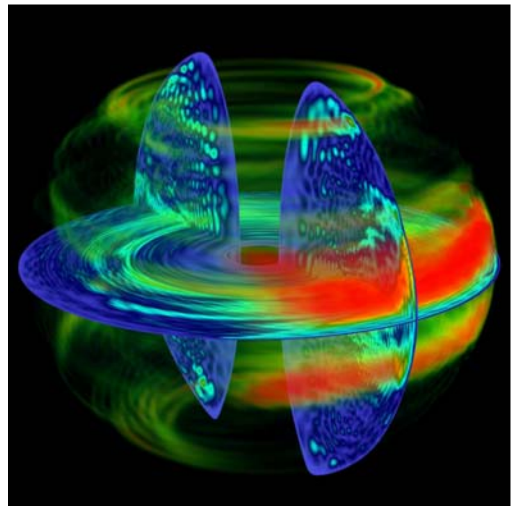
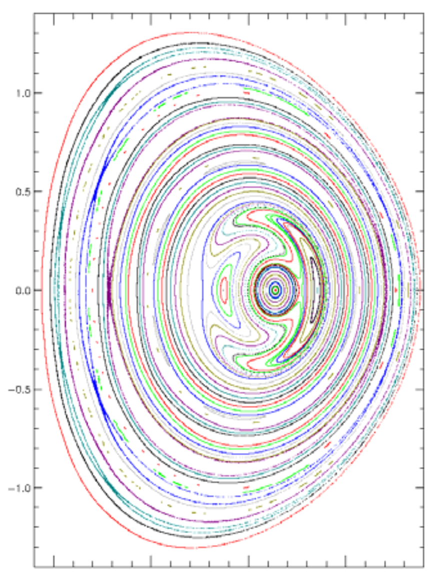
Renewal Proposal for Center for Simulation of Wave Interactions with Magnetohydrodynamics

ABSTRACT



The Center for Simulation of Wave Interactions with Magnetohydrodynamics (SWIM) was begun in 2005 with the scientific objectives of: improving our understanding of interactions that both RF wave and particle sources have on extended-MHD phenomena, improving our capability for predicting and optimizing the performance of burning plasmas, developing an integrated computational system for treating multi-physics phenomena with the required flexibility and extensibility to serve as a prototype for the Fusion Simulation Project, addressing mathematics issues related to the multi-scale, coupled physics of RF waves and extended MHD, and optimizing the integrated system on high performance computers. This work has considerable scientific and programmatic importance since performance of fusion devices is often limited by the appearance of unstable plasma motions that can degrade plasma containment, whereas high-power radio frequency (RF) electromagnetic waves can be used to influence plasma stability—sometimes reducing or eliminating instability. Originally proposed as a five-year project, the present proposal is to complete the final two years of the project. In the first two and one half years of the project our center has built an end-to-end computational system, referred to as the Integrated Plasma Simulator (IPS), based on a framework/component architecture that allows fusion physics codes to be able to function together in a parallel environment, and connects them to utility software components and data management systems. The IPS has been designed and implemented and the required physics functionality has been incorporated at an initial level. The IPS is being employed for verification and validation studies, discharge simulations and scientific investigations of RF interactions with plasma stability. The final phase will emphasize situations in which the coupling between physics functionalities is tighter. This will have implications for the mathematical formulations, the program execution model, and computer load balancing. Ongoing simulation studies will be completed and new studies will be carried out in the areas of benchmarking and validation through experimental comparisons, tokamak scenario modeling, and RF effects on plasma stability.



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1. EXECUTIVE SUMMARY

Comprehensive plasma simulations are essential to the development of fusion energy. Not only does simulation serve to advance science by allowing us to evaluate and test basic theory through comparison with experiments, it also has a direct economic benefit by maximizing the productivity of experimental facilities and by supporting design decisions for new facilities. For a device like the International Thermonuclear Experimental Reactor (ITER), such decisions can have large financial consequences. The need for a comprehensive simulation capability for fusion devices has been emphasized by the fusion research community and by several program evaluation and planning activities [Dahlburg01, Post04, Kritz08]. As stated in the Fusion Simulation Project (FSP) Steering Committee report: "The ultimate goal of the FSP is to simulate the behavior of toroidal magnetic fusion devices on all important time and space scales, and to account for the interactions of all relevant processes. It will serve as an integrated 'standard model' for the community, permitting the exploration of new multi-scale physics and mathematics." The driving focus is to contribute to experimental planning and performance optimization of ITER and to design decisions for devices beyond ITER.

In 2005, as a partnership between the DOE Office of Fusion Energy (OFES) and the Office of Advanced Supercomputing Research (OASCR), two SciDAC centers were started to serve as pilots for a comprehensive Fusion Simulation Project. The purpose of these was to begin the process of multi-physics, multi-scale coupling, at a reduced scope from a full FSP, while addressing problems of programmatic importance, and to develop approaches to large-scale code integration as required for the full FSP. The present project, Center for Simulation of Wave Interaction with MHD (SWIM), was one if these initial pilots.

The scientific rationale of the SWIM project is relatively simple. One of the most fundamental observations in fusion devices is that performance is often limited by the appearance of unstable plasma motions that can degrade plasma containment or even terminate the plasma discharge, with the potential for damage to the containment device. These instabilities can be modeled using extended magnetohydrodynamics (MHD). A second observation is that high-power radio frequency (RF) electromagnetic waves can be used to influence plasma stability—sometimes producing instability, and sometimes reducing or eliminating instability. A capability to understand and predict the effects of RF waves on plasma stability would be of significant scientific and economic benefit.

To this end we assembled a cross-disciplinary, multi-institutional team to create a new capability for integrated modeling of toroidal plasmas, with the emphasis on the interactions between high-power electromagnetic waves and MHD stability. Our Center has built an end-to-end computational system that allows existing physics codes to be able to function together in a parallel environment and connects them to utility software components and data management systems. We have used this framework to couple together several state-of-the-art fusion energy codes to produce a unique and world-class simulation capability. The two broad scientific objectives of the center are:

- **To improve our understanding of interactions that both RF wave and particle sources have on extended-MHD phenomena, and to substantially improve our capability for predicting and optimizing the performance of burning plasmas;**
- **To develop an integrated computational system for treating multi-physics phenomena with the required flexibility and extensibility to serve as a prototype for the FSP, address mathematics issues related to the multi-scale, coupled physics of RF waves and extended MHD, and to optimize the integrated system on high performance computers.**

It is useful to distinguish two regimes of phenomena addressed by extended MHD models in the presence of wave and particle sources:

1. **Fast phenomena** in which the unstable plasma motions are so rapid that energy deposition, currents, flows, and energetic particle populations driven by RF waves or other sources do not directly

influence the rapid motion. Instead, the RF acts indirectly over a longer timescale to drive the slow evolution of the plasma equilibrium and profiles, effectively setting the initial conditions for the fast MHD event. An example of such a phenomenon is the crash phase of the sawtooth oscillation.

2. **Slow phenomena** such that energy deposition, currents, or flows driven by RF waves or other sources do operate on timescales that directly influence the dynamics of the unstable motions. The perturbations of the plasma state by the instability in turn influence the energy, currents or flows driven by the RF. An example of such a phenomenon is the neoclassical tearing mode (NTM), which is an important consideration for the performance of burning plasma such as that of ITER.

The first regime is the traditional one in which RF sources affect the global plasma pressure and current profile and create an energetic particle population. The second regime addresses some very important plasma instabilities in which RF, the kinetic evolution of the velocity distribution, and extended MHD phenomena are all tightly coupled.

The SWIM project consists of three elements.

1. **Development of a computational platform, Integrated Plasma Simulator (IPS)** that allows efficient coupling of the full range of required fusion codes or modules, that is flexible enough to allow exploration of various physics models and solution algorithms, that permits convenient user access and access to experimental data, and that is robust to evolving physics, code development, and developments in computer hardware. The IPS contains components to calculate wave propagation and absorption in all relevant frequency regimes, to calculate the modification of the plasma velocity distribution from sources (RF, neutral injection and a particles), to calculate profile and magnetic evolution (assuming closed flux surfaces), as well as linear MHD stability models and reduced models of non-linear MHD events.

2. **Fast MHD physics campaign—addresses long timescale discharge evolution in the presence of sporadic fast MHD events**. This will involves interface between the IPS and 3D non-linear extended MHD codes. The primary physics focus is to allow the development of optimized burning plasma scenarios and to improve the understanding of how RF can be employed to achieve long-time MHD stable discharges and control sawtooth events.

3. **Slow MHD physics campaign—models the direct interaction of RF and extended MHD for slowly growing modes.** This requires development of new approaches to closure for the fluid equations and the interfacing of RF modules directly with the extended MHD codes and with code modules that implement the fluid closures. The primary physics focus is to improve the understanding of how RF waves, can be employed to control neoclassical tearing modes. Electron cyclotron current drive is the initial focus.

SWIM, originally proposed as a five-year project, was reviewed as a five-year project with uniformly very favorable reviews, and was approved for 3 years subject to intermediate review. The first phase has demonstrated that the original concept was valid and the objectives feasible. The overall goals and approach therefore remain the same. What has changed is that ITER is now underway, giving a new urgency to improving our simulation capability, and available supercomputers are approaching the petaflop range, making the potential for what is achievable by simulation much greater.

Section 2 describes progress achieved in the first phase. The IPS has been designed and implemented. All of the required physics functionality has been incorporated, at least at an initial level, in some cases with multiple implementations. The IPS is being employed for verification and validation studies, for Fast MHD campaign physics studies, and for tokamak simulations. In the Slow MHD campaign a theoretical approach for including the effects of RF in the fluid closure has been developed, a computational approach to coupling MHD with RF has been developed, and initial numerical studies with reduced models have begun. By the end of this first phase we fully expect to have met all of the substantive goals proposed for this period.

Section 3 describes the proposed work for the second phase of the project. While directed to the same final project goals as in the initial proposal, we are now able to be more specific about the tasks remaining to achieve them. By the end of the five-year project we will have:

- Developed IPS so that it provides a computational environment satisfying the SWIM project's needs for concurrency, performance, and data management, and is the tool of choice for those performing tokamak scenario simulations;
- Demonstrated capability of the SWIM system to address important questions of sawtooth instability behavior and their control by RF (Fast MHD campaign);
- Completed the coupling of ECCD, non-linear MHD and kinetic closure for study of RF stabilization of Neoclassical Tearing Modes (NTM), and performed numerical simulations comparing with NTM experiments (Slow MHD campaign);
- Provided a base of experience with framework/component architecture applied to integrated fusion simulation that can be factored into the design of a larger scale Fusion Simulation Project.

As before, we will be leveraging ongoing investments by OFES and OASCR. In particular, we draw on the developments in MHD provided by the Center for Extended MHD Modeling (CEMM) and RF modeling provided by the Center for Simulation of Wave Plasma Interactions (CWSPI). However we have considerably broadened the scope of our collaborations to include the other FSP pilot projects and more of the SciDAC CET centers. The SWIM project unites experts in magnetic fusion, computer science, and applied mathematics in an effective partnership. The funding requested for the team remains at $2M per year.

2. PROJECT PROGRESS

The computational engine of the SWIM project is the Integrated Plasma Simulator (IPS). The core of the IPS is a software framework designed and developed, not only to support the coupled simulations required by the SWIM science plan, but also to explore issues associated with integrated fusion simulation at an even larger scale for future efforts such as the proposed Fusion Simulation Project (FSP). The IPS environment brings together a variety of well-established physics codes, and a Plasma State component to manage the exchange of key simulation data, under a framework that provides a uniform execution environment, services for data and resource management, and integration with a web portal to facilitate tracking the progress of simulations.

2.1 Overall Approach and Philosophy

Design Philosophy. The IPS framework is based on the concepts of components and interfaces as articulated by the Common Component Architecture [CCA Forum; Allan06]. But at the same time, the IPS is designed to minimize the level of effort required to be able to use a physics code in coupled simulations. Since the codes of interest for SWIM physics are under active development, we have adopted the approach of implementing physics components as "wrappers" around the largely unmodified physics codes, with the Plasma State providing a mechanism for interfacing the components. The physics codes of interest have their own well-established input and output files and formats, so we use small "helper" programs within the component wrapper script to serve as adapters between the Plasma State and the physics code's own input and output files.

The IPS has been designed to accommodate multiple implementations of individual physics components, even within the same simulation run. The framework design imposes few restrictions on the types of simulations that can be carried out, allowing the IPS to be used for studies outside of SWIM's physics principle targets of RF interactions with MHD.

A User's View of the IPS. The user's primary interaction with the IPS is through the simulation driver component and the IPS configuration file. The driver is a Python script that orchestrates the integrated simulation: initializing the components, calling them in the desired sequence, typically in a time-stepped loop, testing for convergence and other conditions, and finalizing the simulation. The concept of a driver routine is common, in both component-based and traditionally-structured applications, and provides a great deal of flexibility to the user. Drivers can be reused to carry out similar simulations for different conditions and with different component implementations and different drivers can carry out very different kinds of simulations. A simulation configuration file allows the user to specify which specific implementations are going to be used when the driver invokes each component, to specify certain key input parameters for those components, as well as more general metadata for the simulation.

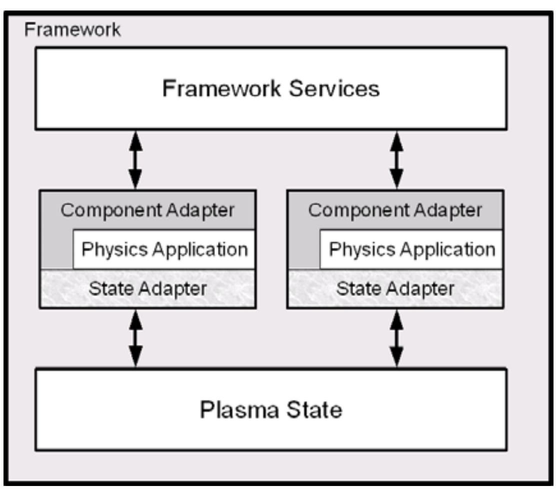

Figure 2.1. The schematic architecture of the Integrated Plasma Simulator environment [Elwasif07].

IPS Implementation. The IPS is implemented as a lightweight framework, written in Python, that provides basic services for physics components. As shown schematically in Figure 2.1, a component consists of adapters around a standalone physics application, which is used essentially without modification. Components exchange data through the Plasma State, which uses netCDF files as its underlying storage medium. In the rest of this section, we describe in more detail the design and implementation of the elements of the IPS environment.

2.1.1 Physics Components

A major task was that of "componentizing" the physics codes; that is to carefully define at an abstract level the mathematical functionality of each component and all of the inputs and outputs necessary to realize this functionality, independent of which code implementation is used. To enforce this abstraction IPS physics components are required to implement a standard interface, and to use the Plasma State to exchange all data needed by other components in the coupled simulations. The minimal interface involves three methods: init(), step(), and finalize(), which provides for any initialization operations required by the component, advancing the time step, and clean-up. There is no intrinsic limitation on the number or nature of method calls supported by the IPS, but these three cover the functionality required for the simulations to date. The Earth System Modeling Framework [Collins05] employs a similar approach. However, we anticipate extending to a richer component interface as we go to tighter component coupling and more complex component interactions.

An extensive set of physics components has been developed, in most cases with multiple code implementations. The Equilibrium and Profile Advance (EPA) component is implemented with the TSC code. It advances in time the plasma density and temperature profiles, plasma current and magnetic equilibrium and retains all of the sophisticated capabilities of TSC discharge programming and control. The EPA component also maintains an interface to the TRANSP code, permitting some of the TRANSP modules such as the NUBEAM neutral injection module to be used directly. ICRF components implementing both the AORSA2D and TORIC codes have been developed. Two Fokker-Planck components have been developed, one for ICRF and one for ECH, both implemented by the CQL3D code. The MHD stability component interface supports both linear MHD stability (PEST2 and BALLOON) and full 3D nonlinear extended MHD (M3D and NIMROD). A number of utility components have been developed that support simulation logic functions, collecting of time series data as the simulation proceeds for monitoring and visualization purposes, and several test components. Several driver components have been written which are tailored for different initialization sequences. Appendix 1 contains more detailed component descriptions and references. A number of new or improved components will be added in the second project phase.

2.1.2 IPS Framework

The IPS framework has been designed to be relatively small, highly flexible, and readily evolvable in response to the needs of the simulations. It works with no change to the underlying physics codes and implements different execution models as needed for different HPC systems utilizing several. It provides developers with an easily understood component environment, a small set of services that components can use, and a straightforward mechanism to orchestrate integrated simulations.

Use of Component Concepts. The IPS framework models the basic concepts of component based software development, as exemplified in the scientific computing field by the Common Component Architecture (CCA) [CCA Forum; Allan06]. Components are well-encapsulated units of computational functionality that interact with other components in the application through well-defined interfaces. Components and interfaces are distinct, in the sense that several different components can implement a given interface. For example, the IPS includes two components for RF modeling, based on the AORSA and TORIC codes, both conforming to the RF interface. The design of the IPS anticipates multiple implementations of nearly every component.

At the same time, SWIM's needs are relatively simple, and would utilize very little of the full generality provided by an environment like the CCA. These environments have problematic implementations on HPCs, and have a relatively steep learning curve. This led us to a simple problem-specific framework implementation that provides a tailored set of services, and supports a particular execution model. This approach has also given us the agility to easily evolve the framework as new needs and opportunities have become apparent.

Execution Model. Since the physics components of the IPS are based on unmodified standalone executables, the underlying physics codes must be run as child processes of the framework, using mpirun/mpiexec (for various MPI implementations), aprun (on Cray XT systems), or similar platform-specific tools to launch parallel physics executables. As a consequence, the framework itself does not "see" the multiple nodes and processes involved in parallel tasks. (From a CCA perspective, this is closer to the typical "distributed" component execution model and the HPC parallel model which is the primary focus of the CCA Toolkit reference implementation.).

The original execution model was that tasks (invocations of methods on components) would be carried out in sequence (as dictated by the driver). Work is now underway to generalize framework to support a "multiple-component multiple-data" (MCMD) style of programming [MCMD; Krishnan05]. In an MCMD environment, multiple parallel tasks can execute simultaneously via the driver invoking component methods in a non-blocking fashion. This provides the flexibility to use computational resources more efficiently by overlapping computations where data dependencies permit. During the first phase, the new framework services required to support MCMD execution were designed and implemented [Foley08]. We anticipate that this new execution model will also allow exploration of novel time-stepping and load balancing approaches.

Framework Services The IPS provides a small, tailored set of services to its components. The Data Manager abstracts the key operations needed to manage the file-based data exchange between components, provide executing components with appropriate workspaces, and capture the results of a component execution for archival purposes. The Task Manager handles component method invocations as well as the launching of the underlying physics application from within the component wrapper. This lower level interface provides an abstraction that hides the various platform-specific task launch mechanisms (mpirun, mpiexec, aprun, etc.) The Resource Manager tracks the computational resources allocated to the current batch job (currently just the number of nodes), allocating and deallocating them in response to the Task Manager launching tasks and terminating them. The Configuration Manager provides structured access to the information provided by the IPS configuration file. For example, the getPort() method returns a handle to the component that implements the requested interface, and the getGlobalConfigParameter() method provides access to individual component parameters specified in the configuration file. Finally, an Event Service is being implemented by our collaborators on the DOE Coordinated Infrastructure for Fault Tolerant Systems (CIFTS) project. The IPS Event Service, which is modeled on the CCA's draft Event Service specification [CCA Event Service], will initially be used to add a fault tolerance capability to the IPS (see below), but we envision that it will eventually be used in SWIM simulations as a means of signaling between components.

Implementation. The IPS framework is implemented in Python. It is high-level, object-oriented, and easily understood by developers, regardless of their background. It is also highly portable, and available on all platforms of interest to SWIM (on the Cray XT, for example, the framework itself runs on a front-end node, launching the physics applications on the compute nodes with aprun).

Significant Sollaborations. The IPS framework has also been a very useful tool in collaborations with other research projects. The IPS MCMD capability provides use cases and implementation experience to efforts underway in the SciDAC Center for Technology for Advanced Scientific Component Software (TASCS) to develop general interfaces and tools to manage MCMD computations in the CCA environment. SWIM participants Bramley (Indiana), Bernholdt, and Elwasif (ORNL) are all involved in TASCS as well as in SWIM. We are also collaborating with the CIFTS project, which is developing a Fault Tolerance Backplane (FTB) to make fault-related information available throughout the software stack running on an HPC system. The IPS is one of two applications CIFTS is targeting to demonstrate how the FTB can facilitate effective application-level responses to hardware failures (as an alternative to killing the entire job and later restarting it). Bernholdt (ORNL) provides the connection between CIFTS and SWIM.

2.1.3 Plasma State

Overview of Plasma State design. The Plasma State functions as a shared repository for time evolving plasma simulation data and as the mechanism for communication between physics components. An instance of the plasma state contains a snapshot of the data at a single point in time. The PS is implemented as a Fortran95 derived data type, the elements of which are elementary Fortran types. Multiple, separately-named state instances can be declared and held in memory simultaneously. Most of the code of the plasma state software is automatically generated by a Python script from a plasma state definition file. This permits modifications and extensions to the Plasma State to be made quickly and efficiently. Typical data residing in the Plasma State includes:

- Tokamak (axisymmetric) MHD equilibrium.
- MHD equilibrium derived flux surface averaged metrics and field quantities.
- Flux surface averaged plasma temperatures, densities, and rotation velocities.
- Flux surface averaged heating, current drive, momentum, and particle source profiles due to various types of RF and neutral beam actuators.
- Tables of results of linear MHD stability analysis.

The Version 1 of the Plasma State Software was released in January, 2007. Version 2 of the Plasma State represented a substantial redesign based on experience of approximately one year's use of version 1. The following table summarizes features added in Version 2:

Feature	Description
Machine description	Separate section for time invariant data describing items "bolted on" to the experimental device. Example: neutral beam geometries.
Shot configuration	Separate section for time invariant data that may vary from shot to shot on tokamaks. Examples: species lists, orientation of toroidal current and magnetic field.
Simulation control	Generally time invariant data characterizing the simulation, such as, grid discretizations of spatial coordinates, determining the spatial resolution of various components of the simulation.
Redesigned I/O	Plasma State files are now transparent, self-describing NetCDF files, improving accessibility of data to generic software e.g. visualization.
Separated fast ion species lists	RF minority, fusion product, and beam ions are handled in separate lists, facilitating mix and match of model components for treatment of the different types of fast ion species.
C interface	C/C++ callable interface based on a mix of machine generated and hand maintained code; allows FACETs driver to use Plasma State.
Toroidal momentum balance	State elements added for sources and sinks of toroidal angular momentum.

Detailed description documents of versions of the plasma state have been committed in the "component description documents" section of the SWIM website http://cswim.org; the most recent such document is Plasma_State_V2.003.doc.

Significant Collaborations. The FACETs SciDAC project is using the Plasma State to couple their C/C++ transport driver to NUBEAM for neutral beam and fusion product sources. Involvement of FACETs has been helpful in the design, implementation, and MPI scalability testing of NUBEAM as a component, as well as parts of the Plasma State itself. The Plasma State is also being used for component-to-component data sharing within TRANSP and PTRANSP; its use is planned for the CPES SciDAC as well.

2.1.4 SWIM Portal

The purpose of the SWIM portal is to provide a simple browser-enabled interface to monitor simulation runs, to discover archived runs through rich metadata, to initiate data movement for subsequent analysis and visualization, and to launch computational runs where allowed (Figure 2.2). The portal is intended as a convenience for physicists, and its use is entirely optional. The SWIM portal is located on a General Atomics server, at http://swim.gat.com:8000/monitor, and is implemented using standard web technologies, backed by an MS SQL database. It is based on the SciDAC-funded monitoring system that has been used to track computational runs on the FusionGrid. The initial version of the production SWIM Portal is operational and it allows real-time tracking of progress of IPS runs made on Jaguar at ORNL and the viz/mhd clusters at PPPL (and in principle any other site that allows outbound HTTP connections).

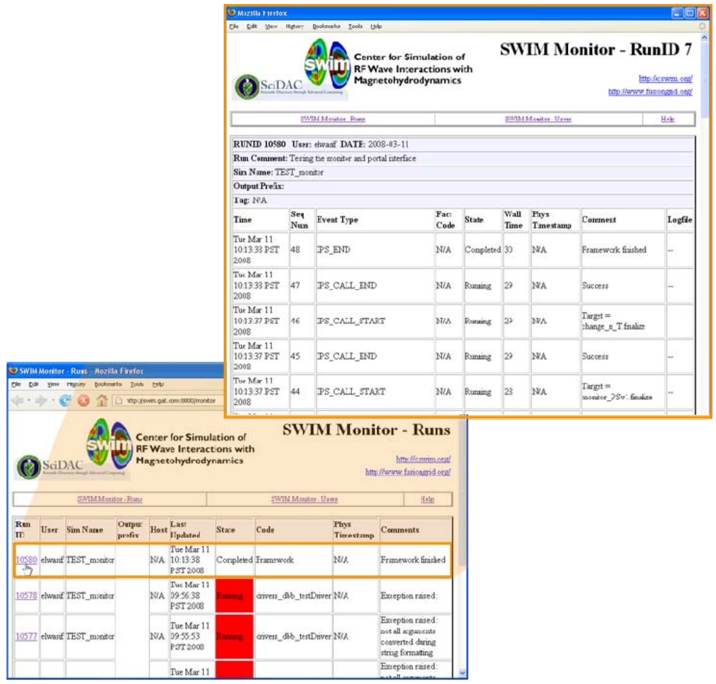

Figure 2.2. The SWIM web portal gives monitoring information on all runs with the ability to drill down into greater detail on specific runs.

The ElVis visualization program has been integrated with the job monitoring system to allow real-time graphical monitoring of data as the simulation progresses (Figure 2.3). ElVis is a display client written in Java. The applet version is launched by clicking on a link in the portal website. ElVis reads variables from the NetCDF file and displays a set of graphs according to a layout template. Graphical techniques were developed so dozens of graphs can be displayed legibly and accessed quickly.

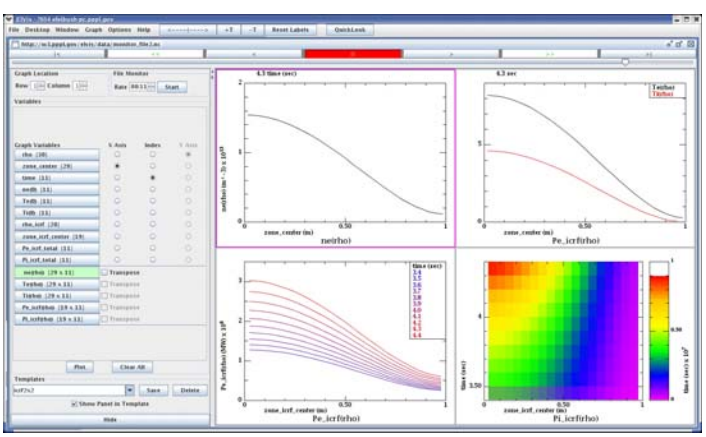

Figure 2.3. The Portal launches ElVis to enable scientists to monitor their simulation runs graphically in real-time from a web browser.

We have carried out additional work aimed at possible future enhancements to the SWIM portal. Our long-range vision for the portal extends to data management and possible online analysis and visualization. This work has included extending the FusionGrid portal framework (which is also used by SWIM) to use the PubCookie single sign-on to support fully federated multi-site web portal solutions. We have also investigated possible use of the

MDSplus data management system, widely used in the experimental fusion community, for large-scale movement of simulation data. Parallel I/O was tested in MDSplus using the XIO BIDI driver from within the Globus Project. Although there were increases in data transfer rates, the increases were not as large as expected and we decided not to pursue an MDSplus based solution.

2.2 IPS Physics Studies and Fast MHD

Here we describe the physics studies that have been performed using the Integrated Plasma Simulator and other studies using the SWIM framework related to fast MHD.

Alcator C-Mod ICRF Minority Heating Simulations. We have begun to use the SWIM framework to simulate the time dependent evolution of the fast ion distribution during hydrogen minority heating in the Alcator C-Mod device. These simulations will allow us to validate the predictive capability of the RF and MHD components, a prerequisite to investigating sawtooth modification in the presence of energetic particles. The TSC EPA component was used to advance the plasma profiles and equilibrium for a specific C-Mod discharge (shot #1080408021), and both the AORSA and CQL3D codes are being used to calculate the 3D fast ion distribution during ICRF minority heating. The simulation is programmed to adjust the OH-coil and other PF coil currents (and thus the loop voltage) to give the experimental values of the plasma current and plasma major radius vs time as well as the line-averaged density, and Z_{eff}. The time history of the total ICRF power was also programmed to match the experimental square wave modulation, 30 msec on-time and 30 msec off-time.

The simulation used the standard TSC thermal conductivity model, which normally provides a good model for L-mode transport at low power, and the Porcelli sawtooth model was used for sawtooth evolution. Model source terms were used for the electron and ion heating associated with the collisional slowing down of the minority ion tail. We are comparing with the experimental values of sawtooth amplitude and crash time, the loop voltage, the plasma shape, and the variation in the electron temperature during different phases in the heating and sawtooth cycles. As can be seen from Figure 2.4, the overall comparison between the TSC simulation and the experiment is reasonable.

Using the RF component (AORSA-CQL3D) we have also performed a standalone simulation of the time evolution of the minority tail energy at a time corresponding to 0.91 sec. in the C-Mod discharge simulation of Figure 2.4. Figure 2.5 compares the minority tail energy from this simulation with the measurement of charge exchange count rate due to energetic minority ions, as detected by a compact neutral particle analyzer (CNPA) diagnostic on C-Mod. The simulated turn-on time of the fast ion tail energy follows the rise time of the CNPA signal quite well for the vertical diagnostic channel viewing at R = 69 cm, corresponding to $\rho \approx 0.1$. The decay time of the energetic tail in the simulation is noticeably longer than the fall time of the CNPA signal however. This difference may be attributed to the fact that no spatial losses were turned on in the Fokker-Planck simulation. Also, the simulation assumed a constant electron and deuteron temperature in time, whereas in reality the background temperatures were evolving during the 60 msec. simulation time, due to the ICRF heating and sawtooth cycle. These latter effects will be captured properly when the model ICRF heating sources used in the TSC simulation are replaced by the AORSA-CQL3D results and the fast ion tail distribution is calculated more frequently.

ITER Approach to Burn. We have used the SWIM framework to perform a high-resolution simulation of the 200s approach to flattop of an ITER hybrid scenario discharge, using the parallel NUBEAM package. In these initial runs, we used 16 processors on the Princeton SGI computer (mhd.pppl.gov). The NUBEAM package exhibited near perfect parallel scaling, indicating that many more processors could be used in future runs. We were able to use a total of 16,000 Monte Carlo particles for the beam and alpha-heating calculations, 16 times more than what is normally used, with essentially no increase in running time.

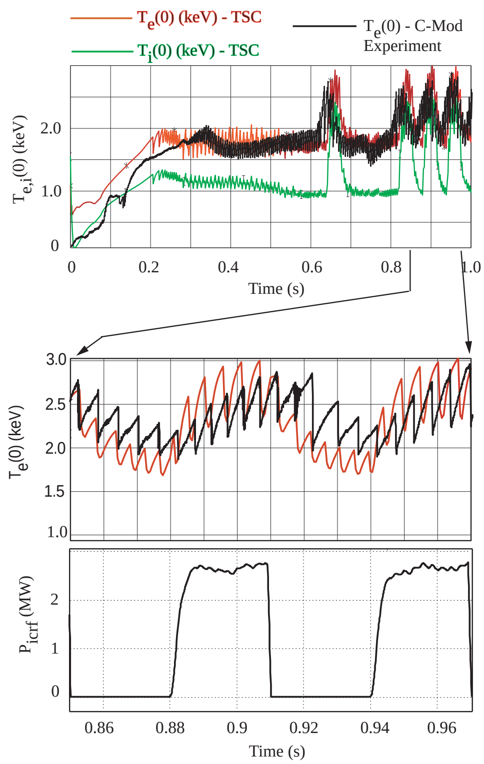

Figure 2.4. Comparison of experimental central electron temperature (black traces) with TSC simulation. Central electron (ion) temperatures from the simulation are shown in red (green). The bottom graph shows an expanded time period with associated ICRF power pulse.

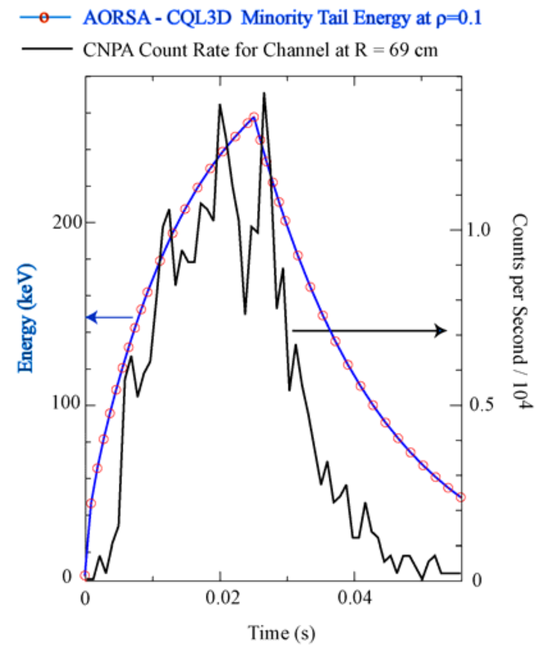

Figure 2.5. Comparison of minority hydrogen tail temperature (keV) versus time (s) from an AORSA-CQL3D simulation with CNPA diagnostic count rate versus time for a channel at R = 69 cm. Plasma parameters correspond to the TSC simulation in Fig. 2.5 at 0.91 sec.

As can be seen in Figure 2.6, we observed broad, double-peaked beam deposition at high densities for the electrons and the energy deposition profiles were significantly smoother than the older 1000 particle runs. The differences in the associated temperature profiles were not as dramatic, but the improved statistics make the calculated distribution functions significantly smoother. The use of even more Monte Carlo particles will make kinetic stability analysis possible in future runs.

In these runs, the temperatures, densities, and the plasma current all reach near steady values within 200 s of simulation time. The GLF23 transport module was used to determine the electron and ion thermal conductivities. The TORIC RF package was used to provide the ICRF heating profiles. A steady state alpha power of about 80 MW is produced with 33 MW of NB and 20 MW of ICRF input power. The pedestal temperature reaches 4.3 keV for electrons.

ITER Radio Frequency Power Propagation and Absorption Benchmarking and Analysis. Transport simulation of ITER plasmas is a key activity for specifying and designing the ITER facility. The fixed boundary transport code PTRANSP, the free-boundary TSC/TRANSP, and more recently the SWIM IPS have been the principal tools used for these simulations. Accurate modeling of plasma heating in these codes is required for reliable discharge simulations.

Heating for the ITER plasma is provided by energetic neutral beams; by radio frequency power in the 150 GHz range for resonant coupling to electrons at the cyclotron frequency (for localized current for plasma stability control); and by 20 MW of power in the 50–60 MHz range for plasma heating. The majority of existing ITER simulations used TORIC for modeling the ICRH. However, more detailed

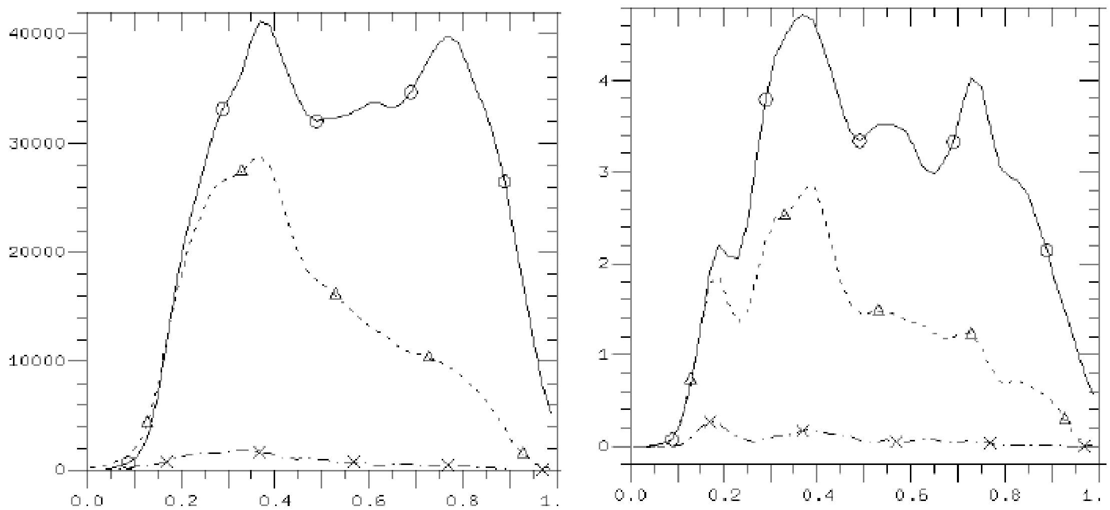

Figure 2.6. Comparison of beam deposition with 1000 (right frame) versus 16,000 particles in NUBEAM calculations at t = 200s. A similar difference was seen in the alpha-power deposition profiles.

analysis of, for example, a particular time slice of a particular PTRANSP ITER run would allow validating the physics used in TORIC and the particular set of resolutions chosen for those runs. These analyses were expedited (and the chances for coding errors significantly reduced) by using the SWIM Plasma State interface to communicate time-slice data to AORSA. Higher resolution ICRH simulations of a PTRANSP time slice using AORSA indicate that the electron damping and ion cyclotron heating predicted by TORIC is qualitatively correct, thus giving confidence in the reduced physics model and numerical resolution used in TORIC in the time dependent PTRANSP work.

The principal conclusion is that the SWIM STATE and framework provide the capability for detailed, standalone analyses of complex, multi-physics simulations. At a technical level, the comparisons indicate that, first, there is a systematic trend for AORSA to show less electron heating than TORIC even though the physics restrictions on TORIC compared to AORSA should not be significant. The reason(s) for this difference are not understood, and are the subject of ongoing analyses. However, the differences between the two RF codes are not likely to lead to significant differences in the overall simulation results. Second the convergence studies for both codes indicate that the resolution used in the PTRANSP simulation is sufficient.

Sawtooth Simulation using NIMROD and M3D. NIMROD and M3D are both parallel nonlinear 3D MHD codes in toroidal geometry that nominally solve the same equations, but that have very different numerical representations and algorithms. These codes can now both be initialized from the same equilibrium configuration that is calculated by the EPA component TSC, with the equilibrium information being transmitted through the Plasma State. Among other advantages, initializing from the same equilibrium file provides a convenient way to benchmark calculations from the two codes. We performed such a benchmark for a discharge in the CDX-U tokamak.

The results of the nonlinear comparison are shown in Figure 2.7. It is clear from the figure that the codes are in substantial, detailed agreement. The codes agree in the relative magnitudes of the various toroidal modes before, during, and after the crashes; on the detailed time behavior of the low-n modes; on the degree of damping of the oscillation in successive cycles, and on the cycle period of ~200 μs.

When we investigate the actual plasma state at various corresponding times in the two runs, we also find detailed agreement (Figure 2.8).

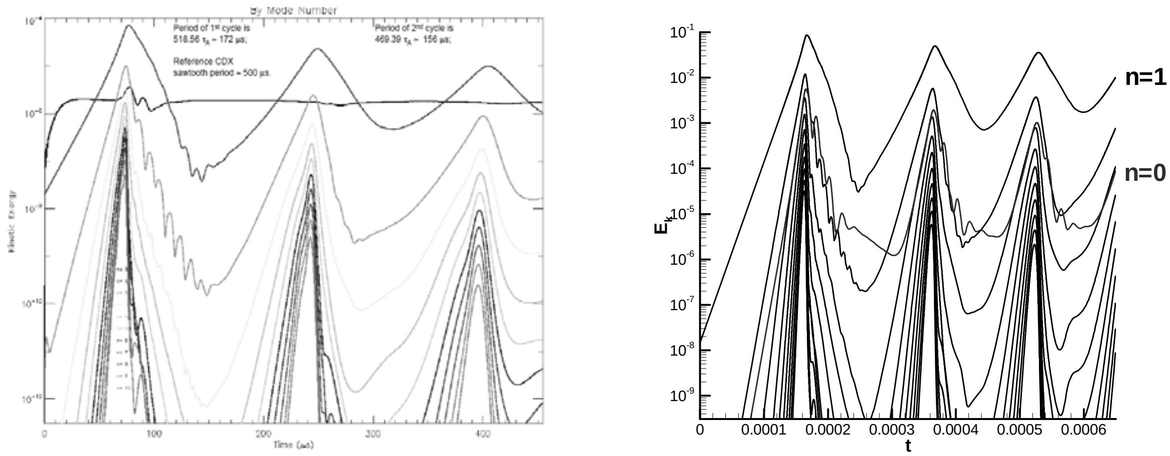

Figure 2.7. Time history of kinetic energy by toroidal mode number during the first three sawtooth crashes in the present iteration of the nonlinear CDX benchmark. Left: M3D result (energy in normalized units, time in μs). Right: NIMROD result (MKS units).

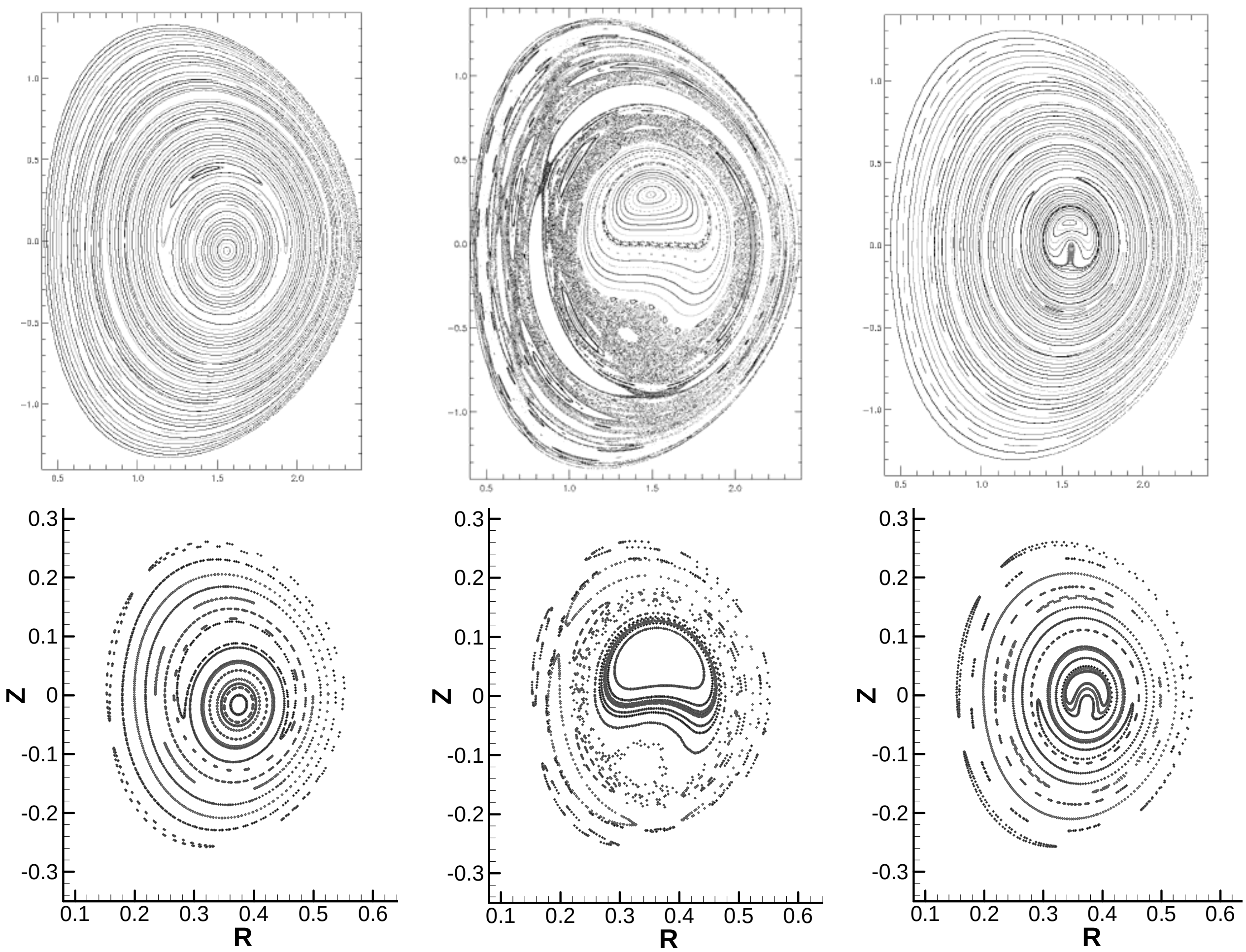

Figure 2.8. Poincaré sections showing magnetic flux surfaces at several time instants during the M3D (top) and NIMROD (bottom) sawtooth cycles. Left: late linear phase. Center: at culmination of crash. Right: Early recovery phase following crash.

This agreement constitutes a successful verification of the two codes. However the modeling is insufficient to produce quantitative agreement with the experimental results for the two predictions that can be compared directly with soft X-ray data from the experiment: the sawtooth period and the crash time. The predicted period of 200 μs is significantly less than the observed 500 μs sawtooth period in CDX, and the predicted crash time is a much larger fraction of the total cycle time than is observed in the device. Hence this study cannot be considered a successful validation of the model. A more refined model and a set of initial and boundary conditions that show greater fidelity to the experimental conditions are required. This is the focus of our future studies.

2.3 Accomplishments in Slow MHD Campaign

The goal of the Slow MHD Campaign is to provide a self-consistent simulation of the effect of ECRF source deposition on neoclassical tearing modes (NTMs) by coupling computational models for RF wave propagation and deposition (GENRAY and CQL3D) with a computational model for extended MHD (NIMROD). Development of such a capability will allow more confidence in projecting current favorable results to NTM stabilization in ITER, as discussed in Appendix 1, Technical Background. Although simulation models have been developed for this interaction [Yu00], the derivation of the models has been somewhat obscure. This makes understanding of the approximations used in the derivation difficult, and limits confidence in the model. In the current work, analytic theorists, computational MHD experts, and RF experts have worked together to ameliorate these problems. We have:

1. Developed a self consistent fluid model that includes effects of ECRF modifying the distribution function in the extended MHD equations;
2. Used a CEL approach to obtain closure relations for pressure tensor and parallel heat flux with RF sources;
3. Developed a staged plan of increasing self consistency that enables us to quickly gain experience with RF effects in extended MHD, initially with phenomenological RF and closure models, and proceeding ultimately to self consistent RF calculation and numerical closure;
4. Performed preliminary studies with NIMROD on classical tearing modes in tokamak geometry, including specified RF driven current perturbation, and demonstrated non-linear island shrinkage.

In the following sections, we detail these accomplishments.

2.3.1 Extended MHD Equations with RF Sources

Consider a kinetic equation in the form

$$\frac{df}{dt} = C(f) + Q(f) \quad , \tag{2.1}$$

where the left side is the usual kinetic operator in phase space, *C(f)* is the collision operator, and *Q(f)* represents the contribution due to RF-induced fields, and is to be obtained from RF codes. Taking moments of our kinetic equation, we are left with the usual fluid equations augmented by additional terms from the RF source. Consider just the momentum equation,

$$m_s n_s \left(\frac{\partial \mathbf{V}_s}{\partial t} + \mathbf{V}_s \cdot \nabla \mathbf{V}_s\right) = n_s q_s (\mathbf{E} + \mathbf{V}_s \times \mathbf{B}) - \nabla p_s - \nabla \cdot \mathbf{\Pi}_s + \mathbf{R}_s + \mathbf{F}_s^{rf} \quad , \tag{2.2}$$

where conventional notation is used. The additional term due to the RF source is given by $\mathbf{F}_s^{rf} = \int d^3\mathbf{v}\, m_s \mathbf{v}_s Q(f_s)$, which is a function of three spatial dimensions and time. A similar term, S_s^{rf} appears in the energy equation.

The above fluid equation is exact. However, we now have the normal closure problem: calculations for the stress tensors and heat fluxes are needed, and these calculations need to include the modifications of the distribution function by the RF sources. In an approach similar to the Spitzer problem, wherein the plasma conductivity in the presence of an electric field is calculated, we apply perturbation theory and use as the small quantity E / E_D, where E_D is the Dreicer electric field, and assume that to lowest order the distribution is Maxwellian with small corrections (reasonable for the case of ECCD). We can then replace $Q(f_s)$ with $Q(f_{Ms})$ and with the identification of a proper quasilinear diffusion operator, $\mathbf{F}_s^{rf}$ and S_s^{rf} are now expressible as functions of low order fluid moments and RF physics.

To complete the description, we also need to understand the changes to the parallel heat flux and stress tensor terms. Using a Chapman-Enskog-like (CEL) approach, a kinetic equation for the distortion F away from the Maxwellian can be derived and subsequently solved to obtain $\mathbf{q}$ and $\mathbf{\Pi}$. Following the usual CEL procedure in which the fluid equations are used to evaluate df_M / dt, we have

$$\frac{dF}{dt} - C(f_M + F) = ... + Q(f_M) - \frac{\mathbf{v}' \cdot \mathbf{F}^{rf}}{nT} f_M - \frac{2}{3}\frac{S^{rf}}{nT}(\frac{mv'^2}{2T} - \frac{3}{2}) f_M \quad , \tag{2.3}$$

where the species subscript is suppressed for simplicity. Since F is a small distortion, the collision operator on the right side can be linearized. The (…) terms on the right denote the “usual” CEL source terms due to temperature and flow gradients, which drive heat flows and viscous stresses [Held04]. The important modifications from the RF enter as additional source terms on the right side.

In order for this model to provide a realistic representation of the NTM-RF dynamics, sufficiently accurate explicit forms of the d/dt operator and the (…) terms are still needed, and require further analytic development. This is not trivial, given the NTM’s slow growth rate and sensitivity to physical effects beyond the single-fluid MHD description, and part of our theoretical effort has been devoted to this issue. We have obtained a new level of accuracy by following a systematic expansion to the second order in the ratio between the ion sound gyroradius and the macroscopic lengths, assuming first-order distortion from Maxwellians and a second-order electron to ion mass ratio. This level of accuracy is important to retain the physical effects that compete with the weak drive for the NTM instability. Our new terms in the d/dt operator include the effect of the parallel electric field and the contribution of inhomogeneous, compressible macroscopic flows. This work will be in a forthcoming publication.

With this approach, the only thing needed from the RF codes is the form for $Q(f_{Ms})$ as a function of the phase space variables. The fluid code hands the state variables of interest to the RF code, where $Q(f_{Ms})$ is calculated. When this information is passed back to the fluid code, the necessary terms $\mathbf{F}_s^{rf}$, and S_s^{rf} can be calculated by the fluid code to determine the closures and fluid evolution. To make further progress, one needs to solve the kinetic equation. The construction of efficient and accurate solutions to equations of this form is also a topic of ongoing interest to the SciDAC CEMM project.

2.3.2 Computational Approach for the Slow MHD Campaign

With this development, our phased approach for accomplishing the Slow MHD Campaign Goals is:

- Phase 0: We postulate an axisymmetric, phenomenological model for the RF interaction. We use an analytic shape $\boldsymbol{F}_{RF} = \boldsymbol{F}_{RF}(R,Z)$.
- Phase 1: Introduce toroidal variation of $\boldsymbol{F}_{RF}$, to more realistically model toroidally localized RF deposition. $\boldsymbol{F}_{RF} = \boldsymbol{F}_{RF}(R,Z,\phi)$, and include equilibrium toroidal flow.
- Phase 2: Pass the NIMROD equilibrium data to RF ray tracing codes, and fit the ray data generated by these codes to the parameters of the phenomenological model (e.g. Gaussian half-width, amplitude, spatial location, etc.).

- Phase 3: Relax the assumption that F_{rf} is constant over the simulation time, recalculating this term intermittently as NIMROD runs. Develop methods for the direct interpolation of RF ray data to NIMROD finite elements, such that phenomenological method is no longer used.
- Phase 4: Fully couple the RF and MHD codes such that $\boldsymbol{F}_{RF}$ is calculated at every time step.
- Phase 5: Incorporate more advanced closures and neoclassical effects.

We have completed Phases 0–2, and discuss these accomplishments next.

2.3.3 Numerical Accomplishments in the Slow MHD Campaign

We have successfully incorporated a non-self-consistent model of RF current drive into the NIMROD code, and have used it to demonstrate the stabilization of resistive MHD magnetic islands by RF radiation. For the calculations reported here, $\boldsymbol{F}_{RF}$ is specified by a Gaussian function.

The equilibration of the RF current over a flux surface is illustrated in Figure 2.9 for a test case in cylindrical geometry with the NIMROD code. The RF current is initially localized as a Gaussian in the poloidal plane. As time proceeds, it spreads over the intercepted flux surfaces and eventually surrounds the plasma core; the time for equilibration is approximately 10 Alfvén times. This result demonstrates that the MHD model that introduces RF effects through a modified Ohm's law reacts in the correct manner to the introduction of a localized RF current source, in distributing the induced current over the affected flux surfaces.

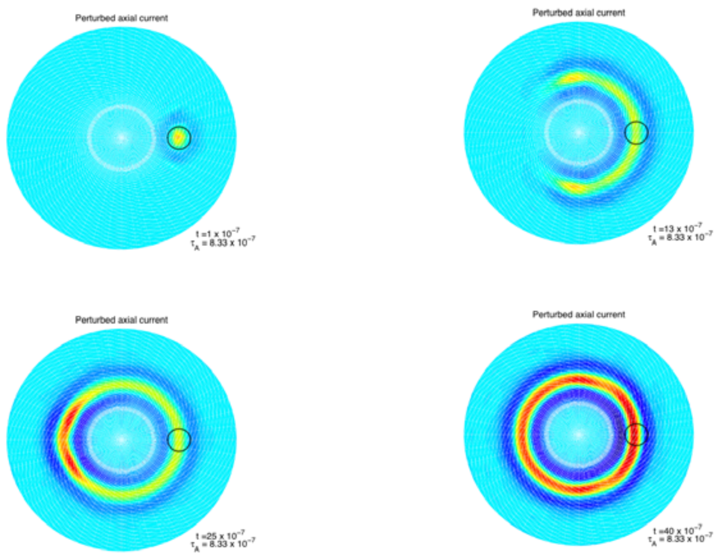

Figure 2.9. Illustration of equilibration of a localized RF current source over a flux surface as a result of modifications to Ohm's law in the resistive MHD model.

The correct equilibration effect also occurs in toroidal geometry for realistic plasma profiles. In Figure 2.10, we illustrate the effect of the RF current source on the evolution of a resistive magnetic island. The equilibrium is unstable to a 2/1 tearing mode that is allowed to grow and saturate. The RF current source is then gradually increased from small amplitude. Comparisons of the subsequent evolution of the magnetic island with and without the RF current source show that the island shrinks in response to the current perturbation. The relative sizes of the magnetic islands in the presence and absence of RF are shown in Figure 2.10.

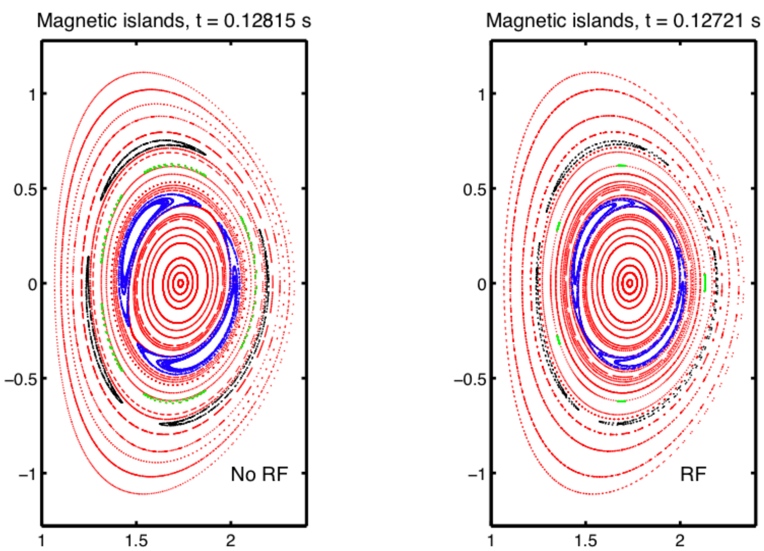

Figure 2.10 Size of the 2/1 magnetic island near the end of the simulations without (left) and with (right) RF current source.

These results demonstrate that we can achieve similar results to previous work without the need for their less rigorous models. These results are also in qualitative agreement with prior predictions [Pletzer97]. More detailed comparisons are ongoing as we work towards a publication of these results. This work shows successful completion of Phase 1 of our goal, and will serve as an excellent baseline as we move onto the other Phases of the project. We are currently in Phase 2.

2.4 Math and Other CS

2.4.1 Tri-Diagonal Newton Solver for GLF23

In solving the 1D (flux surface averaged) transport equations for the temperatures, magnetic fields, and densities in the "evolving equilibrium" description of a tokamak, one increasingly encounters highly nonlinear thermal conductivity and diffusivity functions, such as GLF23, that have a strong and non-analytic dependence on the temperature gradients. These arise from a subsidiary micro-stability based calculation in which the growth rates and hence transport coefficients are sensitive functions of these gradients. When these nonlinear functions are interfaced with an existing transport framework that uses a standard implicit time advancement algorithm such as Crank-Nicolson or backward Euler, large non-physical oscillations can develop and, as a result, non-convergent solutions can occur.

It is known that the non-linear equations can be differenced implicitly (with the spatial differences and the diffusivity at the advanced time) and the system of equations solved with the Newton-Krylov method. However, implementing this technique is a major perturbation to the algorithms of the existing transport codes, and can be somewhat inefficient if not specialized to the difference equations at hand. We therefore developed an algorithm that does a linearization of the GLF23 nonlinearity and applies the multi-variable Newton algorithm to solve the resulting equations. This algorithm keeps the solution matrix in tri-diagonal form, so that the only increase in running time is due to additional evaluations of GLF23 at each node for each Newton iteration in order to form a derivative. The new Newton solver is a great improvement over the backward Euler method, and does not require time or space averaging in order to get convergent results.

We illustrate this improved method in Figure 2.11 where we solve a model equation that exhibits the GLF23 nonlinearity with both the new "Newton" method, using only a single Newton iteration, and with the standard backward Euler method. We plot the result at a particular space-time point as computed by

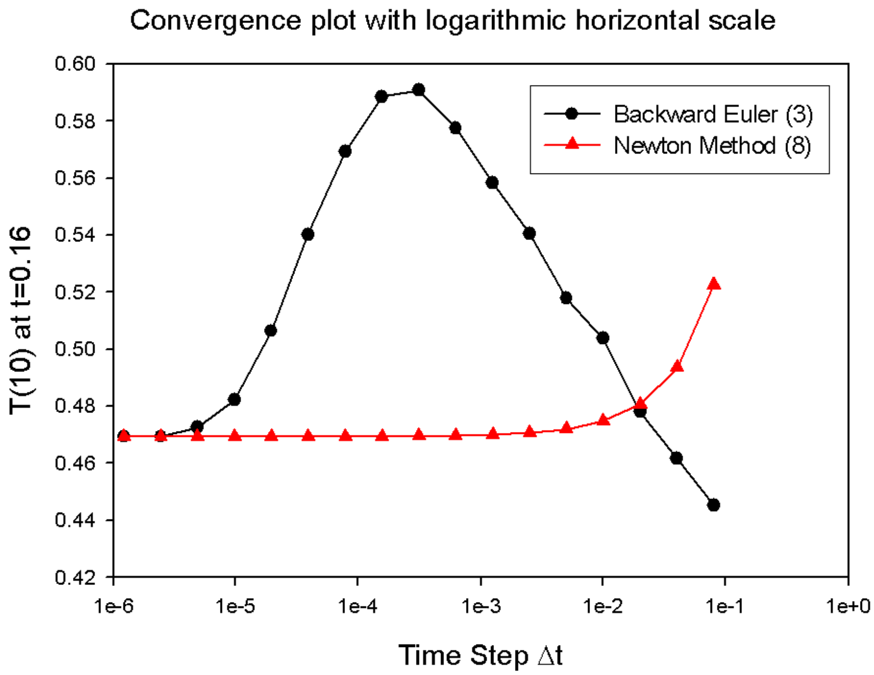

Figure 2.11. Convergence plot comparing the Backward Euler method with the Newton method versus time step using a logarithmic horizontal scale. The Newton method allows a time step four orders of magnitude larger than the Backward Euler method.

the two methods as a function of the time-step, using a logarithmic scale. We see that for small enough time step, the two methods converge on the same result, but that the Newton method can use a time step 4 orders of magnitude larger and still be of acceptable accuracy. This technique has been submitted for publication.

2.4.2 Electric Field Iteration between the EPA and FP Components

Both the Equilibrium and Profile Advance (EPA) and Fokker Plank (FP) module need the parallel electric field, and special care must be taken when interfacing these two components. The FP module can calculate the steady state parallel current associated with a steady state electric field, $J_{||}(E_{||})$, but does not include the effects of magnetic induction, which is important in a time-dependent simulation. (Induction is basically an electric field in the direction to oppose the current increase associated with a time-varying current and magnetic field). Induction is included in the EPA component, however, but the inclusion of induction can lead to an unstable coupling if a linearization is not performed.

In order to stabilize this coupling, the EPA component calls the FP component several times with several values of the electric field that differ slightly so that it can form a derivative: $\partial J_{||}/\partial E_{||} = \left[J_{||}(E_{||} + \delta E_{||}) - J_{||}(E_{||}) \right] / \delta E_{||}$. The magnetic field is then evolved from time n to n+1 in the EPA component using the implicit induction equation:

$$\frac{\partial \mathbf{B}^{n+1}}{\partial t} = -\nabla \times \mathbf{E}^{n+1}. \tag{2.4}$$

Where the new time electric field is obtained implicitly through the linearization:

$$\mathbf{E}^{n+1} = \eta \left[\frac{1}{\mu_0} \nabla \times \mathbf{B}^{n+1} - J_{\parallel}(E_{\parallel}^{n}) - \frac{\partial J_{\parallel}}{\partial E_{\parallel}} \left(E_{\parallel}^{n+1} - E_{\parallel}^{n} \right) \hat{\mathbf{b}} \right]. \tag{2.5}$$

Equation (2.5) is then solved for $\mathbf{E}^{n+1}$, substituted into Eq. (2.4) and solved by standard tri-diagonal techniques. This linearization is observed to stabilize the interface, but may need to be iterated for accuracy.

2.4.3 Vectorized Iterative Solver for the X1E

The centralized mathematical task of most present-day large-scale fluid and magneto-fluid physics codes such as M3D and NIMROD is the frequent, repeated solution of large sparse linear systems arising from implicit finite difference or finite elements discretizations of the equations. This task is made considerably easier by the availability of libraries such as PETSc, which provide flexibility in the choice of solvers and preconditioners while hiding much of the complexity of the parallelization of data structures. However, the introduction of sophisticated vector processors into next-generation parallel architectures, such as in the Cray X1E, imposes new requirements on sparse solver algorithms that are not yet addressed by the PETSc libraries. In particular, the solvers on the X1E will achieve only a tiny fraction of the theoretical peak performance unless they can be written in such a way as to keep the 64-unit vector pipelines full throughout most of the kernel linear algebra operations in the algorithm. Existing PETSc routines are not designed to do this.

In order to run the M3D code on the X1E, we had to develop our own customized sparse linear system solver that was both parallel and that could vectorize. We built this around a relatively old algorithm, called dynamic relaxation, which can be shown to converge to a solution on an N $\times$ N grid in order-N iterations, with a small coefficient if the iteration starts with a good initial guess, as is the case in repeated solutions of an elliptic equation in a time-dependent simulation. Because the algorithm both vectorizes and parallelizes easily, we found it to be over an order of magnitude faster on the X1E for M3D than any of the existing PETSc solvers with their preconditioners .

2.4.4 Solving PDE's in Moving Coordinates

We are supervising a graduate thesis in applied math that is involved with solving partial differential equations in moving coordinates. An especially promising technique is the Monge-Kantorovich approach that generates a mapping relating a pair of configurations. An application of interest to the sawtooth problem is in finding the best coordinates to solve the heat transport equation during the sawtooth crash when the magnetic surfaces begin to break up. It is well known that the use of magnetic coordinates offers many advantages when good surfaces exist, since the plasma thermal conductivity is highly anisotropic, with the value parallel to the magnetic field many orders of magnitude larger than that perpendicular to the field. We find that even though many magnetic surfaces breakup during the crash phase so that a complete set of magnetic surfaces do not formally exist, the temperature does not completely flatten due to the presence of residual surfaces and cantori which form effective heat barriers. The goal is to use these evolving cantori to form the "best" moving coordinate system in which to solve the heat transport equation. Figure 2.12 illustrates these coordinates in a model problem with highly anisotropic thermal conductivity in chaotic fields, and shows how the ghost surfaces formed from the cantori approximate the temperature isotherms.

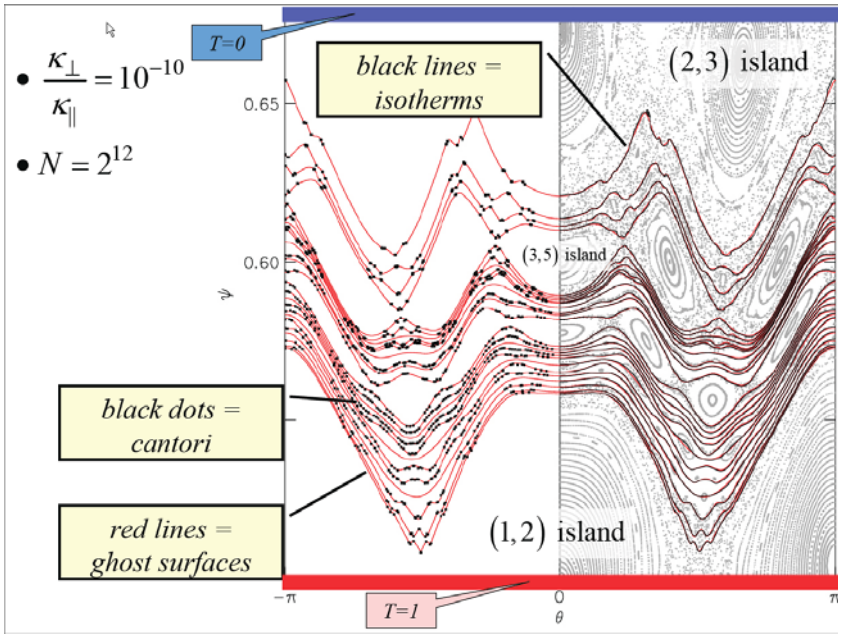

Figure 2.12. The right half of the figure shows the temperature contours obtained when solving the heat conduction equation in a stochastic field with a very large anisotropy ratio on a uniform grid of very high resolution. The left half is a reflection, showing the location of the cantori and ghost surfaces in this field. It is seen that the ghost surfaces (left) are a good approximation to the isotherms (right).

2.4.5 CG/HYPRE Solves in M3D

The most compute intensive part of the M3D code involves solving 13 different 2D elliptic type equations each time step on each toroidal plane. In the original formulation of M3D, these equations were not cast in a symmetric form. The PETSc solver GMRES was used to solve these equations, with an Incomplete LU (ILU) preconditioner. After some tuning of the parameters of the solver, this appeared to be an adequate approach. However, it was found that by a slight reformulation of the underlying finite element equations, the sparse matrices given to PETSc could be cast in a symmetric form that allows use of the Conjugate Gradient (CG) solver rather than the less efficient but more general GMRES. Also, the algebraic multi-grid pre-conditioner HYPRE became available via PETSc on both the ORNL and NERSC centers. We have therefore converted the M3D solves from GMRES/ILU to CG/HYPRE and in doing so have reduced the running time of M3D by a factor of almost 2 for our smallest problem sizes and by over a factor of 7 for the largest problem sizes.

2.4.6 Early Evaluation of AORSA2D on the CRAY XT4 Machine at the National Center for Computational Sciences (NCCS)

Vendor optimized ScaLAPACK achieved about 38% of peak performance on over 10,000 cores. This result was much lower than expected given the performance of high performance computing LINPACK Benchmark (HPL), a widely known benchmark that solves a dense linear system of the sort of interest to us. LINPACK achieved nearly 80% of peak performance.

HPL is a freely available software package developed in 2001 and written in portable C. HPL is designed to solve a randomly generated dense linear system using LU factorization in 64-bits double-precision arithmetic on distributed memory computers. It is used as a benchmark for ranking the world's top 500 fastest supercomputers. ScaLAPACK is a freely available software package for parallel dense matrix computation. It can be viewed as a parallel version of the very successful LAPACK library for serial matrix computation. Both ScaLAPACK and HPL are renowned for their portability within different parallel machines. HPL users are given the option to fine-tune extra parameters to speed up computations. Some parameters control the depth of look-ahead algorithm, the use of hybrid left-looking and right-looking algorithms for panel update, topology of processor grid, and several variants of coding for efficient message passing in MPI. This prompted us to explore the possibility of enhancing the performance of AORSA2D by modifying and adapting the HPL code to replace the ScaLAPACK dense "Lower/Upper" (LU) solver. We converted the HPL source code to solve a given double complex linear system to replace the ScaLAPACK routine PZGESV enabling us to obtain nearly 87.5 TFlops on 22,000 processors on the CRAY XT4 machine, over 75% of peak performance.

2.5 Supercomputer Usage

All of the major IPS codes (on which components are based) have been ported to the National Center for Computational Science Jaguar at Oak Ridge National Laboratory. These include AORSA and TORIC, (source codes); TSC (equilibrium and profile advance) M3D and NIMROD (nonlinear MHD); and CQL3D (Fokker-Planck). The component descriptions in Appendix 1 provide a more detailed description.

Computation of sources for particles and energy are the most demanding components with respect to computing resources. AORSA and TORIC, the two principal RF codes, have demonstrated strong scaling through the tens of thousands processor level. An example of the scaling studies that have been performed is shown below in Figure 2.13.

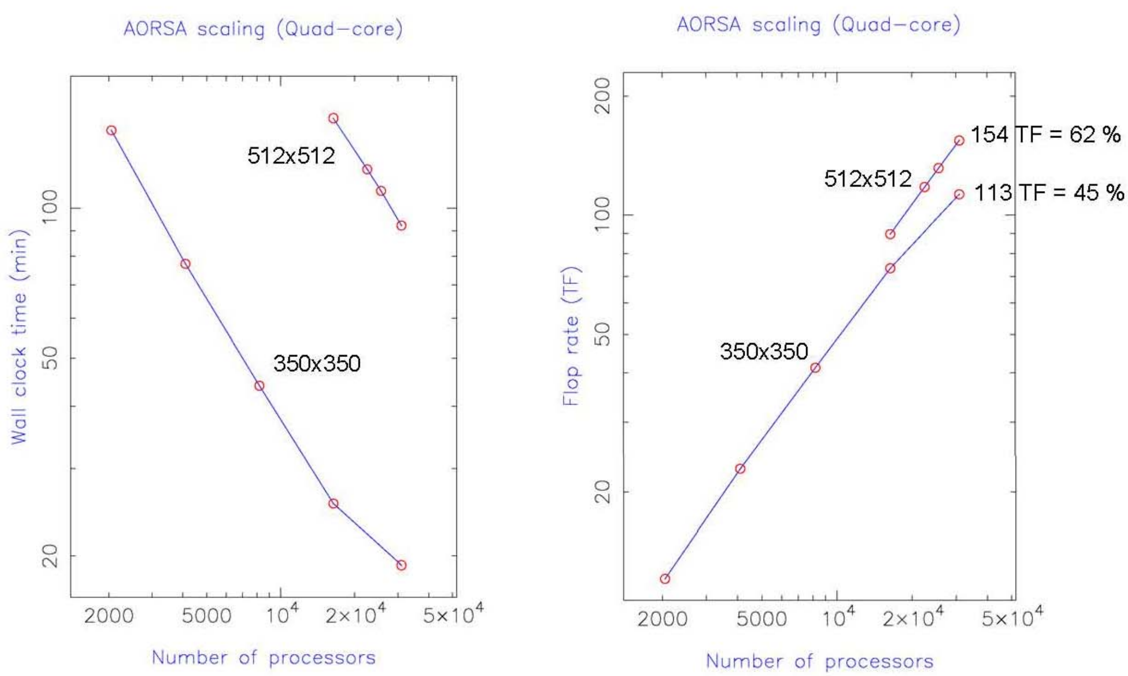

Figure 2.13. Scaling Studies for AORSA on the quad core, ~250 TF Jaguar at ORNL.

Depending on the particular simulation target, resolutions of 256 × 2 56 to 512 × 512 will be required. Past scaling studies for TORIC have demonstrated similar scaling. A parallel version of NUBEAM, a Monte Carlo neutral beam code, is presently being tested on a Linux cluster at PPPL. We expect that NUBEAM's scaling on Jaguar will be very good, as is typical for similar Monte Carlo based simulations.

Nonlinear 3D MHD. The time-dependent, non-linear 3D MHD codes, while posing challenges for efficiency at high processor counts, are making substantial progress. As reported in [Section 2.4.5: CG/HYPRE Solves in M3D], we have recently switched from GMRES/ILU solves to CG/HYPRE in

M3D as they became available through the PETSc interface. This allowed a dramatic increase in the number of processors that M3D can use efficiently. NIMROD has now interfaced to PETSc and has begun initial explorations of different solvers for the NIMROD implicit solves

In addition, the computation of the closure relations required for modeling plasma response to electron cyclotron current provides opportunities for parallelism that is being exploited. As outlined in the proposed work, the calculation of the RF quasilinear operator is calculated on a separate group of processors using the IPS framework. In addition, a new scheme has been implemented in NIMROD to separate the parallel decomposition of the kinetic computations from the decomposition of the fluid advance. In this scheme, a separate group of processors perform the computationally demanding nonlocal closures and exchange data with the fluid processors. This results in overall strong scaling efficiency of over 70% in going from 512 to 4096 processors. As we move to more realistic modeling of RF effects, this capability will become crucial.

3. PROPOSED NEW RESEARCH

3.1 Further Development of the IPS

Our development plans for the IPS are primarily motivated by the needs of the physics being done using the framework. Consequently, much of the detailed development of the IPS will be dynamic, responding to new needs and opportunities as the physics side of the project progresses. However, several of the key strategic directions needed to support planned New Physics (Section 3.2), Advanced Studies (Section 3.5), and Verification and Validation (Section 3.6) are already clear.

3.1.1 Framework

From the beginning, we have anticipated that the framework would need to evolve progressively towards greater levels of sophistication in terms of the interactions between components than it is capable of supporting. The work on MCMD support, already in progress, is one example of more complex interactions and relationships among components. We plan to continue this work, extending and generalizing the MCMD capability as needed to support the various physics and parallel load balancing scenarios currently under development (see below). While our initial MCMD implementation uses cases that (by intent) avoid the complication of multiple components needing simultaneous (write) access to the Plasma State, the issue clearly needs to be addressed for a general MCMD capability. A straightforward solution would be to establish a locking mechanism around updates to the Plasma State. If necessary, a more sophisticated approach involving writing separate updates and merging them into the main Plasma State will be considered.

We also anticipate the need to provide for tighter coupling among some components, primarily in situations where interactions are much more frequent than is the case for present components. One example is componentization of transport models. The present Equilibrium and Profile Advance component internally invokes the TSC code every macro-timestep and performs a calculation involving micro-timesteps that can be 100 to 1000 times smaller, with evaluation of transport coefficients occurring every one or few micro-timesteps. There is a desire to turn the transport coefficient models into components so that the TSC transport solver can readily use a broader range of models for transport coefficients, including a parallelized GLF23 (see Section 3.5.4), a more computationally intensive TGLF model, and other simplified models. Another example is where the interaction of sources with the transport solver requires many iterations, such as performing current drive calculations with CQL3D, but using TSC to perform the magnetic field update. Since this is a very tightly coupled system it can sometimes require 50 or more iterations to converge at a given time point. In situations such as these, we anticipate that the overheads of current task launch and file-based data exchange mechanisms will become performance issues. The desired environment in these cases is much closer to the Common Component Architecture's HPC (or "direct connect") approach, and we will leverage both concepts and tools from the CCA to provide a solution for the SWIM project's needs.

One of the lessons learned so far in the SWIM project is that a clear and complete definition of the interfaces between physics components can be even more challenging to achieve than we anticipated. The primary problem is that by using the Plasma State to exchange data, the interface is implicit rather than explicit, and, therefore, cannot be enforced independently by the execution environment. In traditional programs, or CCA-like component applications, interfaces are explicit, and mismatches between the data provided by the caller and that expected by the callee can in many cases be caught by compilers and/or runtime checks. We propose to explore mechanisms to make the interfaces more explicit and allow them to be independently verified during execution. The basic idea is for the component writer to provide an explicit definition of the component's interface, similar to the Scientific Interface Definition Language (SIDL) [Dahlgren07a] used in the CCA, based on specific entries in the Plasma State. From such a definition, we can automatically generate the code required to verify pre- and post-execution of the component method that the relevant entries are set and have been updated, respectively. This idea is also closely related to design by contract methodologies [Meyer97], and as time permits, we plan to investigate the idea of further annotating the newly-explicit interfaces with pre- and post-conditions to support deeper verification of the data passing through the interface. This work will leverage collaborative connections with the CCA's effort on Software Quality and Verification, which is introducing functional contracts into the CCA environment. [Dahlgren05; Dahlgren07].

3.1.2 Plasma State

Although already in production use, the Plasma State (both the software and the specification of contents) will continue to be developed through the remainder of the SWIM SciDAC project. Priorities will be driven by emerging physics components requirements. It is expected, for example, that the Machine Description and Shot Configuration sections of the State will be modified to include greater details on RF antenna description and operational setup. These sections will also incorporate data on vacuum vessel and coil locations. Higher dimensional data items such as distribution functions will be added according to the requirements of the project. Prototype code now exists for MCMD support: hash code driven "update only" Plasma State file sections can be serially merged by a driver code, to safely receive the output of concurrently executing parallel components. This capability will be hardened with use. The Plasma State update detection facility may be generalized as appropriate to provide data for CCA-like contract methodologies described in the preceding section. Finally, existing prototype standalone capability will be extended to provide a *data component* that will enable time dependent access to measurement profiles as recorded in archived TRANSP runs in experimental archives. The option to constrain elements of a SWIM simulation to use experimental data will be useful and necessary for V&V activities.

3.1.3 Portal

The SWIM portal is a relatively new capability for the project, and we expect that additional experience with it in the coming months will result in valuable feedback to guide further development, along with several thrusts which have already been identified as important.

We plan to enhance the visual monitoring capabilities for IPS runs in several ways. First, we will develop a generalized monitoring component for the IPS, which provides much greater flexibility over what data to export for monitoring purposes. The plasma state contains hundreds of variables for a simulation run. Researchers need a mechanism for choosing the variables to monitor based on the nature of the run. We will develop a user interface, and integrate it with the portal, to select the variables that are available for monitoring. We will also add support to derive and display certain quantities that are not directly available in the Plasma State, but are useful in monitoring the progress of a simulation. Researchers are also interested in comparing plasma states. We will develop a web service and integrate it with the portal for comparing variables in several plasma states. The interface will enable selecting the plasma states and producing graphs for comparison.

We anticipate adding an authentication capability to the portal, to allow personalization of the information presented, notifications, and privacy control. For example, instead of being presented with a long list of *all* recently active IPS jobs and having to pick out the one of interest, we can present users with a list of only *their* jobs, customized to their preferences.

Our most significant thrust in portal development during the remainder of this project will be to bring the metadata management capabilities to a production level. This will allow users to, for example, identify runs of interest which have already been carried out in order to avoid redundant simulation runs. Not only will this be a valuable capability for the SWIM project itself, but we see it as providing important insight into the data management needs of a larger scale Fusion Simulation Project.

3.2 New Physics Capabilities and Physics Studies with the IPS

In this section we describe some of the new physics capabilities and studies that will be performed using the Integrated Plasma Simulator (IPS) during the next 2-year proposal period. We first describe the new physics components that will be added and next the physics studies that will be undertaken using these and the previously described components.

3.2.1 New or Improved Physics Components

Transport Component. A new Transport Component will be written to provide an interface between the Integrated Plasma Simulator (IPS) and the Transport Common Interface Module that is being developed as part of the "Framework for Modernization and Componentization of Fusion Modules" (FMCFM) SBIR project [Vadlamani08]. The new Transport Component is designed to be a kind of switch-yard that will enable the user to combine neoclassical transport models such as NCLASS [Houlberg97] with well-tested anomalous transport models such as GLF23 [Waltz97] or MMM95 [Bateman98] or with new models that are being developed, such as TGLF [Kinsey08]. The Transport Component will provide a clean interface to the transport models that will facilitate the implementation of new finite difference schemes that have improved numerical stability properties [Jardin08, Pereverzev08]. In addition, members of the FMCFM project are parallelizing transport modules, which will then be available for parallel processing as a component in the SWIM IPS.

Monte Carlo Implementation of Fast Ion Components. A prototype Plasma State based interface to NUBEAM [Goldston81] [Pankin04] has been tested in a development copy of PTRANSP. This interface will be hardened and NUBEAM will be made available for use as a SWIM component. NUBEAM provides an MPI-parallelized Monte Carlo model for deposition and slowing down of neutral beam and fusion product fast ions in an axisymmetric tokamak MHD equilibrium flux surface geometry. The Plasma State now includes a detailed description of the neutral beam geometry, as well as the data necessary to drive the beams (powers, voltages, species and energy fraction mixtures). A development version of NUBEAM includes a Monte Carlo RF quasi-linear operator, which can be tested in the context of the SWIM V&V effort. A separate NUBEAM-based component will be built to provide fast ion deposition only, allowing slowing down to be computed in CQL3D in combination with its quasi-linear RF operator, with the goal of cross verification of the Fokker-Planck and Monte Carlo methods for computing this physics.

It is known that energetic particles produced in ICRF heating can have orbits that exhibit large bananas that deviate significantly from flux surfaces. Particle cyclotron resonances and strong quasilinear diffusion take place on surfaces of constant magnetic field, roughly vertical planes. However, the topology of the orbits of energetic particles can move them away from (or towards) resonances that would be sampled (not sampled) in the full-wave solvers. In order to account for this effect we plan to implement the Monte Carlo orbit code—ORBIT RF—that accurately follows particles. This Hamiltonian guiding center drift code models the wave-particle resonant interactions as an RF-induced random walk process to reproduce the quasilinear diffusion in phase space [Choi05, Choi06].

Energetic Particle Stability Component. Understanding and predicting energetic ion driven instabilities is essential for planning self-sustained burning plasma fusion experiments where they can strongly effect the fusion alphas confinement and plasma performance. One distinct property of alpha particles in fusion plasmas is that their distribution function is isotropic, whereas the interpretation of many present day experiments requires accurate modeling of anisotropic fast ion distribution functions such as in the case of beam injection and ICRH of plasmas with a H-minority. Such modeling needs to be included in the numerical simulations of fast ion driven instabilities.

We are planning to incorporate the state of the art codes available to model the plasma evolution and the distribution function of fast ions produced during ICRH and NBI into the hybrid MHD-kinetic NOVA-K code. As a result, the stability properties of various modes such as Toroidal Alfvenic Eigenmodes (TAE) and fishbones can be studied. In order to do this, we need to develop an effective interface between TSC, NUBEAM, AORSA CQL3D, and NOVA-K. This will be done within the SWIM framework by making the existing NOVA-K code into a component that reads and writes information from and to the plasma state. Since the other four codes are already embedded in components, making NOVA-K into a component will allow them to easily communicate the necessary information.

This will require adding some additional information to the Plasma State component to store the required information about the distribution function. The usage of NOVA-K will be similar to what is being done now for the MHD stability packages for the internal kink stability but will require several additional fast ion and plasma parameters. In particular the distribution function needs to be passed through the Plasma State so it can be read by NOVA-K. We also will develop the capability of a proper parameterization of the distribution function to study the trends of the stability as plasma parameters vary. The later task will include the analysis of the Fokker-Plank equation for ICRH ions to describe H-minority behavior during the ICRH and the slowing down.

Improved Physics Capabilities in RF Components. During the next phase, the GENRAY ray tracing code [Smirnov95] will be implemented as an RF component. This will enable the IPS with the capability to treat lower hybrid current drive (LHCD) as well as electron cyclotron heating and current drive (ECCD). Wave propagation in the lower hybrid range of frequencies (LHRF) is described by integrating the ray equations of geometrical optics. The RF electric field is evaluated along individual ray paths and is used to reconstruct the quasilinear diffusion coefficient (D_{rf}) for the Fokker Planck analysis carried out by CQL3D. The coupling between GENRAY and CQL3D then will be accomplished in the usual way by the framework using the Plasma State.

As part of research activity in the SciDAC Center for the Simulation of Wave-Plasma Interactions, the TORIC ICRF solver is being modified to generate the quasilinear diffusion coefficients required for the SWIM Fokker-Planck solvers, and to evaluate the RF plasma response in terms of non-thermal particle distributions produced by the Fokker-Planck component. This advance will facilitate inter-code comparisons between AORSA-CQL3D and TORIC-CQL3D that will help us to understand the limits of validity of the ion FLR conductivity operator employed in TORIC. It could also reduce the CPU and processor requirement for long time ITER simulations that require frequent calls to the ICRF solver, since the TORIC code inverts a much smaller matrix than AORSA.

3.2.2 New Physics Studies to be Done with the IPS

We will make use of the existing components and the new ones described above to perform the following physics studies which make use of the IPS.

ITER Studies for ITPA Tasks. The SWIM IPS is the most comprehensive modeling tool now available to U.S. physicists involved in ITER modeling and International Tokamak Physics Activity (ITPA) modeling studies. We expect that the framework will be heavily used for studies such as the kind reported in Section 2.2.

The coupling of the parallel versions of the source codes TORIC, GENRAY, AORSA, and NUBEAM to the EPA component TSC will allow modelers to perform high resolution runs where they can model effects of the antennas and beam boxes much more faithfully than previously. The CQL3D will be used routinely to calculate the RF coupling much more accurately than in past studies. We will also improve the density prediction model, include a pellet model, and will use this to perform fueling sensitivity studies.

We also plan to improve the rotation model in the EPA component TSC, and to make use of the momentum sources calculated in the source codes mentioned above. This will allow more accurate transport predictions, since some of the transport models depend on rotation shear. This is a requirement for calculating the advanced modes of operation in which transport barrier formation is an issue.

Sawtooth Modification Experiments Using Mode-Conversion Current Drive. Mode conversion (MC) is a plasma wave phenomenon in which EM waves launched from the antenna can change, in a very short distance, converting to very short wavelength electrostatic or electromagnetic waves inside the plasma

[Perkins77]. This is a difficult multi-scale problem that has only been feasible to simulate with MPP computers [Jaeger03, Wright04]. It is known that sawtooth behavior can be modified, that is, the period can be lengthened (stabilizing) or shortened (de-stabilizing) by respectively decreasing or increasing the current gradient at the q = 1 surface [Bhatnagar94, Porcelli96]. Mode conversion current drive (MCCD) in the ICRF is ideally suited for this purpose since the electron deposition layer is relatively narrow. Sawtooth behavior in tokamaks has been seen to be modified, either stabilizing or de-stabilizing, by ICRF under conditions where MC is thought to be present (see Fig. 3.1). We plan to use the RF, EPA, and stability components to simulate these experiments in order to elucidate the physics of the process. These simulations will be carried out using tens of thousands of processor cores, since the full-wave solvers require very high mode resolution to resolve the mode converted waves in these cases.

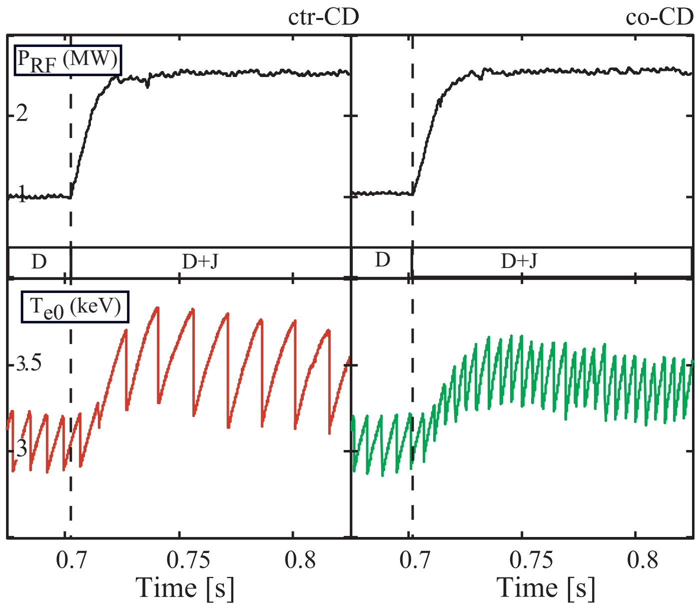

Fig. 3.1. Sawtooth modification experiment on Alcator C-Mod using ICRF mode conversion current drive [Wukitch05].

We plan to use the RF and MHD Components and the TSC implementation of the EPA component to simulate and analyze these experiments. Both AORSA and TORIC can resolve the short wavelength mode converted waves generated in these experiments and can evaluate the driven current density due to the mode converted waves using a parameterization of the local current drive efficiency computed from an adjoint treatment of the Fokker Planck equation [Ehst91]. The resulting current density profiles can then be tested for MHD stability using the MHD Component of the IPS. These simulations will be carried out using tens of thousands of processor cores, since the full-wave solvers require very high mode resolution to resolve the mode converted waves in these cases.

Lower Hybrid Current Profile Control Studies. Off-axis lower hybrid current drive (LHCD) has been shown to be an effective tool for modifying the current profile in a tokamak. Proven applications include optimizing the current profile for access to advanced tokamak (AT) operating modes [Söldner97, Ide98], sawtooth stabilization [Söldner86], and suppression of neo-classical tearing modes (NTM's).

When the GENRAY RF component has been implemented and coupled to CQL3D through the Plasma State, the IPS will have the capability to simulate integrated experiments with both intense ICRH heating and LH current profile control. These types of experiments are currently being conducted in the Alcator C-Mod device, where LHRF power is being used to assess off-axis LH current drive at ITER relevant parameters [Bonoli07]. We plan to use the IPS to simulate these experiments as follows: The TSC code will be used to evolve the discharge subject to a theory-based transport model such as TGLF, while simultaneously invoking two RF and two Fokker Planck components. AORSA or TORIC will be used to compute self-consistent ICRF heating sources through coupling with the ion Fokker Planck calculation in CQL3D and GENRAY will be called to compute LH current drive through coupling with the electron Fokker Planck solver in CQL3D. Finally, the MHD codes will be used to analyze the resulting equilibria for stability to the n=1 external kink mode (when operating near the no-wall β-limit) or for sawtooth modification in experiments where the current profile has been modified locally near the q=1 surface.

Interaction of High Harmonic Fast Waves with Beam Ions. In collaboration with the SciDAC Center for the Simulation of Wave-Plasma Interactions, we plan to apply the IPS to what has evolved into an extremely challenging problem, namely developing an understanding of the interaction of high harmonic fast waves (HHFW) with fast neutral beam ions. This problem is highly relevant to ITER where 20 MW of ICRF heating power will be used in the presence of fast ions from NBI heating and fast fusion alpha particles from fusion reactions.

Implementation of the AORSA and CQL3D codes in the IPS has made it possible to now perform time dependent calculations with a short time advancement (relative to a collision time) of the Fokker Planck equation at each iteration with AORSA, rather than advancing CQL3D to the steady state solution (as was done in the past). Including interim updates of the wave fields and diffusion coefficients in the time dependent Fokker Planck solution is clearly the more accurate approach to the coupled full-wave-Fokker Planck problem and we plan to apply this new simulation capability to HHFW-fast NBI ion interaction experiments in DIII-D.

Over the next two years we also expect the finite ion orbit code ORBIT-RF to be implemented in the Fokker Planck Component of the IPS. With this capability in place it will be possible to repeat the calculations described above that employed AORSA and CQL3D. In this way it will be possible to assess the importance of finite ion orbit effects in the HHFW-fast ion interaction since CQL3D is a zero ion-orbit width code. In these simulations a statistical ion distribution function will be computed by ORBIT-RF and an RF quasilinear diffusion coefficient will be provided by AORSA.

Runaway Electrons during the ITER Startup. Preliminary studies have shown that there is a possible danger of large numbers of runaway electrons being generated during the startup phase of ITER, primarily due to the knock-on effect. We propose to use the IPS framework and EPA components to model and study this phenomenon as realistically as possible. However, because the plasma cross-section is changing during the startup, this will require some modification to the CQL3D code and the associated FP component to accommodate the change since the EPA and Fokker Planck components use different radial grids. We have developed a procedure in which information on the relative grid size in EPA is communicated to the Fokker Planck component through the Plasma State in terms of the time varying total toroidal magnetic flux. We will evaluate under what conditions runaway production will be a problem, and how this is affected by LH and EC wave heating.

3.3 Full 3D Studies of Fast MHD Phenomena

3.3.1 Sawteeth with an Energetic Ion Component (Giant Sawteeth)

Burning plasmas introduce new physics resulting from the interaction between an energetic minority ion species and the fluid plasma. In both NIMROD and M3D this is accounted for by solving the kinetic equations for this species in the presence of self consistent electric and magnetic fields and coupling it back to the fluid equations through the pressure tensor in the momentum equation. [Park99, Kim04]. To simplify the resultant system of equations, it is assumed that the density of hot ions is much less than bulk ion species ($n_h << n_i$) This allows the hot ion inertia to be neglected in the total momentum equation:

$$\rho \frac{d\mathbf{V}}{dt} = \mathbf{J} \times \mathbf{B} - \nabla \bullet \mathrm{P} - -\nabla \bullet \mathrm{P}_h \quad ,$$

where P is the total (electron and bulk ion) stress tensor and P_h is the perpendicular component of the stress tensor contribution from the hot ions.

One effect of the energetic species is to stabilize the resistive internal kink mode in tokamaks. The implication is that burning tokamak discharges may operate well below the resistive MHD limit $q(0) = 1$, at least transiently [Micozzi93], thus creating a "giant sawtooth" [Campbell88] that extends over a large fraction of the cross section. The non-linear evolution of these instabilities will be more violent than the usual sawtooth crash in a non-burning plasma, and may need to be controlled in a fusion reactor (see next section). Both NIMROD and M3D have benchmarked their energetic particle calculation with each other and with the NOVA-K code [Fu94] in the linear regime. We will now have the opportunity to extend these energetic particle benchmark calculations to the fully nonlinear regime as we simulate an entire sawtooth cycle in the presence of an energetic particle component. These simulations will provide a wealth of information on these complex nonlinear phenomena including the triggering events, the subsequent reconnection, the interaction of the energetic particles with the stochastic fields during the crash, the size of the seed islands created, and the redistribution of the alpha particles. These simulations will also provide a unique check on the validity of both the "Porcelli Model" [Porcelli96] that is being used in many transport codes to model sawteeth in a burning plasma in the surface averaged approximation and also on the TRANSP sawtooth hot particle redistribution algorithm.

3.3.2 Study of ICRF Effects on the Sawtooth Mode

In order to avoid giant sawteeth and also to favor ash removal from the core, it may be advantageous to reduce the sawtooth period by reducing the shear around the mode-resonant surface. Another possibility is to operate in a regime where fishbone oscillations replace the internal kink since the fishbone oscillation is a comparatively benign, fast-particle driven version of the internal kink. Control of the internal kink mode with both ion cyclotron heating (ICH) and Lower-Hybrid Current Drive (LHCD) has been demonstrated experimentally, but modeling is needed to extrapolate the system requirements to burning plasma regimes.

The mechanism by which ICRF sources affect the internal kink mode is a resonant wave-particle interaction. This is also true in the ECRF case (discussed in Sect. 3.4), but for ECRF, the dominant wave-particle interaction is at the Landau resonance and is not critical to obtaining the dominant physics of feedback stabilization. In the case of ICRF-generated hot particles, however, the wave-particle resonance of interest to the internal kink mode is the resonances with the precession frequency of the ions. This resonant interaction process with MHD cannot be described as diffusion in velocity space. To model the interaction of resonant interaction of energetic particles with Alfvén waves, the energetic particles are considered as a separate species (even if the ion species is the same as the bulk ion species) with a separate distribution function.

In this proposed work, we plan to study the effect of ICRF-generated hot particles on the internal kink mode. We build upon previous CEMM work of studying the internal kink with a MHD model. To obtain the correct slowing down distribution function, we will use the capabilities developed in the fast MHD campaign to correctly calculate the slowing down distribution function coming from the application of the ICRF sources in ITER. By running AORSA on these equilibria, and using the CGL3D code for calculating the slowing down distribution function, we will be able to systematically study how the ICRF power sources can be changed to control the nonlinear behavior of the internal kink mode. Of particular interest is to study whether the plasma confinement would be improved by destabilizing the internal kink mode to avoid the "giant sawteeth" described above.

3.4 Slow MHD Development, Implementation and Physics Studies

In the first section, we detail our plans for completing the work plan delineated in Section 2.3.2. In the second section, we describe the analytic work that will be done to complete the new formulation outlined in Section 2.3.

3.4.1 Numerical Continuation of Slow MHD Campaign

In Phase 3 of the work plan outlined in Section (2.3.2), we plan to provide a direct interpolation of the GENRAY calculation of the forces onto the NIMROD grid. This will allow us to explore the difficulties of interpolating quantities at arbitrary (R,Z,ϕ) locations onto the NIMROD grid, and calculating the correct finite element basis functions that gives a field that fit the discrete points.

Concurrently with this work, we will use the IPS framework to couple GENRAY and NIMROD in parallel, which will require the newly developed MCMD capability of the IPS framework. It is expected that the RF deposition will change slowly over the time scale of the NIMROD simulation, so we will initially aim to couple the codes such that NIMROD will obtain update sources as fast as GENRAY can calculate them. The procedure is as follows:

1. NIMROD writes the n=0 fields for GENRAY to calculate the RF energy deposition.
2. Framework fields are available and spawns a parallel GENRAY execution.
3. When GENRAY completes, the sources are made available to NIMROD.
4. As NIMROD runs, it inquires if new GENRAY sources exist at each time step. If it does, it reads in the sources, and writes out the n=0 fields. Cycle repeats.

This development can occur independently of the other parts of the proposed work to a large degree, allowing for continuous development. If we find that the results are sensitive to the frequency at which the RF sources are updated, then we will switch to the methods to be developed in the IPS for tighter coupling cases.

After demonstrating that the discrete fields of the GENRAY sources can be imported into the NIMROD representation both accurately and robustly, the next coupling is for NIMROD to import the full quasilinear diffusion operator and perform the velocity space integrals. As this capability becomes available, we can begin to understand how the new mathematical formulation compares to GENRAY for current equilibration. By running an $n=0$ simulation, we can compare the predicted current deposition with the predictions used by GENRAY in transport modeling. This will serve as one test of the importance of the closures.

The final phase of this work is to incorporate the integral closures that include the RF sources. As these closures become available, we will further extend the $n=0$ benchmark described above.

3.4.2 Completion of Analytic Formulation of the Extended MHD Equations with RF Sources

There are a number of outstanding issues with the development of the extended MHD equations with RF sources, especially in the consistency of the assumptions between the RF codes and extended MHD equations. We will continue the theoretical work on the drift-kinetic equations used for the parallel closures of our RF/MHD model. Additional explicit forms will be derived for the phase-space time derivative operator, the collision-independent CEL source terms and the collision operator in the electron equation. The completed analysis of the phase-space time derivative operator and the collision-independent CEL source terms in the electron drift-kinetic equation was carried out under a fast dynamics or MHD ordering, whereby the time derivatives and flows were assumed comparable to the sound transit frequency and the sound velocity respectively, with first-order FLR corrections on the diamagnetic drift scale. However, the realistic time scales and near-equilibrium flows for the NTM are significantly slower and better approximated by a diamagnetic drift ordering. Consideration of the slow dynamics, drift ordering in the electron drift-kinetic equation will be our first new proposed task.

A study of the collision operators is also proposed, aimed at producing explicit, gyrophase-averaged forms to be used in the drift-kinetic equations. These will be based on new asymptotic expansions in powers of the ratio δ between the ion sound gyroradius and the macroscopic lengths. The collisionality ordering adopted in conventional neoclassical transport theory may be too high for a realistic thermonuclear plasma. We propose an alternative, low collisionality ordering such that the ratio between the ion collision and cyclotron frequencies is comparable to δ^2. This is to be complemented by ordering the deviation from Maxwellian distribution functions as first order and the electron to ion mass ratio as second order in δ.

The velocity moments of the distribution functions involved in the macroscopic fluid equations (i.e. the stress and heat flux tensors, the collisional friction force and heat exchange rate, and the RF-induced sources of momentum and energy) are defined relative to the macroscopic flow velocity of the plasma species under consideration. If the drift-kinetic equation is solved in the laboratory frame, this macroscopic flow must be subtracted when taking the relevant velocity moments. We have found it far more convenient to solve the drift-kinetic equation in the moving reference frame of the macroscopic flow. The addition of collisions poses no problem due to the Galilean invariance of the Fokker-Planck operator. The RF quasilinear diffusion operator is normally expressed in the laboratory frame and is not manifestly Galilean invariant. Therefore, unless the flows are sufficiently slow, the transformation to the reference frame where the rest of the drift-kinetic equation applies must be carried out. As an alternative to the brute force application of this change of reference frames, the possibility of a Galilean-invariant form of the quasilinear RF operator will also be explored. ECCD does not affect the ion equations, but a consistent closure of the ion equations is still needed. We also propose an ion drift-kinetic analysis along the lines followed for the electrons.

3.5 Math and Other Advanced Studies

3.5.1 Ongoing Interactions with CETs

APDEC: We will continue to collaborate with APDEC in further developing the AMR MHD code suite to simulate pellet injection and ELMs. These codes will eventually be connected to the SWIM framework. The current emphasis of this work is to implement implicit time stepping, based on the Newton-Krylov (NK) approach. Initial tests of this method (in collaboration TOPS Center) show great promise [Reynolds06].

ITAP: We are collaborating with ITAPS researchers X. Luo, K. Jansen, and M. Shephard at the Rensselaer Polytechnic Institute. This collaboration has led to SCOREC software for adaptive unstructured grids which has been implemented in the M3D-C^1 code. We plan to further expand the capabilities in these areas.

TASCS: Work on the IPS framework continues to be closely associated with TASCS and the Common Component Architecture. The CCA provides models for many of the concepts implements, usually in simplified form, in the IPS, and provides feedback to spur future CCA development directions.

TOPS: We will continue our very fruitful collaboration with TOPS. Both NIMROD and M3D make use of the TOPS linear solvers and we interact frequently with the PETSc and other TOPS developers. A new emphasis is to use a modified version of SuperLU_DIST as an incomplete LU pre-conditioner for iterative solves.

SDM: We are continuing to collaborate with the DOE Scientific Data Management Center in exploring ways to facilitate rapid and seamless data transfer and storage.

VACET: We are collaborating with the DOE SciDAC Visualization and Analytic Center for Enabling Technologies. With the assistance of this center, we plan to make much more use of the VISIT visualization system during this period, and to have some new discipline-specific capabilities made available.

3.5.2 Particles to Distribution Functions

Many plasma physics codes used in the SWIM project use a collection of discrete particles to calculate and provide a numerical representation of a non-Maxwellian distribution function. Examples of this are the NUBEAM calculation of neutral beam injection and alpha particle heating, ORBIT-RF and the hybrid MHD/kinetic calculations in NIMROD and M3D. Other codes, such as the NOVA-K linear stability code and the CQL3D Fokker-Plank code, use a PDE based continuous representation of the distribution function.

We seek to develop standard tools for going from one representation to the other. Obtaining a smooth particle distribution function on velocity grid without much sacrifice in computing time can be beneficial to several key problems in SWIM and to the particle codes in general, and is being developed in the CPES project. SWIM proposes a close collaboration with CPES to leverage this activity, since other particle codes can benefit when particle operations and continuum operations are to be used together. In these techniques, the first step is usually to put the local particle information on a v-space grid. Finiteness of the local particle number is bound to generate noise in the v-space grid information. Smoothing of the v-space information, with conservation of the velocity moments to desired accuracy, can benefit the subsequent mathematical operation. Such techniques, called penalized splines, already exist [Eiler96], and a code has been generated to study this problem by a CPES graduate student (Rao, Columbia). Their code, which interfaces to the PETSc library for nonlinear implicit solves, ensures nonnegative values of the probability density and has required conservation properties, through the matching of higher moments of the particle data in the distribution. The code uses Newton's method, and in any particular context, requires work on the linear system preconditioner. In the context of SWIM's particle-PDF work, we will invest independently on the preconditioning of the linear systems in the Newton implementation.

3.5.3 Parallel Load Balancing

Due to the wide range in parallel scalability of plasma physics codes, it can be very difficult for a coupled simulation to effectively utilize all computational resources allocated to a job throughout the entire course of the simulation. To complement on-going work in SWIM and elsewhere in the community to improve the scalability of individual codes, we are also investigating other ways to improve the parallel load balancing for coupled simulations that can work with existing codes.

The core idea behind our approach is to find ways to increase the number of computational tasks that can run simultaneously, and utilize the framework's MCMD capabilities described above to implement them. Increased parallelism might come from more detailed analysis of data dependencies within simulations, or from creative manipulation of the problem itself to expose more parallelism while achieving the same physics results.

A simple example of the latter involves linear and nonlinear stability analyses. Instances of these components can be run in parallel with source components (sources of heat and particles), and the data from both fed into the next time step of the profile advance component. A more complex example might be a "leapfrog" time-stepping approach, in which the coupling between different components might lag by a step in order to allow the two to be run simultaneously. The possibilities will depend on the specific simulation scenarios, and will have to be carefully analyzed, but if the approach shows sufficiently broad applicability, we would examine more convenient ways to express the drivers for such simulations, for example, based on data dependency graphs.

Another related possibility is to run two (or more) separate simulations simultaneously on the same set of nodes, under a single IPS instance. The simulations would be run out of phase, so that highly parallel components in one simulation share the resources with low parallelism components in the other, and vice versa. Run in this way, each simulation might take longer to complete than it would have run independently, but the overall resource utilization would be much better. This would require extending the IPS framework beyond the MCMD capabilities to support the idea of multiple simulations being run at once, primarily involving data management service, and in the handling of the drivers.

3.5.4 Parallel TSC/TGLF

The TSC code both evolves the plasma equilibrium and evolves a set of 1D surface averaged transport equations for the plasma temperatures, densities, and toroidal rotation, and for the magnetic field transform. The transport part of the calculation uses a block tri-diagonal solution algorithm. TSC is a legacy code that is completely sequential, and this has historically been sufficient since the transport part has not been a very time consuming part of the entire calculation and the tri-diagonal algorithm is very efficient.

However, two developments have changed this picture. One is that TSC is now part of the SWIM IPS, and since many components of the IPS are highly parallel, Amdahl's law can be used to show that the sequential nature of TSC will reduce the parallel efficiency of the entire calculation. The second development is that the transport models that are used to compute the thermal conductivities and particle diffusivities have become compute intensive themselves. The latest model, known as TGLF, involves a complex subsidiary micro-stability calculation at each surface, and can take minutes to return a value for the thermal conductivities at a given surface. Keeping TSC as a sequential code when using TGLF would seriously affect the timing and load balancing of the entire IPS.

We thus propose to parallelize the 1D surface averaged transport calculation in TSC. This will be done by modifying the Tri-Diagonal Newton Solver described in 2.3.1 [Jardin08] so that a parallel tri-diagonal algorithm is used. More importantly, all the evaluations of TGLF will be performed concurrently. Since we typically have 100 flux surfaces, and each surface needs to evaluate TGLF at least six times each iteration in order to evaluate the thermal conductivity and its functional derivatives, we can immediately obtain a factor of 600 speedup if that number of processors are available.

3.6 Verification and Validation (V&V) Strategy and Plan

Verification ensures that a software package correctly implements the planned data flows and algorithms. That is, the programming is correct. Validation confirms that the software, as provided, will fulfill its intended use. Both are essential elements for reliable integrated fusion simulation. For SWIM, V&V for individual components and for their physics and algorithmic interactions is required. For component V&V, SWIM builds on the V&V programs of the two SciDAC projects that provide key physics codes: the Center for Simulation of Wave Interactions with Plasma (CSWIP) and the Center for Extended MHD Modeling (CEMM). The RF codes TORIC and AORSA codes are key elements of CSWIP, while the non-linear extended MHD models NIMROD and M3D are core codes for CEMM. Within CEMM there is an extensive program to benchmark M3D and NIMROD against each other and against experiments. Similarly, the CSWIP is focusing on minority heating on CMOD and interactions with energetic fast ions from neutral beam injection on NSTX and DIII-D. Thus the SWIM V&V program focuses on the framework and on project-specific software (particularly the state) and on the interactions of components, particularly through the IPS. The V&V plan includes the following elements:

Verification. Our verification efforts are focused on the framework, configuration file behavior and driver component performance. The component strategy of the IPS allows "dummy" components to be implemented with little physics content or computational work. This class of components is discussed in Section 2.1.2. When a simulation is run that utilizes these components, the results are trivially known. The Monitor component, with its plotting capability, allows ready confirmation of the expected performance. These verification tests, as discussed below, will be incorporated into regression tests.

Component and IPS Benchmarking. Multiple instances of specific physics components have been implemented and more are planned for the future. Present examples include the TORIC and AORSA wave-plasma codes, the M3D and NIMROD nonlinear stability codes, and multiple linear stability models. The IPS design allows multiple component implementations to be run on the same physics data and also allows direct comparison of their outputs. When, for example, plasma parameters are such that both AORSA and TORIC should be valid, we should expect to see the same or close to the same results.

These interfaces also allow sensitivity studies as to the effects of grid resolution and various options that are specific to an individual code. Results of such studies for an ITER simulation are presented in Section 2.2.3. We propose to continue these studies with emphasis on those components whose validity depends on plasma physics regime. These include ICRF components, Fokker-Planck components, and stability components.

Additional benchmarking studies will be carried out using a systematic protocol for benchmarking the Transport Component in the IPS by comparing simulation results with corresponding simulation results using the PTRANSP integrated modeling code. There are important problems that both the IPS and PTRANSP can address, and we will compare the results for the same problem input.

Comparison with Analytic and Reduced Models. In many cases and for particular parameter regimes, analytic solutions to implement the functionality of a component are possible. For example, the distribution function of a resonant, low density ion species can have an RF-driven tail. If the interaction is assumed to be isotropic, then an analytic solution to the Fokker-Planck equation is possible [Stix92]. In a similar vein, the two-fluid terms in the extended MHD codes have been validated by comparing against analytic results of the gravitational instability in simple geometry [Ferraro06]

Comparisons with Experiments. As described in Section 2.2.1, a campaign is underway to simulate Alcator C-Mod experiments. The plasmas for these experiments are dominantly composed of deuterium with a few-percent hydrogen minority. The minority is resonantly heated by 80 MHz RF power. These experiments exhibit sawtooth oscillations (a manifestation of internal disruptions) whose period and amplitude are affected by the RF power. In addition, the minority hydrogen has an RF-driven non-Maxwellian tail. These experiments are an excellent target for understanding the time-dependent dynamics of such tails and for understanding how RF heating affects internal disruptions. These physics studies depend on the integration of transport, ICRF, Fokker-Planck, and linear and non-linear stability components.

Several experiments have conducted experimental campaigns demonstrating the stabilization of NTMs with ECRH. There is a wealth of data available, particularly on DIII-D. As our modeling in this area matures, we will begin systematic comparison with experimental results, trends, and scalings.

For both campaigns, synthetic diagnostics within the physics components will be utilized for detailed comparisons with data. Fast neutral particle diagnostics provide detailed data on the dynamics of fast ion tails for the fast MHD campaigns (Section 3.2.2). Similarly, soft x-rays and electron cyclotron emission give insight on plasma response for the slow MHD campaign (Section 3.4). The current case is in DIII-D geometry, and initial comparisons of gross measurements such as the required current amount and stabilized island size are underway. Use of a synthetic diagnostic will allow for more detailed comparisons.

Regression Testing. Implementation of routine regression testing major elements of the IPS is proposed for this extension. The structure of the IPS framework allows ready implementation of regression testing and other intercomparisons. New tools will be implemented within the IPS, leveraging existing utilities such as the Plasma State's cstate tool and other tools for the manipulation of netCDF files, to allow easily configured comparisons of data in different Plasma States and reporting of differences. For example, the components, driver, and configuration files needed to run an AORSA reference case have been implemented. The new tools will allow the results of the test run to be automatically compared against the "gold standard" reference result. Thus, after a successful checkout and build, a one-line script is all that is needed to run this case. The percentage of RF power delivered to the plasma species then provides the basis for success/failure decisions. Similar reference cases are available for CQL3D (a Fokker Planck component) and for coupled AORSA-CQL3D simulations. Additional regression targets will be developed as the need is identified.

3.7 Project Milestones

FY 2009	Milestone	Responsible institutions
IPS Development	Full MCMD capability in framework	ORNL, IU, PPPL
	Preliminary implementation of tight coupling capability	ORNL, IU, PPPL, CU
	Add generalized monitoring component and web interface	PPPL, ORNL, GA
	Add authentication and personalization capabilities to portal	GA
	Bring existing portal metadata management capabilities into production	GA
Physics component development	Add NUBEAM component	PPPL
	Add component for experimental data access	PPPL
	Add Transport component	Lehigh, PPPL
	Add GENRAY component	CompX
	Add ORBIT-RF component	GA
	Develop and implement mapping/smoothing algorithms for particle based phase space distributions	ORNL, PPPL, CU
IPS applications	Evaluate runaway electrons in ITER	PPPL, CompX
	Finish time-dependent simulations of ICRF minority ion tail in Alcator C-Mod	MIT, ORNL, PPPL
	Simulate LHCD + ICRF in Alcator C-Mod	MIT, CompX, PPPL
Fast MHD campaign and sawtooth studies	Initial simulation of sawteeth with energetic ion component	PPPL, Wisconsin
Slow MHD campaign and NTM studies	Couple GENRAY's quasilinear operator to NIMROD, using the IPS framework	ORNL, Tech-X, CompX, UW-M, USU
	Perform NTM simulations that explore the effect of the ECCD source modulation	UW-M, Tech-X, CompX, USU
	Complete analysis—electron Chapman-Enskog-like drift-kinetic equation, electron phase-space time derivative operator, and collision operator with diamagnetic drift ordering	MIT, USU

FY 2010	Milestone	Responsible institutions
IPS Development	Full implementation of tight coupling capability	ORNL, IU, CU, PPPL
	Prototype implementation of explicit interfaces for file-based data exchange	ORNL, PPPL, IU
	Enhance and extend portal metadata management capabilities based on user feedback	GA
	Implement a web service utility for comparing plasma states	PPPL
	Develop project documentation	All participants
Physics component development	Parallelize the TSC/TGLF transport advance	PPPL
	Add NOVA-K energetic particle component	PPPL
	Implement non-Maxwellian TORIC as a component	MIT, ORNL
IPS applications	Paper comparing LHCD + ICRF simulations with C-Mod experiment	MIT
	Compare AORSA vs TORIC time-dependent simulations of ICRF minority ion tail in Alcator C-Mod	MIT, ORNL, PPPL
	Simulate LHCD + ICRF in Alcator C-Mod	MIT, CompX, PPPL
Fast MHD campaign and sawtooth studies	Second generation simulation of sawteeth with energetic ion component and ICRF	PPPL, Wisconsin
	Simulate sawtooth modification via MCCD in C-Mod	MIT, PPPL, ORNL
	Simulate interaction of high harmonic fast waves with beam ions	GA, ORNL
Slow MHD campaign and NTM studies	Transformation of RF quasilinear diffusion operator to the macroscopic flow	MIT
	Analyze ion drift-kinetic equation under MHD and drift orderings an expansion of the collision operator	MIT
	Develop synthetic soft X-Ray diagnostic, perform detailed structure analysis of stabilized mode, and compare with experiment	UW-M, Tech-X, CompX, USU
	Perform NTM simulations with integral closures	USU, UW-M, Tech-X, CompX

4. BUDGET SUMMARY

Institution	Primary work elements	Year 4	Year 5	Total
ORNL	All	760	760	**1520**
PPPL	All	585	585	**1170**
U. Indiana	Framework development	72	73	**145**
MIT	RF and Slow MHD theory	100	100	**200**
GA	Portal and Monte Carlo Fokker Planck	125	125	**250**
U Wisc.	Slow and Fast MHD	100	100	**200**
Columbia U.	Applied math	55	55	**110**
Lehigh U.	Transport component and IPS bench marking	50	50	**100**
TechX	Slow and Fast MHD	50	50	**100**
CompX	Fokker-Planck, Geometrical optics RF	75	75	**150**
Subcontracts		28	27	**55**

5. MANAGEMENT PLAN

Project Management Team: D. Batchelor will be the Project Principal Investigator (PI) with three Co-Principal Investigators—S. Jardin (PPPL), D. Bernholdt (ORNL), D. Keyes (Columbia U.)

The PI and Co-PIs will have dual responsibilities to coordinate both within a scientific discipline and also for a project element:

Jardin—Extended MHD and fast MHD campaign

Bernholdt—Computer Science and Architecture development (replacing Randy Bramley)

Keyes—Applied Mathematics and Algorithms

Batchelor—RF-Plasma Interactions and slow MHD campaign

In addition to these project responsibilities, the Co-PIs also are responsible for coordinating SWIM activities with corresponding communities, particularly the relevant SciDAC projects, including CEMM (Jardin), CSWPI (Batchelor), Computer Science CETs (Bernholdt), and Mathematics CETs (Keyes). In addition Batchelor will be responsible for coordination with ORNL CCS and NERSC computer centers.

Advisory Committee. Our user/advisory committee, which was appointed by the PI and Co-PIs, contains a representation from the fusion experimental and modeling community to help us ensure that the system developed meets the simulation needs of the fusion community users, plus members with backgrounds in physics simulation and large-scale code development. The members are Charles Kessel (PPPL), Masanori Murakami (ORNL/GA), Andrew Siegel (ANL), and Alan Sussman (U. Maryland).

Roles and Responsibilities. The PI has responsibility for overall project coordination with authority over resource allocations. The PI has responsibility for formal interactions with DOE. To the maximum extent possible, actions are based on consensus among the PI and Co-PIs. PI and Co-PIs coordinate technical work across the project in their discipline and element of responsibility and assign priorities for work on particular tasks. Task Co-PIs plan the tasks for project elements and monitor the progress of team participants. The PI and Co-PIs jointly identify project issues and develop plans to address them.

Project Meetings and Reporting. Project wide meetings will be approximately three times a year. At least one will be a dedicated project meeting involving the advisory committee. The other meetings may be in association with technical conferences or combined with other SciDAC CEMM of CSWPI meetings. The PI/Co-PIs hold periodic remote collaboration meetings often weekly and at least every four weeks depending on project status.

Outreach and Interaction with the Computer Science, Applied Mathematics and Plasma Physics Communities. Through a program of presentations at technical conferences, workshops, highlight reports, and a project webpage, especially during the first phase, the project will continue to involve the community in the development of fusion-specific standards for data types and code interfaces and will establish a technical presence in order to allow adoption of its models and codes. The project will work to advance project goals by encouraging work in related research areas. The SWIM project supports a post doc and involves 6 graduate students.

Collaborations are an integral part of the SWIM project. Many of the collaborations with the other fusion SciDAC projects and ASCR CSET projects are described in the previous sections. In addition we have established collaborations with related efforts in Europe and Japan through the International Tokamak Physics Activity (ITPA). In particular we have a technical exchange with the Europeans on simulation data structures—the Plasma State on the US side and the Universal Access Layer XML schemas on the European side.

Special mention should be made of the open relationship that exists among the FSP pilot projects (SWIM, FACETS and CPES). We participate in each other's project meetings and include each other on our project email distribution lists. There is an overlap in the project participants. There is also substantive technical collaboration between projects. FACETS is employing the Plasma State for some of their data communication, and it directly supported the development of the C/C++ Plasma State interface. We are also collaborating on development of the Transport Common Interface Module. We are also exploring technical exchanges with CPES on several fronts, including application of the Plasma State to communicate data between the SWIM RF codes and CPES PIC codes and application of the Kepler workflow to the IPS. We regard our respective projects as complementary with respect to developing an experience base for design of the FSP.

6. FACILITIES REQUIREMENTS

The applications being developed by SWIM will require extensive computer resources. The actual resources available will determine the allowed resolution, simulation time, and detail of the modeling. These in turn will determine what range of physical parameters can be realistically modeled and the number of scenarios (particularly important for ITER) that can be realistically simulated. To set the scale, the CEMM and CSWPI projects have utilized 5–10 million cpu-hours (MCPU) per year over the past several years with a combination of INCITE awards at the NLCF at ORNL and OFES awards at NERSC. In addition to these computational resources, SWIM makes extensive use of the collaboration server at ORNL. This server is outside of the firewall, and provides access by team members to both project software and technical documents.

The 32 processor SGI Altix 350 was installed at PPPL and has been the core facility for IPS software development over the past two years. When needed, the greater capability of the 256 processor Loki cluster at MIT has been valuable for RF component development. During FY 2007, the project utilized a two MCPU INCITE award on the NLCF Jaguar for porting and optimizing component codes to meet SWIM requirements. Physics research utilized the SWIM framework for, mainly, single component simulations. This year, SWIM is utilizing a 0.4 MCPU Director's award for framework testing and (now underway) initial physics runs.

The project will require significant storage on intermediate and archival timescales. We estimate 12 Tbyes for source codes, metadata, data exchanged between components, simulations results, and post-run analysis artifacts. Some of this will be supplied by NERSC and the NLCF. For these facilities, I/O files must be staged before and after runs using the Lustre parallel system. Some storage and cluster resources will also be made available at Indiana University and at PPPL.

SWIM resource requirements will rise sharply during for this proposal. We will apply for INCITE and NERSC awards to meet these needs. Our present estimates of two-three MCPU-hours for 2009 and four-five MCPU for 2010 will be refined over the next few months as we complete our first integrated physics runs.

7. CONCLUSION

We have assembled a cross-disciplinary, multi-institutional team that is working very effectively to create a new capability for integrated modeling of toroidal plasmas. Our center has built an end-to-end computational system (the IPS) that allows existing physics codes, essentially without change, to function together in a parallel environment and connect to utility software components and data management systems.

The IPS design is based on a component architecture in which the various required physics functionalities have been abstracted at a high level. Formal interfaces have been defined such that the components can be implemented by any code that provides the required functionality, so that multiple code implementations can be used. The IPS is implemented as a lightweight framework written in Python, which orchestrates the execution of a collection of physics components, primarily written in Fortran90. An important element of the IPS is the Plasma State, a software component that serves as the mechanism for sharing of time evolving data across the various physics models in the IPS. The Plasma State is now being used in several projects outside of SWIM. The IPS has been implemented on an SGI Altix at PPPL as well as on the quad-core XT4 (Jaguar) at NCCS.

The IPS is being used in code benchmarking studies, ITER scenario studies, and simulation studies related to the Fast MHD campaign. Applications include: detailed comparisons using the AORSA full wave ICRF code to verify PTRANSP simulations for ITER; time dependent modeling with AORSA, CQL3D and TSC of energetic minority ion tail formation in Alcator C-Mod and comparison with experimental measurements; a high-resolution simulation of the 200s approach to flattop of an ITER hybrid scenario discharge with TSC using the parallel NUBEAM neutral beam injection package and TORIC for ICRF. In the Slow MHD campaign we have (1) developed a self consistent fluid model that includes effects of ECRF modifying the distribution function in the extended MHD equations, (2) developed an approach to calculate closure relations including RF sources and (3) developed a staged plan of numerical implementation that begins with phenomenological RF and closure models, and proceeds ultimately to self consistent RF calculations and numerical closures. We have also performed preliminary studies with NIMROD on classical tearing modes in tokamak geometry, including specified RF driven current perturbation, and demonstrated non-linear island shrinkage.

The proposed work in the final phase should allow us to meet all of the project goals. For the further development of the IPS, the emphasis is on tighter coupling of codes that for performance or algorithmic reasons cannot are hampered by coarse code granularity and the predominantly file-based communication used so far. Additional work on concurrent component execution will allow exploration of innovative approaches to load balancing and component time stepping. New physics capabilities to be introduced will broaden the scope of possible physics investigations. We will demonstrate capability of the SWIM system to address important questions of sawtooth instability and neoclassical tearing mode behavior and their control by RF in numerical simulations carried out in our Fast MHD and slow MHD campaigns. We are now at a point to explore the possibilities and limitations of our architecture for full integrated plasma simulations and are in a position to gain experience that will be valuable in guiding development of the Fusion Simulation Project.

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BIOGRAPHICAL SKETCHES

OAK RIDGE NATIONAL LABORATORY

Donald B. Batchelor is the Plasma Theory Group Leader at Oak Ridge National Laboratory. He has been at ORNL since receiving his Ph.D. in Physics from the University of Maryland in 1976, and has more than 70 refereed publications. After joining ORNL, he began working on the Elmo Bumpy Torus and developed one of the first geometrical optics codes for a relativistic plasma in the vicinity of cyclotron resonances. In 1984, he formed a group to study a broad range of RF problems including ion cyclotron heating in complex geometries. He was instrumental in initiating the development of the ORION, PICES, and RANT3D RF codes. These models have been central to the design and analysis of RF heating experiments including TFTR at Princeton, DIIID at General Atomics, and JET, as well as for ITER. Other research interests include the development of innovative plasma confinement systems. He led the development of a Small-Aspect Ratio Stellarator-Tokamak Hybrid (SMARTH) that has since developed into the Quasi-Poloidal Stellarator (QPS) experiment at ORNL, an element of the U.S. Compact stellarator program. Don was the principal investigator on the DOE SciDAC project on wave-plasma interactions. Since 2005 he has been the principal investigator for the SWIM SciDAC project. His publication in Physics Today of an article on Fusion Simulation is indicative of his impact in the area. He is a fellow of the American Physical Society.

Lee A. Berry is a Senior Research Staff Member in the Fusion Energy Division’s Theory Group at Oak Ridge National Laboratory. His research experience covers a wide range of experimental and theoretical plasma physics topics including tokamak, bumpy torus, and stellarator experiments and theory. His current plasma research includes stellarator experiments (Deputy Project Manager for the Quasi-Poloidal Stellarator at ORNL), and RF-Plasma theory and computational modeling through the SciDAC RF-Plasma Interactions project. Contributions have been in the areas of neutral beam heating, bumpy torus experiments and design, stellarator design and analysis, fusion technology, semiconductor process tool experiments and modeling, RF flow drive, and algorithm development for the AORSA full-wave code. He received his Ph.D. from the University of California at Riverside in 1970 and has been at ORNL since then. He is a fellow of the American Physical Society, and was awarded the DOE Distinguished Service Award for his leadership on the ORNL bumpy torus program. He has served on a variety of Division of Plasma Physics Committees and on the Office of Science’s Fusion Energy Science Advisory Panel, as well as subpanels under FESAC. He is currently Chair of the Coalition for Plasma Physics, and a member of the UCLA Plasma Science and Technology Institute Ad Hoc Committee.

David E. Bernholdt is a Senior R & D Staff Member in Computer Science at ORNL, where he has worked since 2000. Bernholdt's formal training is in chemistry, with a B.S. in 1986 from the University of Illinois and Ph.D. in 1993 from the University of Florida. He was a postdoctoral fellow at Pacific Northwest National Laboratory 1993–1995. From 1995–2000, he was at Syracuse University, as an Alex Nason Fellow and a Senior Research Scientist in the Northeast Parallel Architectures Center, and a Research Assistant Professor in the Chemistry Department. Bernholdt's primary research focus is on means to improve the performance and productivity of HPC software developers and their software. He is the lead PI of the SciDAC Center for Technology for Advanced Scientific Component Software (TASCS), the leading developers of the Common Component Architecture (CCA). He is also the ORNL lead PI and an Executive Committee member for the SciDAC Earth System Grid Center for Enabling Technology (ESG-CET) and a participant in the Coordinated Infrastructure for Fault Tolerant Systems (CIFTS) project. He is the author of more than 80 peer reviewed publications and has given more than 90 technical presentations.

Eduardo F. D'Azevedo is group leader for the Computational Mathematics Group at the Computer Science and Mathematics Division, Oak Ridge National Laboratory. He is co-author of one book and over 20 refereed publications. His current research includes: optimal mesh generation, vectorized iterative solver, out-of-core dense linear solvers, and application specific preconditioners. He received his Ph.D. in 1989 in the Faculty of Mathematics (Department of Computer Science) from the University of Waterloo, Ontario, Canada. He held an ORISE postdoctoral fellowship from 1990–1991, and has been a research staff member at ORNL since 1991. He is a member of the Society for Industrial and Applied Mathematics.

Wael Elwasif obtained his Ph.D. in Computer Science from the University of Tennessee, Knoxville, in 2004. He joined the computer science and mathematics division, ORNL in 2000, where he conducted research in heterogeneous distributed computing and component models for high-performance computing. Dr. Elwasif's research interests include parallel and distributed computing, component models for large-scale High-Performance Computing (HPC), HPC language interoperability, and large-scale parallel programming models.

E. Fred Jaeger is a senior research staff member in the Plasma Theory Section of the Fusion Energy Division, Oak Ridge National Laboratory (ORNL). He has co-authored over 61 refereed journal articles, seven invited papers, and 63 papers published in major conference proceedings, and has served on several Department of Energy review panels. His research has covered a broad range of topics in plasma physics theory and computation with applications to fusion plasmas, plasma processing of materials, gas lasers, and space plasmas. Most recently, he has developed tera-scale parallel simulations of radio frequency interactions in tokamak and stellarator plasmas. These simulations, developed under SciDAC, have become valuable tools for understanding electromagnetic wave propagation and heating in 2-D and 3-D plasmas. He received his Ph.D. in Nuclear Engineering from the University of California in 1970, and held postdoctoral fellowships at the National Center for Atmospheric Research, Boulder from 1971–72, and at the Joint Institute for Laboratory Astrophysics, Boulder, from 1973-74. He has been at ORNL since 1974.

Vickie Lynch is a research staff member of the Modeling and Simulation Group in the Computational Science and Engineering Division, Oak Ridge National Laboratory. She works with the Scientific Computing group at the Center for Computational Science as primary liaison for two plasma physics projects on the Jaguar parallel computer and is a TeraGrid staff member supporting the Neutron Science TeraGrid Gateway with parallel neutron science simulations and data analysis. In 1979 she received an MS in Applied Mathematics from the University of Tennessee and won the student paper award for the southeast section of SIAM for the presentation of her thesis, "A Comparison of Several Methods for Solving Second-Order Damped Systems of Ordinary Differential Equations." Since 1979 she has worked with the Plasma Theory Section of the Fusion Energy Division doing numerical calculations of turbulence and transport problems using the supercomputers at both NERSC and ORNL. Research interest include numerical calculations of fusion energy turbulence and transport, numerical methods for solving PDEs with fractional derivatives, analysis of experimental data, tracer particles in 3-D parallel turbulence calculations, pictures of quasi-coherent resistive ballooning structures, and calculations of the dynamics of blackouts in electric power systems. She is an author or coauthor of over 100 refereed publications.

Donald A. Spong is a senior research staff member and group leader for stellarator plasma theory in the Fusion Energy Division of Oak Ridge National Laboratory. He is an author on about 100 publications. His current plasma research interests include particle-based closure relations for MHD problems, stellarator neoclassical transport using Monte Carlo and fluid moments methods, fast particle-destabilized Alfven modes in stellarators, and applications of scientific visualization to plasma physics problems.

Previously he has worked in the areas of stellarator optimization, gyrofluid and neoclassical closures for resistive MHD and fast particle instability problems, alpha particle physics, kinetic ballooning modes, plasma processing of semiconductors, hot electron instabilities, and runaway electrons in tokamaks. He has served on the Program Advisory Committee for the National Energy Research Supercomputing Center, the ITER Expert Group on Energetic Particles, and as a reviewer of Plasma Theory proposals for the Office of Fusion Energy, DOE. He received his Ph.D. in Nuclear Engineering (plasma physics and controlled fusion) from the University of Michigan, Ann Arbor, in 1976. He has received the 2001 ORNL Research Team Award for development of the Quasi-Poloidal Stellarator, the 1994 Martin Marietta Author of the Year Publication Award, and the 1988 Martin Marietta publications Award.

INDIANA UNIVERSITY

Randall Bramley received a Master's degree in computational mathematics and then a Ph.D. in computer science at the University of Illinois-Urbana/Champaign in 1989. After three years as research scientist at the Center for Supercomputing Research and Development at UIUC, he moved to Indiana University where he is currently an associate professor of Computer Science, adjunct professor in Informatics, creator and director of the multidisciplinary Scientific Computing Program, and a senior research scientist in the Pervasive Technologies Labs at Indiana University. He currently has collaborations in x-ray diffractometry, astronomical photometry, geophysics, molecular modeling, bioinformatics, and biophysics. His research interests have ranged from numerical analysis to systems development, particularly in distributed scientific computing, direct access to scientific instruments through web services, and large-scale data management. He has co-edited one book on problem solving environments, has over 40 refereed publications, and is a founding member of the DOE Common Component Architecture Forum.

Samantha Foley received a B.S from SUNY Fredonia in 2004, and a Master's degree from Indiana University in 2007, in computer science. She is currently a Ph.D. Candidate at IU working on scientific computing, specifically component coupling frameworks for multiphysics simulations.

PRINCETON PLASMA PHYSICS LABORATORY

Joshua Breslau is a staff research physicist in the Theory department at the Princeton Plasma Physics Laboratory. He received a B.S. in physics from MIT in 1995 and a Ph.D. in plasma physics from Princeton in 2001. His doctoral research, with Stephen Jardin, involved a numerical study of fast collisionless magnetic reconnection with an original parallel semi-implicit fluid code. For this work, he was awarded the Procter Honorific Fellowship by Princeton University, as well as the Grimm memorial prize for achievement in computational physics. For his postdoctoral and subsequent work, also at PPPL, Dr. Breslau joined the group responsible for the development and maintenance of the Multilevel 3D (M3D) code and has become its primary developer. His research topics with this code have included detailed studies of the formation of "current holes" observed in JET discharges; and extensive modeling of resistive internal kink instabilities in tokamaks.

Morrell S. Chance is a Principal Research Physicist in the Theory Department at the Princeton Plasma Physics Laboratory (PPPL). He received his B.S. at Yale University where he was awarded the First Benjamin F. Barge prize in mathematics. He received his Ph.D at UCLA in 1972. After been initially involved in RF research at PPPL, his main interest turned to the MHD properties of tokomak plasmas. He has made major contributions to many of the MHD stability research projects at PPPL including the development of the ancillary numerical codes, with applications to the various devices at PPPL. Some of these codes are included in the MHD stability component of the SWIM project. He has authored or co-authored many scientific publications, and is a co-holder of the patent for the Princeton Beta Experimental (PBX) device. He is Fellow of the American Physical Society.

Jin Chen received a PhD in Applied Mathematics from National Institute for Fusion Science, Japan in 1999; and worked as a Post Doc at Uppsala University, Sweden from 1999 to 2000. She has been employed as a PPPL Computational Scientist since 2001 and mainly cooperated with M3D group. She has had considerable experience in code porting to various advanced computing platforms, optimizing parallel performance, high-order finite elements, and advanced linear solvers.

Eliot Feibush is a scientist in the Computational Plasma Physics Group at the Princeton Plasma Physics Laboratory. He is leading the development of web service software for visualizing data from fusion experiments and simulations. His initial web service, Elfresco, enables scientists to simulate reflectometers and correlate their effects. In collaboration with other members of CPPG, another web service was developed for preparing data and running TRANSP between NSTX shots. A web service for RPLOT enables displaying graphs from TRANSP runs. His ElVis software is deployed on the Fusion Grid Monitor for displaying the input and progressive results of TRANSP runs. The SWIM project is using ElVis for monitoring data from its simulation runs. Web services for other fusion codes are under development. Previously, he has developed graphics, visualizations, and user interfaces for architectural design, medical imaging, and geospatial-situational awareness applications. He has published journal articles on modeling, rendering, and visualization. Eliot received his B. Architecture (1979) and M.S. in computer graphics (1981) from Cornell University. He is a member of the ACM.

Guo-yong Fu is a Principal Research Physicist at the Princeton University Plasma Physics Laboratory. His main research area includes energetic particle physics and MHD stability of toroidal plasmas. He has authored over 60 refereed publications in plasma physics. He received a Ph.D. in physics from The University of Texas at Austin in 1988. After a one-year postdoctoral fellowship at the Institute of Fusion Studies in Austin, Texas, he worked on MHD stability in stellarators at the center for plasma physics research (CRPP) in Lausanne, Switzerland, from 1989 to 1991. He joined PPPL in 1992. He is currently active in the area of MHD stability in compact stellarators and nonlinear dynamics of energetic particle-driven fishbone and TAE. He won the Kaul Foundation Prize for excellence in plasma physics research in 1998.

N.N. Gorelenkov received a BS in physics from Moscow State University in 1988 and a PhD in plasma physics from Kurchatov Institute in Moscow in 1993. He specilized in studies of fusion related wave particle interaction and instabilities driven by energetic particle in toroidal magnetic confinement devices. Dr. Gorelenkov is an author of about 100 papers and made numerous presentations at national and international conferences on plasma physics. More recently he was involved in simulations of Alfvenic instabilities in burning plasmas and ITER.

Stephen C. Jardin is a Principal Research Physicist at the Princeton University Plasma Physics Laboratory. He is presently Co-Head of the Computational Plasma Physics Group at PPPL, and MHD Physics leader for the Theory Department. He has been Lecturer with Rank of Professor in the Princeton University Astrophysics Department since 1986. He holds a BS in Engineering Physics from the University of California, a MS (Physics) and MS (Nuclear Engineering) from MIT, and a Ph.D. in Astrophysics from Princeton University (1976). He has been an APS Fellow since 1986. He was the primary developer of several widely used MHD equilibrium, stability, and transport codes including the Tokamak Simulation Code (TSC). He is currently the lead Principle Investigator for the SciDAC Center for Extended Magneto-hydrodynamic Modeling, which was just renewed for its third 3 year cycle in the summer of 2007. He holds four U.S. patents, has had over 150 refereed publications in plasma physics, and has supervised 9 Princeton University Ph.D. students.

Long-Poe Ku is a principal engineer and an engineering fellow at the Princeton Plasma Physics Laboratory. He received his PhD in Nuclear Engineering and Applied Physics from Columbia University in 1976. Since joining PPPL as a post-doctoral fellow, he has worked on a wide variety of subjects, including providing neutronics analysis for the design of various fusion devices, predicting responses of and providing shielding for detectors and equipment sensitive to nuclear radiation in various experimental facilities, projecting radioactivation and the dispersion of radioactive effluent in TFTR, predicting trajectories of electrons in photoelectron lithography, designing correction magnet for the Superconducting Supercollider, and in recent years he has been involved in the design and optimization of stellarator configurations. He has authored and coauthored more than 80 papers in the above areas. He is the principal architect of the plasma configuration for NCSX now under construction and the stellarator and coil configurations for ARIES-CS.

Douglas McCune is a software engineer and applied mathematician by training and has over 25 years of experience in computational software development at the Princeton Plasma Physics Laboratory. He is the main author and creator of TRANSP, an integrated software package for tokamak fusion plasma simulation, which has been used to analyze and validate experimental results on tokamaks around the world. The TRANSP code pioneered the use of detailed Monte Carlo fast-ion simulation for accurate prediction of the energy content and fusion reactivity of MHD-quiescent tokamak core plasmas, given thermal plasma temperature and density measurements. In recent years, Douglas McCune has co-led the Computational Plasma Physics Group at PPPL. He has played a leading role in numerous successful projects involving collaborative sharing and integration of software, such as the National Transport Code Collaboration Modules Library project, http://w3.pppl.gov/NTCC, and the SciDAC Collaboratory's Fusion Grid project, http://www.fusiongrid.org, by which a production TRANSP facility is made available to both PPPL and remote users as a computational service, producing over 4000 runs in 2007. He is the creator of the Plasma State component, which is being used in the SWIM SciDAC Fusion Simulation Project prototype to exchange data between physics codes. The Plasma State software is also being used in PTRANSP (predictive upgrades to TRANSP), and use is planned in the FACETs and CPES SciDAC projects. Douglas McCune was named a PPPL Distinguished Engineering Fellow in 2001.

COLUMBIA UNIVERSITY

David E. Keyes is the Fu Foundation Professor of Applied Mathematics at Columbia University. He earned a B.S.E. in Mechanical Engineering from Princeton in 1978 and a Ph.D. in Applied Mathematics from Harvard in 1984. He post-doc'ed in Computer Science at Yale and taught there for eight years prior to joining Old Dominion University and ICASE at the NASA Langley Research Center in 1993. He moved to Columbia in 2003. For the past nine years, he has been the (part-time) Acting Director of the ISCR at LLNL. Keyes is author or co-author of over 100 publications in computational science and engineering, numerical analysis, and computer science. He works at the algorithmic interface between parallel computing and the numerical analysis of partial differential equations, across a spectrum of aerodynamic, geophysical, and chemically reacting flows. Newton-Krylov-Schwarz parallel implicit methods, introduced in a paper he co-authored in 1993, are now widely used throughout engineering and computational physics, and have been scaled to thousands of processors. Keyes has been recognized with ACM’s Gordon Bell Prize in 1999 and the IEEE’s Sidney Fernbach Award in 2007. He is currently co-editor of Int J High Performance Computing Applications and SIAM's Computational Science & Engineering book series. He serves as the Vice President of SIAM and on two Directorate-level advisory committees at NSF, for Mathematics and Physical Sciences (MPS) and the Office of CyberInfrastructure

(OCI). Keyes recently co-authored with A. Kritz a major community report on the Fusion Simulation Project.

UNIVERSITY OF WISCONSIN

Dalton Schnack is a computational physicist with over 30 years experience in the analytic and numerical solution of nonlinear, multidimensional problems in hydrodynamics and magnetohydrodynamics (MHD). He has authored or co-authored many papers in the fields of linear and nonlinear resistive MHD, and computational methods related to such problems. He has extensive experience in the supercomputing environment. He is actively involved in studying the nonlinear MHD properties magnetic fusion experiments and the solar corona, and in the highly nonlinear (turbulent) properties of the Navier-Stokes and MHD equations. After receiving his B.S., Dr. Schnack worked for over seven years (1967-1973) for the Pratt and Whitney Division of United Technologies Corporation as a Senior Scientific Programmer/Analyst. There he worked on computational problems of steady flow in nozzles and supersonic exhaust jets, and the performance of axisymmetric compressors. During this time, he completed work on an M.S. in physics, which included a thesis on ultra short optical pulse propagation. Dr. Schnack did his doctoral research at Lawrence Livermore Laboratory under Prof. John Killeen where he began his interest in nonlinear MHD processes in fusion plasmas. After graduation, he served as a staff physicist in the computational physics group at the National Magnetic Fusion Energy (MFE) Computer Center, a supercomputer network funded by the Department of Energy. In 1980, he joined the fusion theory group at Los Alamos National Laboratory where he worked on problems relevant to the reversed-field pinch and compact torus experiments. In July 1982, Dr. Schnack joined the Applied Plasma Physics and Technology Division of SAIC, and in 1996 was appointed Director of the Center for Energy and Space Science. He is presently Principal Investigator for two grants with the U. S. Department of Energy. He is actively involved in research related to the nonlinear fluid dynamics of advanced magnetic fusion devices, and the nonlinear properties of the MHD equations. Dr. Schnack is a member of Phi Kappa Phi, national scholastic honor society, and is a Fellow of the American Physical Society. He is also a member of the American Geophysical Union and the Solar Physics Division of the American Astronomical Society. He has been an active participant in the functions of the international fusion program for many years. Dr. Schnack has co-authored over 70 refereed publications, and one book.

Chris C. Hegna is a Professor of Engineering Physics and Physics at the University of Wisconsin and serves as the director of the University's Center for Plasma Theory and Computation.. His primary field of research is theoretical plasma physics with an emphasis on the area of plasma confinement using magnetic fields. He is the author or co-author of over 100 refereed publications and has advised or co-advised 12 doctoral students. Hegna's current research includes; the role of macroscopic instabilities in high-temperature plasmas; nonideal and nonlinear magnetohydrodynamic instabilities; kinetic theory modifications to fluid-like descriptions of plasmas; plasma dynamics in non-symmetric magnetic systems; the role of magnetic geometry, symmetry and topology on plasma instabilities, turbulence and transport properties; self-organization properties of plasmas; anomalous current and momentum transport; magnetic reconnection in laboratory and astrophysical plasmas and dynamo processes. He received his B. S. from the University of Wisconsin in Applied Mathematics, Engineering and Physics in 1986, his M. S. from Columbia University in Applied Physics in 1987 and his Ph.D. from Columbia University in 1989. He has been employed at the National Institute for Fusion Science (Nagoya, Japan), UKAEA Technologies, Culham Laboratory (Abingdon, England) and Columbia University, working at the Princeton Plasma Physics Laboratory. He is a fellow of the American Physical Society.

Thomas G. Jenkins is a Research Associate at the University of Wisconsin-Madison. He received his Ph.D. from Princeton University (working at the Princeton Plasma Physics Laboratory) in 2007, where his research focused on fundamental numerical issues which arise in gyrokinetic particle-in-cell simulations (e.g. discrete particle noise, discrete-to-continuum interpolation issues, Monte Carlo integration, and growing weights). Several of these issues also find application in the development of the NIMROD code (to enable interfacing with various RF propagation and deposition codes); Dr. Jenkins has been involved with this development for much of the past year.

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Paul Bonoli is a Senior Research Scientist at the Plasma Science and Fusion Center at the Massachusetts Institute of Technology. He specializes in theoretical and computational plasma physics in the areas of radio frequency heating and current drive in toroidal confinement devices (tokamaks). He has developed detailed simulation models for radio frequency heating and current drive experiments, which include wave propagation and Fokker Planck calculations. Paul Bonoli received the BS and MS degrees in electrical engineering from Cornell University in 1976 and 1978 respectively. He received the Ph.D. in electrical engineering from Cornell University in 1981, under Professor Edward Ott. He then joined the Physics Department at the Massachusetts Institute of Technology as a post-doctoral associate under Professors Bruno Coppi and Miklos Porkolab. In 1984 he became a research scientist at the Research Laboratory of Electronics at MIT. He then joined the research staff at the MIT Plasma Science and Fusion Center (PSFC) in 1986 and rose to the rank of principal research scientist in 1989. Dr. Bonoli is the co-author on over 45 papers in refereed journals and he is currently the principal investigator for the SciDAC Center for Wave – Plasma Interactions (CSWPI) and for the NSTX High Harmonic Heating and Current Drive Project at MIT. He is also currently serving as the co US Team Leader of the ITPA Working Group on Steady State Operations. Dr. Bonoli is a fellow of the American Physical Society.

John Wright After graduating with a B.S. in Applied Physics in 1991 from Columbia University, John Wright received his doctorate in astrophysics at Princeton University in 1998 under the supervision of Dr. C. K. Phillips for a thesis titled, “Fast Wave Current Drive Modeling in Tokamaks.” He then served a three year post doctoral position and one year as a staff scientist in the plasma physics group at the University of Wisconsin-Madison under Dr. Stewart Prager. He worked on magnetohydrodynamic modeling with emphasis on current drive techniques within that fluid model. He returned to radio frequency research with a position in the Plasma Science and Fusion Center at MIT in the theory group working with Drs. Paul Bonoli and Peter Catto. Since arriving at MIT he has developed a parallel version of the TORIC code in collaboration with E. D' Azevedo at Oak Ridge National Laboratory under the RF SciDAC Initiative. His present work at the PSFC focuses on applying advanced parallel RF models to experimental and theoretical RF issues. Close on-going collaborations with the RF group on Alcator C-Mod have a direct impact on the direction of the experimental program. He continues to be involved in several international and multi-institutional domestic collaborations focusing on various modeling integration and algorithm development issues in RF simulations including the US RF-SciDAC and pre-FSP Computer Simulations with Waves in MHD (CSWIM). He pursues interests in advanced algorithms and novel mathematical algorithms in computing through membership in IEEE Computing in Science and Engineering Division. He has an interest in beowulf computing and has helped design and maintain the current PSFC theory group 256 core cluster.

Jesus Ramos is a Principal Research Scientist at the Plasma Science and Fusion Center of the Massachusetts Institute of Technology. He has a Ph.D. in Physics from the "Universidad Complutense" of Madrid, Spain. He has made extensive contributions to the magnetohydrodynamic theory of fusion plasmas and has participated in the design teams of Alcator C-Mod, CIT, ARIES, TPX, and ITER. He has authored or co-authored over 60 refereed publications.

Linda E. Sugiyama is a principal research scientist in the Research Laboratory of Electronics at the Massachusetts Institute of Technology. She has worked in many areas of the theory and numerical simulation of magnetically confined plasmas, including equilibrium, stability, transport, auxiliary heating, and nonlinear simulation. She first proposed and, with W. Park, developed the two-fluid MH3D-T code for axisymmetric confined plasmas, based on the existing MH3D MHD nonlinear code developed at PPPL. These codes formed the basis of the M3D project. She received a B.S. from the University of Wisconsin in 1975, and a Ph.D in Applied Mathematics from the Massachusetts Institute of Technology in 1980. Since then, she has worked at MIT, with brief sojourns at other institutions.

GENERAL ATOMICS

David P. Schissel is the Manager of the Data Analysis Applications Group at the DIII-D National Fusion Facility and the Director of the Advanced Imagery Laboratory at General Atomics. He has over 20 years experience in fusion plasma physics and management with over 75 fusion-related publications from plasma confinement research to advanced computer science research. For the DIII-D National Fusion Facility, he is responsible for coordinating computer hardware and software resources to support the scientific staff's data analysis requirements. As the principal investigator of the USDOE SciDAC funded National Fusion Collaboratory Project, he is responsible for coordinating advanced computer science research among seven distinct institutions to deliver a persistent collaboration infrastructure to transform fusion research. As principal investigator for basic confinement studies on the DIII-D tokamak, he has been responsible for creating and implementing experimental proposals to study the global energy confinement and local energy transport properties of neutral beam heated fusion plasmas. He has been a visiting scientist at the JET Joint Undertaking Tokamak (Culham Laboratory) in the United Kingdom and at Tore Supra Tokamak (Cadarache Laboratory) in France. He received his B.S. degree in Nuclear Engineering from the University of Wisconsin Madison in 1979, his M.S. degree in plasma physics from the Massachusetts Institute of Technology in 1982, and is a fellow of the American Physical Society.

Gheni Abla is a Senior Software Developer at Theory and Computational Science Division of General Atomics. He has many years of experience in software development and research. Recent years he has designed, and implemented a number of software packages, including distributed image processing tool in the Linux cluster environment and large scale scientific unstructured grid data visualization tool. At General Atomics, he has developed software tools for signal analysis, visualization and computer-assisted collaboration for fusion experimental research. He also has developed interactive 3-D data visualization tool for High Temperature Gas Cooled Reactor (HGTR) simulations. He currently writes data analysis, scientific visualization and web portal programs for DIII–D experiments. He also supports remote collaboration software tools and large format shared display wall-based collaboration for the Fusion Group of General Atomics. He received his B.S. degree in Physics from Xinjiang University, China in 1991 and M.S degree in Computer Science from South Dakota School of Mines and Technology in 2002.

Myunghee Choi is a staff scientist in the integrated modeling branch in the theory and computational science division in energy group at General Atomics. She received her B.S. and M.S. degrees in physics department from Pusan University in Korea in 1983 and 1987, and her Ph.D. degree in nuclear engineering in Purdue University in U.S.A. in 1993. Prior to joining GA, she had a research opportunity at the CEA Cadarache Magnetic Fusion Research Center in France from 2000 to 2002. While at CEA Cadarache, she worked in the research area of fast electron losses due to toroidal magnetic field ripples during lower hybrid current drive and heating experiments in Tore Supra. She joined General Atomics in August 2002 and has been working on improving the TORAY-GA electron cyclotron current drive and heating ray-tracing code and developing the ICRF simulation package ORBIT-RF to self-consistently model the plasma interaction with the electromagnetic wave in the ion cyclotron frequency range in order to resolve several important physics problems related to the finite banana width effect of energetic ions that is absent in the conventional linear full wave and Fokker-Planck solver. Her current research interests include studying the effect of ICRF wave induced energetic ion tails on non-inductively driven fast wave current drive (FWCD), MHD stabilization/destabilization, RF driven plasma rotation and momentum transport, and control of turbulence and transport barrier formation by energetic ions at their high harmonic resonance.

COMPX

Robert (R. W.) Harvey is an expert in fusion energy computations, specializing in in-depth development and application of computational models for interpretation of auxiliary heating and transport in fusion energy plasmas. Dr. Harvey conceived and led development of several major computer codes used for physics interpretation of fusion energy experiments, while working at General Atomics, San Diego for twenty years, and then at CompX, Del Mar, California, which he founded in 1995. For the past twenty years, he has focused primarily on the development, application, and dissemination of the CQL3D collisional/rf-quasilinear Fokker-Planck code for simulation of microwave and neutral beam heating in tokamak fusion energy plasmas. The code has led to many collaborations, nationally and internationally, for interpretation of experiments, playing a direct role in more than one hundred research publications. Dr. Harvey has contributed to design of the International Tokamak Experimental Reactor, primarily in regard to requirements for electron cyclotron current drive systems to stabilize neoclassical tearing modes. He has also worked as a leader of a GA/Russian Theory Collaboration Program (1989–1995), an Associate Editor of Physics of Fluids (1986–1988), and a lecturer at the University of California, San Diego. Dr. Harvey is an author or co-author on 184 papers. He obtained his Ph.D. in Applied Physics at the University of California, San Diego, 1973.

TECHX

Scott Kruger is a Principal Scientist at Tech-X Corporation. Scott Kruger received his doctorate at the University of Wisconsin-Madison in 1999 under the supervision of Drs. J.D. Callen and C.C Hegna. After his doctorate, he joined Science Applications International Corporation, where he became a senior developer of the NIMROD nonlinear, initial-value magnetohydrodynamics code, which is part of the Center for Extended Magnetohydrodynamic Modeling U.S. Department of Energy SciDAC project. He continued as a NIMROD developer upon joining the Tech-X Corporation in January 2004. Dr. Kruger is a computational plasma physicist with extensive experience in analytic development of fluid models for plasmas, and the application of those models in massively-parallel numerical simulations. He collaborates extensively with scientists at the DIII-D National Fusion Facility and his simulations have been driven by their experimental results. He is also interested in the coupling of disparate codes, and the associated numerical and computational challenges associated with that coupling.

LEHIGH UNIVERSITY

Glenn Bateman is a senior research scientist at Lehigh University with more than 40 years of experience in magnetic fusion research and 86 publications in refereed journals. Dr. Bateman has strong interests in numerical analysis and the comparison between simulation results and experimental data. Over the years, he has taught courses on advanced numerical analysis (including finite difference, finite element, Monte-Carlo and particle in cell techniques), programming in C++ and Fortran, and plasma physics. In 1965, Dr. Bateman earned a BA degree in mathematics and physics at Yale University and, in 1970, he earned a PhD degree in astrophysical sciences at Princeton Unversity. He worked on MHD stability theory at the NYU Courant Institute of Mathematical Sciences and MHD instability simulations at the Max-Planck-Insitut fűr Plasmaphysik and the Oak Ridge National Laboratory. In 1978, Dr. Bateman published the book *MHD Instabilities,* which was subsequently translated into Russian and Chinese. While he was an

Associate Professor in the Nuclear Engineering department at the Georgia Institute of Technology, he developed a model for computing saturated tearing modes as well as engineering techniques for reducing magnetic ripple in tokamaks. While working at the Princeton Plasma Physics Laboratory, Dr. Bateman developed the Multi-Mode transport model. During the last 24 years, Dr. Bateman has concentrated primarily on predictive integrated modeling simulations of tokamak plasmas and comparison of simulation results with experimental data. He is a fellow of the American Physical Society.

APPENDIX 1. IPS PHYSICS COMPONENT DESCRIPTIONS

A.1 Equilibrium and Profile Advance (EPA) Component

We have made the equilibrium and profile advance parts of the Tokamak Simulation Code (TSC) into a SWIM component. In doing this, we have preserved all of the existing functionality of TSC and have greatly extended its capabilities by giving it access to all the advanced heating and current drive packages via the plasma state.

The EPA component has the following functionality: It initializes all the plasma profiles and equilibrium variables, and defines adiabatic variables for the subsequent time advance. Each time step it invokes one of several transport modules to define the electron and ion thermal conductivities. It then uses these thermal conductivities and the heating source functions that it reads from the Plasma State to advance the profiles one macro timestep in time. It also uses the circuit equations and feedback systems to advance the coil currents and vessel currents in time. It then calculates the equilibrium configuration at the advanced time on a 2D (R, Z) grid using the dynamic relaxation method. A flux-surface mapping is done to compute flux-surface averaged metric coefficients.

The EPA component also has the capability of accessing the TRANSP source routines using the pre-existing TSC/TRANSP communication mechanism. This capability has been used within the SWIM framework, but we expect to phase this out once all the TRANSP energy and current drive sources become SWIM components, as they can then be accessed directly through the SWIM framework.

A.2 MHD Stability Component

We have created a MHD stability component that communicates strictly through the plasma state. The component performs the following steps in order to analyze the MHD stability of the current equilibrium state of the plasma: (1) It runs GEQ2EQDSKA in order to obtain the plasma equilibrium from the plasma state in GEQ format, and convert it to EQDSKA format to be processed further. (2) It next runs JSOLVER to read in the EQDSKA file, recomputes the equilibrium to a higher tolerance using a flux coordinate solver, and writes out the EQB1 file for subsequent processing. (3) One or both of two mapping codes can then be invoked. The MAPCK code reads the EQB1 file, calculates all the necessary quantities in an appropriately new flux coordinate system for subsequent ballooning analysis and writes these out to the files MAPDSK and MPOUT1. The MAP2 code also reads the EQB1 file, and performs a similar function relevant to the PEST2 code. (4) The stability analysis is then performed by invoking either or both the BALLOON and PEST2 ideal MHD stability codes. The BALLOON code is used to analyze high-toroidal-mode-number stability, the ideal Mercier criterion, D_I, and also checks for the resistive counterpart, D_R. The PEST2 code calculates the low-mode-number stability. (5) The final step is to place the results of the stability codes back into the Plasma State using the module PS_UPDATE_LMHD. This stability information is then available to be viewed or to accessed and acted upon by other components. We have also extended the MHD stability component to write an equilibrium file to initialize the M3D and NIMROD nonlinear MHD codes. We expect this new capability to be heavily used in the next proposal period.

A.3 RF Component

During the past three years, an RF component was created as part of the Integrated Plasma Simulator (IPS). This component consists of two advanced full-wave electromagnetic field solvers, the AORSA [Jaeger, 2002] and TORIC [Brambilla, 1999, Wright, 2004] codes, valid in the ion cyclotron range of frequencies (ICRF). These simulation codes solve a wave equation of the form:

$$\nabla \times \nabla \times \vec{E} = \frac{\omega^2}{c^2}\left(\vec{E} + \frac{4\pi i}{\omega}\overline{\overline{\sigma}} \bullet \vec{E} + \vec{J}^{ANT}\right) , \tag{A.1}$$

where $\overline{\overline{\sigma}}$ is the local conductivity tensor and $\vec{J}^{ANT}$ is the antenna current. The conductivity is a non-local integral operator on the wave electric field in AORSA and the integral form of Eq. (1) is solved with no restriction on perpendicular wavelength relative to orbit size and no limit on the number of cyclotron harmonics. The conductivity operator in TORIC is formulated in the ion finite Larmor radius (FLR) limit where $(k_\perp \rho_i)^2 < 1$. AORSA also treats arbitrary (non-thermal) particle distributions whereas the version of TORIC currently implemented in the IPS treats all species as Maxwellian.

Incorporation of AORSA and TORIC into the IPS was performed without making any changes to the solvers themselves. Each code was implemented as a component of the IPS through scripts, where each script calls initialization, pre-processor, and post- processor programs that allow the codes to communicate with the Plasma State. Each script executes a "prepare input" file that retrieves species-dependent density / temperature profiles and MHD equilibrium data from the Plasma State. After each solver is run, the component executes a "process output" script that writes the direct electron and ion heating profiles from the solver to the Plasma State. AORSA accepts a 3D fast ion distribution (when available) from which it computes a 4D quasilinear diffusion coefficient that is used by the Fokker Planck code CQL3D. Transfer of the fast ion distribution function and quasilinear diffusion coefficient between AORSA and CQL3D is accomplished through files stored on disk. TORIC is not as yet coupled to CQL3D, thus the damping on any minority species is written directly to the Plasma State as an ion heating source term. Both codes write 2D electric field information to files also stored on disk.

A.4 Fokker-Planck RF Minority Component

The distribution function of a plasma species under the influence of RF power and Coulomb collisions evolves according to a Fokker-Planck equation of the form

$$\frac{df}{dt} = \vec{\nabla}_v \bullet \overleftrightarrow{Q} \bullet f + \vec{\nabla}_v \bullet \overleftrightarrow{C} \bullet f + S$$

Where the time derivative of f is total convective derivative and, respectively, $\overleftrightarrow{Q}$, $\overleftrightarrow{C}$, and S are the RF quasi-linear operator, Coulomb collision operator, and particle and particle source rates. Under the assumptions of axisymmetry (a tokamak), RF and gyro time-scales much shorter than particle orbit times and collision time-scales, this can be reduced to the 3D so-called bounce- and gyro- averaged Fokker-Planck equation. The CQL3D code, with the additional assumption of small departure of particles from flux surfaces implements a solution to this model appropriate for following the evolution of RF-driven distribution functions [Harvey, 1992]. Such RF-driven tails are possible for species whose RF heating per particle is sufficiently high. Fusion alphas, fast ions from neutral beam heating, and low density ion components have all been observed in previous simulations to have such interactions. Plasma profile data are communicated though the state, while files are used for the communication of the 3D distribution function (from CQL3D to AORSA) and the 3D Quasi Linear Operator (from AORSA to CQL3D).

A.5 Fokker-Planck Runaway Electron Component

With different input parameters, the same Fokker-Plank solver that follows ion distribution functions can also follow the electrons. The toroidal electric field is now important (but typically not for ICRF heated ions) and a term that reflects this drive, $\vec{F}_{em}$, must be included.

$$\frac{df}{dt} = \vec{\nabla}_v \bullet \vec{F}_{em} f + \vec{\nabla}_v \bullet \overleftrightarrow{C} \bullet f + S$$

The runaway electron component has been implemented, and simulations started to model electron runaway during the ITER startup.

A.6 References

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