Quarterly Progress Report of the PSI-Center (April-June 2008)

by

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The Plasma Science and Innovation Center (PSI-Center) has accomplished a great deal this quarter. The PSI-Center is organized into four groups: Boundary Conditions and Geometry, Two-Fluid and Transport, FLR and Kinetic Effects, and Interfacing. Each group has made good progress and the results from each group are given in detail. On June 23 the PSI-Center had its annual meeting in Reno in conjunction with the ICC meeting. Presentation can be found on our website.

Progress Report for the BC&G Group (*U. Shumlak, W. Lowrie, V.S. Lukin, G. Marklin, and E. Meier*)

Accomplishments:

- Extended the 2D SEL code to the 3D HiFi code, including the complete machinery of an arbitrary topology-preserving logical-to-physical mapping;
- In both codes, generalized and simplified the implementation of boundary conditions to allow for explicit specification of normal flux through the boundary;
- Added Parallel and Serial HDF5 I/O capabilities to SEL code.
- Added HDF5 I/O capabilities to SEL and HiFi post processing.
- Added the capability for 2D SEL and 2D HiFi post processing to write XDMF files for VisIt visualization (points to HDF5 data).
- Investigated curvature with respect to CUBIT grids with uniformly spaced grid mapping points (rather than default Jacobi spacing).
- Investigated how the number of quadrature points affects curvilinear grids.
- Benchmarked SEL versus NIMROD has been conducted for an FRC translation problem. Total computational effort is comparable for SEL and NIMROD. The average axial velocity within the FRC predicted by SEL is within 10% of the NIMROD prediction throughout the run. Work is in progress to identify the cause of the 10% difference.
- Multi-fluid physics models, including a Spitzer/Chodura combined model and an atomic physics model, have been developed and tested. Simulations with multi-fluid physics give results that are physically consistent when compared to visco-resistive MHD results.
- A Hall MHD FRC simulation has been developed in SEL. The Hall MHD model incorporates the diamagnetic and Hall terms in the generalized Ohm's law, and hyper-resistivity is applied to the toroidal current. Initial Hall MHD FRC translation simulations have been performed, and boundary condition development for Hall MHD is in progress.

- A set of mimetic numerical operators for a 3D tetrahedral mesh have been installed into the T4 Taylor state code which was also upgraded to Fortran90 and parallelized with OpenMP. The new code is called MT4 and is much faster and more accurate and the computed Taylor states exactly satisfy div(B)=div(J)=0.
- Work is in progress to incorporate mimetic operators into the M4 3D tetrahedral mesh resistive MHD simulation code. Application to the induction equation is straight forward and should enable a consistent implementation of the insulated conductor boundary condition. A trial end error approach will be used to determine if mimetic operators can be directly applied to the momentum equation or if a more traditional approach such as the discontinuous Galerkin method will give better results.

Scalability work (*Alan Glasser*)

The following recent progress has been made in the implementation of a scalable parallel solver for the extended MHD codes. It is being developed initially on the 2D SEL code, using high order spectral elements, with plans to port the results to other codes such as the 3D HIFI, M3D, and NIMROD codes.

Accomplishments:

- Interfaced to nonlinear PETSc SNES Newton solver, incorporating selective Jacobian update and adaptive time step. This results in a 30% increase in the speed of the code, relative to the previous method using our own Newton solver. The real motivation for this work is to use the previous linear solvers as preconditioners, preparing the way for the development of a physics-based Schur complement preconditioner.
- A second code module has been written and is in the course of debugging, implementing the physics-based preconditioner. This will be tested on a sequence of problems, including linear sound waves, ideal MHD waves, and Hall MHD waves, to verify its scalable properties. It uses FETI-DP for scalable solution of the parabolic preconditioning equations.

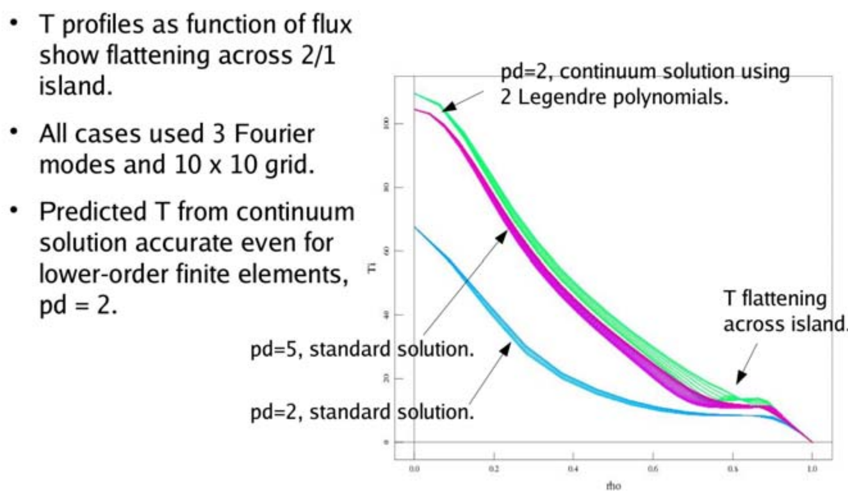
Two-fluid and Transport Group (*C. R. Sovinec, E. D. Held, R. A. Bayliss, and J.-Y. Ji*)

Over the quarter of funding ending on 6/30/08, the Two-fluid and Transport Group has prepared a paper on the convergence of the moment approach for electron heat flux over the entire range of collisionality. We have also completed development for the mixed finite element method for parallel heat flux, and we have tested solving the drift kinetic equation (DKE) directly within the NIMROD framework. We have also completed MHD simulations for a study of weakly relaxing conditions in HIT-II.

Accomplishments:

- Derivation of electron parallel heat flux with our moment method for the exact linearized Landau collision operator is complete. A manuscript that is nearly ready for journal submission shows that the results agree well with Braginskii in the limit of high collisionality and that the computation converges to the collisionless limit with an increasing number of moments. An application to heat flux in the SSPX spheromak in conditions with chaotic magnetic field-lines shows how the moment approach captures the integral nature of free-streaming particles, smoothing over fine-scale gradients in temperature that influence misapplied local closures.

- Our implementation of the mixed finite element for diffusive parallel heat flux has been improved. With suitable scaling of the algebraic systems, our solvers now converge in both cylindrical and slab geometry. A relatively realistic cylindrical test case with a large magnetic island and large parallel thermal conductivity confirms results from a simpler slab test in that the mixed method converges with considerably fewer degrees of freedom than the standard expansion for temperature alone.
- Motivated by success with the mixed method, we are testing direct implicit numerical solution of the DKE with coefficients for the kinetic distortion (from the Maxwellian) solved simultaneously with temperature. Initial results are promising. As shown in the figure below, the results reproduce important physical features, such as flattening of temperature across the island. Moreover, the computational cost is much closer to calculations without any kinetic effects, and the approach can be generalized to include time-dependent kinetic effects, unlike our integro-differential approach.



- Comparison of temperature profiles from a cylindrical computation solved with the diffusive closure and with the DKE expansion.
- Our MHD simulation study of weakly relaxing conditions in HIT-II is nearly complete, and results on current multiplication compare well with experiment and a simple scaling of the force-balance relation. A manuscript has been drafted; though, we decided to include a three-dimensional case that shows a nontrivial degree of relaxation for completeness. Resolving this case at realistic S-value required substantial computing time, delaying the completion of the manuscript.

FLR and Kinetic Effects Group ***(R. Milroy, C. Kim, and G. Cone)***

The FLR and Kinetic effects group continues its collaboration with the MST group on FLR effects on RFP tearing modes, and on improving the performance of including particle effects in NIMROD. In addition, we have begun FRC formation and translation simulations including calculations with a shaped radial boundary. All Ψ-Center supported FRC experiments (TCS, FRX-L and PHD) employ translation and a shaped radial boundary.

Accomplishments:

- The paper "Impact of velocity space distribution on hybrid kinetic MHD simulation of the (1,1) mode" by Charlson Kim, has been accepted by PoP and will appear soon.
- Charlson spent two weeks with the MST group at the University of Wisconsin, working on FLR effects on tearing modes in RFPs.
- Work has begun on the implementation of high order polynomials for particles in NIMROD. This work is required to implement the full energetic particle pressure tensor, rather than the current CGL like, pressure tensor.
- We have completed modifications to boundary conditions that allow us to begin formation and translation studies. We can now perform FRC calculations with a shaped radial boundary and have performed some initial simulations of the PHD experiment at the University of Washington. These calculations will continue in the next quarter.
- We have modified boundary conditions on the radial wall appropriate for FRC θ-pinch formation calculations. Some initial calculations have been performed with the Hall term included. So far, all formation calculations have been performed in a cylindrical chamber, but the effects of an immediately translated FRC can be accounted for by firing coils sequentially to accelerate it out of the formation chamber. The generation of some net toroidal flux and rotation is observed. These calculations will continue, as we compare code results with past experiments.

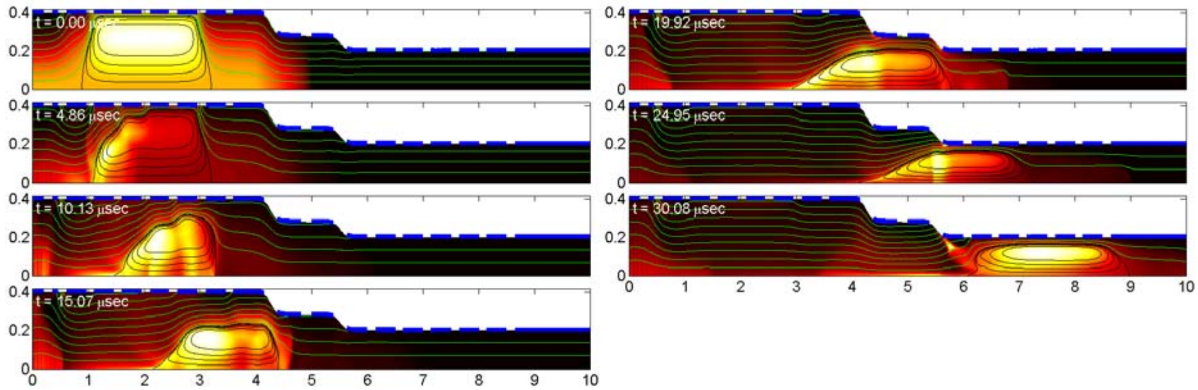


Illustration of FRC translation in the PHD experiment's shaped flux conserver.

Interfacing Group (*B. A. Nelson, C. C. Kim, A. P. Cassidy, S. D. Griffith*)

Accomplishments:

- The IG is tasked with assisting in computational support for the twelve collaborating ICC experiments (along with the three physics groups).
- Working with Jay Kesner of MIT to set up LDX runs:
  - improve equilibrium generation
  - study impact of diffusivity vs. heating rate
  - allow more flexibility in LDX grid generation
- Beginning work with Swarthmore postdoc Tim Gray to study stability properties of SSX
- The Python-based "NimPy" post-processor has been improved, working with suggestions and feedback from Drs. Carlos Romero Talamás and Bick Hooper of LLNL. NimPy now can read current density, divergence of **B** error, toroidally-averaged poloidal flux, and lambda parallel from the standard NIMROD post-processing code "nimplot" output files. A Python script runs nimplot for each NIMROD dump file, writing and renaming the nimplot output files for each dump file. If appropriate flags are set in the NimPy resource file (.nimpyrc) NimPy reads both the NIMROD dump and nimplot files, and converts these quantities to the Visualization Toolkit (VTK) format, which can then be read by the LLNL VisIt visualization program (http://www.llnl.gov/visit/). All 3D quantities can be broken into individual mode structures in the VTK file. "Proper" connectivity between NIMROD "rblock"s (which becomes an unstructured mesh in VTK) has been implemented to allow full use of VisIt functionality. Drs. Romero Talamás and Hooper are examining NIMROD SSPX output using NimPy and VisIt, and presented a poster and invited talk of their results at the recent ICC meeting in Reno NV. This method, of using Python scripts to "steer" the "standard" NIMROD post-processing codes allows collaborators to use their NIMROD installations without requiring code modification or re-compiling.

- Carleton College undergraduate student Ben Haynor is working with the PSI-Center this summer to improve NimPy.