NIMROD Team Meeting Minutes, August 1-3, 2018
Logan, Utah

Computational developments:

Carl Sovinec started the meeting with a discussion of several computational projects. He provided an update on formulating and implementing a least-squares version of the Hall magnetic advance. With the exception of boundary conditions, the linear version of a formulation with **B** and **J** as dependent variables has been implemented. It runs compressional wave problems with $\omega \sim \Omega_i$, but at present it does not converge on a tearing mode with rotation. A formulation with **B** and vector potential **A** would be more straightforward, but it requires edge elements for **A**. Another computational project is a generalization element-side seaming to allow arbitrary orientations of blocks of elements with polynomial degree larger than two. A third project presented here is checking energy conversion and conservation in slab-geometry tearing computations. Jacob Maddox and Sovinec have quantified energy loss from artificial particle diffusivity and are investigating whether hyper-resistivity is needed to maintain resolution during plasmoid-mediated reconnection.

Eric Howell summarized the discontinuous Petrov-Galerkin method that is designed to be a stable representation for hyperbolic problems. It casts the system of equations in first-order form and integrates by parts to move all derivatives onto the test functions. A couple of applied math groups have been developing this method, which is unique in that it solves an auxiliary problem to identify optimal test functions. Howell went through the steps for a Poisson problem and showed results from a computation of sound-wave propagation with flow. He implemented the DPG method in the Apollo framework, which is built on the Camellia toolkit (not NIMROD). The sound-wave computations run without any signs of numerical instability at very large values of the flow CFL condition.

Dan Barnes gave an update on developments for the boundary-integral approach for resistive-wall modeling. The motivation is to provide high-order accuracy without the computational cost of a meshed external vacuum region. Matrices are based on free-space Green's functions and have the form of elliptic integrals of (integer-1/2) order and can be computed during pre-processing. Barnes is using numerical integration that was described in a paper by Young and Martinsson, which is Gaussian over all element sides, except for element sides that are adjacent to the source/observation point singularity. Special quadrature rules are used there, but the rules in the arXiv version of the YM paper have an error. Barnes was able to contact Jim Bremer, who provided a code for generating the necessary integration rules, and tests for n=0 and n=1 show high-order convergence. Barnes will next apply recursion to generate matrices for n>1.

Jacob King and Brian Cornille led a discussion on the development of abstract blocks to increase NIMROD's flexibility. They started with a Gitlab tutorial, which is where the development is being done to facilitate unit testing. They approach the move to abstraction through a concept of layering to ensure that dependencies are satisfied. Planned work includes solving a Poisson problem as a test case, checking performance, and implementing H(curl) vector elements to verify the expected flexibility. Cornille went into more detail for the H(curl) implementation, noting how Jacobian information for the element mapping appears differently than what is used for H1 elements. This forces a tighter coupling between interpolation and mapping.

Physical model development:

Jeong-Young Ji reviewed the moment approach for kinetics and the meaning of closure relations for a finite set of moments. He noted that parallel closure relations in the absence of inhomogeneous and nonlinear terms can be solved, and he compared results from Hankyu Lee's NIMROD implementation with from theory. Ji is considering inhomogeneous magnetic field and is testing convergence with an increasing number of moments. His presentation then changed focus to partially ionized gas and noted that the distribution of electrons produced from ionization is still an open theoretical research topic. Present modeling relies on empirical approximations. Moments of the charge-exchange operation are also used in Ji's theory. Progress has been made by summing the ion and neutral kinetic equations, decomposing each species into Maxwellian and non-Maxwellian parts, and applying approximations for the non-Maxwellian parts. He compares contributions from charge-exchange, ionization, and recombination and has evaluated coefficients of closure terms as functions of temperature.

Hankyu Lee has implemented equations for solving the moments that are needed for parallel heat flux, parallel viscous stress, and parallel friction. The present implementation assumes sinusoidal variation of the drives, which is used for testing and comparison with analytical results. He has made the implementation general, so that the number of moments used for these closures can be set at runtime. He has run computations that solve all moments simultaneously with the $\Delta/\Delta t$ term removed and computations that keep the time-change term with even and odd moments staggered in time. His results for these three closure terms agree well with Ji's analytical computations.

Eric Held gave an update on development of Eulerian ("continuum") drift kinetic computation in NIMROD. He and Joseph Jepson had worked out and implemented all of the linearized terms for the Chapman Enskog-like (CEL) system in order to run genuinely linear computations. Recent work includes merging separate kinetic-modeling developments back into the main trunk of the nimdevel repository. The separate branches were "electron_cel" for CEL testing and "newpart" for running PIC computations using the map_mod agglomeration of grid blocks. Applications work includes preparing a publication on continuum energetic particle modeling, a separate publication that compares continuum with PIC, assisting flow-damping studies, and starting global neoclassical computations. Development work includes parallelization over the speed grid and implicit nonlinear coupling of the CEL-DKE computation with the temperature equation.

Joseph Jepson reviewed the status of his flow-damping study from the time of the Sherwood meeting and reviewed how a closure for electrical potential is found from conservation of angular momentum. A flux-surface average is required. He has run flow-damping computations with two sets of initial conditions, one with a narrow Gaussian in pitch-angle and the other with a flow-shifted Maxwellian. The evolution is qualitatively correct with flow damping to zero when $dT_{i0}/d\psi=0$ and damping to a non-zero level, otherwise. He is making comparisons with simplified analytical relations and is checking numerical convergence.

Applications:

Ping Zhu summarized a number of projects that his group at USTC is studying for the design of China's CFETR tokamak, which is expected to lie between ITER and DEMO, performance-wise. His topics include VDE assessment, MHD stability, and energetic-particle modes. The group uses plasma profiles that result from 1.5D transport studies, and operation scenarios include reversed-shear and hybrid profiles. They find that the hybrid profile is unstable to resistive kink and are assessing the threshold for mode locking with error fields. They use the modified Rutherford equation to examine neoclassical tearing and the AEGIS code to search for stability gaps for resistive wall modes (RWMs). NIMROD computations with a profile from EAST show vertical displacement as a result of MHD-induced pressure loss. Computations of massive gas injection (MGI) for CFETR using Val Izzo's implementation of the KPRAD radiation code show familiar phenomenology with respect to radiation/MHD synergies, but the CFETR computations also exhibit radial shifts of the profile. A study of edge-localized modes (ELMs) is checking whether the planned profiles are in the desired "grassy" ELM regime. Energetic-particle computations for the hybrid profile finds TAE modes for n>1 and fishbone modes at n=1.

Xingting Yan is applying NIMROD to tokamak equilibria with negative triangularity, which are expected to have better properties with respect to particle and heat exhaust. This summer, he is working with Linjin Zheng of UT-Austin and is running linear computations of DIII-D discharge 171421. Recent studies have shown that turbulence and transport can be reduced with negative triangularity, but MHD stability has been a concern. Zheng's recent work shows that ideal stability can be achieved at fairly high plasma beta. Yan's non-ideal computations with fixed viscosity show an n=1 mode whose growth-rate scales with $\eta^{1/2}$. For all n=1-5, ELM-like mode growth and structure are evident. He is also running computations that compare stability for equilibria with no triangularity, positive triangularity, and negative triangularity. He is also considering an advanced scenario that represents high bootstrap.

Jacob King gave an update on his modeling of broadband quasi-harmonic (QH) operation in DIII-D and discussed edge transport modeling. His previous QH simulations reproduce important features, such as density pump-out, but comparisons are challenged by the limited time-span that is computationally affordable with flow. Because drifts are important, adding two-fluid effects would be a significant step for the modeling. A new discharge, 163518, has been selected for analysis to help distinguish standard edge harmonic oscillation (EHO) from broadband behavior. To model the flows in this and other applications more self-consistently, King is considering more detailed modeling of sources for the n=0 flows, such as beams, interactions with neutrals, and coupling to walls. He has done some preliminary investigations with the neutral model that was implemented by Sina Taheri; the evolution of the neutral density in a slab case seems counter-intuitive and needs to be checked.

John O'Bryan gave an overview of a relatively recent application to model possible self-organization from dynamo activity in the shallow solar convection zone. Most studies of the convection zone consider field resulting from dynamics at the base of the zone. The shallow zone has the unique property of being buoyancy-unstable, and this gives rise to the granulation and super-granulation that is observed on the photosphere. The orders of magnitude variations in density and temperature are important considerations for numerical modeling. O'Bryan has addressed these issues by solving equations for the logarithm of each of these variable. He finds that not applying dealiasing is best for avoiding unphysical overshoot. He has also incorporated the implicit gravitational force due to compression in the semi-implicit operator. Initial simulations show that fast growing modes in the buoyancy-unstable region quickly develop into turbulence. Scaling the guide field in these computations demonstrates the feasibility of self-organization into larger-scale structures.

Urvashi Gupta presented her work on modeling quasi-single helicity (QSH) states in the Madison Symmetric Torus (MST) experiment. The objective is to provide information on flows in toroidal QSH configurations for comparison with experimental observations from MST, eventually considering warm-ion effects identified by King in his PhD research. Gupta described her computational setup, which models all of the discharge by applying loop-voltage to vacuum (toroidal only) field. The voltage is adjusted to maintain a prescribed level of plasma current. She forces QSH by computing a 1/5 toroidal slice of the torus. Magnetic fluctuation energies suggest that the (m=1,n=5) distortion dominates, as expected, but in some cases n=10 perturbations dominate the kinetic energy spectrum, possibly consistent with laboratory observations of m=2 flows. With resistive MHD, contours of flow patterns from given toroidal angles in the simulations are complicated and do not resemble a single island.

Torrin Bechtel described recent progress on his nonlinear computations of a (l=2,m=10) toroidal stellarator configuration subject to heating. Using high toroidal resolution to represent fields from external helical coils and then filtering reduces problematic divergence errors near the domain surface by a factor of 50. Following that with a short cleanup computation that allows the surface-normal component of **B** to relax reduces error by another factor of 20. With these errors reduced, the computations are now more sensitive to temperature evolution, due to its influence through Spitzer resistivity. Increasing the number of elements helps. Bechtel has also improved his computation of the toroidal flux function. He is now using pressure profiles to indicate flux surfaces, and following contours of fixed pressure values at a given toroidal angle provides a means of integrating vector potential to get the toroidal flux function.

Ge Wang presented his initial work on modeling RWMs with a goal of simulating nonlinear evolution using increasingly detailed modeling. He reviewed characteristics of RWM instabilities and the externally meshed implementation of resistive-wall modeling in NIMROD. He presented new linear benchmark results for the cylindrical constant-J_z equilibrium, which differ from Sovinec's previous benchmarking in that Wang's computations use the cylindrical-polar r-θ mesh instead of the rectangular r-z mesh. Wang has used NIMEQ to create a comparable, large aspect-ratio equilibrium in toroidal geometry. The linear mode structure is dominantly m=2, n=1, and scans of wall resistivity and the radius of the external conducting shell show variations in growth rate, similar to what is expected from cylindrical theory. An initial nonlinear computation runs into numerical instability, however, which may stem from noise along the plasma-vacuum surface of the equilibrium. After solving this issue, he will examine the physics of RWM saturation.

Sovinec presented modeling of asymmetric vertical displacement. The work was presented at the Theory and Simulation of Disruptions Workshop at PPPL in July, and some updates on computational results were included here. Sovinec described the problem setup for vertical displacement that is forced over the resistive-wall timescale. The nonlinear 3D computations produce a sequence of progressively more virulent external modes. He compared the magnetic topology evolution produced in new case having rounded corners with that from a previous case having sharp corners, where unphysical topologies resulted. The 3D computations show the thermal quench proceeding faster than the current quench, and there is a bump in current that occurs with relaxation during the thermal quench. Sovinec also discussed new results on the NSTX-based linear benchmark with M3D-C1, and there is better agreement than what had been obtained by Sherwood. Bunkers' work on including sheath effects in the nonlinear modeling was also covered. Lastly, Sovinec quickly described recent simulations of the TREX experiment at Wisconsin, which uses internal coils to drive reconnection at Alfvénic rates.