Advances in simulation of wave interactions with extended MHD phenomena

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Abstract: The Integrated Plasma Simulator (IPS) provides a framework within which some of the most advanced, massively-parallel fusion modeling codes can be interoperated to provide a detailed picture of the multi-physics processes involved in fusion experiments. The presentation will cover four topics: 1) recent improvements to the IPS, 2) application of the IPS for very high resolution simulations of ITER scenarios, 3) studies of resistive and ideal MHD stability in tokamak discharges using IPS facilities, and 4) the application of RF power in the electron cyclotron range of frequencies to control slowly growing MHD modes in tokamaks and initial evaluations of optimized location for RF power deposition.

1. Introduction
The Center for Simulation of Wave Interactions with Magnetohydrodynamics (SWIM) has 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.

The SWIM Center consists of three elements: (1) Development of a computational platform referred to as the Integrated Plasma Simulator (IPS) that will allow efficient coupling of the full range of required fusion codes or modules and carrying out a program of research on as optimizing burning plasma scenarios, (2) A physics campaign addressing long timescale discharge evolution in the presence of sporadic fast MHD events. This involves interfacing the IPS to both linear and 3D non-linear extended MHD codes and improving the understanding of
how RF can be employed to achieve long-time MHD stable discharges and control sawtooth events, and (3) A physics campaign for modeling the direct interaction of RF and extended MHD for slowly growing modes. The primary physics focus of this campaign is to improve the understanding of how RF can be employed to control neoclassical tearing 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.

2. New developments in the Integrated Plasma Simulator

The computational core of the SWIM project is the Integrated Plasma Simulator (IPS), 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 design of the IPS is based on concepts from the Common Component Architecture, expressed in a simplified form that satisfies the project’s needs without introducing unnecessary complexity [1, 2]. For example, the IPS itself, as well as computational driver components, are written in Python, which is readily modified and extended in response to new scientific needs. The physics components of the IPS are generally wrappers around standalone physics codes. The physics codes used by the IPS are routinely used as stand-alone models, and are under continual development. So the ability to use them unmodified in the IPS for integrated simulations is a major advantage. Likewise, with the help of a Plasma State component as a central store for key simulation data, file-based data exchange remains adequate for current IPS applications.

A major focus of recent development in the IPS has been support for the execution of multiple components concurrently, where individual components may be parallel [3]. There are several motivations for this “multiple-component multiple-data” (MCMD) execution model, which can ultimately be traced back to the fact that in this field, existing codes vary widely in their level of parallel scalability. One illustrative use for the MCMD-style of execution arises in the slow MHD campaign, where a scalable long-running MHD code such as NIMROD [15] requires updates to certain quantities as it evolves the system through time. In this case, updates, which couple only loosely to the MHD, are done by the GENRAY code [14], which has only a small degree of parallelism. Stopping a large-scale MHD task in order to run a small-scale GENRAY task would leave the majority of compute nodes allocated to the job idle during this phase of the simulation. The MCMD execution model allows the small GENRAY task to be run on a small number of additional processors while the MHD code keeps iterating, resulting in a much more efficient use of resources. Only a small number of nodes are idled between GENRAY executions. Another example of MCMD execution comes from the fast MHD campaign. In this case (see figure 1) each iteration of the simulation consists of a phase in which one or two scalable simulation codes run (in this case the AORSA full wave ICRF code [8] and the NUBEAM neutral beam code [5, 12]), followed by a phase in which several less scalable codes must be run. Fortunately, their data dependencies allow several of the non-scalable codes to be run concurrently – in this case CQL3D [6], and TSC [9, 10], which in turn may require several GLF23 evaluations [16]. Additionally, many of the stability analyses of the plasma from the just-completed time step can easily be run concurrently over the many toroidal modes of the plasma (DCON, PEST-II, ELITE, and BALLOON in this example; see for example [4]). The IPS MCMD capability even allows for several distinct simulations to be run simultaneously as a single job, interleaved so that scalable components in one simulation run concurrently with unscalable components of the other. With judicious allocations of resources, designed to produce similar execution times for the scalable and unscalable components, it is possible to achieve a more efficient overall utilization of the computing resources than would be possible running either simulation individually.
3. Applications of the Integrated Plasma Simulator to ITER

Integrated modeling of projected ITER discharges already plays a very important role in the ITER program, both for the purpose of finalizing the design of auxiliary systems and for planning the research program. Presently a single run of an integrated model can take a month or more of continuous running time if the most powerful physics models are employed. The number of such runs that will be needed is quite large, particularly when surveys of various discharge parameter values are required such as for optimization studies.

Figure 2. IPS results for an ITER simulation. Power sources include two neutral beams and ion cyclotron heating. In this case the plasma heating is dominated by fusion alpha particles.
The SWIM project has adopted a near term goal of demonstrating the capability to use massively-parallel computers to greatly accelerate the integrated simulation process for ITER, while also improving the level of physics fidelity of the simulations. To this end we are using the SWIM IPS with TSC/GLF23 coupled to the AORSA full-wave ICRF code and the NUBEAM code. Figure 2 shows IPS results for an ITER H-mode scenario that has been previously studied using the TSC/PTRANSP code with serial versions of the heating and transport modules. For this run the ICRF power deposition was calculated with AORSA using 2056 processors and the neutral beams and fusion physics was calculated with parallel NUBEAM running on 512 processors on the Franklin computer at NERSC. The number of Monte Carlo particles used by NUBEAM was $10^6$ for neutral beam injection and $10^6$ for fusion products, while the AORSA calculations used 256×256 Fourier modes for the radial and poloidal angle grids. These are much higher resolution calculations than were feasible previously. We expect soon to do similar studies with the parallel TORIC code for ICRF [17], to begin the process of benchmarking against the PTRANSP simulation, and to work on optimizing the running time using the MCMD capability.

4. Progress in fast MHD campaign

We are evaluating the ideal and resistive MHD stability of a CMOD discharge simulated using the IPS. The stability codes read the equilibrium from the plasma state as the simulation proceeds. Shown in figure 3 is the linear phase of a n=1 resistive instability as calculated by the new toroidal MHD stability code M3D-C1. We are able to use realistic values for the resistivity and other parameters by packing the mesh points around the magnetic flux surface where the magnetic island forms (using routines provide by the RPI SCORE Center). Shown in the figure is the perturbed part of the toroidal current density for a resistive instability in CMOD with magnetic Lundquist number $S=10^7$. The configuration is ideally stable.

![Figure 3. Perturbed toroidal current density for a resistive instability in CMOD with Lundquist number S=10^7. Equilibrium file is read from the plasma state and analyzed by M3D-C1.](image)
5. Progress in slow MHD campaign

Tokamaks have achieved their high performance by relying on strong magnetic fields to create a nested set of surfaces on which the magnetic field is confined. Near rational surfaces, where the magnetic field lines close on themselves rather than cover the surface, the plasma is susceptible to instabilities which can break the magnetic field into island structures. The break in topology allows particles and energy to escape the plasma more readily and reduces the plasma performance. The most promising technique to control this process uses localized radiofrequency (RF) current drive to stabilize the islands. One of the key control parameters of the stabilization experiments is the location of the RF current deposition relative to the location of the rational surface. Numerical experiments have begun to understand the influence of this parameter.

Initial numerical simulations with the NIMROD code have reproduced many of the qualitative features seen in experiments, including the stabilization or destabilization of the instability. Stabilization is sensitive to the location of the RF current deposition is changed as seen in figure 4. Nonlinear effects complicate attempts to deposit current directly at the rational surface, as the position of this surface shifts in response to the deposited current, figure 5. Simulations suggest that the goal of inducing current at the island center (enabling suppression) is best achieved by depositing current at a point initially just outside the island, and that robust, safe approaches to island stabilization will need to take the motion of rational surfaces into account (especially at high RF powers). These preliminary calculations provide useful guidance as we move to more quantitative predictions.

To make more quantitative predictions, future work will include coupling the NIMROD and GENRAY codes. The mathematical formulation for this coupling has been developed under the SWIM project [7, 13] and work on...
completing this coupling is underway. The coupling makes use of the Plasma State component to transmit the appropriate quantities from NIMR OD to GENRAY without modification of the GENRAY component (which was developed under the fast MHD campaign) and utilizes the recently developed MCMD capabilities described in Section 2. Once the full coupling is complete, truly quantitative predictions of RF feedback stabilization of magnetic islands will be possible.

References
[1] D. Batchelor, C. Alba, G. Bateman, D. Bernholdt, L. Berry, P. Bonoli, R. Bramley, J. Breslau, M. Chance, J. Chen, M. Choi, W. Elwasif, G. Fu, R. Harvey, E. Jaeger, S. Jardin, T. Jenkins, D. Keyes, S. Klasky, S. Kruger, L. Ku, V. Lynch, D. McCune, J. Ramos, D. Schissel, D. Schnack, and J. Wright, Simulation of Wave Interactions with MHD, in Rick Stevens, editor, SciDAC 2008, 14-17 July 2008, Washington, USA, volume 125 of Journal of Physics: Conference Series, page 012039, Institute of Physics, 2008.
[2] Wael R. Elwasif, David E. Bernholdt, Lee A. Berry, and Don B. Batchelor, Component Framework for Coupled Integrated Fusion Plasma Simulation, in HPC-GECO/CompFrame 2007, 21-22 October, Montreal, Quebec, Canada 2007
[3] Samantha S. Foley, Wael R. Elwasif, Aniruddha G. Shet, David E. Bernholdt, and Randall Bramley, Incorporating Concurrent Component Execution in Loosely Coupled Integrated Fusion Plasma Simulation, in Component-Based High-Performance Computing (CBHPC) 2008.
[4] A. H. Glasser, American Physical Society, 45th Annual Meeting of the Division of Plasma Physics, October 27-31, 2003, Albuquerque, New Mexico, MEETING ID: DPP03, abstract QP1.109
[5] R.J. Goldston et al., "New Techniques for Calculating Heat and Particle Source Rates due to Neutral Beam Injection in Axisymmetric Tokamaks", J. Comp. Phys. 43 (1981) 61
[6] R. W. Harvey and M. G. McCoy, The CQL3D Code, Proc. IAEA TCM on Thermonuclear Plasmas, Montreal (1992), p. 527, available through USDOC/NTIS No. DE93002962.
[7] C. C. Hegna and J. D. Callen, to be published, Phys. Plasmas 2009
[8] E. F. Jaeger, L. A. Berry, E. D’Azevedo et al., Physics of Plasmas 9, 1873 (2002).
[9] S. C. Jardin, N. Pompfrey, and J. Delucia, "Dynamic Modeling of Transport and Positional Control of Tokamaks", J. Comput. Phys. 66 481-507 (1986)
[10] S. C. Jardin, M. G. Bell, and N. Pompfrey, "TSC Simulation of Ohmic Discharges in TFTR", Nucl. Fus. 33 3710382 (1993)
[11] “Fusion Simulation Project Workshop”, Journal of Fusion Energy, Eds. A. Kritz and D. Keyes, 28 (1) 1-59 (2009).
[12] A. Pankin, D. McCune, R. Andre et al., "The Tokamak Monte Carlo Fast Ion Module NUBEAM in the National Transport Code Collaboration Library", Computer Physics Communications Vol. 159, No. 3 (2004) 157-184
[13] J. J. Ramos, Phys. Plasmas 15, 082106 (2008)
[14] A. P. Smirnov and R. W. Harvey, Bull. Am. Phys. Society 40, 1837 (1995); “The GENRAY Ray Tracing Code”, CompX Report CompX-2000-01 (2001).
[15] C.R. Sovinec, A.H. Glasser, D.C. Barnes, T.A. Gianakon, R.A. Nebel, S.E. Kruger, D.D. Schnack, S.J. Plimpton, A. Tarditi, M.S. Chu and the NIMROD Team, "Nonlinear Magnetohydrodynamics with High-order Finite Elements," Journal of Computational Physics, 195, 355 (2004)
[16] R. E. Waltz, G. M. Staebler, W. Dorland, G. W. Hammett, and M. Kotschenreuther, Phys. Plasmas 4, 2482 (1997).
[17] J. C. Wright, P. T. Bonoli, M. Brambilla, F. Meo, E. D’Azevedo, D. B. Batchelor, E. F. Jaeger, L. A. Berry, C. K. Phillips, and A. Pletzer, "Calculations of fast wave mode conversion and lower hybrid propagation in tokamaks", Phys. Plasmas, 11(5), May 2004