NIMROD Team Meeting Minutes
August 12-14, 2014, Logan, Utah

The team meeting began with an informal discussion of features that would be beneficial for applications and for development. Participants were encouraged to offer ideas, regardless of feasibility and generality. The following items were discussion, and comments that were recorded during the conversation are noted. Also, see the slides prepared by Jake King for this discussion.

- More general meshing capability would be useful for modeling real boundary structures.
  - A general 3D mesh would provide more flexible geometric capabilities.
  - Coupling to external EM solvers like VALEN would be easier.
  - General 3D meshing requires changes to operators (Fourier rep. is assumed) and to pre- and post-processing.
  - Gridded phi-direction but similar poloidal planes is more tractable but less general.
  - An extension of the Fourier rep. to include Fourier-expanded metrics is another possibility.
- Better preconditioning over the toroidal direction would improve computational performance.
  - Algebraic multigrid is an option, possibly over just the toroidal direction. Effectiveness of basic smoothers depends on operators.
  - Dense solves over toroidal couplings could be used via additive Schwarz with existing poloidal-block solves. Matrix generation via trigonometric cardinal functions is possible.
- On a framework level, Fortran03 object-oriented extensions allow abstract blocks.
  - Modifications would eliminate block-type-specific looping.
  - Development of new block types would be easier.
- New asynchronous collective communication can be used to overlap communication and computation related to FFTs and pseudo-spectral operations.
- Take advantage of new accelerator hardware, somehow.
  - Coding or coupling of matrix software that uses accelerators
  - Coding OpenACC directives
  - New external solvers with accelerator capability
- A more robust 2-fluid advance is needed.
  - Discussed further during presentations
- Documentation needs attention.
  - Tutorial needs to be updated.
  - Some code comments are out of date.
  - Particle coding needs to be commented.
- Reuse of temporary memory in integrand routines is confusing to new developers.

<u>Computational topics:</u>

In an effort to improve the two-fluid advance, Carl Sovinec has recently investigated a vector potential formulation to replace the advance of the magnetic field. The modified code eliminates div(**B**) as a possible source of error, but the advance needs to impose a gauge condition for solvability. Separating electromagnetic and electrostatic contributions is different in the two formulations. Development and tests are only linear resistive MHD. While a resistive tearing mode runs relatively well, an internal kink case does not. Implications for the two-fluid advance are not clear at this point.

Dan Barnes presented a new semi-characteristic method for solving the Vlasov equation with a delta-f method for an evolving background. He first reviewed prior algorithmic development for implicit PIC with noise reduction. The early efforts used particle information to close moment equations but numerical synchronization is not satisfactory. Switching the kinetic system to a *particular velocity*, $\mathbf{v} - \mathbf{V}_{\text{fluid}}$, eliminated circular implicit couplings between the moments and the delta-f equations, and symmetry properties provided energy conservation. Recent efforts take advantage of Hamiltonian properties to use different characteristics without changing the delta-f evolution: subtracting the equilibrium contribution to the characteristics removes shot noise. There is a remap step but only in 1D. Results for a small-amplitude wave demonstrate order of magnitude improvement in the evolution.

Jake King discussed computational improvements for different parts of the NIMROD suite. The first is parallel I/O via the HDF5 library. His development has all processors on processor-layer 0 collect all Fourier components, then write their set of blocks to the new-format dump file in parallel. This improves speed with more than 10 Fourier components, and direct use of viz schema graphics is possible. The second is replacing NIMROD's FFT routines with the FFTW, which does its own optimization. The FFTW use is not parallel, and the purpose of the development is to allow an arbitrary number of toroidal mesh points. The third topic is a proposed coupling of FLUXGRID and NIMEQ to iterate meshing with Grad-Shafranov solves. The primary intent is to refine externally provided equilibria for more accuracy and to remove jumps along the separatrix. The FLUXGRID meshing then makes it easy to distinguish the closed- and private-flux regions. The coupling will add X-point functionality that has been missing.

<u>Physical model development and analysis:</u>

Eric Held presented results and plans for his continuum kinetic modeling for NIMROD. He showed results on bootstrap current, particle flux, heat flux, and parallel ion momentum for a high-beta low aspect ratio NSTX case. The results show good quantitative agreement between NIMROD and GA's NEO code. Held also reviewed application of the kinetic modeling to energetic particles and the internal-kink/fishbone computation. A paper on cross-code comparisons is fully drafted and nearly ready for submission to PoP. Held is now considering an energetic-particle case on Alfven eigenmodes for comparison with TAEFL.

Jeong-Young Ji presented work on his general moment method of plasma kinetics for the two topics of integral parallel closures with a straight magnetic field and for conditions of inhomogeneous field. His method separates the background Maxwellian part of the distribution and uses orthogonal polynomials to represent the kinetic distortion. The parallel moments are expressed in matrix form, and Ji has formulated a relatively simple fitting that matches numerical results with up to 6400 moments and limits to the collisionless result. He is presently studying the effect of inhomogeneous magnetic field numerically, solving for heat flux as parameters for magnetic field and temperature fluctuations are varied.

Andrea Becerra reviewed the resistive-wall formulation for the external Green's function solver GRIN and presented results for the ideal-plasma limit. Careful consideration of geometric coefficients shows helpful cancellations in the weak form of the normal-component evolution. An example application is an NSTX test case with the NIMROD domain extending to the experiment's copper plates. The ideal plasma limit is conditionally stable with an ideal wall. There is some question as to the accuracy of the equilibrium. With Spitzer resistivity modeling, the ideal wall case shows a growing mode with significant divergence error. There was discussion of how to best use the piecewise-constant information on magnetic potential from GRIN. King has been working on the coupling and has tried several different approaches.

Peter Norgaard provided an update on his implementation of the Shumlak-Meier model of dynamic neutrals. The model includes the effects of ionization, recombination, and charge-exchange collisions. The plasma is affected by sources, drags, and accretion terms. His development fits with NIMROD's implicit leapfrog algorithm, as achieved in 4 stages: 1) explicit, 2) time-centered linear implicit, 3) explicit nonlinear, and 4) time-centered nonlinear via iteration. The neutral density advance is solved simultaneously with the plasma density advance so that particle source terms can be coupled implicitly. Spatially uniform test cases verify the behavior of the neutral-plasma interaction terms and show the benefits of the implicit implementation.

Jake King presented analytics and numerical computation for drift-tearing. He has prepared a manuscript that has been split into two sections, the first of which has been submitted for publication in PoP. He reviewed the beta/skin depth parameter space for two-fluid tearing and noted how previously published results appear in this space. He also identified the experimentally relevant regime and where different analytical approximations are applicable. He has obtained 3 new dispersion relations from analytics using the transformation method of Ahedo and Ramos but with extensions to include drift effects. NIMROD computations have been performed for four sets of conditions with varying degrees of drift. The scans inherently move the parameters in the beta/skin depth space, and this is taken into account in comparisons with theory. Complete stabilization is predicted and effectively realized in the physically relevant regime. The growth-rate increases with drift in the electron MHD regime, but this may be an unphysical consequence of dropping electron advection and gyroviscosity. One of the scans helps verify NIMROD's diamagnetic heat implementation. Future steps include nonlinear evolution.

Applications:

Eric Howell described his extended-MHD studies of interchange modes in cylindrical pinch/spheromak equilibria. The cases are motivated by SSPX conditions that had relatively low magnetic shear. His modeling compares results with MHD, MHD plus gyroviscosity, MHD plus GV plus two-fluid Ohm's law, all of previous plus two temperatures with diamagnetic heats and flow. At low Suydam parameter (D_s), there is a transition through resistive instability to ideal instability, as expected from previous results of Fatima Ebrahimi. Adding GV to MHD is stabilizing for $D_s<1/2$, and it affects resistive scaling. Including the two-fluid Ohm's law always increases growth rates. When the Hall parameter is scanned by changing the elementary charge, there is initially a stabilizing effect then a destabilizing effect as eigenmodes acquire a drift character. The 2-temperature results show significant stabilization but are only tractable at larger particle and thermal diffusivities. Howell provided a table to summarize numerical tractability. Cases with 2 temperatures are the most problematic.

Josh Sauppe presented two-fluid RFP simulation results and comparisons with experiment and analytical relaxation theory. His simulations are run at S=20,000 with Pm=0.1 or 1. An important issue is the relative sign of the fluctuation-induced Lorentz force (and hence Hall dynamo) and the change in parallel flow in the core. Some experimental papers indicate one relation and others imply the opposite, and a group effort with experimentalists is underway to sort the discrepancy. Simulations always show that the Hall and MHD dynamos work constructively during the first relaxation event. However, some later events show destructive contributions with MHD dominating. For comparison with two-fluid relaxation theories, Sauppe constructs a vector potential and then species helicities, paying attention to gauge invariance. When using the species relative helicities of Seth You, it is clear that the ion relative helicity is not conserved well in relation to magnetic energy. Also, gyroviscosity strongly affects the evolution of cross helicity.

Ping Zhu presented recent analysis of his simulations of the magnetotail, which produce plasmoids through the nonlinear evolution of ballooning. The reconnection that occurs is necessarily 3D, so identifying reconnection is nontrivial. He is using computation of the squashing degree and bald spots to identify quasi-separatrix layers. The squashing degree is from field-line integration, so finding it is computationally intensive. In contrast bald-spot analysis is local. His results show bald-spot development prior to the formation of plasmoids, although plasmoids do not appear after all bald-spot occurrences. Zhu also presented his recent work on the resonant magnetic perturbation (RMP) benchmarking exercise. His latest computations eliminate all toroidal harmonics except 0<=n<=3. With the applied RMP fields, his computations develop into resistive ballooning, i.e. the expected linear saturation is not found. The quality of the equilibrium and parameters used for the internal vacuum region need further investigation.

Tom Jenkins described his efforts to continue Dalton Schnack's work on the DIII-D giant sawtooth study. He has been able to gain access to Schnack's NERSC repository and has found files for the internal kink benchmark and for GS computations. He will be repeating some of the computations to verify that previous capabilities can be recovered before extending the study to more realistic energetic particle distributions. He will also work on two-fluid computations for the GS in collaboration with the Wisconsin group.

Jonathan Hebert presented his study of current evolution in the CTH stellarator-tokamak hybrid. An important experimental result is the hesitation of current as low-order rational surfaces move into the plasma from the outside. His NIMROD simulations show significant island development at or after these times and hesitation in the edge rotational transform value, but the current does not show the hesitation despite being driven with representative loop voltage. The simulations show sensitivity to number density and the simulation parameters have been adjusted for agreement with the overall current rise of the experiment. Hebert has investigated how varying the resistivity affects magnetic fluctuations of toroidal harmonics 5j+-1 and 5j+-2, where j is an integer, and '5' reflects the toroidal periodicity of the imposed stellarator fields.

Nick Roberds described two efforts with the NIMROD code. He has tested 1D shock problems with NIMROD's non-shock-capturing algorithm using the code's nonlinear numerical particle and temperature diffusivities for upwinding-like smoothing. The results are surprisingly good for both the unmagnetized Sod shock tube and for the magnetized Brio-Wu shock tube. His second effort is a new study of CTH's low-q disruptions. He will be studying the MHD dynamics starting from VMEC fields fitted to the experiment prior to disruption. For that he has developed capability to read VMEC output into NIMROD. VMEC does not provide the vacuum fields outside the last closed flux surface, so Roberds uses Biot-Savart computations for that information. There is a double interpolation process to get the VMEC fields into the NIMROD representation, and Roberds is checking flux surfaces and current-density profiles.

Torrin Bechtel is using CTH-like equilibria to investigate the effects of heating with enhanced stellarator transform. He increases the magnitude of the applied n=5 fields and the vertical field to make the configuration more like a conventional stellarator. The modeled heating is over a circular cross section and relies on large parallel conduction to spread the thermal energy over flux surfaces. The rotational transform evolves with the heating due to diamagnetic effects. He has modified NIMFL to generate puncture plots at multiple surfaces for a single set of field-line traces. Next steps include larger heating rates and adding a source of momentum density to investigate flow effects on magnetic islands.

Charlson Kim described his new work for simulating the General Fusion approach to spheromak compression. He made updates to bring NIMPSI code development into the main NIMDEVEL trunk. He performed linear computations to verify the spheromak tilt instability threshold with aspect ratio. He has also investigated stability with a central rod, as used in the GF configuration. For nonlinear computations, compression is modeled through the application of time-dependent boundary conditions on electric field, magnetic field, and flow along the outer boundary. In a straight cylindrical geometry, the nonlinear 3D results become unstable near the time when the tilt-instability aspect ratio is obtained. He has also started modeling a cylindrical wedge geometry and has added a gun region to the bottom of the domain. A filtering function is used to smooth corners.

Val Izzo presented her validation study of massive gas injection (MGI) for disruption mitigation in tokamaks. She characterized the simulated evolution as pre-thermal quench (TQ), early TQ, late TQ, and then current quench (CQ). Stochastic mixing from m>n MHD activity occurs during early TQ, and the radial mixing effect of the 1/1 occurs during the late TQ. She presented information on the influence of localized high-field-side (HFS) vs. low-field-side (LFS) injection. The modeling shows preferential migration of impurities toward high field as a result of dilution and radiative cooling and subsequent forcing from pressure. In DIII-D experiments, the 1/1 mode always appears 180 degrees away from the point of injection, as predicted by Izzo. Izzo also showed results from synthetic diagnostics that show how experimental measurements tend to average-out the actual extent of toroidal peaking of radiation. She has made a prediction that the diagnostics will be able to discern toroidal peaking when the experiment is run with opposite helicity, and this is planned for DIII-D. With two gas jets, the sign of magnetic helicity matters, because it dictates whether the two injectors are at the same phase or the opposite phase with respect to 1/1 activity.

Kyle Bunkers and Carl Sovinec are working on a new simulation study of VDEs. This study uses a numerical implementation of the external vacuum region, and separate computational regions are linked by thin-wall interfaces. Sovinec reviewed the numerical implementation with implicit coupling of regions. Test cases include large aspect-ratio VDEs for comparison with the Mukovatov-Shafranov "decay-index" criterion. NIMROD computations are run from NIMEQ equilibria, where a symmetry boundary condition is used to generate vertically unstable equilibria. The linear results agree well with the decay-index criterion, provided that conducting walls are sufficiently far from the tokamak. Results with a resistive wall provide scaling of linear growth rates with wall resistivity. Nonlinear results demonstrate evolution with large vertical displacement. Next steps include more complete vacuum-region geometry and ExB-governed flow boundary conditions.

To follow-up on the discussion of two-fluid computations and vector-potential formulations, Dan Barnes reviewed an idea for a symmetric stabilizing operator for the Hall advance, which he proposed in 2011 and tested in 2D. The formulation uses an auxiliary vector field through a constraint equation. The operator can be tested in NIMROD when an auxiliary vector is solved simultaneously with the B-advance. Similar coding was needed when using the Harned-Mikic semi-implicit algorithm for the Hall advance, so the development is tractable.