NIMROD Team Meeting Minutes, August 17-19, 2017
Tech-X Corporation, Boulder, Colorado

Computational topics:

Carl Sovinec reviewed the limited investigations of the first-order systems, least squares (FOSLS) method for NIMROD. Most of this work had been presented previously at the 2016 APS-DPP meeting. The primary motivation is to find a more stable formulation for cases with strong advection. That the formulation leads to symmetric algebraic systems helps the implicit advances of stiff systems. Sovinec reviewed basics of the NIMROD spatial and temporal discretizations and how FOSLS has been tested in time-split advances of the ideal parts of the continuity, temperature, and magnetic-field equations. Results from simple 1D tests and 3D external kink, as computed with the test implementation, were shown.

Tom Manteuffel of UC-Boulder presented some of his group's research efforts on applying FOSLS to plasma-fluid and kinetic models with a focus on how well multi-grid solvers perform for the implementations. He started with an impromptu mathematical description, noting that LS is a Petrov-Galerkin method and why it is both continuous and coercive. The appropriate space for a formulation can be identified by generating the "formal normal" for the system. His group has investigated the two-fluid plasma model as a preconditioner for implicit Vlasov computations. Light waves are eliminated with the Darwin approximation. The implicit system is solved using algebraic multigrid (AMG) as a preconditioner for conjugate gradients (CG). The formulation has all fields in the H^1 function space. Manteuffel's group has shown that nested iteration through adaptive mesh refinement works well with the AMG solver. Diagonal scaling of the system is important, and the error reduction per solver step can exceed an order of magnitude. Test applications include wave propagation and magnetic reconnection. Manteuffel also presented ideas on applying FOSLS to the Vlasov-Maxwell system.

Jacob King presented work on three topics -- code optimization for vector processing, infrastructure for 3D elements, and a possible numerical instability from curved flow. He first covered aspects of the Intel AVX-512 optimization capabilities that are important for good performance on Cori Phase II at NERSC. He demonstrated this with a small test code run on Phase I and Phase II with different levels of OpenMP parallelization and with Open MP SIMD enabled. These tests point to the importance of array index ordering. King noted that NIMROD may do better on its finite element computations with different array ordering, but there are tradeoffs. The effort could be part of broader NIMROD infrastructure work with abstract blocks to facilitate 3D elements for kinetic computations (2D spatial, 1D pitch-angle) with an efficient memory layout. Regarding the possible numerical instability, King noticed dramatic changes in short wavelength components of EHO computations with reduced time-step in cases with flow (but not in those without flow). This prompted a study of rotation in a simple cylindrical configuration and von Neumann type analysis using a local approximation. The group discussed the role of magnetic divergence cleaning in the simplified test and whether it was being applied to a sufficient extent.

Brian Cornille described development work that he is doing at LLNL this summer for his Computational Sciences Graduate Fellowship. He is adding the magnetic remap step to the arbitrary Eulerian-Lagrangian (ALE) code BLAST. The code uses H(div) and H(curl) function spaces for vector fields, and Cornille first gave an introduction to what they are and how they are described in the mathematical de Rahm sequence. Their discrete forms can be found from nodal representations of different degree and continuity in the different directions, but one must then be careful with metric information. Cornille's most recent work on BLAST had not been cleared for public release, so he covered what he presented at the annual CSGF meeting. Tests of his remap implementation include pulling the mesh through fixed fields and the anisotropic, Sedov blast wave problem.

Physical model development and analysis:

Jeong-Young Ji presented an overview of his recent work on improving closure relations through analysis from the general moment method for describing particle distributions. He has been focusing on parallel closures, relaxing various approximations that have been made previously. He uses large numbers of moments to describe the behavior of closure coefficients in the transition regime from strong to weak collisionality, then applies fitting procedures to the collisionless limit in order to guarantee correct asymptotic behavior. When applied to the Spitzer electrical conductivity problem, Ji notes that the Landshoff-Spitzer theory over-predicts conductivity in the short wavelength limit. This may have bearing on magnetic reconnection, including fast reconnection effects. Ji has also been developing kinetic theory for partially ionized plasma, including information on ionization and recombination. His student Hankyu Lee is working on implementing general moment equations in NIMROD.

Eric Held described recent work on continuum (Eulerian or mesh-based) kinetic modeling for NIMROD. At present his group is maintaining two lines of development. One of them is δf kinetics, where the background distribution does not evolve, so the perturbation includes all velocity moments. This has been useful for modeling minority species and for benchmarking, and it is simpler. The second is Chapman-Enskog-like, where low-order moments are evolved with fluid equations, and the kinetic distortion represents all high-order moments. This provides closure information for the low-order majority-species fluid moments, but the implementation is more complicated. Held has used Ramos's analytical formulation for the second approach. To facilitate initial testing, Held is considering applications where certain effects are not important. These applications include the Spitzer electrical conductivity problem, poloidal flow damping, and electron parallel heat transport over magnetic islands.

Applications:

Ping Zhu presented computations of toroidal Alfven eigenmodes and energetic particle modes using the PIC simulation-particle module for the minority energetic ions, originally implemented in NIMROD by Charlson Kim. The first application is the ITPA-EP benchmark case with circular cross section and large aspect ratio. At lower values of hot-particle pressure, the dominant unstable mode is a TAE that bridges the m=10-11 gap in the Alfven continuum spectrum. At larger hot-particle pressure, the dominant mode is an EPM. There is good agreement between the NIMROD eigenvalue results and those from other codes when equilibrium temperature is scanned at fixed density. However, scans at fixed hot-particle fraction indicate a quantitative gap in growth rates. Zhu's group is applying this simulation capability to investigate the so-called "long-lived mode" in the HL-2A tokamak, which appears during neutral beam injection. Zhu finds that a slowing-down distribution of energetic particles drives 1/1 modes and harmonics of it. Other applications include a double kink mode in DIII-D and TAEs and reversed-shear AEs in the projected profiles for CFETR, a follow-on step to ITER.

Matt Beidler summarized his previous simulation work on forced magnetic reconnection and described efforts to model transient forcing--motivated by observations of edge-localized modes subject to resonant perturbation in DIII-D. The usual plasma-flow/perturbation-amplitude hysteresis curves show the bifurcation of nonlinearly possible equilibria, but previous studies do not address where the system goes when subject to a transient perturbation. Beidler uses time-dependent boundary conditions in slab-geometry computations to address this question. He has scanned both amplitude and duration of the transient perturbations and how the threshold for mode penetration depends on them and on the initial equilibrium state. Beidler is also deriving an analytical description of the response to a transient and will compare its predictions with his NIMROD computations.

Tom Jenkins described a new synthetic diagnostic that he is developing for NIMROD that has technical connections to his VSIM work on modeling RF propagation and deposition in tokamaks. The diagnostic is motivated by King's edge harmonic oscillation simulations. Laboratory observations of EHO dynamics have been through microwave imaging reflectometry, and the signals are not direct measurements of what happens; optics and plasma dielectric effects influence the signals. Jenkins is porting 3D fields from NIMROD into VSIM in order to model the physics of the diagnostic, itself. This is work in progress, and initial results are expected by the time of the APS-DPP meeting in October.

Dan Barnes presented work at Tibbar Plasma Technologies to develop plasma-based high-power transformers. The concept uses externally imposed axial magnetic field in a cylindrical chamber that is surrounded by helical electrodes. Cihan Akcay and coauthors have published a first paper on DEBS simulations of the concept, but DEBS assumes periodicity in the axial direction. NIMROD is being developed and applied to describe end effects. The development part includes new boundary conditions that induce normal current density through a surface Poisson equation to obtain E-tangential. A separate code solves the surface-potential equation, and the gradient of the solution is ported into NIMROD. The surface solver uses a Green's function that is integrated with an accurate numerical algorithm, which handles the singularity, produces a symmetric matrix, and leads to second-order convergence.

Torrin Bechtel gave an update on his computations of pressure-related limits in stellarators, focusing on an $l = 2$, $m = 10$ configuration that will be the subject of comparison with HINT2 relaxation computations. Most of his computations use toroidal harmonics of $m = 10$ to reduce resolution requirements. They model a source of heat, and heat transport is via anisotropic thermal conduction. Bechtel has scanned both and sees evidence of an equilibrium beta limit, but he has had difficulty following the resulting dynamics through an energy crash. He is developing a toroidal flux diagnostic and has investigated ideas on field-line following integrals to obtain the toroidal flux without prior knowledge of flux-surface cross-sections. However, a proper formulation has proven more elusive than anticipated. He has also traced-out the shape of flux surfaces, triangulated the resulting shape and applied numerical integration.

Jacob Maddox is investigating energy conversion and conservation in computations of magnetic reconnection. Discrepancies between computed and laboratory measured temperatures in Pegasus prompt the numerical checking, but he is using slab configurations for simplicity. Computations with the equilibrium transferred into NIMROD's solution field conserve energy as well as one part in 100,000, but having sufficient scale-separation between reconnection and global diffusion is not trivial, and most of the energy conversion in the cases run so far is likely due to global diffusion. Cases that retain the equilibrium in separate data arrays effectively represent sources and sinks, so energy is not conserved. They also develop holes of negative temperature at the island O-points, and this will be investigated further.

Eric Howell presented his simulation-based study of disruptions in low-q conditions in the Compact Toroidal Hybrid experiment, the Auburn stellarator-tokamak hybrid. Experimentally, it is found that increasing the fraction of externally imposed (vacuum) transform suppresses disruptive activity. However, with sufficiently low vacuum transform, discharges with $q(a) \approx 1.7$ almost always disrupt during current rampdown. Howell is modeling these cases by taking the current density from 3D VMEC equilibria and using it as a source-density profile. Attempts to apply simulated loop voltage do not reproduce the experiment's current profile with sufficient accuracy, likely due to simplifications in modeling transport. When modeling conditions that disrupt, an *n*=1 kink couples with the five-field period stellarator fields, driving $5j \pm 1$, where *j* is an integer. The $5j \pm 2$ fluctuations are from nonlinear coupling. The nonlinear evolution destroys 5-field period symmetry-preserving islands, leading to stochastic regions and significant loss of internal energy. Computations with larger vacuum transform but the same $q(a)$ value show the instability saturating at small amplitude without significant loss of heat.

Simon Woodruff presented three topics. The first is a simulation study of spheromak compression for a DARPA grant. His group has used information from the SSPX experiment to help calibrate parameters without compression. Compression is then modeled through an applied time-dependent field from two Helmholz coils. With a polarity switch, the computations develop a hot spot on the outboard side of the spheromak, which is possibly of interest in its own right. The second topic is the computational bootcamp event that has been held annually for the past few years. Woodruff is considering holding one overseas. The third topic is modeling a plasma "spring" in a reconfigured SSX experiment at Swarthmore. The initial conditions are an isolated compact torus localized to an end of a drift tube. After expansion, the CT evolves to a lower energy state with more twist. Woodruff's group has ported the simulation output to software for virtual-reality postprocessing, and a demonstration was given.

Kyle Bunkers covered two topics: 1) verifying a repository update of John O'Bryan's development for collisional closures with variable magnetization and 2) axisymmetric vertical displacement event studies. Bunkers solved the dispersion relation for planar waves with anisotropic viscosity and thermal conduction to provide analytical results for benchmarking. He found that the numerical reference-temperature parameter had not been used consistently in all terms, but after correcting that, he was able to verify all wave branches. For the VDE work, generating starting conditions for a CMOD computation without a conformal wall had been a problem. Free-boundary NIMEQ solves would not converge on an unstable profile when using the experiment's coil information and EFIT pressure and current profiles. However, finding the plasma current distribution from FLUXGRID and using it, along with the external coils, to generate the flux distribution along the domain boundary and then performing a fixed-boundary NIMEQ solve does work. Bunkers is revisiting the influence of flow-velocity and particle density boundary conditions using recent VDE computations as a basis. There is little difference between setting the normal component of flow to the E_{wall}xB drift speed or to 0. More significant changes result late in time when changing the density condition from diffusive flux to advective flux.

Carl Sovinec presented computations of VDE with toroidal asymmetry; most of this talk was the same as that given to the Theory and Simulation of Disruptions Workshop at PPPL in July. Two up-down symmetric, double-null equilibria are considered with the primary difference being the safety factor profile. Only one of the profiles is below 2 at the magnetic axis. Both are initially unstable to edge modes, with all modes except the n=1 in the lower-*q* case having growth rates of order $10^{-3}\ \tau_A^{-1}$. When run nonlinearly with the upper divertor coil turned off to force vertical displacement on the wall time, the edge modes grow more virulently in both cases. Scrape-off induced from wall contact leads to strong edge current layers, which likely enhances the instability. Sovinec is checking numerical resolution, particularly with respect to the number of Fourier components. Follow-on computations will impose floor values for density and temperature to make the computations more robust with respect to local overshoot, which has remained a problem despite improvements on numerical advection.