NIMROD Team Meeting Minutes, August 15-16, 2015
Tech-X Corporation, Boulder, Colorado

Computational topics:

Carl Sovinec started the meeting by presenting the motivations for and development of free-boundary Grad-Shafranov (GS) solves with NIMEQ. Simulations of dynamics that displace or distort the entire plasma over timescales longer than the wall time need equilibria that are consistent with actual external current distributions. Free-boundary solves avoid unphysical equilibrium eddy currents and provide consistent equilibria. Unlike fixed-boundary computations, free-boundary computations need the surface flux distribution to be consistent with internal current distributions and external coil currents. The initial implementation updates surface flux at fixed intervals in the nonlinear GS iteration. This leads to slow convergence, and an approach to solving surface flux simultaneously at each GS iteration-step has been formulated. The existing implementation has been used to initialize vertical displacement event (VDE) computations, and an example was presented.

Val Izzo described her work on incorporating NIMROD into the OMFIT workflow software, developed by Orso Meneghini. Many different codes have been made compatible with OMFIT, and it can store data in different formats. The software allows a user to send computational jobs to remote locations. It also helps automate running parameter scans and assembling data from scans. It is written in PYTHON, and a new GUI for NIMROD input is part of the PYTHON code. Izzo's presentation slides include a tutorial on how to run NIMROD through OMFIT.

Jacob King reported on his efforts to achieve performance on the Mira IBM Blue Gene Q machine. The challenges with the many-core environment are the relatively weak performance of each core, the 4x threading, and the small memory of 16 Gb per node for 16 cores. King has tried SuperLU_DIST 4.0, which uses threading during factorization (of NIMROD's preconditioner matrices), but it hangs for some problem sizes. MUMPS does better with threading. Node allocation is best utilized for jobs where the number of cores is a power of 2, so King sets the number of Fourier components to a power of 2 and has FFTW run with a nonstandard number of real-space mesh points. The NIMROD finite-element assembly scales well, whether using MPI only or mixed parallelism with OpenMP. However, memory limitations are more problematic with MPI-only computation. King also described memory fragmentation difficulties and his efforts to use the HYPRE algebraic multigrid solver.

Physical model development and analysis:

Eric Held gave a summary of recent work by Jeong-Young Ji, who was not able to attend. In collaboration with colleagues in Korea, Ji has extended his parallel electron closure analysis to consider ions of arbitrary charge. The derivations for heat flux, friction, and viscous stress are complete. The closures are for arbitrary collisionality and are expressed in integral form. Ji's approach to obtaining accurate kernels for arbitrary collisionality is to use his general-moment relations to find behavior at finite collisionality in a simplified configuration and to develop fits that extend to collisionless results. He is now working on ion closures and more complicated geometry to incorporate trapping effects.

Held then presented his work on applying "continuum" methods to solve the drift kinetic equation (DKE) in the Hazeltine form together with fluid moments. For hot-particle computations, Held uses the linearized form of the DKE. He thinks that it will be possible to also apply DKE for the thermal ions to include the Kruskal-Oberman contribution. The primary application is the giant sawtooth (GS) validation case from DIII-D shot 96043. The energetic particle computations now include both the slowing distribution from beam-injected particles and the tail component that is induced by RF. Held uses the equilibrium from G. Fu that is based on canonical momentum, although only the hot-particle current in the equilibrium seems to be important. Held also finds that the fishbone behavior is sensitive to background number density, and refitting the MHD equilibria with FGNIMEQ has been very helpful. He is starting to get numerical results with the RF tail component.

Applications:

Tom Jenkins reported on computing the GS cases with the PIC module in NIMROD. In the cases he has run with recent versions of nimdevel, there appears to be a normalization error, either in the coding or in the input parameters that are based cases run by Dalton Schnack. There may also be a sign issue with respect to the flux function, as drift orbits seem inconsistent with the expected directions. From the coding, it appears that the perpendicular components of drift velocities are based on the lowest-order **E**x**B** drift only, although the two-fluid electric field has been incorporated. [There has been some progress on the input parameter selection in the week since the team meeting.]

Eric Howell has been working on cases for verifying internal kink computations, starting with MHD but with the intent of verifying two-fluid internal kink. He reviewed MHD kink theory, noting that while the drive is throughout the volume inside the resonance, the resonance is only broadened by inertia or other physics in the inner layer. His screw-pinch computations with NIMROD at β=0 are in good agreement with linear theory at sufficiently large S-values, including the transition from resistive to ideal kink. At finite β, there are quantitative discrepancies with NIMROD growth rates being less than the analytical ones, possibly due to the finite layer width. Howell described the challenges of finding two-fluid cases where drift is appreciable yet parameters are within the limits of the Ara, Basu, and Coppi analysis. He is also considering the Zakharov and Rogers derivation, which is valid at moderate beta. So far computational results are in qualitative agreement and may need more spatial resolution. Increasing aspect ratio may also help.

Nick Roberds presented his study of sawteeth, motivated by observations in CTH. He initializes nonlinear computations with VMEC equilibria that have $q(0)>1$ and uses applied loop voltage to drive $q(0)<1$. He does observe sawtoothing and finds that m=2 modes can develop near the wall after the first crash. Whether periodic behavior occurs is sensitive to thermal conductivity, resistivity, and other parameters. In cases with repetitive sawteeth, the characteristic inversion of temperature traces, inside and outside the inversion radius, is reproduced. At larger current, behavior after the first crash, which reconnects completely, appears to switch to quasi-interchange. Sawtoothing is also observed with CTH vacuum fields (harmonics of n=5), and the kinetic energy evolution indicates coupling of sawtoothing with the n=5 fields.

Val Izzo reported on her initial work on including plasma rotation in simulations of massive gas injection (MGI) for disruption mitigation. The injection is modeled as a localized initial distribution of neon in the tokamak edge and off the midplane. Toroidal spreading of the impurity is asymmetric due to a Bernoulli effect from the magnetic geometry and parallel thermal conduction; the impurities tend to move more to the high-field side. This affects the phase of the 1/1 kink that is destabilized by changes in the equibrium profile from the edge cooling. Comparison of phases with results on DIII-D is improved when rotation is included. The direction of impurity spreading is reversed by the rotation, and the rotation enhances the spreading. Izzo is also considering the simulated transport of momentum from the core to the edge. In particular, flow profiles show a fairly sudden change in core rotation as MHD activity changes. However, computations with rotation need more toroidal resolution than those without it, so results are considered preliminary at this point.

Jake King presented an update on his numerical study of edge harmonic oscillation (EHO). He first noted considerations when using fitted profiles and trying to match transport-related physics. Using the fitted density profile is important; so are the fractions of electron pressure and Z-effective. Modeling of EHO also requires appropriate flows, including **E**x**B** and drifts that only appear with two-fluid modeling. Refining equilibria with FGNIMEQ is important, and the edge pressure profile is smoothed by allowing scrape-off-layer current. King is using profiles taken from the broadband phase of an EHO discharge, where fitting quality may be best. However, it is not clear whether the simulations will correctly induce the oscillations when using profiles that are fitted to conditions where they are already established in the experiment. King observes a transition to turbulent transport, and the homoclinic tangle off the initial separatrix is apparent from field-line tracing. Particle transport is also enhanced due to correlated fluctuations of density and flow. Future work includes more modeling of transport and sources and identifying the saturation mechanism.

Ping Zhu presented recent work on neoclassical toroidal viscosity (NTV) that is associated with resonant magnetic perturbation (RMP). Previous analytical results are obtained from the bounce-averaged DKE, and the net torque is analytically tractable in extreme limits. Other regimes are evaluated by fitting or by numerical computation. The NTVTOK code by Sun is one implementation for NTV, and Zhu has had his undergrad student Yan couple NIMROD output on magnetic fields into NTVTOK. The rotation for the torque computation is specified and is also used in the nonlinear NIMROD computations. The NTVTOK code predicts torque for each flux surface, and values peaks off axis in the cases that Zhu and Yan have run. The torque is insignificant at low β, but at 9% β and a maximum Mach number of approximately 10%, the torque is substantial. The spectrum of toroidal harmonics that contribute to the torque is broad.

Torrin Bechtel gave an update on his finite-β stellarator computations, where the goal is to examine pressure-driven topology evolution. He starts with a field distribution from CTH but alters coil currents to increase rotational transform without loop voltage. He is now using T-dependent resistivity and is applying heating in a region that is not aligned with flux surfaces but does not extend beyond the closed-flux region. MHD dynamics lead to concentrated temperature and density, especially when using T-dependent thermal conductivity. Ballooning is evident in computations with T-independent (but anisotropic) thermal conductivity. Bechtel also presented his use of Delauney triangulation to compute the volume of closed flux from NIMROD results.

Joshua Sauppe provided an update on his study of relaxation dynamics in reversed-field pinches (RFPs). He reviewed experimental results from the Madison Symmetric Torus and the two-fluid model that he uses for his study. His computations are at S=20,000 and include single- and two-fluid cases, where the latter are run with and without gyroviscous stress (GV). All cases start from the same paramagnetic pinch profile with uniform plasma pressure. The total dynamo effect, i.e. the sum of MHD and Hall contributions that is equivalent to $-\left\langle \tilde{\mathbf{v}}_e \times \tilde{\mathbf{b}} \right\rangle$, is comparable among single- and two-fluid results. A computation with GV and Pm=1 shows weaker relaxation events after the first event, unlike the single-fluid and no-GV computations, although they are somewhat stronger when Pm is 0.1. Parallel flow remains relatively small in the MHD results. The two-fluid cases produce more significant flow. The two-fluid case without GV shows periodic relaxation events, and the parallel flow generated during different events changes direction. Through analysis of fluctuation-power transfer terms, Sauppe finds that the role of the (1,-6) mode differs among events where the induced parallel flow has different directions.

John O'Bryan is revisiting SSPX results and is performing more detailed simulations for the purposes of validation and optimization of future spheromak experiments. His computations prescribe injector and bias fluxes only, and applied voltage is a result of the computation and depends on the spheromak dynamics. O'Bryan is focusing on the multi-pulse experiments that were performed in SSPX. He is using both single- and two-temperature modeling with Braginskii thermal conductivity and viscosity closures. Results are similar, although two-temperature modeling predicts higher electron temperature. The discharges were considered lower-performance discharges, and the simulations show that initial pulses do not excite the n=1 column mode that leads to relaxation. That mode arises in later pulses, however. At greater injection, helicity builds over multiple events. O'Bryan is using the Trellis software to mesh more complicated geometries for new designs. He is comparing three configurations: SSPX, one with a lengthened injector, and another with a thinned injector.

Kyle Morgan presented his numerical investigation of the HIT-SI experiment at Washington. The NIMROD modeling was developed by Val Izzo and Cihan Akcay. The focus of Morgan's study is the frequency scan performed during the last series of 2-injector HIT-SI experiments. Morgan finds that two-fluid simulations with pressure evolution are in better agreement with experimental results than β=0 simulations. Specifying the injector asymmetry and flux-current phase relation from the experiment also helps. At low injector frequency, the two-fluid results are somewhat insensitive to viscosity, but they are more sensitive at high frequency. The artificially large electron mass used to facilitate the magnetic advance also affects results, so Morgan keeps ω_{inj}/Ω_e constant when scanning ω_{inj}. Finite pressure tends to move the core region outward in radius to an increasing extent as frequency is increased. The high frequency simulations get to very large $\beta \sim 60\%$, which is probably twice that of the experiment, though the trend is consistent. There is also an increasing tendency to induce n=2 activity with increasing frequency, also consistent with experimental results. The new experimental configuration has three injectors, which allows three operating modes via different phasings. Morgan already has simulations results for all three phasings.

Aaron Froese described General Fusion's (GF) work on the magnetized target fusion (MTF) concept. Their intended approach is to merge two spheromaks within a vortex of liquid metal that is then subject to a compressive pulse via hydrodynamic forcing. The spheromaks would also be compressed by a factor of 4 prior to entering the vortex. GF is using a series of smaller experiments to test formation and compression. With guidance from Charlson Kim, Froese is using NIMROD to study why n=1 modes apparently terminate the spheromak in compression experiments. However, his computations usually encounter n=3, possibly due to the chosen *q*-profiles. He is scanning parameters of the RB_ϕ profiles that are available in NIMEQ and generating stability maps with NIMROD. He is also investigating spherical tokamak profiles and is changing NIMEQ to specify eddy currents along the central column.

Kyle Bunkers presented a set of parameter scans that are motivated by our initial VDE computations. His new NIMPLOT diagnostic shows that parallel flow of the order of the local ion acoustic speed develop along opening magnetic field-lines as the simulated position-challenged tokamak encounters the resistive wall. The computations use prescribed anisotropic thermal conductivity. Bunkers first checked numerical resolution by changing the polynomial degree of the basis function and by changing the number of elements, and results are generally well resolved. The results are also insensitive the artificial particle diffusivity parameters. There is sensitivity to viscosity and parallel thermal conductivity, however. The largest Mach number over the domain increases as viscosity is decreased and as parallel thermal conductivity is increased.

Alexei Pankin described his work on H-mode pedestal and edge localized modes (ELMs) in the Korean KSTAR experiment. In comparison with other experiments, there is relatively little diagnostic data to specify equilibrium profiles in the edge region. Others have applied the BOUT code to edge dynamics in KSTAR, but they adjust equilibrium profiles to improve agreement with measured fluctuations. Pankin has used the BALOO and DCON codes to map the stability of moderate-n modes over edge current and pressure-gradient parameters. He is also applying XGC0 to predict the bootstrap current in the edge of KSTAR. He is comparing linear computations from NIMROD and BOUT++, checking MHD and two-fluid models from each code. He is also running nonlinear ELM computations with NIMROD.