Project Overview

Don Batchelor
SWIM Project Meeting
September 23-25, 2008

D. B. Batchelor, L. A. Berry, S. Diem, D. Green, E. F. Jaeger, D. A. Spong – *ORNL Fusion Energy*

D. E. Bernholdt, E. D'Azevedo, W. Elwasif, V. Lynch (NCCS) – *ORNL Computer Science*

S. C. Jardin, E. Feibush, D. McCune, J. Chen, L. P Ku, M. Chance, J. Breslau – *PPPL*

G. Abla, M. Choi, D. P. Schissel – *General Atomics ,* **R. W. Harvey** – *CompX*

R. Bramley, S. Foley – *Indiana University,* **D. Keyes** – *Columbia University,* **D. Schnack, T. Jenkins** – *U. Wisconsin*

P. T. Bonoli, J. Ramos, J.Wright – *MIT,* **S. Kruger** – *TechX*, **G. Bateman** – *Lehigh University*

Unfunded participants:

J. D. Callen, C. C. Hegna, C. Sovinec – *University of Wisconsin,* **E. Held** – *Utah State*

H. St. John – *General Atomics,* **A. Kritz** – *Lehigh Univ*.

- **Project goals and strategy**
- **Highlights of accomplishments**
- **Objectives for this workshop**

***See our fun website at:* www.cswim.org**

Remember what we set out to do

Study effects of RF on Macro-stability

- **Use of RF (and other sources) to control slow plasma evolution and affect fastMHD events, $\tau_{MHD} \ll \tau_{Heating}$ → sawteeth**
- **Use of RF (primarily ECH) to control slowly growing modes, $\tau_{MHD} \sim \tau_{Heating}$ → Neoclassical Tearing Modes**

Be a prototype for a comprehensive FSP

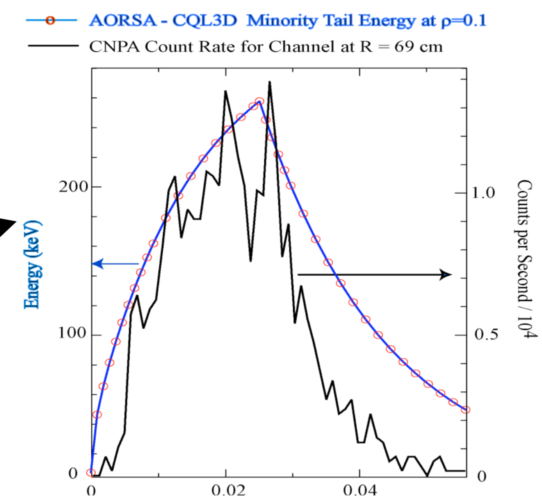
- **Learn about physics and math of integration of multi-scale, multi-physics phenomena arising from RF/transport/MHD**
- **Learn to couple state-of-the-art codes that describe multiple plasma phenomena on state-of-the-art computers**

Develop a powerful integrated plasma simulator

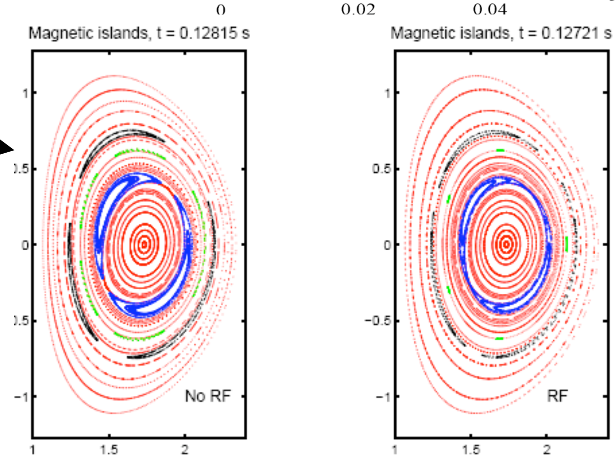
- **A system that is sufficiently extensible to include any fusion code that conforms to the specified interfaces**
- **A system that has high standards of useability, data integrity and accessibility**
- **A simulation system that will be the tool of choice for modelers studying present experiments, ITER, and beyond**

Where we are in the project – details in following talks
(from review presentations)

- **SWIM framework and associated utilities designed, built and work on PPPL clusters and Jaguar (should also work on Franklin at NERSC)**
- **Developed a simulation data exchange mechanism, Plasma State – becoming *lingua franca* of fusion simulation, adopted by several projects outside SWIM**
- **We have a complete set of physics components (i.e. at least one of each functionality) running in the framework**



- **We have developed the analytic basis for Slow MHD**
- **We are doing physics runs**
  - **Detailed, quantitative, time-dependent modeling of ICRF energetic minority tail formation on Alcator C-Mod → also serve as validation studies**
  - **preliminary studies with NIMROD on classical tearing modes in tokamak geometry, including specified RF driven current perturbation, and demonstrated non-linear island shrinkage**



Summary of Recent Progress – IPS Environment

- IPS in production in both Cray XT (ORNL Jaguar) and SGI Altix (PPPL Viz/MHD) environment
  - Various internal improvements to support evolving physics requirements, user experience with IPS
- Web portal for job monitoring in production
  - Monitoring job progress, key results
- Plasma State improvements
  - Additional data elements
  - Back-end netCDF storage restructured
- Design and initial implementation work on MCMD execution model for IPS framework
  - Needed for more complex and efficient use of parallel computing resources
  - Detailed explanation follows
- Development of additional physics components

Progress on Scientific Goals – physics studies

- IPS simulations directed to validation and verification
  - RF power propagation and absorption benchmarking
  - Time dependent energetic minority tail formation in Alcator C-Mod
  - Sawtooth simulation benchmarking M3D/NIMROD (Fast MHD campaign)

- ITER scenario modeling

- Progress on analysis of RF terms in fluid equations, RF effects in kinetic closures. Initial simulations of RF effects on classical tearing mode evolution with NIMROD (Slow MHD Campaign)

- Improvements to mathematical algorithms and improved libraries
  - Tri-diagonal Newton solver for EPA/GLF23
  - Electric field iteration between EPA and Fokker Planck components
  - Introduction of HYPRE and HPL solvers. HPL with AORSA specific modifications

Where we expect to be by end of 3rd year (October 2008)

- **Limited release of Integrated Plasma Simulator – studies by non-project participants supported by project members *(doing now)***

- **IPS ported to NERSC and maintained at NERSC, ORNL-NCCS, PPPL clusters *(if Franklin is completely compatible with Jaguar this is done)***

- **Fully coupled, time dependent simulations of ICRF energetic minority populations in C-Mod with TSC, AORSA2D, CQL3D, MHD stability, with synthetic diagnostic of NPA measurements – on Jaguar XT4 *(in progress)***

- **Slow MHD: effect of RF on classical tearing mode studied with NIMROD *(initial numerical studies completed)***

- **Initial sawtooth simulation with IPS *(done)***

Where we expect to be by end of project

- **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 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) (Slow MHD campaign) and performed numerical simulations comparing with NTM experiments**
- **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.**

Outline of approach to achieve objectives – (This is from our review panel presentation)

High Level Goal	Specific objectives	Principal Supporting Tasks
Develop IPS to satisfy science needs	IPS becomes simulation tool of choice	Metadata management, generalize monitoring, improve load balancing (MCMD), streamline job setup and submission
Demonstrate IPS capability for Tokamak modeling	Ensemble of validated, coupled simulations Support ITPA activities	New and improved physics components (ray tracing RF, NBI, Monte-Carlo Fokker Planck, Transport interface, experiment data access
Demonstrate capability to study RF effects on Sawtooth	ICRF sawtooth modification exp on C-mod. Energetic particle effects on JET and others.	Non-linear MHD initialized by IPS, linear stability analysis, improved reduced 'Porcelli like' model, Nova-K component, particles-to-distribution transform
Demonstrate capability to study ECCD effects on NTM	NTM simulations with coupled non-linear MHD, ECCD, kinetic closure.	Couple ECCD quasilinear operator to NIMROD, implement tight (in memory) coupling in IPS, couple kinetic closure
Serve as basis for FSP design decisions	Evaluate limits of coarse-grain factorization. Study achievable tight coupling with component/framework.	Explore ability of MCMD to accommodate range of SWIM physics components, optimize transport/transport-coefficient and slow MHD coupling, investigate math issues of stability and accuracy with coupled models

Plans for Coming Year – IPS Environment

- Complete MCMD implementation
- Generalized monitoring component and web interface
  - More flexibility, easier configuration of what is exported for monitoring
- Add authentication and personalization capabilities to portal
- Bring prototype metadata management capabilities into production
- Preliminary implementation of tight coupling capability
  - Support components coupling more frequently, exchanging more data
  - Task launch overheads become too high
  - File-based data exchange may be insuficient
  - Conceptual model: CCA-like environment with tightly-coupled components in a single parallel job, exchange data through subroutine calls
  - Implementation will be more intrusive into physics codes than current components
  - Pay-off is generality, reusability of new components in other IPS contexts

Verification and Validation Strategy

The major projects providing SWIM components have V&V programs. We benefit from that (CEMM, CSWPI, TRANSP, PTRANSP)

SWIM Verification

- **“Dummy” physics components permit verification of IPS framework, Portal, and monitoring functions**

Component benchmarking

- **SWIM plug-and-play architecture plus Plasma State data exchange facilitate component V&V efforts – AORSA/TORIC, M3D/NIMROD, many more planned**

Comparison with reduced or analytic models

- **SWIM supports easy substitution of reduced models which can be compared to more complete models in overlapping range of validity – e.g. ICRF Stix model compared to CQL3D, ORBIT-RF in collisional (isotropic) limit.**

Validation – comparison with experiment

- **Example: C-Mod time dependent tail formation comparisons**
- **Synthetic diagnostic development a priority**
- **Experimental data access component is facilitating simulation validation**

Validation of coupled simulation is a challenge. But the ability to couple the most sophisticated physics models is essential to approaching that challenge

Role of leadership class computing

Major codes ported to Jaguar

- **M3D, NIMROD, AORSA, TORIC, CQL3D, ORBIT-RF, TSC, Plasma State**
- **Have had issues with availability, stability, utilities (like the compiler)**

Porting to PPPL SGI cluster

- **A gateway for development and testing SWIM invested in 32 SGI processors on PPPL cluster**
- **All major codes also ported to PPPL cluster**

INCITE project Simulation of Wave Interactions and MHD

- **Early years mostly CEMM and CSWPI → SWIM later years *(i.e. now)***
- **Renewed in 2007**
- **Not renewed in 2008, despite uniformly favorable reviews**
- **Presently completing C-Mod simulations and MCMD studies on Jaguar under directors discretionary account**
- **Will move everything to NERSC**
- **Will be applying for INCITE next call**

Workshop objectives

- **Refine the definition of the final objectives of the project – What will we have two years from now? There are CS and Math answers to this as well as physics.**
- **Assure that we have a plan to get to the final objectives**
  - **Where do we stand on each element of the project?**
  - **What are the additional steps needed to get there? Who is responsible?**
- **Develop a clear plan for the physics target we will address this year**
  - **Complete and publish our present initial physics studies**
  - **Gain much more experience with using IPS → make improvements to IPS**
  - **Get on with the new physics studies in the proposal, or select better ones**
- **Identify near/long term improvements to IPS and framework**
  - **Issues of usability, documentation, incompatibilities, changes to file structure**
  - **Plan for development of new infrastructure – meta-data handling, provenance, monitoring, visualization, portal, build system, regression testing**
  - **Plan for more advanced time stepping capability and expansion of component interface**
- **Identify opportunities for closer collaborations with Math community**

Questions for physics study discussions

1) **What are the physics issues to be addressed?**
2) **What experimental data is to be compared, or what validations studies will be done?**
3) **What components are needed for the work?**
4) **What development is needed to complete the studies? – physics code development, component script development, generalization of IPS time stepping logic ...**
5) **What are the major milestones toward completion and what is the schedule?**
6) **Who is going to do what in the study and when will they do it?**
7) **What publications/presentations are envisaged? What is the schedule for that?**

We will revisit these questions later and boil the answers down to:

Where can we have the highest physics (CS and Math) impact?

What are the dependencies? What has to done to complete the studies

What is the manpower and schedule?