ohm's law [19].

The 3-D nonlinear code was used extensively to model the CTX gun-injected Spheromak at LANL [17]. These simulations were carried out in toroidal geometry. For the decaying Spheromak the initial conditions consisted of a linearly unstable equilibrium together with toroidal eigenmodes. Calculations were performed for various values of Lundquist number S and Hall parameter, various initial perturbation levels, various mesh sizes and mode numbers, etc. The 3-D magnetic fields were then evaluated with a field line tracing code. It was demonstrated that saturation occurs, followed by reconnection and formation

of a new magnetic axis, the new configuration being closer to a Taylor minimum energy state than the original one.

The 3-D nonlinear code has been modified to include implicit differencing [20-22]. For the purposes of economizing computer time, a multitasked "semi-implicit" technique has been implemented. Hall terms have also been included in the semi-implicit formalism. Generally a one-to-two order of magnitude speed improvement is realized. A study of the effectiveness of the semi-implicit method in accurately modeling Hall term effects in toroidal geometry is in progress [23].

The 3-D code has recently been used to model the internal tilt mode in a Field Reversed Configuration [24]. Preliminary results show agreement with the code of Milroy, et al. in the linear regime for cases without Hall terms. Calculations with Hall terms are in progress.

The most recent application of TEMCO has been to model the injection of compact toroids into a tokamak plasma. For simplicity, the CT is initialized at rest in a uniform magnetic field modified to exclude the CT. The rate at which the CT reconnects with the tokamak determines when and where the fuel and flux are dumped. This is measured using a field line tracing code. Calculations to date indicate that the CT will last 7 to 10 CT-Alfven times before reconnecting, which is much shorter than anticipated [25]. This means that larger than expected CT's will have to be injected, but less often.

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PROJECT OVERVIEW

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Plasma Turbulence and Anomalous Transport

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Turbulence is a primary candidate to explain anomalous transport and the resulting loss of confinement in tokamak plasmas. Fluid-equation based turbulence models have had qualitative success in explaining some observed trends in the scaling of energy confinement times in tokamaks. However, detailed studies of these equations are needed to provide an adequate understanding of the underlying dynamics. We have investigated and developed a number of techniques for the numerical study of plasma turbulence. We use both closure theory and direct simulation to study the coupled sets of nonlinear equations. By reducing the complexity of the physical problem, we have been able to test and develop a number of schemes based on the standard closure approximation theory developed originally for the study of Navier-Stokes turbulence. We have modified and rederived these theories in order to incorporate properties of the plasma equations not contained in related Navier-Stokes turbulence modeling. The primary differences are the occurrence of complex field quantities, the presence of linear damping and driving via complex linear terms, and the non-diagonal coupling of two or more field quantities in the system. By combining our study of closure theory with direct numerical simulation, we are able to have some measure of the accuracy and applicability of the closure. We note that since closure theories for strong turbulence are not based on standard perturbation theory, but rather renormalized perturbation theory without a small parameter, it is not possible to estimate *a priori* the error in a given closure theory. Thus, numerical simulation of the primitive (unclosed) equations is necessary to validate the applicability of the closure theory.

We have augmented our analytic development of the closure theory equations with sophisticated numerical techniques to handle their computational solution. A standard closure theory which can be applied to our system is the direct interaction approximation (DIA) of Kraichnan. However, naive application of the DIA for complex physical systems would not be computationally feasible. We have therefore investigated several means of simplifying both the time history integrations and the spatial convolutions present in full DIA calculations. One of these procedures is based on using Pade approximates to the characteristic-time integral parametrizing correlations in the system. This method eliminates the need for the introduction of ad hoc parameters (usually based on estimates of the eddy viscosity) in models of the Markovian type. Other approximations based on the physics of the turbulent steady state are

useful for simplifying the numerical computation. In particular, we have shown that the fluctuation-dissipation relation is a reasonable approximation for a damped-driven system in steady state. One scheme (FDDIA) incorporates this approximation, and in doing so, eliminates costly integrations which are present in full DIA calculations. Finally, in order to make full DIA calculations possible for certain anisotropic problems, we implement fast transform methods for the spatial convolutions. Together with our collaborators from the Center for Compressible Turbulence at LLNL, we are developing a full-DIA code to study two-field plasma turbulence equations. The development of this code will be a multi-year effort, but it should be sufficiently general to handle a variety of equations.

In the area of direct numerical simulation, we are developing and using a two-field simulation code, written primarily by our post-doctoral researcher, to study the dynamics of the Hasegawa and Wakatani model of drift wave turbulence. We are in the process of bench-marking this new code, adding graphics and analysis packages, and applying it to study the statistical dynamics of the system. Preliminary results show the importance of the cross-correlation between the density and potential fields in determining relaxation rates. We note that the cross-correlation has been traditionally neglected in analytic estimates of transport coefficients and in certain closure theories. Eventually, we hope to be able to compare results of the DIA code with the direct numerical simulation code.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Plasma Simulations Using a 3-D Particle Code

D.E. Shumaker and D.V. Anderson
February 1990

It is well-known that certain instabilities on the MHD timescale cannot be treated by the fluid models of MHD theory but require detailed modeling of the kinetic effects of the ions to get reasonable agreement with experiment. In the case of the tilting mode in Field-Reversed Configurations [1], a full 3-D treatment is required as well.

The estimated requirements of memory and calculational speed of such a calculation are well-matched to the Cray-2 capabilities. Consequently, a 3-D plasma particle simulation code, QN3D, that exploits most of the new features of the Cray-2 has been constructed [2,3]. To eliminate inessential high frequency physics the code uses a zero mass fluid model to represent the electrons and a reduced set of Maxwell's equations to model the electromagnetic fields.

Unlike earlier particle codes that required disk memory and scalar interpolation, new algorithms that allow every phase of the calculation to be vectorized and multitasked have been developed. Tedious coding of buffered disk memory and the concomitant waste of CPU time have been eliminated. The interpolation of grid data to the particles and the interpolation of particle data to the grid have been coded in terms of indirect indices and execute in vector mode via the hardware gather and scatter instructions. A particle sorting scheme to satisfy the vectorization constraint that scatter operations must be one-to-one has been developed [4]. The parallel algorithms in this code are executed using both vectorization and multitasking. Typically, the parallel work is partitioned into k subsets or tasks, where k is the number of processors. Within each subset or task, vectorization is employed to further optimize the calculation. Exploiting both forms of parallel computation results in a computing speed about 16 times that of a Cray-1.

QN3D successfully modeled the normal modes of a cold plasma [7]. It was also applied to the rotational instability of a rigid rotor [8]. In the latter case the growth rates generally agree with those computed from Harned's 2-D PIC code [9]. We also observed the nonlinear saturation of the rotational instability.

More recently, simulations of the internal tilt mode have been carried out [10,11]. It is found that in the small gyroradius limit, the rate of growth agrees with MHD predictions, but that at large gyroradius, kinetic effects have a stabilizing influence.

Some problems were encountered when FRC tilt mode simulations were run for a long time (a few MHD tilt mode times). These problems were mainly due to failure of the field solver to converge and also the appearance of an $m=4$ distortion. The $m=4$ distortion is associated with the use of Cartesian coordinates. This problem could be eliminated by using a larger number of grid points in the x-y plane; however in a 3-D problem this is not a practical solution. Research is under way to eliminate these problems.

One alternative approach is to solve the field equations in cylindrical coordinates. The code using this approach is called HQC. In either version, the field solve has recently been simplified by the elimination of the vacuum region; instead a uniform background density is used in the entire computational domain.

Another method that is being tried is modification of the field equations to include some electron inertia effects. This leads to an evolution equation for the electron current [12]. This approach was recently introduced by E. Horowitz.

The 3-D MHD code, TEMCO, also developed at NERSC, has been used to compute growth rates in the MHD limit. The comparison of the growth rates from these two codes can give an indication of the importance of ion kinetic effects.

These codes may also be used to model the formation dynamics of the FRC. This would involve initializing with some cylindrical distribution of particles and fields and tracking the evolution of the field lines. The translation experiment, in which the FRC is formed in one region and then moved into another region, could also be modeled. This could be simulated by starting with an FRC equilibrium and then applying a magnetic field which is asymmetric about the $z=0$ plane. This would accelerate the FRC in the z direction. The effect of the acceleration on the plasma and field line structure could then be studied.

QN3D is also being used to model the expansion of a high energy plasma surrounded by a plasma of lower energy. This study has direct bearing on several others, including compact torus injection into a tokamak and dynamics of the Earth's magnetotail. Particularly in this latter application kinetic effects are important since the magnetic field is low, and thus the ion gyroradius is usually large compared to the size of the plasma.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Efficient Calculation of 3D Toroidal MHD Stability of Fusion Plasmas

D.V. Anderson
February 1990

In magnetic fusion research the most popular plasma confinement devices use a toroidal chamber and externally applied magnetic fields to restrain the plasma. In the tokamak a large toroidal current driven in the plasma produces a large poloidal field which supplements the applied fields. The stellarator, on the other hand, has no toroidal plasma currents but relies entirely on the externally applied fields for confinement.

Since several 3D equilibrium codes are available to generate model equilibrium configurations, we have restricted our interest to the analysis of their stability properties. In our new code, TERPSICHORE, developed in collaboration with European colleagues, we use the relatively simple model of ideal magneto-hydrodynamics (MHD) to investigate the linear stability of these configurations [1,3]. TERPSICHORE generalizes previous treatments in which the stability of two-dimensional equilibria were studied. While earlier and even present tokamaks have small deviations from axisymmetry, proposed reactor designs will have much larger departures from axisymmetry. Thus, to be realistic, one must perform a full 3D analysis to ensure that all possibly unstable modes are evaluated. In the development of TERPSICHORE, our contribution to the collaboration has been mainly in the areas of building eigenvalue solvers and in developing efficient algorithms for the computationally intensive portions of the code [2]. Evidently, we have succeeded in optimizing this code because TERPSICHORE had the distinction of placing first in the 1989 Gigaflop Performance Awards Contest sponsored by Cray Research, where it achieved 1.7 Gigaflops sustained speed averaged over the run.

To get started we use the equilibrium code of Hirshman, VMEC [4], to provide the plasma equilibrium configuration. From it TERPSICHORE reads input data specifying equilibrium quantities such as the geometry of the flux tubes and the magnetic fluxes contained therein. The flux tubes are specified by their R and Z coordinates expressed in terms of the Fourier coefficients of the double finite Fourier series of these cylindrical components. The first phase of the calculation reconstructs the input equilibrium and tests its validity. Since the coordinate system optimum for the stability analysis differs from that best for the equilibrium calculation, a mapping from the equilibrium coordinates to the Boozer coordinates, of the stability analysis, is done next. After applying the energy principle to obtain the corresponding Euler-Lagrange

equations, these are discretized by double Fourier series (over the angle-like coordinates) and by finite elements radially. This results in a matrix eigenvalue problem in which the matrix elements depend on combinations of double flux tube integrals. Since similar flux tube integrals comprise the overwhelming proportion of the work in the reconstruction and mapping phases of the calculation, it is important to optimize their evaluation. The matrices encountered in this analysis consist of multidiagonal structures with dense blocks. We evaluate the elements of these matrices a block at a time by using the MULFI technique which exploits the matrix-matrix product routine (MXM) to great advantage. In fact these matrix blocks can be evaluated in parallel at speeds up to 1.7 or 2.0 gigaflops for the Cray-2 or Cray Y-MP computers, respectively.

The last phase of the calculation is the solution of the eigenvalue system by the method of inverse vector iteration. In doing this it is necessary to solve a linear matrix system which we accomplish either by employing the PAMS or PAMERA algorithms [2]. Although this solution phase of the calculation typically requires less than five percent of the arithmetic operations, we also use optimal BLAS3 type routines (MXM and MINV) here.

TERPSICHORE, in its present form, is being used to study the stability of stellarators, particularly the Helias stellarator design for the Max Planck Institute in Garching, FRG. It is proving to be a very efficient tool in the Helias design where, for example, it took only 20 seconds of wall time on the Cray Y-MP to execute 35 billion floating-point operations to complete the stability analysis of each prospective design. With this kind of efficiency we can do extensive parameter studies of many candidate designs of fusion experiments and reactors. We are keen on using it to explore the feasibility of constructing the "race-track Tokamak" which could not be analysed with previously available tools [5,6]. Thus TERPSICHORE represents a big advance in the theoretical modelling of fusion plasmas as well as a very efficient tool for making these studies affordable.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

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

A.A. Mirin
February 1990

In the mid-to-late 1970's and very early 1980's the National Energy Research Supercomputer Center (NERSC) Physics Group did extensive modeling of neutral beam heated tokamaks. Our first application was that of investigating the Two Component Torus with our 2D nonlinear Fokker-Planck code [1,2]. Shortly thereafter this same code was used to model the Counterstreaming Ion Torus [3].

As successful as these calculations were, it was clear that a zero spatial dimensional model could not supply sufficiently accurate results. In 1975 the Fokker-Planck/Transport Code (FPT) was written. This code was revolutionary in that it was the only radial transport code to treat the nonlinear evolution of the energetic ion distribution functions in 2-D velocity space [4,5].

The FPT code was first applied to the Counterstreaming Ion Torus [6]. In order to accurately and efficiently determine the fusion rate, a very efficient algorithm was developed to perform the five-fold velocity-space integration necessary for the determination of the fusion reactivity [7,8].

In 1977 it was proposed that extra beam lines be added to PDX. Extensive parameter studies in support of this proposal were carried out using FPT [9]. At the same time a substantial effort was undertaken to include self-consistent treatments of neutral transport and neutral beam deposition. Monte Carlo codes of Hughes and Post [10] and Lister, et al. [11] were acquired, improved and incorporated into FPT, culminating in presentations at Grenoble [12] and Innsbruck [13].

In late 1978 the question of whether or not neutral tritium beams should be injected in TFTR was addressed, and results were presented at a TFTR review meeting chaired by John Clarke [14]. It was shown (see [15]) that for D on T operation with tritium gas puffing, the continuous deuterium fueling of the central region would result in a thermal plasma dominated by deuterium, and that it would be necessary either to inject tritium neutral beams or pellets in order to properly fuel the central region. It was also shown that fusion performance was very sensitive to the assumed diffusion rate of bulk ions and

*The studies reported here assume a uniform magnetic field.

moderately sensitive to the ion thermal conductivity and the energetic ion diffusion rate.

In 1979 and 1980 the FPT code was used to model the PLT experiment [16,17]. Time dependent simulations of the beam injection phase of PLT were carried out, assuming a uniform concentration of carbon and iron impurities and a gas puffing rate dynamically adjusted to match experimental measurements of the line averaged density. Neutron fluxes generally to within thirty percent of the experimentally measured values were predicted, with best agreement at low density and high power. It was demonstrated that most of the fusion neutrons result from beam-target reactions, and at low density almost as many are produced from beam-beam reactions.

In 1982 and 1983 FPT was used to model the DITE experiment at Culham Laboratory [18]. Injection of hydrogen into both hydrogen and deuterium plasmas was considered. The effects of both high and low Z impurities were modeled, along with the effect of beam impurity charge exchange on the radiative power loss. Transverse diffusivities and conductivities were derived which accurately represent the experimental data both with and without injection over a wide range of discharge parameters.

More recently FPT has been used to model the energetic ions in TFTR [19]. The transport mechanisms have been ignored, and instead experimental profiles of electron density and temperature and estimates of ion temperature have been specified. The neutron flux has been compared with experimental measurements. Equally important, the origin of the fusion neutrons has been analyzed. In a number of the cases the majority of the neutrons have come from beam-beam reactions. For the 1986 supershots excellent agreement between code and experiment is obtained [20].

FPT has also been used to study neutral beam current drive in TIBER [21]. Here too the transport mechanisms have been ignored and profiles of electron density and electron and ion temperature have been specified. Values of current drive efficiency comparable to those of rf scenarios have been obtained. A poloidal field and bootstrap current consistent with steady-state current drive are calculated.

Over the past couple of years a number of tokamak simulations concentrating on rf heating and current drive and utilizing a bounce-averaged/quasilinear model CQL have been carried out. This work is described in a separate document.

The FPT and CQL models are discussed in a recent book [22].

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Simulations of the Davis Diverted Tokamak

D.E. Shumaker
January 1989

The Davis Diverted Tokamak (DDT) is a small toroidal device which is being constructed by the University of California, Davis and located at LLNL. It has a major radius of 45 cm. and a minor radius of 15 cm. Poloidal divertor coils are placed outside of the vacuum chamber on the top and bottom. The plasma current will be 10 kA, and the maximum toroidal magnetic field will be 9 kG. DDT will use lower hybrid current drive at 800 MHz. Some of the experiments to be done with the DDT are:

- (1) beat-wave current drive;
- (2) current drive and profile shaping due to a lower hybrid wave;
- (3) low-high mode transition; and
- (4) MHD stability of the axisymmetric mode.

The NERSC Computational Physics Group has been providing some computational support for the DDT experiment. Numerical studies of equilibrium and axisymmetric MHD stability have been carried out [1]. Both of the studies use a code developed at Princeton, TSC [2]. TSC can simulate both active and passive feedback systems in plasma devices which contain divertors and the associated separatrix in the magnetic field structure. Flux-surface-averaged transport equations are used to model the evolution of plasma parameters. A free plasma boundary separates the plasma and vacuum regions. Ohmic heating coils can also be included [3,4].

Another area which we intend to study is the effect of lower hybrid current drive on the stability of the axisymmetric mode. Lower hybrid current drive has been shown to produce electron distributions which appear to contain an anisotropic high energy tail [5]. The shape of the plasma current profile can be controlled by the input frequency or the plasma density. In previous experiments the tail of the distribution near the surface of the plasma seemed to be more energetic, which should lead to a more highly conductive plasma on the outside of the device. For a given loop voltage this could result in a redistribution of the current with a larger fraction of the current flowing on the plasma surface. This change in the current profile would produce a large change in the plasma inductance and the resulting redistribution of current could then have a significant effect on the axisymmetric mode. By making changes in the resistivity profile in the TSC code we hope to study this

phenomenon. The effectiveness of passive stabilization depends on the closeness of the conductors to the plasma, or more exactly, how close the eddy currents in the passive conductors are to the currents in the plasma. Thus a redistribution of the current profile to the outside could make passive stabilizations more effective.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Equilibrium and Transport of the Field-Reversed Configuration

D.E. Shumaker
January 1989

The National Energy Research Supercomputer Center (NERSC) has conducted numerical studies of the Field-Reversed Configuration (FRC). This document describes 2-D equilibrium calculations and 1-1/2-D transport simulations. Nonlinear particle simulations of ion kinetic effects on the tilt mode are described in a separate Project Overview, "Plasma Simulations Using a 3-D Particle Code." Some of this work has been done in collaboration with Los Alamos National Laboratory in support of the FRX-C and FRX-C/T experiments [1].

The 2-D axisymmetric MHD equilibrium code (EIV) uses finite elements and a flux-surface coordinate system [2]. Adiabatic quantities are used to specify the equilibrium. This method has been quite successful in generating elongated equilibria similar to the ones seen in the FRX-C experiment at Los Alamos [3]. These equilibria are difficult and/or more time-consuming to produce by other methods. Diagnostics from the code have been shown to give close agreement with side-on interferometry data from the FRX-C experiment. Since this code uses adiabatic variables, it is easy to simulate compression studies of the FRC by computing a series of equilibria with different boundary conditions.

A code (EQV) has also been developed which determines a 2-D axisymmetric Vlasov equilibrium for the FRC. The distribution functions for the ions and electrons are assumed to be given in terms of the Hamiltonian and the canonical angular momentum. The code can also compute equilibria for zero electron temperature plasmas. In this case the electrostatic potential is an input quantity. This latter version of the code is used to generate initial conditions for the 3-D hybrid particle simulations. These equilibria also can have ion flow, which may be important in the stabilization of the tilt mode.

The transport code CTT assumes that the plasma evolves through a sequence of equilibria. This calculation proceeds by alternating between solutions of the 2-D equilibrium equation and the simultaneous solution of three 1-D transport equations [5,6]. It can be shown that some plasma quantities such as density, temperature and pressure are functions of the flux surface label. One-dimensional transport equations for these quantities are obtained by averaging the 3-D transport equations over the flux surfaces. The code presently solves equations for ion density, electron entropy and ion entropy. Two-dimensional equilibria are needed to determine the position of the flux surfaces and certain flux surface averaged quantities which appear in the

transport equations. Various physical processes have been added to the transport equations, including classical transport, collisional transfer of energy from ions to electrons, radiation cooling due to impurities, loss on the open field line region due to flow along the field lines, and lower-hybrid drift anomalous diffusion.

CTT has been useful for studying the effect of various processes on the confinement times. Comparisons have been made between CTT simulations and FRX-C experiments. For the high density experiments (20 mTorr) there is good agreement when the electron-ion collision frequency used in the simulation is multiplied by a factor of about 9 at the o-point. For the low density experiments (5 mTorr) this factor must be 22, and in order to increase the electron energy transport the electron-electron collision frequency must be increased by a factor of 70.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Fokker-Planck Analyses of Mirror Systems

A.A. Mirin
December 1987

Since its inception in 1974, the Computational Physics Group of the National MFE Computer Center has been carrying out Fokker-Planck studies of mirror systems. Much of this work has been in collaboration with the Mirror Program at LLNL; a more recent effort has involved the joint participation of SAIC (La Jolla).

Virtually all of these studies have utilized the general Fokker-Planck package FPPAC [1]. This widely-used package, developed at the NERSC in the late 1970's and available over the network, computes the coefficients of the complete nonlinear, multispecies, 2-D velocity-space Fokker-Planck collision operator and time integrates the corresponding finite difference equations. In addition to the mirror applications discussed here, FPPAC has been used to analyze toroidal systems. (A study completed in 1982 concluded that fusion reactivity in TFTR would not be appreciably affected by distortions of the bulk ions from Maxwellians [2].) Our Fokker-Planck models are discussed in a recent book [3].

A chronological summary of our mirror applications follows.

Collisional Loss of Electrostatically Confined Species

Our 2-D nonlinear Fokker-Planck code has been used to compute the endloss rate of electrons and electrostatically confined ions in a multispecies, multiply-charged plasma with the intention of comparing the results with analytic formulae developed by Cohen [4]. It has been found that the code results and the theoretical results scale quite similarly with the potential to temperature ratio for $Z\phi/T \geq 2$, but that the generalized Pastukhov expressions tend to vary more slowly with mirror ratio R , especially in the case of ions [4]. The prediction that the only Z -dependence is through the product ZR has been verified by the code results.

Classical Ion Confinement in a Tandem Mirror Plug

Our 2-D nonlinear Fokker-Planck code has been used to develop a heuristic model for classical ion confinement in a magnetic mirror, the idea being to replace expensive 2-D Fokker-Planck computations with simple expressions describing particle and energy confinement [5]. The resulting formulae involve an appropriate weighting of drag and pitch angle scattering times, and are

valid to within 10% over a wide range of mirror ratio, temperature, potential, injection energy and injection angle.

Electrostatically Trapped Electrons in Thermal Barrier Tandem Mirrors

Results of our 2-D nonlinear Fokker-Planck code have been compared to analytic expressions for the density and energy of electrostatically trapped electrons in the thermal barrier of a tandem mirror, valid for small to intermediate mirror ratios, with and without passing particles [6]. The objective has been to ascertain the range of applicability of those analytic formulae. It has been found that the numerical results and the theoretical predictions agree to within 20% for most values of mirror ratio, energy, and passing-to-trapped density ratio. Further calculations have been carried out which demonstrate electron heating and detrapping by strong rf diffusion for parameters appropriate to TMX-U.

Plasma Performance of the Central Cell of a Cat-D Tandem Mirror Reactor

A particle and power balance assessment of a conceptual tandem mirror reactor has been carried out using our 2-D nonlinear Fokker-Planck code [7]. This has required solution of the Fokker-Planck equations for the distribution functions of the five ionic species. Results have compared favorably with those of a 0-D simulation code of SAIC [8]. It has been concluded that the central cell of a Cat-D fueled reactor can achieve ignition with a reasonable confining potential in the 45-70 keV temperature range provided alpha ash buildup is strictly controlled.

Trapping Rate of Passing Ions in Tandem Mirror End-Cells

The trapping rate of passing ions in tandem mirror end-cells has been studied using our 2-D nonlinear Fokker-Planck code. A generalization of the Futch-LoDestro Scaling law [9] which takes into account the dependence on potential-to-temperature ratio has been developed [10]. It has been found that the dependence on ϕ/T , which was ignored in Ref. [9], can be quite strong. It has also been found that in multi-ion mixtures, the drag between ions of differing charge-to-mass ratio is as important as angle scattering in determining the trapping rate [11].

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Tandem Mirror Equilibria Studies

D.V. Anderson
December 1987

Members of the NERSC physics group have played a predominant role in the calculation of mirror equilibria - even prior to the establishment of the Computer Center [1-2]. The VEPEC [3-5] program (Vector Potential Equilibrium Code) has been evolving over the last several years in concert with the progression of the experiments from simple mirrors to the tandem configuration, with the improvements in the field of numerical analysis, and with better theoretical models. An overriding emphasis in these calculations has been to build realistic models that include the important effects without too many unsubstantiated idealizations which limit other models to small regions of parameter space.

For example, we wish to compute accurately both in paraxial regimes (where $\lambda \gg 1$) and in short-fat configurations (where $\lambda \sim 1$). Here, λ is the aspect ratio, defined as the ratio of the axial gradient scale length to the radial one. This is an important issue because mirror devices tend to be of the latter variety while many methods of computing their equilibria are restricted to the former.

In its first version, VEPEC computed the equilibrium of a single minimum-B mirror on a 3D uniformly spaced Cartesian grid using finite difference techniques to solve the nonlinear Ampere's equation of the theory. Electrostatic effects were ignored and only one species of plasma was permitted. Its pressure was obtained in an ad-hoc fashion. The fields of realistic coil sets were computed precisely by the ABCXYZ code, and the boundary conditions were self-consistently derived from the multipole expansion. The Douglas-Gunn algorithm efficiently solved the resulting system of nonlinear equations. Confinement properties of single particles were studied with the orbit code ORBXYZ.

Studies were done of simple mirror devices that have aspect ratios of order unity ($\lambda \sim 1$), such as the 2XIIB and the MFTF-A single cell configuration. They demonstrated the modified long thin mirror ratio enhancement formula, confirmed the assumption of omnigenous drift surfaces for fusion energy deuterons, and validated the superiority of using the vector potential instead of the alternative magnetic induction as the dependent variable [3].

With the introduction of tandem mirrors the code was extended to represent multiple plasma species in a multi-region device on a nonuniform Cartesian grid. To maintain good accuracy a finite element collocation method, based on tri-cubic B-splines, was introduced to perform the discretization. In this process the old 7 point operator stencil was replaced by a 27 point operator. The physics of tandem mirror ion confinement required inclusion of electrostatics on an equal footing with magnetostatics. The zero dimensional code ESTEQ was developed to do special electrostatic equilibria.

Calculations of tandem mirror magnetostatic and electrostatic equilibria for the TMX and the TMX-Upgrade demonstrated the existence of plasma sheaths [5], as predicted by others. Good fits to experimentally determined electrostatic potentials were computed.

Theoretical and experimental developments regarding sloshing ions, thermal barriers, ECH, and ICH have required that the models represent the very highly anisotropic distributions that are associated with these phenomena. Collaborations with MIT have resulted in better ad-hoc pressure models [6], while a more recent effort with the mirror program at Livermore has led to the inclusion of self-consistent Vlasov models [7] in the latest 3-1/2 D version of the code. No other mirror equilibrium code to date can model these complicated features of tandem mirrors. Very detailed studies of complex configurations are now underway on the Cray-2. Its memory would allow realistic studies of TARA to proceed.

Recently, very careful comparisons have been made with equilibria determined from the paraxial theory. In calculations of radial transport, knowledge of the detailed shapes of the drift surfaces is critical. The drift surfaces obtained from the paraxial equilibrium calculations have been compared to those of VEPEC. It has been estimated that the paraxial calculations become inaccurate below aspect ratios $\lambda \sim 100$; very few realistic mirror configurations have larger aspect ratios. We have computed very good agreement between VEPEC and the high beta paraxial theory for $\lambda = 250$. The low beta model of Pearlstein, Kaiser and Newcomb has been installed in the code itself for more detailed comparisons [9].

In the areas of numerical analysis, algorithmic developments and optimization, VEPEC has been revised to make best use of new methods and features. It is now highly vectorized. The iterations converge very rapidly compared to most codes using the reduced MHD formulation. Multitasking has been introduced to the implicit solver and to other portions of the code. Where implemented the resulting speedup factor is typically 3. All other time consuming portions of the code are multitaskable and may be so treated as circumstances permit.

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PROJECT OVERVIEW

National Energy Research Supercomputer Center
Computational Physics Group

Computation of Vacuum Magnetic Fields - Application: HELIAC

A.A. Mirin
January 1986

A method has been developed for computing the vacuum magnetic field inside a toroidal domain created by helically winding a poloidal cross-section about a circle [1]. A nonorthogonal coordinate system conforming to the shape of the torus is used. The magnetic scalar potential is Fourier analyzed in the poloidal and toroidal directions. Finite differencing is used in the radial direction. The resulting system of difference equations is block tridiagonal, the order of each block equal to the total number of Fourier harmonics.

This technique has been applied to helical axis stellarators [2]. The boundary of the domain is taken to be an outer magnetic surface. The aim is to produce realistic configurations possessing magnetic wells (for stability), favorable transform with low shear (to avoid resonant rational surfaces), and small variation of

$$Q = \int d\ell/B$$

(to minimize parallel currents). The resulting magnetic field, which is generated by skin currents flowing along equipotential contours on the boundary, is analyzed using a field line integration code. Configurations having a shallow well and favorable beta limitations and Q variations have been constructed.

This method is quite efficient for scanning large ranges of parameter space since expensive Biot-Savart integrations need not be performed. For some of the more optimistic cases, the skin currents have been discretized into a modular coil system and the resulting magnetic field compared to that of the continuum. This discretization has usually resulted in a magnetic field of the same transform and Q variation but having less favorable well properties.

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II. Computational Models Developed at NERSC

This section lists the various computer programs developed by the Computational Physics Group.

TABLE 1. NERSC TIME INDEPENDENT CODES

<u>CODE</u>	<u>CONTACT</u>	<u>CHARACTERISTICS AND APPLICATIONS</u>
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	D. V. ANDERSON	Auxiliary codes for VEPEC
TPSIC		
HILLSV	D. V. ANDERSON	Auxiliary code for CYLEQ
EIV	D. E. SHUMAKER	2D, Flux Coordinates, Finite Elements, Open and Closed Field Lines; Compact Toroids
EQV	D. E. SHUMAKER	2D, Kinetic Equilibria, 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
STABCRIT	D. V. ANDERSON	2D (R,Z) Ballooning Modes, Energy Principle
TERPSICHORE	D. V. ANDERSON	3D Displacements of 3D Toroidal Equilibria; Tokamaks, Stellarators

*Currently in CP-Division (LLNL)

TABLE 2. NERSC TIME DEPENDENT MHD CODES

<u>CODE</u>	<u>CONTACT</u>	<u>CHARACTERISTICS AND APPLICATIONS</u>
TEMCO	A.A. MIRIN	3D (R, ϕ ,Z), Nonlinear, Semi-Implicit, 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, Tensor Viscosity, Tensor Thermal Conductivity, Hall terms, Two-Fluid; Tokamaks, RFP

*Currently in CP-Division (LLNL)

TABLE 3. NERSC TRANSPORT CODES

<u>CODE</u>	<u>CONTACT</u>	<u>CHARACTERISTICS AND APPLICATIONS</u>
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. NERSC FOKKER-PLANCK CODES

<u>CODE</u>	<u>CONTACT</u>	<u>CHARACTERISTICS AND APPLICATIONS</u>
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 A.A. MIRIN	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 G.D. KERBEL	2D (V, θ), Nonlinear, Bounce Average, Multispecies Ions, Quasilinear rf, Relativistic, Noncircular Cross-sections; Tokamaks
CQL3D	M.G. MCCOY G.D. KERBEL	3D (r, V, θ), Nonlinear, Bounce Average, Multispecies Ions and Electrons, RF with Wave Damping, Relativistic, Noncircular Cross-sections; Tokamaks
RFT	G.D. KERBEL	Trajectory Integral Propagator and Data Base Generator for CQL
ORB	G.D. KERBEL	Guiding Center Hamiltonian Orbit Code used in Conjunction with CQL

TABLE 5. NERSC PLASMA TURBULENCE CODES

<u>CODE</u>	<u>CONTACT</u>	<u>PURPOSE</u>
SIMU	A.E. KONIGES	Ensemble Averaging
SCAT	A.E. KONIGES	3-Wave Closure
HAWC	J.A. CROTINGER*	Drift Wave Simulation - Hasegawa and Wakatani Model
MFDIA	A.E. KONIGES P.A. AMALA W.P. DANNEVIK+	Multifield DIA Closure Code

* Plasma Physics Research Institute, Postdoctoral Researcher

+ Center for Compressible Turbulence

TABLE 6. NERSC ITERATIVE MATRIX SOLVERS

<u>CODE</u>	<u>CONTACT</u>	<u>PURPOSE</u>
ICCG2	D.V. ANDERSON	2D Symmetric, Scalar
ICCG3	D.V. ANDERSON	3D Symmetric, Scalar
ILUCG2	D.V. ANDERSON	2D Asymmetric, Scalar
ILUCG3	D.V. ANDERSON	3D Asymmetric, Scalar
ILUBCG2	A.E. KONIGES	2D Asymmetric, Scalar
CPDES2	D.V. ANDERSON	2D Asymmetric, Vector
CPDES3	D.V. ANDERSON	3D Asymmetric, Vector
MTBCG2	A.E. KONIGES	2D Asymmetric, Scalar
MTCS2	A.E. KONIGES	2D Asymmetric, Vector
MTCS3	A.E. KONIGES	3D Asymmetric, Vector
ILUBCG2-11	A.E. KONIGES	2D 11-Banded

TABLE 7. NERSC MULTITASKING CODES

<u>CODE</u>	<u>CONTACT</u>	<u>PURPOSE</u>
VEPEC	D. V. ANDERSON	Plasma Equilibria
MTBCG2	A. E. KONIGES	Iterative Matrix Solvers
MTCS2		
MTCS3		
QN3D	D. E. SHUMAKER	Particle Code
HQC		
SIMU	A. E. KONIGES	Turbulence
PAMS	D. V. ANDERSON	Direct Matrix Solver
TEMCO	A. A. MIRIN	MHD Evolution/Stability
TERPSICHORE	D. V. ANDERSON	MHD Stability

III. Publications

This section lists publications of the NERSC Computational Physics Group. They are arranged according to ten categories.

Category 1 - Time Independent Equilibria and Stability References

Papers and Invited Talks

R.P. Freis, C.W. Hartman, J. Killeen, A.A. Mirin and M.F. Uman, "Calculations of Combined Stellarator-Multipole Toroidal Magnetic Field Configurations," Nucl. Fusion 17, No. 2 (1977), 281.

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