# Progress report for Plasma Science and Innovation Center (12-2-05)

by

*Thomas Jarboe, Brian Nelson, Richard Milroy, Uri Shumlak, and Carl Sovinec*

The Plasma Science and Innovation Center (PSI-Center) has accomplished a great deal since it started on March 1, 2005. We have found some outstanding computational plasma scientists to work in the Center. The hiring is complete and everyone was on board by September 2005. The new SGI350 parallel processing computer, for code development, has been installed. It is running and NIMROD and MH4D are being used on it routinely. 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 very good progress and the results from each group are given in detail.

## ***Boundary Conditions and Geometry Group*** (U. Shumlak, G. Marklin, S. Vadlamani)

The BC Group has made progress in developing MH4D and general plasma simulation techniques using tetrahedral meshes. In developing MH4D, the group has made significant progress in learning the code and in implementing new boundary capabilities.

**Accomplishments**

- The code was modified to produce graphical output files that can be read with a widely available visualization software.
- A Taylor state initialization method has been implemented on tetrahedral meshes.
- MH4D has been applied to HIT-SI and ZaP, which tests the ability of the code to handle re-entrant geometries.
- A testbed code M4 has been written that allows component and algorithm testing in a simplified, serial code.
- The MH4D code along with the required software packages (MPI, PETSc, and ParMETIS) have been installed on the local SGI parallel computer.
- Preprocessing routines have been written that prepare tetrahedral meshes produced by T3D and initial equilibrium configurations (e.g. Taylor states) for use with MH4D.
- The code was modified to produce output/restart files in a format readable by the GMV (General Mesh Viewer) visualization software.
- MH4D was used to simulate a tilting mode in a spheromak in a cylindrical flux conserver.
- With the help of Roberto Lionello, external field conditions were added to MH4D.
- Simulations of HIT-SI and ZaP were attempted using external fields with MH4D and tetrahedral grids generated by T3D. The code was run in an explicit time stepping mode and the time steps were unreasonably small. The time step computation was investigated in detail to understand the algorithm and determine the usefulness of the code for explicit calculations. The semi-implicit method is presently being investigated to alleviate the time step limitation.

- General plasma simulation techniques have been investigated with the testbed code M4 that was developed by the BC Group.
    - Boundary conditions that model conducting walls with insulating surfaces have been implemented by computing the electrostatic potential in the volume assuming the Coulomb gauge. Simulations of a decaying spheromak in the HIT-SI geometry were performed.
    - The Taylor state initialization routine was also implemented in M4.
    - Recently, appropriate boundary conditions assuming the MHD gauge have been derived and are expected to work better because the method only requires calculating the electric and magnetic potentials at the domain surface.
        - The numerical implementation in M4 is currently in progress.
        - A generalization of the method will make it applicable to electrode driven configurations where an external RLC circuit is connected to the plasma to drive plasma current and inject magnetic flux.
- The Taylor state initialization code was also used to investigate flux surfaces in the HIT-SI geometry for various ratios of spheromak flux to injector flux. Taylor states were also computed for HIT-SI with different size midplane gaps to estimate the helicity loss in the experiment.

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

Over the first six months of funding for the PSI-Center, the Two-fluid and Transport Group has made progress on the implicit leapfrog algorithm, the implementation of collisional heat flux, and the analytical formulation of collisionless transport on open magnetic field-lines. Here, we briefly review what has been accomplished in these areas.

**Accomplishments**

- For simulating EC experiments, numerical stability in the presence of significant flows is required. In conjunction with SCIDAC-supported work, we have performed a numerical analysis of the implicit leapfrog algorithm [T1] for the two-fluid plasma model with flow and electron drift represented.
    - We find that implicit advection is required when there is electron drift; the standard predictor/corrector advection algorithm in NIMROD does not suffice.
    - There is no additional complication from gryoviscous terms, provided that they are centered in the velocity step.
    - These results have been reported at the 2005 Division of Plasma Physics Meeting.

- We have written a matrix-free solver for non-Hermitian linear systems that couple Fourier components. These systems arise with nonlinear two-fluid and implicit-advection computations.
    - The routine applies matrix ‘splitting,’ solving approximate matrices that have fully computed elements while using matrix-free computations to update the residual.
    - Tests show the new solver to be effective on the velocity advance in nonlinear MHD computations with three-dimensional variations in the number density.

- The two-fluid advance is being verified on tearing-mode computations in slab geometry (see Fig. TFT.1), where there are analytical results on growth rates and on quasilinear dynamo effects from MHD and Hall terms.

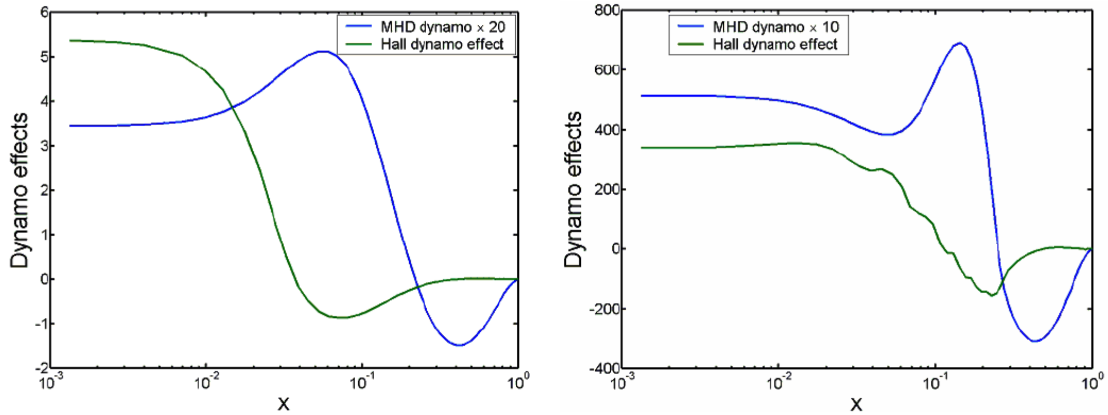



Figure TFT.1. Comparison of NIMROD results on MHD and Hall dynamo effects from a large-Δ´, finite-$\beta$ tearing mode in slab geometry in quasilinear (left) and nonlinear (right) conditions. [From 2005 DPP presentation by H. Tian, U. Wisconsin.]

- We have recently derived a general scheme for quantitatively assessing parallel transport for all regimes of collisionality (collisional comparisons are given in the table below). In this approach, we:
    - Include temperature and flow gradient drives simultaneously.
    - Treat a portion of the collision operator using moment expansions for the distribution functions.

Comparison of Coefficients from Braginskii and the Collisional Limit of the General Closure

| | electrical conductivity, $\sigma$ | parallel ion thermal diffusivity, $\chi_{\|i}$ | parallel electron thermal diffusivity, $\chi_{\|e}$ |
|---|---|---|---|
| Braginskii | 1.96 | 2.76 | 1.60 |
| General | 1.98 | 2.78 | 1.56 |

- We are preparing papers on the treatment of the collision operator as well as the solution to the plasma drift kinetic equation for submission to *Physics of Plasmas*.
- Careful tests of the Braginskii parallel thermal conductivity were performed using a magnetic-field distribution computed previously with NIMROD.
    - The explicit number density dependence has been removed from the thermal conductivity, as appropriate for parallel collisional transport.
    - The temperature dependence of the Coulomb logarithm has been incorporated in Braginskii's thermal conductivities.
    - The temperature profile computed for an SSPX discharge (see Fig. TFT.2) shows a 10 eV increase at its peak over the previous result.

- Drs. Ji, Held, and Sovinec reported on this work in “Nonlocal parallel heat transport and energy confinement in SSPX,” a poster at the Denver APS-DPP meeting.
- Experimental results for the SSPX discharge series 46XX are approximately 30-40 eV higher, and this discrepancy will be examined in future work involving the nonlocal parallel heat flow closure.

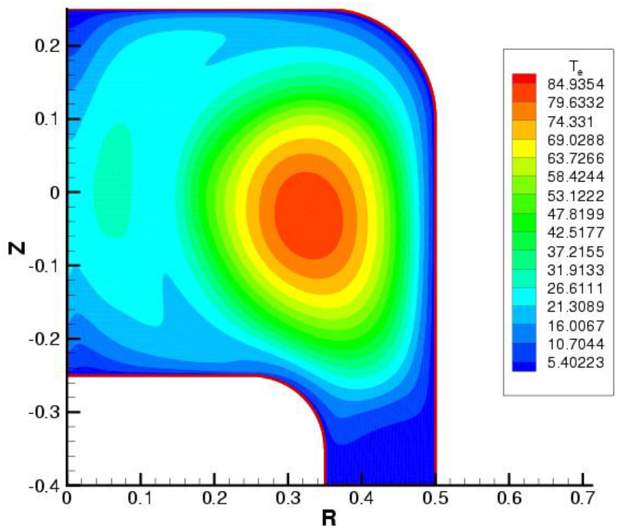



Figure TFT.2. Electron temperature profile (in eV) of SSPX 46XX-series discharges computed by NIMROD, including temperature-dependent Coulomb logarithm factors and density-independent thermal conductivities.

**Reference**


[T1] C. R. Sovinec, D. D. Schnack, A. Y. Pankin, D P. Brennan, H. Tian, D. C Barnes, S. E. Kruger, E. D. Held, C. C. Kim, X. S Li, D. K. Kaushik, S. C. Jardin and the NIMROD Team, “Nonlinear Extended Magnetohydrodynamics Simulation Using High-Order Finite Elements,” Journal of Physics: Conference Series 16, 2005 (IoP, London, 2005).


***FLR and Kinetic Effects Group*** **(R. Milroy, A. Macnab, C. Kim)**

Because of its high $\beta$, the lack of a toroidal field, and the presence of a field null, the FRC has the strongest FLR and kinetic effects of any fusion concept. Thus, one of the first tasks for the “FLR and Kinetic Effects Group” is to model FRCs with NIMROD’s extended MHD capabilities. At the same time, we are working to implement a fully kinetic minority species in NIMROD. A bulleted list of accomplishments to date is shown below.

**Accomplishments**

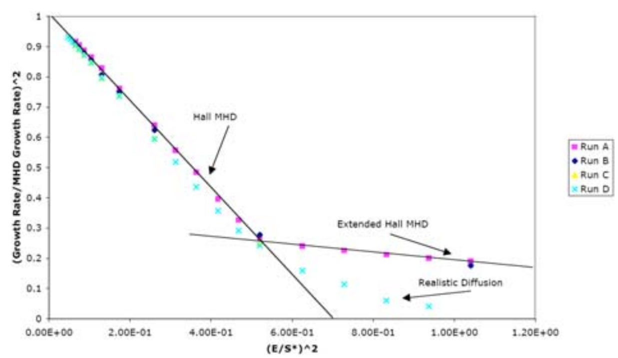
- Hire 1.5 post-docs. Angus Macnab joined the PSI-Center in early August followed by Charlson Kim (shared ½ time with the interface group) in early September.

- Work through the many problems associated with *coming up to speed* with NIMROD including; compiling it and its associated libraries on both a standard Linux box and more recently on the new SGI cluster; start familiarizing ourselves with the codes data structures and algorithms; modifications to the initialization routines to allow us to read from an FRC equilibrium file to initialize either a linear or nonlinear FRC calculation; and developing our own post-processing methods including both Tecplot and Matlab

- Gain familiarity with Dan Barnes FRC equilibrium code and port it with graphics to the SGI cluster.

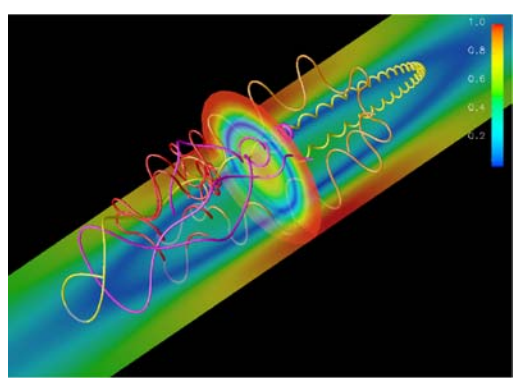
- We have worked with 4 different development versions of NIMROD, and worked through the problems of getting each of them to run on our computers, including the SGI cluster when it came online. We have made some progress in assimilating these versions into a single PSI-Center version.

- We have collaborated with Dan Barnes to calculate the linear growth of the FRC tilt mode with an accurate treatment of the Hall term included. We have performed a series of linear calculations to map the growth rate as a function of $E/S^*$, and characterize the sudden change in the mode complexity when $E/S^*$ exceeds a critical value. This was documented in the APS poster CP1-81; "Verification of a Hall MHD Algorithm in Nimrod for an FRC" by Barnes, Macnab, Milroy and Sovinec. A key figure, showing $(\gamma/\gamma_{MHD})^2$ vs. $(E/S^*)^2$ is shown here.




- Perform nonlinear 2-fluid calculations on a relaxing FRC using the axisymmetric (n=0 only) option. This study has just started, and is helping us benchmark NIMROD's current capabilities for FRC simulations. For example the default end boundary condition sets the tangential component of the electric field, $E_T$ to zero. This corresponds to an end-shorted boundary condition, and with the Hall term turned on it leads to a spin-up of the open field line plasma, which through viscosity leads to a spin-up of the FRC. NIMROD is capable of modeling a highly anisotropic thermal conductivity unlike previous FRC codes, and we have begun to examine the implications of this feature for our calculations.

- We have made progress in implementing a fully kinetic minority species into NIMROD including:
    - Import drift kinetic particles into the U. of Wisconsin version of NIMROD.
    - Implement the full kinetic equations of motion using the Boris algorithm. The figure to the right illustrates some particle orbits in an FRC.



- Apply subcycling time stepping for pushing the full kinetic equations of motion. i.e. push particles multiple times for each MHD timestep.
- Currently working on implementation of the hot particle pressure tensor gather to include it into the right hand side of NIMROD's momentum equation.
- Present this work as APS poster CP1-81; "Extension of Drift Kinetic Hot Particles to Full Orbits in NIMROD.

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

**Accomplishments**

- Hiring of Personnel:
  - Two half-time Research Consultants, Andrew Cassidy and Susan Griffith, joined the IG in August 2005. They maintain the Computational Facility, Communications Network, and assist in programming tasks.
  - Dr. Charlson Kim joined the IG as a half-time Research Associate (shared with the Kinetics Group) in September 2005. Dr. Kim is actively modifying the NIMROD code for use on the collaborating EC experiments.
- Computational Facility Installed:
  - A 16-processor (1.5 GHz Intel Itamium2 CPUs w/6MB L3 cache) SGI Altix 350 cluster with 32 GB shared memory has been installed and commissioned. It is running SUSE Linux, and has the following software: Intel FORTRAN 90 and C/C++ compilers, the Totalview debugger, and the PBS Pro scheduler. The software and hardware of this system is being fine tuned to the needs of the PSI-Center.
- Communications Network Installed:
  - A gateway/logical firewall computer has been installed for network security. All PSI-Center workstations are behind the firewall, or use virtual private networking to access the PSI-Center cluster. Secure wire access points and a stub-office router have been installed for personnel in other buildings. The gateway also serves the PSI-Center web-site (http://www.psicenter.org).
  - Networked disc storage is provided by a dataserver with 2.1 TB of RAID5 SATA drives. Two sysadmin workstations are employed as system loggers/monitors, additional data backup, and are "hot spare" replacement boards for the gateway and dataserver. In addition, four new Linux, one Mac, and two Windows workstations are in use by PSI-Center personnel.
- NIMROD Support:
  - The IG is tasked with providing computational support for the nine collaborating EC experiments. All collaborating PIs have been contacted, and development of plans for proceeding with simulations is ongoing.
  - Modifications to NIMROD are being made for particular groups of collaborating EC experiments. These include generalized applied voltage BCs, and a generalization of specifying external coil sets for NIMSET.

- Initial NIMROD modeling has been performed on SSX. The SSX grid has been made and refined. Initial SSX simulations are being run to test NIMROD's ability to run with the SSX grid and boundary conditions. Of particular concern are the reentrant grid and convex corner boundary conditions. Neither seems to be an issue for NIMROD nor the associated solver SuperLU. These initial test runs were done with the simplest NIMROD options; axisymmetric (n=0 only), flat and constant density ($10^{19}$ $m^{-3}$), zero beta, electric diffusivity=100, kinetic viscosity=1000, with a parabolic diffusivity profile in the gun region with a maximum amplification of 100. Vacuum magnetic field is applied to approximate experimental conditions.
- Gridding of MBX has been done, with the next task to modify the generalized applied voltage BCs for the MBX annular rings.
- Post-processing of NIMROD data have been helped by Python objects and MATLAB scripts (the latter written by Richard Milroy) to read and plot NIMROD dump files. These objects and scripts can be used to convert the FORTRAN binary data into formats suitable for other analysis programs used by the collaborating EC experiments.