Quarterly Progress Report of the PSI-Center (Jan – Mar 2007)

by

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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.

Boundary Conditions and Geometry Group ***(U. Shumlak, G. Marklin, W. Lowrie, E. Meier)***

A cylindrical domain with periodic ends has been used to simulate screw-pinch instabilities. To facilitate periodicity for this case, MH4D was modified such that boundary triangle information can be passed to MH4D from the loader. Comparison of instability growth rates with analytical models is pending.

- Domain reflection routines have been implemented in the MH4D loader. Reflection is used to ensure matching vertex patterns on periodic surfaces such that arbitrarily high resolution can be attained with the mesh generator (T3D). This feature is used in benchmark comparisons of MH4D ZaP simulations with MACH2 results, which are under way.
- MH4D is compiled and running on Bassi.
- Designed potential data structure for new FEM plasma code.
- Researched Hexahedral mesh generators and decided get a copy of CUBIT from Sandia National Labs for further study.
- Researched PETSc implementation.
  - Assembled 2D scalar Laplacian operator in PETSc for simple mesh.
  - Assembled adjacency matrix for a simple meshes.
  - Performed timing study for solving 2D Poisson's equation in parallel with PETSc.
  - Assembled 3D scalar Laplacian operator for a structured mesh.
  - Solved 3D Poisson's equation on a simple mesh with various solvers included in PETSc.
  - Researched optimization methods for assembling sparse matrices in PETSc.
- Researched using SuperLU with PETSc.
- It was discovered how to set up the insulated conductor boundary condition as a self-adjoint system of equations. Now the resistive diffusion term can advance together with the surface potential equation and the circuit equations as a single coupled SPD system. This will greatly simplify the numerical solution process.
- The new version of the M4 code, which will solve resistive MHD with the insulated conductor boundary condition using fully implicit time steps and a Pseudo-Finite-Element spatial representation, is nearly finished. The PFE method assembles the matrix representation of an equation by first construction matrix representations of the basic differential operators using standard finite element methods (e.g. FEMLAB) and assuming that the matrix of any product can be approximated by the product of the matrices. (e.g. matrix(J X B) = matrix(J) X matrix(B) with the matrix of J and B in terms of A computed by FEMLAB using elements of any order) This allows us to use

commercial software such as FEMLAB to define the geometry, construct the mesh and compute some basic matrices which are then fed into M4 and assembled into the full matrix system and advanced implicitly in time. The first version of the code will be parallelized with OPENMP. A later version will use PETSC.

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 3/31/07, the Two-fluid and Transport Group has improved our simulations of coaxial helicity injection in low-aspect ratio configurations by providing better control of the electrostatic part of the voltage and by shaping the cross section to better approximate HIT-II. We have also begun applying our new approach for the Coulomb collision operator when solving kinetic closure terms for the fluid-moment equations.

Accomplishments

- We have derived analytical expressions for general parallel closures from the linearized two-fluid moment equations with arbitrary numbers of moments and studied the convergence properties of these closures as higher-order moments are added. In addition, we are developing the cross and perpendicular heat flow and stress moments using a generalized formalism that provides corrections and modifications from previous theories such as Braginskii's. Two papers are being prepared in conjunction with this work.
- We have also developed a hybrid approach for the exact, linearized Coulomb collision operator that inverts the angular scattering part of the operator but uses a moment approach for the remaining terms. Tests of parallel closures derived from a kinetic equation involving this operator show quantitative agreement with previous collisional and collisionless results. This complete closure scheme is being implemented in NIMROD and a paper on the analytical formulation is nearing completion.
- On the computational side of the kinetic closure work, we have recently implemented an approach that allows NIMROD to use large numbers of processors (1000's) to perform closure calculations independent of NIMROD's fluid advance. This included splitting MPI communicator groups and developing additional routines for data passing. This work is leveraged by code development for the Center for Extended Magnetohydrodynamic Modeling.
- Preliminary work has begun on the implementation of an implicit parallel electron stress in NIMROD. An implicit formulation of the local, collisional electron stress has been derived. The implicit operator will also be used as a semi-implicit operator to stabilized the nonlocal parallel stress closure, once it is introduced into NIMROD's Ohms Law. This work is also in conjunction with research for CEMM.
- Our simulations of coaxial helicity injection relevant for HIT-II and NSTX have been improved. We have modified the simulated absorber boundary to set the electrostatic potential through an $\mathbf{E}\times\mathbf{B}$ drift. This avoids previous difficulties with losing injected current in boundary layers, and we are now able to 'dial-in' current multiplication with the electrostatic potential. We have also shaped the outer wall to better represent HIT-II, and flux amplification now appears more symmetrically with respect to the mid-plane. Results at the threshold of flux amplification from a three-dimensional simulation with HIT-II-relevant parameters are shown in Fig. TFT.1.

Future Work

- Work related to the two-fluid algorithm to be completed within the next quarter includes:

- Compare MHD simulation results on flux amplification with HIT-II-relevant parameters to published data from the experiment.
- Complete testing of the temperature-dependent parallel viscosity coefficient.

- Work on parallel closures to be completed within the next quarter includes:
  - Implement parallel heat flow closures derived using (i) full moment approach and (ii) hybrid moment/kinetic-distortion approach and apply in SSPX transport calculations.
  - Continue implementing a full closure model for parallel heat flows and stresses and identify interesting applications for EC experiments and the PSI-Center.

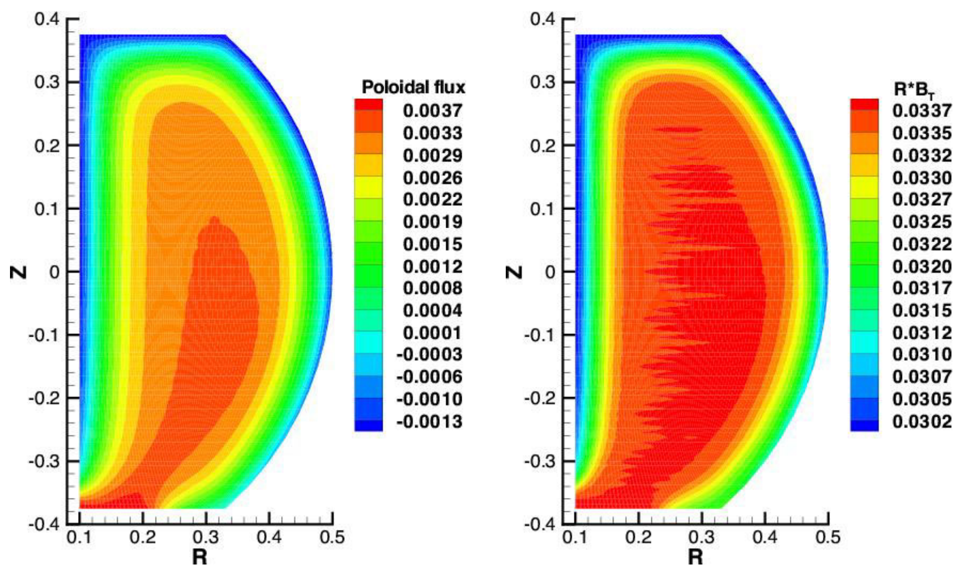


Figure TFT.1. Contours of toroidally averaged poloidal flux (left) and toroidal averaged RB_ϕ (right) from a simulation of coaxial injection in small-aspect-ratio tori with improved absorber modeling.

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

Over this quarter the FLR and Kinetic Effects group has focused on finishing up work started earlier on simulations of FRC spin-up, and on the continued enhancement of particle simulations with a focus on FLR effects on the RMF tearing mode.

Accomplishments

- Work has continued on an in depth examination of the origin of rotation in field-reversed configurations via the end-shorting process.
  - We have demonstrated that a conducting wall is not required for this process. An insulating wall combined with physical processes that prevent the plasma from spinning rapidly near the wall (viscosity, charge-exchange, etc.) will also lead to FRC spin-up.
  - Simulations have demonstrated that the spin-up process leads to a residual toroidal field in the open field line region after the system has settled into a Hall MHD equilibrium.
  - The calculated rotation profiles compare favorably with published measurements from the STP-L device.
  - A paper has been prepared, for submission to Physics of Plasmas.

- We have simulated coil induced translation of FRCs, using the latest version of NIMROD. These simulations include an inflow boundary condition in the region of the coils and employ implicit time stepping for the advection terms in the MHD equations.

The results are much more numerically stable than previous simulations, showing good conservation and convergence with Mach >1 flow.

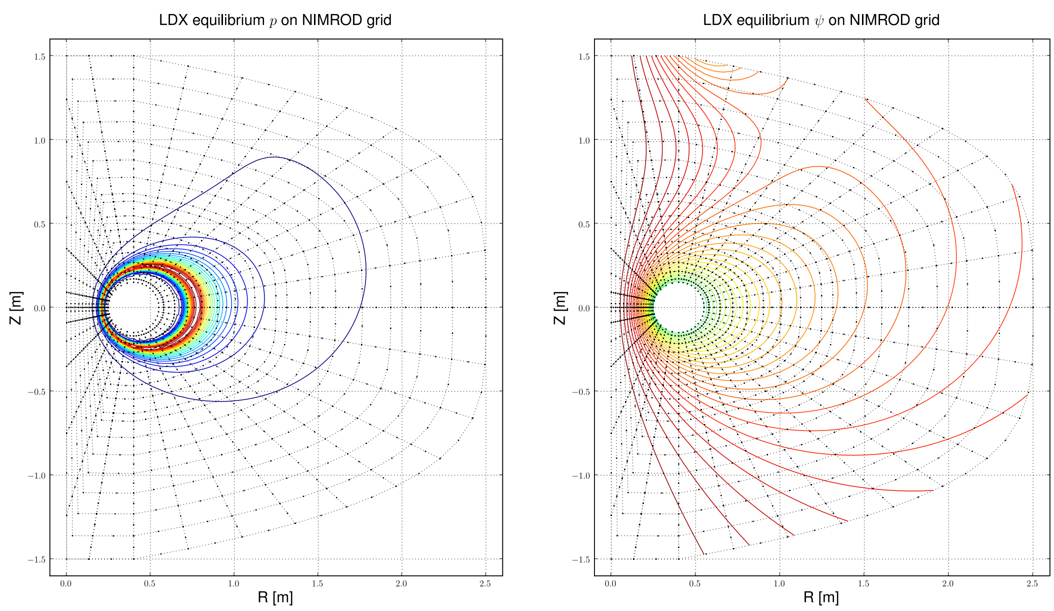
- Particle subroutines were rewritten and reorganized to unify code for the various particle types that are supported by NIMROD to ease usability and further development.
  - In the process of rewriting the particle subroutines, the efficiency and performance were optimized, leading to approximately a 30% improvement.
- In benchmarking the rewritten particle subroutines, we were initially unable to recover the (1,1) internal kink benchmark, neither with the hot particle pressure nor in the ideal MHD case. Upon further exploration of this issue, it was discovered that this discrepancy was most severe for small time steps, in particular the time-step necessary to satisfy the particle's CFL. The culprit was tracked down to the calculation of the pressure (using the ideal gas law) at the quadrature point (for use in the right-hand-side of the momentum advance). This was a recent change introduced into NIMROD with the implicit field advance subroutines. Prior to this change, pressure was calculated at the finite element nodes and interpolated to the quadrature points. Reverting back to calculating the pressure at the nodes and interpolating to the quadrature points resolved this discrepancy and the internal kink benchmark was recovered.
  - This may be a disturbing indicator of a pervasive issue. Locally calculated quadrature quantities are used extensively throughout NIMROD. It is conjectured that the direct calculation of field values at the quadrature point may introduce higher spectral content that is inconsistent with the order of the finite element basis function. Calculation at the node and interpolation eliminates this inconsistent higher spectral content by taking advantage of the orthogonality properties of the basis functions. Further exploration of this issue is necessary.
- We presented two talks at the ICC meeting in February, and have submitted manuscripts to be published in a special issue of Journal of Fusion Energy as the proceedings. The two talks were:
  - "Preliminary Simulations of FLR effects on RFP tearing modes", by Charlson C. Kim.
    - The talk demonstrated that FLR effects of full orbit particles can stabilize tearing modes in RFP in qualitative agreement with V. Svidzinski, et al.
    - More realistic particle phase space distributions result in a modest stabilizing influence at low density.
    - There are also indications that higher hot particle densities may lead to excitation of, an as yet unidentified, fast growing mode.
  - "FRC Simulations using the NIMROD Code", by R.D. Milroy, A.I.D. Macnab, C.C. Kim, and C.R. Sovinec.
    - This talk summarized progress in three areas. 1) The acceleration and super-sonic translation of FRCs. 2) FRC spin-up due to end-shorting. 3) Understanding the influence of toroidal fields and the Hall term on the n=2 rotational instability.

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

Accomplishments

- The IG is tasked with assisting in computational support for the twelve collaborating EC experiments (along with the three physics groups). All collaborating PIs have been contacted, and development of plans for proceeding with simulations is ongoing.

- The Levitated Dipole Experiment (LDX) has joined the PSI-Center's list of collaborators. Drs. Jay Kesner and Darren Garnier and the Interfacing Group are working to set up studies of the non-linear evolution of calculated LDX equilibria at marginal stability. An LDX NIMROD grid, coded by Carl Sovinec *et al.*, has been incorporated into the PSI-Center versions of NIMROD (NIMPSI and NIMlite). An initial equilibrium from the Columbia/M.I.T. DIPEQ code has been bilinearly interpolated onto the LDX grid (see figure below), and is nearing initial runs.



DIPEQ equilibrium pressure (left) and poloidal flux (right) interpolated onto the LDX NIMROD grid, (meshed by Sovinec et al.*). (Values of* $\boldsymbol{B}_R$ *and* $\boldsymbol{B}_Z$ *derived from the poloidal flux are the fields actually advanced in NIMROD.)*

- Progress has continued on the NimPy post-processor, which outputs NIMROD data to the Visualization Toolkit (VTK) format, that can be read by the LLNL VisIt visualization program (http://www.llnl.gov/visit/). Progress was reported at the 2007 ICC meeting.

- NimPy is being extended to be a "steering program" for existing NIMROD post-processors, including nimplot and nimfl. Present efforts are to call nimplot from NimPy to calculate **J** and poloidal flux, dumping them to Tecplot files, which are then read by NimPy, for subsequent output to VTK files for VisIt.

- Development of a version of NIMROD, "NIMlite" (to replace NIMPSI), is proceeding with removal of vestigial elements of old coding and reorganization of the code for more efficient compilation. Several initialization routines have been added, including bessel function spheromak in a can, merging spheromaks, FRCs, LDX, and "Bellan's box".

- Spheromak formation simulations have continued with "Bellan's box", with progress in adding additional physics (density evolution, *etc.*) and boundary conditions (diffusivity shape, *etc.*). These results were presented at the February 2007 ICC meeting. Extensive discussions regarding how to proceed were made with Prof. Bellan and Dr. R. Adam Bayliss (of the PSI-Center MHD Group) at the ICC meeting.

- Work is continuing on hot particle stabilization of tearing mode in RFPs, exploring the parameter space and convergence studies.