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The Numerical Tokamak Project (NTP)

Simulation of Turbulent Transport in the Core Plasma: A Grand Challenge in Plasma Physics

Prepared by the Executive Committee
of the
Numerical Tokamak Project

December 1993

Lawrence
Livermore
National
Laboratory

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THE NUMERICAL TOKAMAK PROJECT (NTP)

SIMULATION OF TURBULENT TRANSPORT IN THE CORE PLASMA: A GRAND CHALLENGE IN PLASMA PHYSICS

Prepared by the Executive Committee of the Numerical Tokamak Project
December 15, 1993

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ABSTRACT:

The long-range goal of the Numerical Tokamak Project (NTP) is the reliable prediction of tokamak performance using physics-based numerical tools describing tokamak physics. The NTP is accomplishing the development of the most advanced particle and extended fluid models on massively parallel processing (MPP) environments as part of a multi-institutional, multi-disciplinary numerical study of tokamak core fluctuations.

The NTP is a continuing focus of the Office of Fusion Energy's theory and computation program. Near-term HPCC work concentrates on developing a predictive numerical description of the core plasma transport in tokamaks driven by low-frequency collective fluctuations. This work addresses one of the greatest intellectual challenges to our understanding of the physics of tokamak performance and needs the most advanced computational resources to progress. We are conducting detailed comparisons of kinetic and fluid numerical models of tokamak turbulence. These comparisons are stimulating the improvement of each and the development of hybrid models which embody aspects of both.

The combination of emerging massively parallel processing hardware and algorithmic improvements will result in an estimated 10^{**2} - 10^{**6} performance increase. Development of information processing and visualization tools is accelerating our comparison of computational models to one another, to experimental data, and to analytical theory, providing a bootstrap effect in our understanding of the target physics. The measure of success is the degree to which the experimentally observed scaling of fluctuation-driven transport may be predicted numerically. The NTP is advancing the HPCC Initiative through its state-of-the-art computational work. We

are pushing the capability of high performance computing through our efforts which are strongly leveraged by OFE support.

Some of the most important HPCC accomplishments of the NTP to date are as follows.

- * A suite of fluid and kinetic, three-dimensional plasma simulation codes have been developed and optimized for various massively parallel (MPP) computers.
- * We have tested and compared the performance of various MPP hardware and programming paradigms, identifying the strengths and weakness of each.
- * We have improved code performance by factors of 10-100 with careful MPP optimization (depending on the machine and number of nodes) and by additional factors of 10-100 as a result of using optimized grids to better resolve the strong spatial anisotropy induced by magnetic fields. Additional significant factors of improvement in simulation efficiency have been obtained from development of advanced algorithms, e.g., perturbative, implicit, and hybrid methods.
- * The combination of code performance improvements and focusing of effort has enabled toroidal simulations of greater relevance to experiments than ever before.
- * The NTP consortium has simulated a TFTR shot as a test case, resolved initial differences in results from gyrokinetic and gyrofluid models, and obtained thermal heat diffusivities and nonlinear fluctuation spectra whose magnitudes and features are very similar to experimental measurements. Encouraged by these results, we are adding additional physics to our models.
- * Use of the MPPs, e.g., the CM-5 at LANL, is enabling simulations with much higher spatial resolution and/or larger plasmas.
- * With the computational resources at the Advanced Computing Laboratory at LANL and help from their support staff, we have developed tools to handle storage and retrieval of very large data sets generated by NTP simulations on the CM-5 and to post-process and visualize the data interactively (simultaneously) with AVS using HPCC resources distributed nationwide. The designation of the NTP as a DOE Grand Challenge has made these accomplishments possible by providing necessary resources and by unifying our consortium. The NTP has fostered strong intergroup activities and tighter collaborations resulting in more rapid research progress.

DOE PROGRAM: Office of Fusion Energy
 Dr. David Crandall
 Dr. Walter Sadowski
 Dr. Mary Anne Scott

RELEVANCE:

Fundamental Significance

- * Fusion as an energy source
- * Effects of turbulence on tokamak performance
- * Computational physics of particle/Monte Carlo and hydrodynamic simulations on high performance computers

Fusion Energy Source

Fusion is the best energy source for the next millenium as indicated in the National Energy Strategy, because of its vast supply of fuel and its environmental advantages (it avoids greenhouse gases and has relatively low radioactivity). The goal of the Numerical Tokamak Project (NTP) is to develop realistic nonlinear three-dimensional simulations of tokamak plasma turbulence in order to understand anomalous transport in present experiments, to increase the confidence of projections to future fusion reactors, and perhaps to aid the search for further enhanced confinement regimes. This goal is coming closer to reality because of the dramatic growth of massively parallel computing, and because of significant advances in algorithms and in theoretical advances in reduced descriptions of plasma dynamics that efficiently represent plasma behavior on the turbulence time scales.

Effects of turbulence on tokamak performance

The applications area of turbulence-driven core transport has great significance and high leverage in its influence on tokamak performance. Our study of plasma turbulence is providing a valuable testbed for methods of profound importance in both basic and applied plasma physics. Because of the very large ranges of time and space scales, and the importance of three-dimensional modeling in understanding turbulent transport in magnetic fusion devices, our simulation needs demand the most advanced high performance computing and communication resources. Our optimization of both kinetic and fluid computational models on high performance computing platforms using high performance tools (new algorithms, advanced software, and visualization techniques) is leading to real progress on understanding turbulent transport and how to better model it, and is providing new technologies of immediate and direct use to plasma physics and controlled fusion in general and to many closely allied fields.

Parallelization of particle and fluid simulations

NTP work has focused on the development and implementation of parallel algorithms for three-dimensional particle-in-cell and fluid turbulence codes on a variety of parallel computers (Intel Delta, Paragon and Gamma; CM200 and CM5; YMP C90) to be used for the implementation of NTP physics models. However, these computational models are widely used in other areas of plasma physics, astrophysics, weather science, and fluid dynamics; and it is expected that the algorithms developed here will be used by many researchers working in other application areas of interest to DoE, NASA, NSF- and DoD research programs and industry.

Economic Competitiveness

- * Support of US supercomputer hardware and software vendors
- * Implications of fusion energy on economy and environment
- * International competitiveness in fusion research
- * Industrial applications of NTP-related plasma research

The NTP will continue MFE direct developmental software support to US supercomputer vendors. For example, in our work with message-passing algorithms on massively parallel machines we are helping to create a generic form of message passing that will produce more efficient and portable code. We are working with several vendors to provide the support necessary so that these algorithms can be easily transferred from one machine to another. This will make these vendors' systems more attractive to those users favoring generic message passing, and, hence, improve the competitiveness of these vendors. Additional examples of our aid to the supercomputer industry are given in the following paragraphs. NTP-related research

also has industrial applications in the area of plasma processing. A longer-term economic benefit will derive from the contribution of the NTP to making the use of controlled fusion as an energy source a reality. Fusion energy has the potential to be a secure, plentiful, and environmentally attractive energy source. The combined European and Japanese fusion research budgets exceed \$1B/year. The NTP will maintain and enhance the US preeminence in theory and computation in the international Magnetic Fusion Energy (MFE) program. This helps to support our competitive position in the ITER international fusion research project.

Support of US supercomputer vendors

NTP researchers at UCLA have been involved with IBM in a joint study of parallel computing using workstation clusters and IBM's new parallel computer the SP1, which also involves the NSF supercomputer center at Cornell. Numerous bugs and problems in all of the new massively parallel systems have been identified in order to help the vendors (Thinking Machines, Intel, IBM, CRI, etc.) improve the software and performance. Skeleton codes developed by UCLA have been adopted by vendors to test the performance of their systems and have been requested by Rice University for use in the Fortran D project.

Kerbel (NERSC) has cooperated closely with a number of hardware and software vendors to test and improve their products while using them for NTP work. One area of interest has been the TMC CM5 and Cray C90 Scientific Software Library. High performance FFT kernels are a necessary ingredient for our spectral and pseudospectral techniques. Kerbel has worked with CRI to enable high performance parallel operation of their vector kernels on the C90. He has also worked with the TMC CMSSL team to test their high performance FFT's, and with individuals at TMC, AVS, and the ACL-IPCCRC to create code where it was necessary, to improve and fix software.

The JPL/Caltech participants have continued to work closely with computer hardware (Intel via Caltech, Thinking Machines via LANL/ACL) and software (Parasoft) vendors, and have repeatedly helped them eliminate unwanted "features" in their state-of-the-art systems. In the next year, via a formal agreement with Cray Research, the JPL/Caltech participants will be among the first users of the JPL 256-processor T3D, Cray's parallel supercomputer, with peak speed of 38 Gflops and 512 megawords memory. Under the umbrella of the joint Caltech/JPL-Cray Center for Excellence in Parallel Computation, we will be working closely with Cray personnel to provide them with early feedback on their new system.

The IFS NTP group is collaborating with the Microelectronics and Computer Technology Corporation (MCC) in developing and deploying advanced parallel computing technologies for application to NTP and other Grand Challenge problems. These efforts revolve around the development of high performance, cost-effective parallel hardware and advanced object-oriented parallel systems software. It is expected that this pioneering research may have a significant impact in shaping the direction of scientific workstation hardware and distributed concurrent processing software technology deployed by US computer firms during this decade.

LANL NTP researchers have collaborated with Cray Research (CRI) to obtain performance data for particle simulations on the T3D. They obtained 43 MFlop per node on a three-dimensional linear interpolation template.

Industrial applications of NTP-related plasma research

An example of a collaboration between fusion and industry involving particle simulation of plasmas to increase competitiveness is the NTP-relevant CRADA proposals submitted to DoE by H. Okuda at PPPL. These efforts include 1) investigations of Low Energy Electron Beam Behavior in Air and 2) investigations of an Advanced Parallel Plate Etching Device. The first project utilizes 3D particle simulations to predict the behavior of electrostatic spray atomizers. This can provide important information for improving present methods for paint spraying, auto-

fuel injection, and crude-oil refining. The industrial partner is Charges Injection Corporation (CIC) of Monmouth Jct., NJ. The second project utilizes 2D particle simulations to study plasma uniformity and ion acceleration in the sheath region of a parallel plate etcher. This supports the development of an advanced etching device proposed by industry partner, Foresyte Technologies, Inc. (FTI) of San Diego, CA. Although Dr. Okuda is not an NTP researcher, he is part of the group of particle simulation specialists at PPPL and exchanges particle simulation technology with NTP researchers. Furthermore, the simulation models involved in these CRADAs are relevant to divertor modeling in tokamaks. Similarly, Prof. Birdsall's group at UC Berkeley contributes particle simulation codes and algorithms to the NTP and has an active research program in plasma processing for industrial applications.

DoE Mission

The NTP is a cost-effective way to advance the OFE goal of the economical development of fusion energy. Furthermore, because of the strong dependence of the MFE program on supercomputing for many other calculations of importance, the computational skills and technologies acquired by the NTP and infused into the rest of the MFE program provide additional benefit to the OFE mission.

Enabling Technologies

The goals of the NTP are unthinkable without the most advanced MPP environment of the coming decade. The current generation of the most advanced supercomputers and MPP machines are enabling the first three-dimensional simplified simulations of reasonably large tokamak core plasmas. The next generation of machines coupled with algorithm improvements that are an important component of our HPCC research will permit simulations involving physics parameter and scaling studies, the use of more sophisticated plasma physics models, and the addressing of larger plasmas of interest.

There are numerous examples of the improvement in modeling power that have already been achieved by NTP researchers. Use of the 512-Node Intel Delta Touchstone with 16 Mbytes per node has allowed the JPL participants to increase the particle-in-cell problem size that can be run dramatically. Particle-in-cell codes with 110 million particles and 16 million grid points have been run on the Delta with a parallel efficiency of over 95%. The time per particle for one time step is 120 nsec versus 10,000 nsec for the same code on a one processor Cray YMP. (For more examples, see the section entitled "Accomplishments" in the following.)

At Supercomputing '93 in Portland Kerbel(NERSC) demonstrated software he has developed in cooperation with TMC, AVS, and the ACL-HPCCRC. The software was used interactively to generate movies of NTP time-resolved data, using an SGI ONYX Reality Engine, a TMC-CM5 and an IOSC Hippi Frame Buffer. This is an example of how the technologies of distributed computing, massively parallel computing, high speed networks, specialized high performance graphics hardware and scientific visualization software can cooperate to enable NTP researchers to process the massive amounts of data coming from our simulations.

Also at Supercomputing '93, John Reynders, in collaboration with the ACL staff, demonstrated a prototype distributed object-oriented particle simulation that was transparently running over a heterogeneous collection of workstations linked together over a 1000 miles with a 100Mbit/second network. This was perhaps the most sophisticated example of transparent heterogeneous distributed computing done at the show. It combined an AVS-driven interface for constructing the input data and for assembling and displaying the output.

Interdisciplinary Approach

The NTP research program and its personnel overlap with inertial confinement fusion, fluid turbulence, computational fluid dynamics, plasma processing, space physics, and plasma astrophysics, as indicated by the specialties of the participants. The NTP researchers are composed of national laboratory and university computational physicists, computer scientists, plasma physicists, and applied mathematicians. At each NTP site, NTP researchers interact routinely with mathematicians, physicists, computer scientists, and engineers in some cases routinely. As an example, the JPL/Caltech participants, all computational physicists, collaborate routinely and effectively with computer scientists and computational scientists at Caltech, JPL and LANL, with visualization experts at JPL, and with physicists at UCLA and LANL. PPPL researchers interact with Prof. S.A. Orszag and his group (supported by an OFE-APT contract) in the Program in Applied and Computational Mathematics at Princeton on renormalization group methods for large eddy simulation techniques and general turbulence issues, and with Prof. N.J. Zabusky and his group at Rutgers on advanced tools for visualization of 3-D vector fields and quantification of characteristics of turbulent flows. Zabusky's group is supported by contracts from DoE:OSC for "Visualization and Quantification of Evolving Data Sets" and from ARPA for "Hypercomputing and Design" including visiometrics and modeling.

Support Leverage

OFE theory support for NTP-related activities is \$7-8M/yr (including NERSC resources). There is an additional leverage from the \$2B/yr world MFE program. Outside collaborators representing additional leverage include the NSF-funded computer center at Cornell, the NASA-funded JPL center, and an LLNL Director's Initiative to support a comprehensive tokamak simulation model in which a plasma turbulence simulation would be a module or provide a database (\$600-750K/yr). Two JPL/Caltech participants (Paulett Liewer, JPL and Steve Roy, Caltech) are both partially supported by the NSF Center for Research in Parallel Computation via Caltech, which also provides access to the Intel Delta, Gamma and Paragon at Caltech. Liewer and Roy are also partially supported by internal JPL research funds for space physics parallel computations, and, as part of the Caltech/JPL Cray Center for Research in Parallel Computation will have access to the Cray T3D at JPL. The gyrofluid approach is relatively new, and received \$60k in FY93 to aid startup from the Laboratory Program Directed Activities fund at PPPL. Other support leverage has been derived through collaborations with Prof. S.A. Orszag and Prof. N.J. Zabusky, which are listed in the section on interdisciplinary approaches. Bill Dorland (Ph.D., Princeton, September 1993) was awarded a DoE Fusion Energy Postdoctoral Fellowship (only two in the nation were awarded this year), which he has just begun at the U. Texas Institute for Fusion Studies, where he will continue his involvement with NTP activities.

Technology Leverage

- * Developments in MPP hardware, software, and advanced algorithms dramatically improving tokamak modeling
- * Interaction with other Grand Challenge computational projects
- * Beneficial spin-offs

The NTP tests the capabilities of current computing resources with regards to cpu power, data handling and visualization and those in the foreseeable future. Recent advances in computing power and algorithm development are resulting in quantum improvements in our modeling power. As a result of our NTP efforts, we are now undertaking simulations of fusion plasmas which have unprecedented relevance to fusion experiments and have the technical means to do even better with the new MPP hardware coming on line. We are making especially large computational gains in the areas of gather/scatter algorithms in kinetic codes and large linear system solvers that benefit many other grand challenge calculations and areas of major

computational effort, e.g., climatology, computational fluid dynamics and fluid turbulence, molecular dynamics, and diverse applications of Monte Carlo methods. Our MFE researchers have a history of frontier projects with vendor participation, including current work with INTEL, Thinking Machines, and IBM.

NTP researchers at UCLA and JPL collaborate closely with the NASA ESS HPPC Grand Challenge projects sharing information about algorithms, problems, and software. An example of a joint undertaking has been the shared development of a parallel FFT algorithm optimized for coarse-grained message-passing systems (Ding and Ferraro at JPL, and Decyk at UCLA). Porting this algorithm to other systems, including the Cray T3D, using PVM is straightforward. Several researchers from NASA laboratories have obtained copies of the UCLA skeleton codes.

The participation of Liewer and Roy (JPL/Caltech) in the NSF Center for Research in Parallel Computation (Rice-Caltech-Syracuse-Argonne-UTenn) provides technological leverage via strong interaction with other CRPC scientists at Caltech and the other sites. The JPL/Caltech participants are also able to obtain technology leverage from the JPL Supercomputing Visualization Project. Collaboration with a JPL visualization expert at JPL has led to the development of a module for reading NetCDF files into AVS for scientific visualization of NTP results. This module is available to NTP participants as part of the software-sharing component of the NTP.

LANL NTP researchers are working with the internally funded National Information Infrastructure project (Sunrise) to leverage some of their technology. Two significant areas of overlap are in visualization and database management. There are several object-oriented approaches under consideration in these areas, and some will be implemented this year. This will provide an environment that makes the actual location and form of the data storage transparent to both the user and the graphical interfaces. LANL researchers also routinely exchange algorithms, visualization tools, data analysis, and base library implementations across several of the Grand Challenges. Applications of PIC to a wide variety of technologies are being explored, including medical, printer design, and other fluid dynamics problems.

Applications outside of magnetic fusion are being found for the Landau-fluid approach initially developed for Numerical Tokamak applications (Hammett and Perkins, 1990; Hammett, Dorland, Perkins, 1992). The Landau-fluid equations provide a way to reduce the dimensionality of the kinetic equations, while retaining approximate models of important kinetic effects like wave-particle resonance (Landau damping) which are missing from traditional collisional fluid equations. Variations of the Landau-fluid approach have been used to study strong Langmuir turbulence in space plasmas (Goldman, 1993) and laser-filamentation in inertial confinement fusion (Berger, et al., 1993).

Accomplishments

HIGH PERFORMANCE COMPUTING

- * Optimized MPP algorithms for particle and fluid codes achieving large speed improvements in 3D production codes on various platforms
- * Comparative MPP performance analyses and scaling studies
- * Portable code development for MPPs and clusters
- * Class libraries and modular code development for MPPs and clusters
- * Evaluation of common data file formats
- * Parallelization of input/output
- * Development of adaptive-grid and smart-coordinate methods
- * Optimized parallel FFTs, elliptic equation matrix solvers, and convolution routines

LLNL Gyrokinetics

T. Williams (LLNL) has developed a parallelized, domain-decomposition, 3D slab, delta-f, electrostatic gyrokinetic particle code for use on several platforms (BBN TC2000, CM200 and CM5, 16-processor C90, and a cluster of workstations using PVM). The code is fully parallelized including general parallel FFT package and parallelized NetCDF for all input/output calls. Williams also has developed in collaboration with D. Hewett (LLNL inertial fusion and plasma processing programs) a parallel dynamic alternating-direction-implicit elliptic equation solver that is widely applicable to many computational physics problems.

UCLA and UCLA/JPL Collaboration

Decyk and co-workers (UCLA, JPL) have developed one, two, and three-dimensional skeleton particle-in-cell codes designed for rapidly exploring new parallel architectures. These are fully functional PIC codes with FFT field solvers. Optimized code has been written for Cray, CM-2 and CM-5, Intel IPSC/860 and Paragon, and clusters of workstations. After considerable experimentation in collaboration with Lyster, Liewer, and Huang (JPL), it was determined that 1D partitioning of data across processors is most efficient for all codes, but 2D partitioning can work well also. The 3D FFT routines are available to all NTP participants as part of the parallel software exchange component of the NTP. Detailed performance comparisons among the different platforms has been documented and scaling of performance with the number of processors has been tested. Message-passing algorithms have been developed and much experience obtained. Performance with FORTRAN 77 and message passing was significantly better than CMFORTRAN, for example. An order of magnitude improvement in wall-clock turn-around was obtained in the multi-tasked Cray C-90 version of R. Sydora's (UCLA) 2D and 3D gyrokinetic codes run at NERSC. Using PVM, Sydora's 2D code has been run on 4 IBM RS/6000 workstations at UCLA to allow a series of large simulations testing statistical convergence with respect to particle number in the range of 0.5 - 12 million particles. As a consequence of porting particle codes to a variety of parallel computers, the UCLA-JPL collaboration has learned how to write nearly portable code for most platforms as described in the Decyk 1993 Computers in Physics paper.

PPPL Gyrokinetics

PPPL's gyrokinetic researchers began implementing gyrokinetic particle codes on the CM2 at NRL in 1989 and the Intel iPSC/860 at Princeton (Applied Mathematics) in 1991. Reynders has pioneered some of the original SIMD and MIMD algorithms for particle pushing on these machines (Ph. D. thesis, 1992, Princeton). Parker and Santoro (Ph. D. thesis, 1993, Princeton) have subsequently parallelized 3D gyrokinetic codes on the CM200 and CM5 at LANL and the C90 at NERSC. These codes have been used extensively for production runs for the past two years supporting the gyrokinetic particle simulation program at PPPL. More specifically, the 3D sheared slab and magnetic field-line following (flux tube) gyrokinetic codes have been developed and optimized for the 16 processor Cray C90 vector-parallel supercomputer at NERSC. Using all 16 processors on a dedicated C90 gives a speedup of approximately 15 over the serial speed for particle pushing. The charge density accumulation routine is parallelized by scattering the particle data to multiple copies of the grid. This routine is most efficient when there are many particles per grid cell, and it can approach the parallel performance of the push in that limit. For the most part, the field solve consists of 3 multiple one-dimensional vectorized multi-tasked FFTs. A speedup of approximately 12 over the serial speed has been obtained with their parallel FFT, which is a substantial improvement over the Cray MCFEFT and other known parallel FFTs. Overall, a speedup of 14 over the serial speed has been obtained for the production code including all diagnostics. The current speed is 0.43 microsec/particle/timestep for 4 point gyrophase-averaged ions and adiabatic electrons. The

parallelization effort at PPPL like that at the other NTP sites has benefitted directly from sharing of techniques and algorithms among the NTP sites.

A full cross-section 3D toroidal gyrokinetic code and 3D sheared-slab code have been developed at PPPL for the CM200 and CM5 massively parallel supercomputers. The codes are written in CM FORTRAN, and use the DATA PARALLEL MODE on the CM5. The parallelization of the particle push is accomplished using the CM FORTRAN FORALL statement. The accumulation routine is once again slightly more complicated to execute in parallel because of multiple memory updates of the same memory location so TMC had to write a special library (CMF_SEND_ADD) routine that would be callable from CMFORTRAN in order to accomplish this. A parallel 3D FFT is used for the field solve. The speed for the 3D toroidal code is 2.5 microsec/particle/timestep on the CM200 (2048 floating-point nodes) for 4 point gyrophase-averaged ions with the NGP interpolation and 0.6 microsec/particle/timestep on the CM5 (1024 floating point nodes). The CM200 sheared slab code speed is 7.4 microsec/particle/timestep for 4 point gyrophase-averaged ions with 7 point linear interpolation at each of the 4 points and adiabatic electrons. The corresponding CM5 code speed is 1.8 microsec/particle/timestep.

NERSC

Milovich and Kerbel (NERSC) have increased the speed of the C90 version of the nonlinear gyro-Landau fluid code TRB by an order of magnitude by using a carefully developed multitasked pseudo-spectral method to evaluate the nonlinear convection terms. Another factor of 3 to 5 was obtained by multitasking the evaluation of the different contributions to the right-hand side of the gyroviscosity equation. The code is a three-dimensional time evolution solver based on a fully implicit technique to deal with stiffness problems associated with the large ion-electron mass ratio. This has led to an additional increase in speed by a factor of 2. Finally, the NERSC group is porting this code to the T3D architecture using the work-sharing parallel programming paradigm. This new version currently runs on the T3D simulator available in NERSC computers.

ORNL

In pursuit of the goal to use a common file format throughout the Numerical Tokamak Project, the ORNL team has tested and implemented various portable, platform independent binary file formats. The BDX suite of Fortran routines from NASA Lewis relies on the machine-independent XDR binary format. BDX has proved easy to use and easy to implement on different platforms, from workstations to the Intels. The need for BDX arises from having to transfer large amounts of data (640 Mbytes per dedicated period so far) from the Intels to another platform for analysis, since no online capability exists on the Intels. The NetCDF package from NCAR has also been tested. The NetCDF is much more sophisticated than BDX since it can be implemented in both C and Fortran and allows for self-describing data structures absent in BDX. NetCDF is clearly the long-term solution of choice, but it is not yet supported on the ORNL Intels, so that BDX will have to be used in the short term. The feasibility of porting NetCDF to the Intels is currently being investigated in collaboration with the LLNL team. Williams (LLNL) has parallelized the use of NetCDF in a parallelized three-dimensional gyrokinetics code to take care of all input/output required for any platform supporting NetCDF.

The ORNL team has carried out performance optimization studies for plasma fluid turbulence calculations on a large number of parallel machines. They include the BBN Butterfly, the Intel family of MIMD mainframes (iPSC/860, Touchstone Delta, Paragon XPS5 and XPS35), clusters of IBM RS6000 workstations and the C90. These studies were performed to assess which of these configurations leads to an optimal path towards the ever higher resolutions

required by the experimental relevance of the calculations and also to determine the algorithmic and computational requirements for future generation parallel machines.

The ORNL team's benchmarks on the Intels indicate that there is an optimal number of processors for a given problem size. The optimal number of processors increases with problem size. For this optimal number, a factor of 5 improvement in performance has been achieved on the iPSC/860 over a single processor of the CRAYII (running the serial version of the message passing plasma fluid turbulence code KITE) and a factor of 13 improvement on the Delta has been realized with the largest size that fits in node memory, namely 512 modes and 1025 grid points [Lynch et al., 1992].

Clusters of workstations offer a large memory per node, which is a problem on the Intels for the most efficient convolution algorithm. This has prompted the ORNL team to implement the KITE code in parallel on an array of IBM RS6000's using PVM. Clusters do represent an affordable path to higher resolution if they are connected by a network of adequate bandwidth. This exercise has also enabled the ORNL team to be ready for the CRAY T3D which operates with PVM. By far the best parallel performance with the ORNL codes has been achieved on the CRAY Y-MP C90 using microtasking. With parallelization over the number of modes, the CPU time per step turns out to be linear with number of modes even though the number of operations scales as the square of the number of modes. This is because more processors are accessed concurrently with increasing number of modes. Tests in dedicated mode show that this linear scaling holds up to the full 200 Mword machine capacity. Even in non-dedicated mode where the 80 Mword memory cap limits overlap to 7 concurrent processors, production runs with the KITE code have been carried up to saturation in a few days instead of the few months it customarily took before the advent of the C90 at NERSC. Moreover, the version of KITE optimized for the C90 averages 2 CPU seconds per step while the optimized version for the iPSC/860, for the same problem size, averages over 1 minute per step. It is only by increasing the problem size (beyond that feasible on the C90) towards that required for optimal use of all processors that comparable performance is expected on the fully configured Paragon [Lynch et al., 1993].

JPL/Caltech

The focus of the JPL/Caltech portion of the Numerical Tokamak Project is the development of parallel algorithms for plasma particle-in-cell (PIC) codes which will be used to implement NTP gyrokinetic physics models on high performance computers. For plasma PIC codes, there are many more particles than grids (10-1000 particles per cell) and the particle portion of the computation dominates. Parallel algorithms have been developed and implemented on MIMD (Intel Delta, Paragon and Gamma), SIMD(CM200) and mixed SIMD/MIMD(CM5) parallel computers. The work has been done in collaboration with UCLA, and UCLA will use some of these algorithms to implement a gyrokinetic code in the next year. LLNL has already used some of the algorithmic ideas for parallel implementation of an NTP physics model and has helped UCLA/JPL with parallelizing the charge/current deposition on the grid.

The JPL/Caltech NTP group has completed development and implementation of an electromagnetic, parallel, three-dimensional plasma particle-in-cell codes for message-passing parallel computers (e.g., Intel). The code is implemented using the General Concurrent PIC (GCPIC) algorithm previously developed by Liewer and Decyk. In the GCPIC algorithm, the particles are divided among the processor using a domain decomposition of the simulation grid. Since the particles and their nearest grid points are in the same processor, the gather/scatter operations can be done with no interprocessor communication. The 3D GCPIC code has a very high (>95%) parallel efficiency. On 512 nodes of the Intel Delta Touchstone, particle-in-cell codes with 110 million particles and 16 million grid points, the time per particle for one time step is 120 nsec versus 10,000 nsec for the same code on a one processor Cray YMP. This code is written using Parasoft's EXPRESS FORTRAN environment and can be easily ported to message-

passing system using PVM including the Cray T3D scheduled to arrive at JPL in late 1993. (JPL in collaboration with UCLA.)

JPL/LANL Collaboration

JPL/Caltech and LANL NTP researchers have collaborated in the development of PIC algorithms for 3D adaptive grid PIC including SIMD particle-sorting PIC algorithms on CM200 and CM5. Parallel algorithms have also been developed and implemented for SIMD 3D PIC codes using adaptive, deformable hexahedral grids. More sophisticated physics models of the future, such as the implicit PIC model of Brackbill (LANL) will require the use of such adaptive grids to improve grid resolution in areas of steep gradients or to align the grid to the geometry of the magnetic field to properly treat transport. For the case when the grid is irregular, new algorithms were needed for locating the particles in a new cells when cell boundaries are crossed and we have developed and implemented a simple search algorithm for this. A 3D electrostatic adaptive grid PIC code was implemented on the CM5 and CM200 using CM-FORTRAN in collaboration with LANL (Brackbill and Forslund, LANL) to study SIMD PIC algorithms.

JPL/Caltech and LANL have begun work on the development of a highly modular, portable three-dimensional deformable grid code that is flexible enough to allow changes in physics models or changes in architecture without massive re-writes of the code. This year, the basic framework for the modularity and portability has been developed. Four "levels" of modules have been identified. The lowest level modules are architecture-specific modules which handle the message passing and other strongly machine and/or architecture-dependent functions. The next level is a "numerics" level with generic computational physics modules (such as matrix multiplication, etc.) and geometric factors) which are used by many physics models. The highest two level are specific to a specific physics model and problem. Using this four-level structure, a simple modular, deformable grid fluid code has been implemented in parallel using Fortran plus PVM message passing.

LANL

To ease maintenance of codes across a variety of platforms, LANL NTP researchers have been developing a class library to do particle simulations on arbitrarily connected logically rectilinear grids which works on a PVM cluster and also on the CM5 (as well as a uniprocessor). They also are working with CRI to optimize gather/scatter kernels for the Alpha chip on the T3D and plan to collaborate with Sandia on the Paragon computer. They are porting Brackbill's multi-domain 3D adaptive-mesh algorithm, working on a version of their virtual domain decomposition scheme, are establishing an object-oriented database management protocols for the library, and have recast their graphical interfaces into an object-oriented paradigm.

IFS

Furnish and Gray of the IFS have worked with MCC to use advanced computer science technologies in support of the heavy demands of the Grand Challenge NTP. They have exploited MCC capabilities in object orientation and parallel execution to develop a prototype one-dimensional particle code, obtaining scalable performance on inexpensive parallel RISC-based multiprocessing technology.

PPPL Gyrofluids

Beer, Dorland, and Hammett (PPPL) have optimized a 3D nonlinear pseudo-spectral gyrofluid turbulence code for parallel performance on a 16 processor CRAY C-90. Spinoffs include developing a multitasking FFT routine which was 5 times faster (for large FFT's on a 16

processor CRAY C-90) than the original CRAY multitasked FFT routine, and made this routine available for general use at NERSC, and identifying and reporting bugs in the CRAY parallelization utility ATEXPRT.

VISUALIZATION

- * Distributed visualization
- * Real-time animations
- * Use of AVS, CMAVS, PVWave, X-Windows

Very large three-dimensional data sets from particle codes require visualization in order to interpret and present results in compact form. A series of modules have been developed at UCLA (Bollens and Sydora) in collaboration with Cornell U. using the visualization package Data Explorer on an IBM RS/6000 and facilities at Cornell. Modules have been developed to contour the electric potential surfaces with various opacities and for tracing magnetic field lines in toroidal geometry. The data originated from Sydora's 3D gyrokinetic simulations.

Kerbel(NERSC) has been active in the development of an interactive scientific visualization system for the NTP. This activity is at the leading edge in high performance computing and communications in a number of areas. The data sets comprise typically 10^{*9} gridpoints and the visualization system is designed to allow animated navigation through parts of the sets in a 'virtual reality' sense. The requirements point to the need to develop (1) schemes for information storage and retrieval which is standardized, highly compressed, and efficient and (2) the use of distributed computing systems where remote high capability compute servers are connected by high bandwidth networks to high performance graphic workstations. To address (1) Kerbel has developed a scripted production mode of operation using adaptive time step adjustment and automatic checkpointing. Special attention was given to creating the smallest consistent set of self-describing regenerative data sets possible for auto-restarting and for recreating intermediate results. For distributed computing systems, Kerbel has used the underlying computer graphics subsystems and communications protocols that are provided by CMAVS, AVS and X-Windows. He designed high performance massively parallel rendering algorithms and navigation tools for the NTP but these are generally applicable to other GC projects as well. Kerbel's visualization system is designed to create composite images quickly enough for real-time animation. Multi-image scenes including geometrical cues (such as magnetic field lines) and surface projections of turbulent field quantities can be composed and viewed interactively. The composition parameters can themselves be animated and reapplied. For example, if the parameters set the viewer position, the result is a sequence of images moving through the data. A research collaboration to develop the technology to store these animations in holographic stereogram format is under way with researchers at the MIT Spatial Imaging Laboratory. Kerbel demonstrated the value of these combined efforts in close collaboration with TMC, AVS, and the ACL-HPCRC at the 3rd SuperComputing Conference in Portland, November 1993.

In collaboration with NERSC staff as part of NERSC's DCE Pilot project, the ORNL team is making use of the scientific visualization tools such as PVWAVE and AVS available on the SAS HP workstation at NERSC and locally on one of the IBM RS6000 workstations. AVS has proven to be difficult to run remotely over ESNET at T1 speeds. PVWAVE and AVS make it possible to probe features of the data which could not be rendered with sufficient details, dimensionality or meaningful colors by other means. Recently, the ORNL team has collaborated with ORNL's Scientific Visualization Laboratory to produce videos of AVS data from large-scale toroidal calculations of Alfvén wave instabilities induced by energetic particles in tokamaks [Spong, 1993].

A portable, freely distributable X-windows based graphics library was developed by LeBrun at IFS (PLPLOT). It is currently in use by three groups of the NTP (IFS, LANL, ORNL)

as well as numerous users worldwide, and is an excellent tool for facilitating collaborative work. PLPLOT is available by anonymous ftp from hagar.ph.utexas.edu in the pub/plplot directory.

ADVANCED ALGORITHM DEVELOPMENT

- * Delta-f perturbation methods
- * Magnetic-field-following coordinates
- * Implicit methods for particle and fluid models
- * Extensions to include electromagnetic and kinetic electron effects
- * Collision algorithms
- * Object-oriented programming
- * Adaptive-grid methods

Advanced algorithm development is at least as important as increases in supercomputing hardware performance in leading to significant improvements in simulation capability. The experience over many years in computational plasma physics and controlled fusion research has been that major advances in modeling capability have resulted from the combination of both algorithm improvement and increased computing power. Algorithm improvement has involved an interdisciplinary approach with physicists, mathematicians, and computer scientists cooperating to make major contributions. An important aspect of the computational side of the NTP is advanced algorithm development.

Delta-f perturbation methods and quasi-ballooning coordinates

Several groups have used partially linearized or delta-f particle algorithms and quasi-ballooning coordinates to achieve improved grid resolution in both fluid and particle codes. This has contributed to much more efficient simulation of toroidal ion-temperature-gradient instability. Resolution is improved by factors of 10-100 in specific cases. Groups at PPPL, UCLA, LLNL, and IFS have tested fully nonlinear particle codes against delta-f codes to confirm the reliability of the latter and to demonstrate their ability to reduce noise while achieving much more efficient simulations.

Delta-f collisions

Dimits and Cohen (LLNL) have developed and tested an improved delta-f gyrokinetic ion collision operator in both two and three-dimensional implementations. In so doing, the theory of collisional effects on the ion-temperature-gradient instability was elaborated and previous published work corrected. A realistic simulation of tokamak transport should include a good model for collisional dissipation. This collision model has been used by Lee and co-workers (PPPL) to study neoclassical transport with their gyrokinetic code.

Implicit methods

Barnes and co-workers (LANL) and Cohen, Xu, Dimits, and Williams (LLNL) have formulated, analyzed, and implemented a new class of implicit-moment, delta-f algorithms for particle simulation of turbulent transport in both electrostatic and electromagnetic models. These methods take advantage of the natural disparities in time scales between the more mobile electron and slower ion species, and between the highest-frequency normal modes and the lower frequency modes thought to dominate the transport and have used time-step splitting, orbit-averaging, implicitness, and the delta-f perturbative method to allow the use of bigger time steps and fewer particles in achieving quieter and more efficient simulations.

LANL researchers have developed an iterative solver for coupled implicit-moment, electromagnetic field equations using conjugate gradient and GMRES methods. They have developed adaptive grid algorithms for toroidal grids and have introduced schemes for dynamically controlling the number of particles per cell for load leveling and for multiple length-scale problems for MPP and other supercomputers. They also have synthesized algorithms for insuring accurate particle motion in boundary-fitted coordinates.

Kerbel, Milovich and Shumaker (NERSC) have been working to relax the constraints which limit the semi-implicit predictor-corrector time advancement algorithms developed for the CM5/C90 gyro-Landau fluid turbulence simulation code TRB. The large $E \times B$ advection velocity present in our tokamak simulations cause a stringent limitation on the time step. This Courant condition limitation becomes worse as the grid size is reduced. In the current version of the code the convection terms are computed by evaluation of convolutions using a pseudospectral method. This convolution, in addition to limiting the time step, is one of the most computationally costly parts of the simulation. Shumaker and Kerbel are developing an alternative scheme which uses a semi-Lagrangian advection method. This method computes the changes due to advection in real space instead of Fourier space. It computes the change in a quantity at a grid point by interpolating along a stream line to the position of the fluid element at the previous time. Since the prior position will generally not be on a grid point, another interpolation method (4th order Lagrangian) is used to determine the function value from the grid point values at the previous time. The semi-Lagrangian method has been shown to operate stably at large Courant numbers, thus we anticipate being able to use a much larger time step. Since this advection algorithm computes in real space, it can be adapted to aid in the visualization of the $E \times B$ flow field. Milovich and Kerbel have implemented (C90) a fully implicit time advancement technique based on a preconditioned Krylov iteration scheme. This technique is expected to overcome two major concerns: a) severe time limitations due to the Courant condition, and b) extending the model to include electron dynamics which stiffen the differential equations significantly.

Kinetic electron and electromagnetic effects

Extensions and generalizations of the gyro-Landau-fluid technique to allow inclusion of kinetic effects in fluid-like treatments of most electrostatic and electromagnetic instabilities of relevance to plasma turbulence and transport in magnetic confinement devices has been worked on by NTP groups at GA, NERSC, ORNL, and PPPL.

Advanced algorithm development at IFS

LeBrun has further developed TPC (Toroidal Particle Code), with completion of its gyrokinetic module and various other technical improvements. TPC uses a true toroidal coordinate system for global simulation. TPC has to some extent succeeded in creating a software environment for doing tokamak simulation, independent of the algorithm or dynamics. Advanced algorithms may be substituted as they are developed without extensive change to the underlying diagnostics package and user interface, which represent the bulk of the actual code. TPC is currently written primarily in MPPL with a shell in C++; the code is being gradually converted over to C++ in order to exploit modern object-oriented technology.

Kotschenreuther (IFS) has developed a fully gyrokinetic, implicit grid code in ballooning coordinates. Both the distribution function time step and the field solution are fully implicit, so there are no time step restrictions for stability. Full electron dynamics are included. The algorithm has been demonstrated to accurately include effects such as resonances and bounce-averaged trapped particle effects even for time steps much longer than a bounce time. The code is presently linear, but planned nonlinear extensions should have excellent stability at long time steps. The code also includes a realistic Lorentz collision operator, electromagnetic effects and

full toroidal (annular) effects. The code has been benchmarked against a similarly comprehensive eigenvalue code of Rewoldt and Tang with good agreement. The code has been modified to include self-consistent nonlinear flow, which has been found to be an important saturating effect in recent gyrofluid simulations. The long-time behavior of these flows is overly damped by present gyrofluid models, a difficulty avoided in this fully kinetic treatment. Aydemir(IFS) has developed a general description of low-noise techniques, such as the delta-f method, in terms of well-known Monte Carlo variance reduction methods. This point of view explicitly recognizes the source of "noise" in particle simulations as the Monte Carlo sampling error in low-order moment calculations and points to various ways of further reducing the noise by using other methods developed in the Monte Carlo community.

Furnish(IFS) is working (in collaboration with LeBrun) to develop a next-generation tokamak modeling code employing advanced MCC technologies for object oriented programming and parallel execution. This code uses modern C++ features to provide a flexible environment for evaluation of software components embodying various physical models.

PLASMA PHYSICS APPLICATIONS

- * Larger three-dimensional toroidal gyrofluid and gyrokinetic simulations using the CM-5 relevant to experiments and relevant simulations also on C90
- * Simulated thermal diffusivity and fluctuation spectra agreeing more closely with experiments
- * Code cross-comparisons leading to closer agreement between gyrofluid and gyrokinetic simulations on TFTR test case, and scaling studies
- * Identification of importance of nonlinearly self-generated sheared flows in influencing
 - * Simulations of ion temperature gradient, trapped electron, and alpha particle driven toroidal Alfvén eigenmode instabilities
- * Inclusion of more physics in simulations: impurities, collisions, kinetic electrons, velocity shear, toroidicity, curvature drifts and resonances, magnetically trapped particles

During the first stages of the NTP, the most important development affecting the physics applications has been the inclusion of three-dimensional toroidal geometry with adequate resolution. There are toroidal gyrofluid or particle codes now in use at most of the NTP sites. Toroidal effects, e.g., unfavorable magnetic curvature on the outside of the torus and trapped particle effects, introduce additional destabilizing forces on the turbulence that can degrade confinement. Our toroidal simulations have seen a significant increase in microturbulence over the same simulations in slab geometry and something like an order of magnitude increase in the turbulent transport bringing the simulation transport rates considerably closer to the corresponding values inferred from experimental data. Because of our successful porting and optimization activities on MPP machines, we now have codes with performance that matches and in some cases exceeds that on the C90. Because we have had access to large blocks of dedicated time on MPP machines, in particular the CM-5, we have been able to do large gyrofluid and gyrokinetic simulations that would have been too painful to carry out at NERSC. These MPP simulations have yielded important new physics results, which are identified in the following. The two most important examples are the PPPL gyrokinetic simulations of TFTR on the CM-5 showing agreement with the beam-emission-spectroscopy-measured fluctuation spectrum and the NERSC/GA gyrofluid simulations and visualization work on the CM-5. Because our researchers also benefit from having access to large amounts of C90 time and because our C90 codes have been greatly improved through our NTP efforts, we also have obtained important new physics results from C90 simulations contributing to the NTP. This is additional leverage for the project. Now that we have the improved capability enabled by the HPCC effort, we expect that a greater share of our new physics results will come from MPP

simulations; and we can take real advantage of the increased MPP capability now coming on line.

PPPL Gyrokinetics

The highlights of the NTP gyrokinetics research activities at PPPL for the past two years have been in the following areas. (1) Development of fully nonlinear weighting delta-f scheme. A newly developed fully nonlinear weighting scheme based on the perturbation expansion (Parker and Lee, 1993) together with the quiet-start techniques have given us the tool to carry out simulations with minimal noise, making comparison with linear theory and simulations of a larger plasma volume easier. (2) Toroidal ion temperature gradient drift instability simulation. This work has been carried out using the CM200 and CM5 (with assistance from LANL NTP researchers) at LANL. As reported in a recent article (Parker et al., 1993), the resulting fluctuation spectra (Fig. 1) resemble those of the TFTR plasma obtained by the beam emission spectroscopy (BES) [R. Fonck et al., Phys. Rev. Lett. 70, 3736(1993)]. This comparison together with simulations with different minor radii may suggest a non-Gyro-Bohm scaling which is currently an issue of high interest in the fusion community. The simulations confirm linear theory regarding the ballooning characteristics of the instability and demonstrate the existence of these elongated structures in the nonlinear stage. (3) Impurity transport due to microturbulence. This is the doctoral research of R. Santoro. It has been demonstrated that microturbulence can be the origin for the inward pinch of the impurities observed in tokamaks. It is further shown that the pinch is the result of ExB convection and acceleration along the field line. In toroidal geometry the pinch velocity is rather insensitive to the Z/m scaling. PPPL experimental physicists are looking for this property in the upcoming trace tritium experiments. (4) Finite-beta effects. In order to extend the gyrokinetic particle simulation into more relevant tokamak operating regime, PPPL is now incorporating the magnetic perturbations and induction electric field into existing gyrokinetic particle codes in a doctoral research project. Finite-beta stabilization of microinstabilities in simple geometry has been confirmed. Work accommodating more complicated geometries is in progress. (5) Neoclassical transport. A new nonlinear weighting scheme for the equilibrium plasma using the gyrokinetic formalism has been developed for studying neoclassical transport. With appropriate collision models (Dimitis and Cohen, 1993), PPPL NTP researchers have confirmed the theoretical predictions on the particle and energy transport and on the bootstrap current in a doctoral research project. (6) Comparisons among gyrokinetic particle codes, gyrofluid codes, and gyrokinetic Vlasov codes have been carried out by Parker, Dorland, Beer, Santoro, and co-workers at PPPL and NTP researchers at other sites [S. Parker et al., APS invited talk (1993)]. (7) Gyrokinetic-MHD hybrid simulation. This effort seeks to understand energetic particle effects on MHD modes. The simulation model uses the pressure coupling and the current coupling between the background MHD and gyrokinetic particles [W. Park et al. Phys. Fluids 4, 2033 (1992)]. The first application of the code by Fu and Park is the investigation of the nonlinear saturation of the TAE modes. The results indicate that the nonlinear saturation is mainly due to wave-particle trapping. Moreover, a new $m=0$ high frequency mode is found to be induced by the hot particles, which may be related to the GAE modes observed in the TFTR experiments [K. L. Wong et al., Phys. Fluids B, 4, 2122 (1993)]. (8) Related physics issues. A proper theoretical foundation for the systematic kinetic analysis of sheared flow effect on plasma microturbulence has been provided by a derivation of the nonlinear gyrokinetic equations in the presence of sheared flows [M. Artun, PhD Thesis]. The influence of velocity shear on ITG modes have been studied, and comprehensive results for sheared slab geometry have been obtained [M. Artun and W.M. Tang, Phys. Fluids B, 1102 (1992); M. Artun, et al., Phys. Fluids B, in press (1993)]. Toroidal applications to trapped-particle modes have also been carried out, and the stabilizing trends assessed. The thermal fluctuation properties for a finite-beta gyrokinetic plasma has been investigated by Krommes (see publication list). This effort may help us to understand the

numerical difficulties encountered in the simulation. Rath and Lee have been studying the entropy balance in the gyrokinetic simulation to understand the nature of the observed transport. For a collisionless plasma, their study reveals that the stochastic particle motion plays a dominant role. Hu and Krommes studied an extension of this problem to include collisional effects. Mynick and Parker have analyzed the gyrokinetic particle simulation data and their conclusion is that the observed transport is weak turbulence in nature.

Gyrofluids

"Gyrofluid", or "gyro-Landau fluid", equations provide a way to reduce the dimensionality of the gyrokinetic equation to a small set of fluid equations, while retaining models for approximating important kinetic effects such as wave-particle resonances (Landau damping) and gyro-orbit averaging. The gyrofluid approach is relatively new. The original model developed by Hammett and Perkins (PPPL) included only Landau damping effects for electrostatic modes, and has been extended by Dorland (PPPL) to include finite-Larmor-radius effects, by Waltz, Dominguez and Hammett (GA and PPPL) to include a basic model of toroidal grad-B and curvature drifts, and by Beer (PPPL) to higher accuracy toroidal models including some trapped particle effects. The ORNL group has produced other extensions of the gyro-Landau fluid model described in the following paragraphs. Chang, Callen and co-workers at Wisconsin independently developed a type of gyro-Landau fluid model, including MHD-like instabilities.

GA/NERSC Gyrofluid Collaboration

The GA/NERSC toroidal field line following gyrofluid code has been used (Waltz and Kerbel 93a and 93b) extensively to map the scaling of toroidal ITG heat diffusion with respect to tokamak variables like shear, safety factor, toroidicity, and temperature gradients. Radial modes or nonlinearly generated shear flows reduce the transport by tenfold to linear mixing length model levels. The scaling follows the standard linear mixing length model only near the critical gradient threshold for moderate to strong shear. The transport saturates at weak shear and very strong temperature. Only gyroBohm scaling with respect to the relative gyroradius has been found. Extensive studies of the effects of equilibrium sheared rotation show that easily achievable shear-flow rates comparable to linear mode driving rates can dramatically reduce ITG transport in the core plasma. This offers the possibility of practical improvements in tokamak confinement now being tested on DIII-D. Most of Kerbel's simulation activity with the gyrofluid code has been at the ACL. The computing environment to support bigger calculations is superior to the C90, and Kerbel had done simulations on the CM-5 that would have been too painful to contemplate on the C90. All of the supporting visualization work done by Kerbel for the gyrofluid simulations has used the CM.

PPPL Gyrofluids

The PPPL gyrofluid group and collaborators at GA and NERSC have generalized the gyrofluid equations to include more toroidal effects and are testing them against established gyrokinetic results while at the same time developing a nonlinear toroidal gyrofluid code and carrying out initial simulations. Highlights of the technical progress in the past two years include the following. (1) Completion of the finite-gyro-radius models in the gyrofluid equations, including important nonlinear gyro-radius terms, with successful linear comparisons with full gyrokinetic codes in slab geometry (Dorland93a, Dorland 93b). (2) Successful benchmarking of nonlinear gyrofluid and gyrokinetic codes in typical parameter regimes (reported in Dorland's Ph.D. Dissertation, Dorland93b, and in an invited talk at the 1993 APS-DPP meeting by Parker, Dorland, Santoro et.al., Parker93). Excellent agreement in turbulent heat conduction was found,

though a 40% disagreement in the saturation level of electric fluctuations remains which is not yet well understood. Some special parameter regimes have been found where the gyrofluid approach needs many moments (and would be inefficient) for accuracy (Mattor92, Dorland93b, Hammett93). (3) Extension of toroidal gyrofluid equations (Waltz92) to higher moments (for more accuracy near marginal stability), and to include neoclassical trapped particle effects important in controlling poloidal rotation (work done primarily with M.A. Beer, reported in Hammett93). (4) Generalization of our nonlinear gyrofluid turbulence code to a flux-tube in toroidal geometry, using a field-line coordinate system proposed by Cowley for efficient representation of nonlinear tokamak turbulence problems (with M.A. Beer and S.C. Cowley, reported in Hammett93).

At present, the PPPL gyrofluid code models toroidal ITG-driven turbulence which is probably dominant in the core of many tokamaks. They intend to add non-adiabatic electron dynamics to destabilize the drift-wave branch which is important in many experimental regimes. They also intend to do more detailed parameter scans with higher resolution, but initial nonlinear results have found two important physics results illustrated in Figs.(2-3) (reported in an invited talk at the 1993 Sherwood Fusion Theory conference, published in Hammett et al., 1993: (1) An important nonlinear mechanism is the generation of sheared zonal flows by the turbulence, and the stabilizing feedback of these flows on the turbulence itself. (This effect has been noted in H-mode studies and edge-turbulence simulations by others, but the PPPL work was the first to show it is important for core turbulence as well. The proper adiabatic electron response is crucial to allowing strong generation of these sheared flows (Dorland92b). Previous ITG simulations had used an electron response which allowed radial flow of electrons to strongly short-out the radial electric field associated with ExB flows.) It appears crucial to properly treat all of the flow generation and damping mechanisms (including neoclassical toroidal effects). If the sheared flow is artificially suppressed, then elongated streamers form and the heat transport increases without bounds (Fig. 2). The importance of these sheared flows in ITG turbulence has been seen in slab gyrofluid (Dorland et.al., 1993 US-Japan Workshop Proceedings, AIP press) and gyrokinetic simulations by the LLNL NTP group (Cohen et.al. Phys Fluids B 93) and other toroidal gyrofluid simulations (Waltz and Kerbel, 1993 US-Japan workshop Proceedings, AIP Press). (2) The nonlinear spectrum is peaked at significantly longer wavelength ($k_{\theta} \rho = 0.15$) than the fastest growing linear instability ($k_{\theta} \rho = 0.4$), producing a spectrum (Fig. 3) with qualitative features like BES measurements on TFTR. More work needs to be done to understand what controls the scaling of the peak $k_{\theta} \rho$ in our simulations (experiments appear to have a Bohm transport scaling, which suggests that k_{θ} should scale independently of ρ , the ion Larmor radius). Nevertheless, it is encouraging to see that nonlinear effects can produce long-wavelength features similar to the experiments. Similar long-wavelength spectra with features like the BES measurements have also been seen in particle simulations in a full tokamak geometry (Parker's 93 PRL). Access to large amounts of time on the NERSC Cray C-90 has made it possible to explore the sensitivity of the results to the size of the simulation box. As shown in Fig. 3 and 4, the typical size of the turbulent eddies (and therefore the shape of the spectra) appears to be insensitive to doubling the box size. This result, also obtained in Waltz' gyrofluid simulations, differs from the first large gyrokinetic simulation results reported by Parker, et al., and will receive more attention by the NTP in the coming year.

ORNL gyrofluids

A version of the Landau-fluid technique, with inclusion of finite Larmor radius effects for the ions, has been applied by the ORNL team to develop analytical and computational models specific to dissipative trapped electron mode (DTEM) instabilities which are deemed to be responsible for fluctuations at the core of toroidal fusion devices, such as tokamaks and stellarators. Models have been developed with various degrees of complexity for the description of the ion dynamics and of the trapped electron response. These models have been implemented

in the three-dimensional, slab geometry, initial value FARDTEM code. Landau-fluid linear results from the FARDTEM code are in excellent agreement with kinetic theory results, regardless of which ion description is used. Preliminary nonlinear results with a reduced resolution model and an i-delta description for the trapped electrons show that saturation of the fluctuations can be achieved without any additional dissipation but for shear and ion Landau damping and that the fluctuation levels are commensurate with simple mixed length estimates.

ORNL/UCLA Collaboration

A gyrokinetic counterpart to the gyro-Landau fluid model has been developed by an ORNL/UCLA collaboration. In the particle model, the ions are treated as particles following the characteristics of the gyrokinetic equation. This low-frequency treatment naturally incorporates linear and nonlinear ion Landau resonances and finite ion Larmor radius effects. The electrons are treated analytically: the passing electrons have a Boltzmann response and the trapped electrons are represented by an i-delta phase shift between the density and potential to mock up inverse Landau damping. The gyrokinetic model has been implemented in the 2D GYRO/DTEM code. The object of this activity was to incorporate important electron effects without being constrained by the small time step required to resolve circulating electrons and to produce a gyrokinetic model as close as possible to its gyrofluid counterpart in order to perform careful comparisons. Test results so far indicate good code agreement on linear growth rates for the dissipative trapped electron mode.

ORNL Toroidal Alfvén Eigenmode Research

A new application of the Landau-fluid technique is being used by the ORNL team to treat plasma instabilities induced by a dilute population of energetic particles [Hedrick, Leboeuf, Spong, 1992; Spong, Hedrick, Carreras, 1992; Spong, 1993]. The model is a hybrid one in the sense that the background plasma is described by the reduced MHD equations, while the energetic particles are treated as a Landau fluid. The Landau fluid description gives an accurate representation of the destabilization of the Alfvén waves in the background plasma by the energetic particles through the parallel velocity Landau resonance needed to model the toroidal Alfvén eigenmode (TAE). The model has been implemented in the three-dimensional, nonlinear, full toroidal geometry, finite beta, initial value TAE/FL code. Linear results from TAE/FL are in excellent agreement with kinetic, analytical predictions. Nonlinear calculations performed with TAE/FL reproduce many of the features, such as fluctuation levels and frequency spectra, observed experimentally in beam-driven discharges on the TFTR and DIII-D tokamaks, as well as the WVII-AS stellarator. TAE/FL has also been used as a predictive tool to assess the linear and nonlinear stability of the International Tokamak Experimental Reactor (ITER) device in the presence of fusion products. The advantage of the Landau fluid technique as implemented in TAE/FL is that it makes possible realistic and high resolution calculations which are currently out of reach with a particle representation for the energetic species with presently available computer resources.

LLNL Gyrokinetics

The LLNL gyrokinetic group has made a careful study of the convergence properties (in time step, particles, and grid resolution) of the three-dimensional gyrokinetic delta-f code to understand the computational requirements independent of computing platform. With the use of quasi-ballooning coordinates, spatial grid-resolution constraints have been relaxed by factors of 10-100 for ion-temperature-gradient (ITG) instability. The LLNL group helped direct and participate in the NTP TFTR test case and code cross-comparison. The LLNL gyrokinetic study (Cohen, et al., 1993) helped identify the importance of nonlinearly self-generated shear flows in

saturating ITG turbulence. Their fully parallelized gyrokinetic code is now sufficiently optimized that its performance on the CM-5 should exceed that on all 16 processors of the C90. With access to the CM-5, the LLNL group can now undertake physics simulations of a size and scope not previously possible.

IFS Kinetic Simulation

Work at IFS has continued primarily on kinetic simulation of ITG mode and comparisons to experiment. There are several code efforts, each with a particular approach. The gyrokinetic delta-f Vlasov code (toroidal annulus) developed by Wong is being used to investigate stability of large amplitude ITG eigenmodes. The full-torus TPC simulation code by LeBrun has been used in a systematic study of ITG transport in collaboration with Tajima and Kishimoto. Novel computational techniques have been employed to investigate ITG stability with experimental parameters additional relevant effects in the effort of Kotschenreuther.

The code of Kotschenreuther has been run with parameters taken from about twenty TFTR shots. L-mode shots are found to be within 20%-30% of marginal stability on the inner half of the minor radius. The modes which are unstable have been found to correlate very well with turbulence spectrum measurements on TFTR using beam emission spectroscopy. Strong discrepancies have been found between the trends for heat transport in the experimental data and the linear stability trends. Estimates indicate that higher-order effects in the ballooning expansion (recently included in the code) are important and could make the theoretical micro-instability predictions consistent with the experiments. Quantitative examinations of this are proceeding as well as comparisons with other groups codes which perform related (but less complete) calculations. Kotschenreuther's gyrokinetic ballooning mode stability code has been extended at GA to include many graphical features, quasilinear flow calculations, linear mixing length models, and real (experimental) magnetic geometry (Dominguez et al 93) along the field lines. It is being used as a transport data analysis tool on DIII-D discharges.

Simulation runs of ITG mode fluctuations and transport were made using IFS' TPC with a nonlinear PIC ion and adiabatic electron model in a full torus. Large scale "streamer" structures in the electric potential were observed coupled with greatly enhanced ion heat transport. The ion temperature profiles were observed to relax toward a marginally stable state, and the resulting ion heat diffusivity showed a radially increasing character strikingly similar to that in published tokamak data.

Figure Captions:

Fig. 1: Comparisons of the BES measurements on the TFTR plasma and the 3D toroidal gyrokinetic particle simulation of the ion temperature gradient instabilities.

Fig. 2: Turbulent heat diffusivity χ_i vs. time when poloidal flows are suppressed (dashed line) or allowed to self-consistently evolve (solid line), from 3-D nonlinear gyrofluid simulations of toroidal ITG turbulence (Hammett, Beer, Dorland, Cowley, Smith, 1993).

Fig. 3: Time-averaged fluctuation spectrum vs. k_θ (with self-consistent poloidal flows) showing that the spectrum is downshifted from the fastest growing linear mode, in good qualitative agreement with BES measurements on the TFTR tokamak. (Hammett, Beer, Dorland, Cowley, Smith, 1993). Doubling the computational box size indicates that the k-spectrum is insensitive to the box size.

Fig. 4: Contour plots of the electrostatic potential (essentially the stream function for the turbulent eddies) at an instant in time, from a small and large run, showing that the size of the eddies does not appear to be tied to the size of the computational box.

Turbulent Spectra in simulation and experiment: $S(k_r)$ and $S(k_\theta)$ in a.u.

- TFTRBES Measurement
Fonck, Crosby, Durst, Paul, Bretz, Scott, Synakowski, and Taylor, Phys. Rev. Lett. **70**, 3736 (1993).
- Gyrokinetic Particle Simulation
Parker, Lee, and Santoro, Phys. Rev. Lett. **71**, 2042 (1993).

Future Progress

High Performance Computing

- * Expanded use of existing and new MPPs
- * Continued MPP code optimization and advanced algorithm development, e.g., implicitness, adaptive grids, electron kinetics, hybrid models, electromagnetics
- * Expansion of library of MPP routines for general applications

The research activities of the NTP in high performance computing are being driven by the continued improvement in hardware and software delivered by the vendors, and by improved new algorithms developed by us. Considerable work remains in the area of increasing the sophistication of our physics models, e.g., adding nonadiabatic electron effects and electromagnetic modeling. Furthermore, the current level of computing power does not allow us to simulate as big a tokamak as we would like even with our simplified physics models. Because access to more powerful systems will be realized in the next two years and with the significant improvements in both the efficiency of our algorithms and their physics content, we are in a position to achieve dramatic improvements in our modeling capabilities in the next two or three years. In the following are given a few examples of the future progress that we expect.

It is expected that NERSC will acquire an MPP supercomputer in the next two years. The suite of NTP gyrokinetic and gyrofluid codes will be ported to this machine and optimized; and physics applications will be undertaken.

Williams (LLNL) and Walt (GA) on the parallelizing tokamak ballooning-mode-representation model with gyro-Landau closure based on the Kotschenreuther Vlasov-fluid model algorithm will lead to the inclusion of electromagnetic effects and electron dynamics in an improved kinetic/fluid physical model.(FY94-95)

Williams (LLNL) will integrate the LLNL toroidal gyrokinetic code using ballooning coordinates with the MPP three-dimensional slab code he has written.(FY94) Use of NetCDF and AVS for graphics and visualization will be expanded.(FY94) Xu, Cohen, and Dimits (LLNL) will complete advanced algorithm development of an electromagnetic gyrokinetic algorithm with kinetic electron effects.(FY94-95)

Algorithm development remains to be carried out for the convolutions over poloidal and toroidal modes used in the nonlinear part of ORNL's fluid calculations. The compact mode convolver developed for the CM-2 is being retrofitted to the message passing version of the fluid turbulence codes to minimize storage requirements and be able to use all processors of the fully configured Paragon in an optimal way. A less compact version will be used in performance optimization studies on MIMD machines. [2nd Quarter FY94] For the convolutions, the ORNL team also plans to adapt the Fast Fourier Transform package developed by the NERSC/GA team for their pseudo-spectral gyrofluid models. This package should soon be available as part of the massively parallel software exchange component of the Numerical Tokamak Project. [3rd Quarter FY 94] The ORNL team will continue optimization of performance of its plasma fluid turbulence codes on the Intel Paragon XPS35 which has 512 processors with 32 Mbytes of memory per node, this in preparation for the fully configured Paragon with 2048 processors. [FY 94 throughout] The ORNL team will be porting its PVM implementation of the plasma fluid turbulence codes to the recently arrived CRAY T3D at Caltech. This work will be carried out in collaboration with the JPL/Caltech team [2nd Quarter 94]

Access to the C90 in dedicated mode is a prerequisite to further optimization studies for many of the NTP codes. Large scale nonlinear production calculations with more physics and more resolution await access to the C90 in dedicated mode. [FY 94 and 95 throughout]

The main focus of the future JPL NTP work will be to continue the development of the modular, portable deformable grid fluid and PIC code. It has been recognized that because of the

complexity, diversity, and rapid evolution of parallel computers and the codes that run on them, it is usually not easy for a scientist to be able to utilize the vast potential that is offered by the hardware. We propose to continue to develop a framework, described above, and a modular code that will help NTP scientists more rapidly implement new physics models on new computers. The near-term goal of this work is to implement both a fluid and implicit PIC code, which share many modules, on several parallel systems using Fortran 77 with message-passing (Intel Delta and Paragon, the Cray T3D and workstation clusters using PVM). The PIC code to be implemented is the NTP implicit PIC model developed by J. Brackbill (LANL) which will be used to model tokamak turbulence. The fluid model to be implemented will be a resistive MHD model. This dual on multiple parallel systems implementation will be a "proof-of-principle" of the portability/modularity framework.

The degree of modularity possible using FORTRAN is limited and the longer term goal is to develop a C++ implementation using its object oriented constructs. Inheritance may be the key concept that distinguishes an object oriented language like C++ from a procedural one like FORTRAN or C. Because C++ allows you to define new objects, it is more extensible and more powerful for the large, complex, retargetable applications we expect to see in the future. A C++ implementation would have stronger boundaries between module levels and the task of porting between architectures, models, and people should be correspondingly smoother. Moreover, the more distant promise of object oriented programming is that libraries of objects build by completely separate projects can also be easily integrated into the Numerical Tokamak Project. With a large library of objects, it will be possible to build a simulation code the way many graphics programs, such as AVS, are built today: with an interface builder that lets you graphically place objects that perform computations and draw links that show how they call one another. This would accelerate tremendously the turnaround from seeing the results of a simulation, making a change to the physics or numerics, running a new simulation and gaining new insights.

A much shorter term goal for the JPL/Caltech group in the next year will be to port the 3D Cartesian PIC code, now running on the Intel Delta, to the Cray T3D, expected at JPL in late 1993, and to compare the performance. Also, since the JPL/Caltech participants will be among the first users of the T3D, feedback to Cray Research on this new system will be an important component of this effort.

The PPPL gyrokinetics group is working closely with the personnel at ACL (LANL) to optimize their CM5 codes and to contribute to the effort of improving the CM5 software. They are also in the process of gaining experience on other massively parallel machines, particularly, the Cray-T3D.

IFS plans further work in developing object-oriented parallel simulation codes for the NTP. These efforts will have many payoffs, including: (a) the development of a substantially more productive software development environment, (b) codes that are more robust, better tested, and easier to understand and modify, and (c) involvement from mainstream computer science (e.g. MCC).

Additional simulation runs using TPC at IFS are aimed at improving their relevance to tokamak plasmas. Effects to be considered include heating and loss effects, collisions, and parameter regimes and geometries closer to that of tokamak plasmas. Longer time scale and higher resolution runs are planned. Improvements to diagnostics and data visualization are in progress to facilitate physical understanding.

LANL researchers intend to extend dynamic particle control to a three-dimensional code. They also intend to port parallel PIC codes to the Cray T3D. They will complete the development of their toroidal quiet implicit PIC algorithm by the end of FY94 and model Coulomb collisions.

Visualization

All of the NTP sites will continue to work on visualization. Because of the large amounts of data involved with time histories of three-dimensional fields in both gyrofluid and gyrokinetic simulations, and additional large amounts of data for the phase space quantities in the kinetic codes, some of the visualization processing must of necessity be done on the massively parallel platforms to reduce the quantity of data in the graphics to a point where it can be transported to either workstations for additional processing or direct to output devices. As the hardware and software from the vendors to support visualization evolve, our visualization efforts are evolving to keep pace. Some examples are given in the following paragraphs.

Thinking Machines continues to improve software on the CM5 to realize better performance. Kerbel (NERSC) will continue to work closely with them using CMAVS to allow general use by NTP codes for coordinated data analysis and comparison. An image indexed storage and retrieval system based on a data base of image files will be created using the facilities of the National Storage Laboratory at NERSC subject to adequate bandwidth being available (T3 minimum). Further development of the distributed post-processing system based on CMAVS will lead to a collection of remote parallel visualization modules designed for use by NTP codes. These modules will be accessible to AVS networks running local AVS-server graphics workstations. Kerbel intends to demonstrate the technology of transferring stereograms by creating animation of current results of NTP simulations. These efforts will extend through FY94 and FY95.

Scientific visualization has so far been applied by the ORNL team in post-processing mode. This sophisticated way of probing the data from large scale nonlinear calculations needs to be carried over to the run-time environment. This will bring to bear common file formats for smooth data transfer from the calculation platform to the analysis platform and network capacity in excess of 100 mb/sec available T3 bandwidth. [FY 94 and 95 through 96].

Plasma Physics Applications

- * Simulations of bigger plasmas more relevant to tokamak program
- * Applications including electromagnetic and kinetic electrons effects
- * Expanded fluid and kinetic simulation studies of trapped particle modes and toroidal Alfvén eigenmodes
- * Transport scaling studies
- * More detailed code cross-checking and comparison to experiments

The NTP as a whole will be addressing the extension of our algorithms to include both kinetic electron effects and electromagnetic field perturbations in our physics models. This will necessitate the continued parallel development of advanced algorithms to cope with the additional time and space scales introduced by the physics. A comparison of NTP code predictions testing whether gyro-Bohm scaling does or does not adequately predict the scaling of the turbulence with increased scale size in terms of the ion Larmor radius. The scaling of the turbulence with some of the other important dimensionless physical parameters will be investigated, e.g., ratio of the magnetic shear to density or temperature scalelength, aspect ratio. Comparative studies of dissipative trapped electron and/or trapped ion modes will be conducted. All of these activities will begin in FY94 and extend into FY95.

The ORNL team will carry out three-dimensional gyro-Landau fluid calculations of DTEM turbulence with its recently developed ion description with magnetic drift effects included, as well as with the more sophisticated trapped electron model. [2nd Quarter FY 94]. Comparisons will be performed by the ORNL team and the UCLA team between gyro-Landau fluid and gyrokinetic implementations with a suitable set of commonly accessible parameters for DTEM. [2nd and 3rd Quarter 94]

The gyro-Landau fluid model implemented in the TAE/FL code to study destabilization of Alfvén waves by energetic particles is being extended by the ORNL team to include an

evolution equation for the temperature fluctuations of the energetic species. [2nd Quarter FY 94]

Model development and implementation is also being carried out to enable the ORNL team to treat cases in which the magnetic drift frequency of the energetic species is larger than the frequency of the MHD modes. This frequency ordering is expected to lead to stabilization of the modes, an effect considered important for ITER. [1st Quarter FY 95]

The gyrokinetics groups at PPPL, LLNL, UCLA, and IFS will continue work on the plasma physics applications already listed. A particular emphasis is the efficient implementation of the electron dynamics and the finite-beta effects in the existing codes. The NTP consortium will focus on electron dynamics and finite-beta effects in the next year so that this research will be done collaboratively. Because one primary purpose of the NTP is to understand core transport in tokamaks, it is imperative to continue close interactions with the experimentalists. One of our ultimate goals is to simulate the tokamak discharge (both the MHD and the kinetic effects) using gyrokinetic particle codes.

In the work of Kotschenreuther (IFS), novel parameter regimes are being explored utilizing simultaneous flow-shear stabilization and q-profile tailoring, aimed at stabilizing microinstabilities. Nonlinear simulations including self-consistent shear-flow effects are being pursued. These will include electron dynamics, impurity and beam dynamics, and electromagnetic effects. Improved grid discretizations are being examined which incorporate some concepts from gyrofluid methods.[FY94]

LANL researchers intend to apply their class library in support of physics applications in the next year. For example, they will conduct 3D suspension flow simulations, 3D electrostatic gyrokinetic and 3D toroidal electromagnetic implicit-moment simulations, and compare vortex simulation methods to classical fluid simulation techniques.[FY94-95]

Anticipated Requirements

In order to fulfill the extremely demanding computational requirements of Grand Challenge scale computing projects such as the NTP, significantly expanded computational resources are needed. Our resource needs fall naturally into several categories: software, hardware (e.g., workstations), allocations at the HPCRC's and NERSC, and support for personnel.

NTP experience so far has been that the in-core memory on both the Paragon and the CM-5 limit physics applications, and faster CPU speeds are needed. For example, to perform three-dimensional gyrokinetic simulations that can resolve on the order of the ion Larmor radius (using the electron temperature) over the entire TFTR minor cross section would require about 8-10 times the amount of in-core memory that is currently available on the CM-5. Also, the runtime on such a grid to nonlinear saturation in a 1-2 days of real time would require a tera-flop computer (also about 8-10 times faster than the CM-5).

Because of the heavy emphasis on advanced computer science issues in NTP, researchers require significantly improved tools for software development. Although a variety of different software engineering paradigms are employed as reflected by the backgrounds and inclinations of the participants, it is clear that an increasing emphasis on advanced object-oriented programming methodologies and parallel execution is a significant requirement of NTP. Improved availability of advanced, professional software development tools such as ObjectCenter and CodeCenter by Centerline and Energize by Lucid Corp. would be a significant boon to development of advanced robust software modeling systems. In the area of visualization, there is a need for licensed software packages like AVS, PVWave, IDL, etc.

In order to make the most effective use of the national resources (CM-5, Paragon, C-90) etc, NTP researchers require the ability to design and prototype their advanced simulation codes on local workstation clusters and medium-scale parallel execution environments. Something on the order of \$200K/yr per institution designated for computer hardware outlays would facilitate a significant improvement in the local development environments available to NTP researchers,

and would tremendously expedite the efficient and effective use of the larger national resource computers at the HPCRC's and NERSC. For example, the IFS desires hardware money for development of advanced object oriented multiprocessing "super workstations" in collaboration with MCC for prototyping and verification of advanced parallel applications destined for production usage on national resource computers.

In order to carry out the computer science, computational physics and plasma physics components of the Numerical Tokamak Project, the NTP consortium requests access to the CRAY Y-MP C90 at NERSC in dedicated mode with its 200 Mword of memory, to all 2048 processors of the fully configured Paragon at the ORNL CCS, to the CM5 at LANL, and to the CRAY T3D computer at Caltech. The required computer time, estimated for the highest resolution calculations that can be performed on each machine by extrapolation of current data is as follows:

	FY93(actual)	FY94	FY95
NERSC C90 (SPP)			
cru hrs:			
IFS		2000	3000
JPL/Caltech			
LANL		2000	2000
LLNL	test queue	200	200
NERSC/GA		1000	1000
PPPL	2500	6000	7500
UCLA	test queue	2000	3500

scratch/permanent memory in Gbytes:

IFS	10/100	10/100
JPL/Caltech		
LANL	2/10	2/10
LLNL	10/100	10/100
NERSC/GA	2/20	2/20
ORNL	2/100(per run)	2/100
PPPL	10/100	10/100
UCLA	8/100	8/100

CM-5 at LANL

node-hours/yr

IFS		5000	20000
JPL/Caltech			
LANL	4000	500000	500000
LLNL	4000	205000	205000
NERSC/GA	50000	100000	100000
ORNL			
PPPL	100000	300000	350000
UCLA	4000	90000	90000

scratch/permanent memory in Gbytes:

IFS	2/20	10/100
JPL/Caltech		
LANL	30/100	30/100
LLNL	10/100	10/100
NERSC/GA	2/20	2/20
ORNL		
PPPL	10/100	10/100
UCLA	10/100	10/100

Paragon at ORNL

node-hours/yr		
IFS	5000	20000
JPL/Caltech	25600	25600
LANL	2000	5000
LLNL	51200	51200
NERSC/GA	2000	5000
ORNL	10000	10000
PPPL		
UCLA	20000	20000

scratch/permanent memory in Gbytes:

IFS	2/20	10/100
JPL/Caltech		
LANL	10/100	10/100
LLNL	10/100	10/100
NERSC/GA	2/20	2/20
ORNL	5/250(per run)	5/250
PPPL		
UCLA	10/100	10/100

Cray T3D*

node-hours/yr		
IFS	12800	12800
JPL/Caltech	3000	20000
LANL	0	51200
LLNL	5000	20000
NERSC/GA	2000	2000
ORNL	50000	50000
PPPL	2000	8000
UCLA		

scratch/permanent memory in Gbytes:

IFS
JPL/Caltech

LANL	10/100	10/200
LLNL	10/100	10/100
NERSC/GA	2/20	2/20
ORNL	2/100(per run)	2/100(per run)
PPPL	10/100	10/100
UCLA	10/100	10/100

* This assumes that there will be DOE-sponsored access to a Cray T3D.

Budget Requirements:

In the following table are enumerated budget requests for OSC funding (\$K) of NTP activities for FY94 and FY95. The participating NTP groups have received smaller total budgets to support both fusion and related computational research (including the NTP) in each of the last several years. Without some net increase in funding from the OSC and the OFE to support the NTP, progress on NTP research will slow down.

Our budget requests already have been documented in Field Work Proposals and Grant Proposals submitted to DoE by the individual institutions in most cases. The dollar requests are for operating expenses unless otherwise shown. Acquisition of workstations and the supporting local-area-networks with adequate bandwidth necessitates a modest level of capital funds; however, detailed requests for capital funds have not been presented in this document (see the current individual Field Work Proposals and Grant Proposals from the institutions). Many NTP members feel an acute need for more network bandwidth, both locally and between their sites and the major computing centers. However, budget requests to improve network bandwidth are not included here.

	<u>FY94</u>	<u>FY95</u>
GA	0	0
IFS	100*	100*
JPL/Caltech	75	85
LANL	85	92
LLNL/NERSC	450	480
ORNL	150	165
PPPL	105	109
UCLA	55	55

*\$50K operating + \$50K capital for hardware and software at IFS

Project Integration

The research activities of the NTP consortium are coordinated jointly by the Office of Fusion Energy, through its APT Division headed by Dr. David Crandall and his staff including Dr. Walter Sadowski and Dr. Mary Anne Scott, and by the Executive Committee of the NTP composed of nine representatives of the major participating institutions with an elected chairman and a scientific leader. The charter for the Executive Committee is included as an Appendix. The Executive Committee gives guidance to the many closely coupled collaborations within the NTP, defines and directs group efforts such as the NTP test case simulating a TFTR tokamak shot and the compilation of a suite of code modules for use on vector supercomputers and massively parallel machines, and coordinates applications by NTP members for resource allocation at the DoE HPCRC computers. We have working groups in gyrokinetic simulation, gyrofluid simulation, implicit and hybrid methods, and high performance computing tools and technology. The NTP has held contributed oral and poster paper sessions at the 1992 and 1993

American Physical Society Plasma Division Annual Meetings, and holds a workshop following the International Sherwood Theory Meeting each spring. The Executive Committee has meetings at both the APS and Sherwood Meetings, and communicates by e-mail regularly and by conference calls as needed during the rest of the year. The NTP is also represented at the annual Supercomputing meeting and at Grand Challenge reviews schedule by the OSC.

Budget Summary (existing)

No capital funds have been allocated.

Operating funds by source (OFE and OSC) and by institution (\$K)

	FY92			FY93			FY94		
	OFE-a	APT-b	OSC	OFE-a	APT-b	OSC	OFE-a	APT-b	OSC
GA	150	0	0	150	0	0	150	0	0
IFS	438	12	0	498	32	0	438	32	0
JPL	0	0	50	0	0	60	0	0	75
LANL	100	0	0	100	100	27	105	106	85
LLNL	400	10	0	450	30	0	500	30	0
NERSC	375	0	30	375	0	90	270	0	90
ORNL	150	0	50	300	0	120	300	0	95
PPPL	685	105	0	660	105	0	685	105	0
Princeton/ Rutgers	0	0	0	0	0	0	128	0	0
UCLA	200	0	12.5	200	0	25	200	0	?

OFE-a = \$K from OFE, other DoE, and ARPA programs base budget funding research related to NTP

APT-b = \$K from APT/OFE specifically labeled by DoE as NTP

OSC = \$K from OSC for NTP

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APPENDIX 2: Publications

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APPENDIX 3: Charter of the NTP Executive Committee

Membership

The Executive Committee (EC) of the Numerical Tokamak Project (NTP) consortium consists of one representative from each of the principal member institutions of the consortium, an experimentalist elected by the EC, and an ex officio representative of the Office of Fusion Energy (OFE) Applied Plasma Physics Division. The principal member institutions having representation on the EC are:

IFS/University of Texas
Jet Propulsion Laboratory/California Institute of Technology
Lawrence Livermore National Laboratory
Los Alamos National Laboratory
NERSC
Oak Ridge National Laboratory
Princeton Plasma Physics Laboratory
University of California, Los Angeles

The EC members will be designated by their home institutions, and the constituency of the EC will be reviewed by the EC and DoE at their discretion. The EC will elect a chairman to serve a one-year term. Each member of the EC will have one vote, and a simple majority will be required to approve any motion. The EC may also elect a scientific leader to serve an unspecified term. The chairman of the EC can invite additional attendees to attend its executive meetings at his discretion.

Purpose

The general purpose of the EC is to provide coordination, oversight, and review of the activities of the NTP. Some of the specific functions of the EC are as follows:

1. Define the scope of the NTP-
 - identify and encourage the addition of new activities and deletion of others;
 - identify areas of duplication and urge appropriate action;
 - identify areas of deficiency of activity and urge appropriate solutions.
2. Recommend priorities for near-term NTP work.
3. Encourage communication and comparison of NTP calculations.

4. Coordinate the submission of a composite work plan for the NTP consortium in accordance with DoE specifications. This will include a summary of research requests and the identification of important research areas and needs.
5. Promote availability of resources from DoE and HPCRC's for NTP work.
6. Identify, promote, and facilitate educational opportunities and functions of the NTP consortium.
7. Assure that internal and external review and reporting requirements are met. At its discretion, the EC may form an external oversight committee to review the progress of the NTP.

Function and Procedures

The EC will function in the following manner. The EC will meet at least twice per year at the Sherwood Theory and American Physical Society Plasma Division Meetings. Electronic mail will be used to maintain additional communication. An annual general meeting of the NTP will be held in conjunction with the Sherwood Theory Meeting. The NTP will also hold a poster or contributed oral paper session at the APS Plasma Division Meeting. The EC will organize additional focused technical meetings as appropriate. The EC will ensure reporting of NTP research activity at other meetings as directed by OFE and SCS. The EC will have representation in the Transport Task Force and coordinate NTP research activities with TTF. The Chairman of the EC will establish a calendar regularizing the schedule of meetings, conference calls, and electronic mail exchanges.

Available Codes and Source Codes

As part of the Numerical Tokamak Project, code modules have been documented and shared within the consortium and to other researchers using high performance computing resources. The following is a list of codes that UCLA NTP researchers have made available: these are a set of documented, skeleton particle-in-cell codes for a variety of parallel computers to be used for education and as templates for further development. So far the UCLA source codes have been requested and distributed to researchers at LLNL, LBL, NERSC, PPPL, Rice U., U. of Iowa, MIT, U. Texas, JPL, GSFC, MFSC, Cray RI, and Cray CC.

1. BABYB1.F

This is a standard reference version for a serial (sun) computer. A version for vector processors (Cray, IBM ES/9000) also exists.

2. BABYB1.MP

This is a multi-tasked version for the Cray which implements a particle decomposition scheme. This means that different tasks are given different particles to work on, but the field calculations are not done in parallel and the charge densities are replicated for each task. This is a very simple decomposition which can be quickly implemented, but is only useful if there is enough memory to replicate the density and there are not too many processors. It gives excellent performance on the Cray C-90. A version for the IBM ES/9000 also exists.

3. BABYB1.FCM

This is a straightforward, data-parallel version written in cmfortran for the CM-2. Also runs on the CM-5.

4. BABYC1.INTEL

This version implements the domain decomposition for the Intel IPSC/860. Both particles and fields are distributed across processors, using the scheme described in p. c. liewer and v. k. decyk, j. computational phys. 85, 302 (1989).

5. BABYC1.PVM

This version implements the domain decomposition for a cluster of IBM RS/6000 workstations running the PVM message passing library, version 2.4.2. It is the same as the version for the Intel except that the message passing calls have been changed.

6. BABYC1.CM5

This version implements the domain decomposition for a Thinking Machine's CM-5 using fortran 77 with the CMMD message passing library. It is the same as the version for the Intel except that the message passing calls have been changed. It does not use the vector processors.

As part of the Numerical Tokamak Project, UCLA is making available useful subroutines originally developed for skeleton particle-in-cell codes for a variety of parallel computers, as described below. Versions of each subroutine exists for the Intel Paragon (using NX calls), CM-5 (using fortran 77 and CMMD calls), and workstation clusters (using pvm 2.4.2), except as noted.

1. ISUM

This subroutine performs a sum of multiples instances of a vector across processors. It is equivalent to Intel's gssum call (or the generalization of TMC's CMMD_reduce_float to vectors).

2. PFFT1C

This subroutine performs a one dimensional complex-to-complex fft.

3. PFFT1R

This subroutine performs a one dimensional real-to-complex fft.

4. PTPOSE

Thus subroutine transposes a 2D matrix where the second index is initially distributed across processors to a matrix where the first index is distributed across processors, and vice-versa.

5. PFFT2C

This subroutine performs a two dimensional complex-to-complex fft.

6. PFFT2R

This subroutine performs a two dimensional real-to-complex fft.

7. PVINIT

2.4.2 This subroutine initializes a cluster of workstations for parallel processing, using PVM

APPENDIX 5: Parallelized convolution calculations at ORNL

ORNL NTP researchers have been developing high performance, generic modules for block-tridiagonal matrix solvers and Fourier mode convolutions. These modules are common to all of ORNL magnetohydrodynamics (MHD) and turbulence models and represent their most computationally intensive components. The block-tridiagonal solvers arise from the implicit linear part of the calculations, while the convolutions stem from the terms due to the convective derivatives in the explicit nonlinear part. Both of these modules have been optimized for MIMD machines with message passing, such as the BBN Butterfly and the Intel iPSC/860, Touchstone Delta, Paragon XPS5 and XPS35. The same paradigm is also used on clusters of workstations using PVM, with native message passing calls replaced by PVM ones.

The convolutions are relatively straightforward to carry out on these massively parallel machines. A radial region is allocated to each processor and the convolutions over mode numbers in each radial region are performed in parallel. The communication between the processors is then limited to the boundary values for each region. The memory configuration used in this implementation is a ring. The parallelization of the matrix inversion is not so easy. After the convolutions have been evaluated, the memory allocation is redistributed. Several modes are allocated to each processor for all radial grid points. In each processor, the block-tridiagonal matrix is inverted for each of the allocated modes. After the inversion, the solution must be returned to all the appropriate processors for each radial region. The actual inversion involves no communication between processors. The inversion is computed with the Block-Tridiagonal Linear System Solver, Minimal Storage, version 3.1.1.0 of [Lynch et al., report UCID-30150, LLNL, 1977]. The matrix elements are computed as they are needed with BTMS so the matrix need not be stored in the (usually very small) memory of the node. [Lynch et al., 1992].

In addition, a Fortran 90 version of the convolution module has been produced by the ORNL team for use on the Connection Machines [Walker, 1992]. The mode data in the convolutions was re-arranged in a more compact form in order to take advantage of the array syntax in Fortran 90. In particular, the need for the memory-taxing indirection arrays, where information regarding which modal interactions contribute to a given mode is stored, was eliminated. This seminal effort has had a great impact on the ability of the ORNL team to reduce the memory per processor needed as the calculation size is increased towards experimentally relevant resolutions on MIMD machines.

The block-tridiagonal matrix solver and mode convolution modules have also been optimized for parallel operation on the CRAY Y-MP C90. Compared to the algorithm development and extensive code modifications necessary to obtain efficient massively parallel code for MIMD machines, few changes are required for the code to multiprocess effectively on the C90. Contrary to the massively parallel version, the matrix and right-side vector needed by the block-tridiagonal solver were stored in memory for all the modes. Tests quickly indicated that the autotasked version of the code produced automatically by the CF77 compiling system was not as efficient as microtasking. The microtasked version was produced using the parallelizer tool FORGE to detect parallelism, and microtasking compiler directives were inserted where parallelism was found. For both the matrix solver and the convolutions, the parallelization is performed over the number of modes. Each variable in the do-loops over modes must be declared to be shared with all the processors or private to each processor. The inner loops, over the number of equations for the matrix solver and over the number of grid points for the convolutions, were already as vectorized as they could possibly be in the serial version and were left untouched. In all, 50 lines needed to be inserted in the serial version of the ORNL team's plasma fluid turbulence code KITE to obtain efficient parallel code on the C90 [Lynch et al., 1993].

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