Minutes of the NIMROD Team Meeting
held online May 5 and 6, 2021

Session on May 5

Shiyong Zeng is using NIMROD with the KPRAD radiation model to investigate the interaction of massive gas injection (MGI) deposition with magnetic island evolution in the EAST experiment. He finds that edge deposition of impurity gas excites a sequence of islands, corresponding with the rational surface to which the gas has penetrated at a given time. He has related the current-sheet perturbation that excites the islands to the perturbed Pfirsch-Schlüter current at the respective rational surfaces.

Haolong Li is simulating asymmetric VDE evolution in the EAST experiment using the resistive wall model with meshed external vacuum. He compared results where the resistive wall has either square or rounded corners. The initial equilibrium is unstable to edge modes, which disrupts the simulated discharge, followed by partial re-healing of core flux surfaces after the thermal quench (TQ). This MHD activity has a large impact on the VDE evolution and causes it to deviate from 2D evolution.

Urvashi Gupta presented her computational study of magnetic relaxation and energy transport in cylindrical pinch configurations. Her "steady-state" data fields are self-consistent with the parameters of the time-dependent problem, including thermal conduction and Ohmic heating but excepting a small amount of particle diffusion. The relaxed state of her high-current computations have long-wavelength tearing activity, and fluctuating parallel heat flux along the fluctuating magnetic field dominates energy transport in the core. Reducing plasma-β increases reversal, as expected from previous studies on compressibility.

Tyler Markham is implementing a relativistic nonlinear collision operator for the relativistic electron drift-kinetic equation (DKE) model that will be applied to studies of runaway electron (RE) effects. He is working with the Braams and Karney formulation of the relativistic Beliaev-Budker relativistic Landau collision operator, which has potentials like the Rosenbluth potentials, albeit more (5) of them. Markham summarized the state of implementation and testing.

Alex Sainterme has implemented a reduced fluid-based model for the macroscopic effects of runaway electrons, similar to Bandaru's work with JOREK. Sainterme has implemented Dreicer and avalanche source terms, both of which are nonlinear. The NIMROD time advance has a double iteration loop to converge the sources and the interaction between the magnetic evolution and the RE density. Sainterme showed test results for implicit RE advection and for decay of a resistive axisymmetric resistive current into conditions where a large fraction of the current is carried by the REs.

Valerie Izzo presented an update on her simulation of dispersive shell-pellet disruption mitigation that is being tested in DIII-D. The experimental study led by Hollman found four trends as the injection velocity of the shell pellet is increased: 1) better TQ mitigation, 2) smaller I_p spike, 3) more RE production, and 4) faster current quench (CQ). Izzo's new set of simulations reproduce the first three (for the RE production, this is inferred by the rate electric-field increase), but the faster CQ is not reproduced. The smaller I_p spike is associated with more core cooling, hence more poloidal flux dissipation there, and therefore less flux compression in the edge.

Charlson Kim summarized his recent work on shatter-pellet mitigation simulation with NIMROD. The radiation and impurity density tracking are from Izzo's development including the KPRAD coupling, and marker particles are used to deposit impurity along the pellet trajectory according to the Parks' ablation model. Kim's simulations are based on DIII-D discharge 160606, and scans have viscosity and toroidal deposition width varied. He noted that MHD activity is important for mixing, and it is influenced by use of multiple injectors. The development of REs is an important consideration in experiments, and Kim is investigating models for them at different levels, including possible coupling with CQL3D.

Eric Howell has been modeling neoclassical tearing mode (NTM) evolution and is analyzing energy transfer among fluctuations and with respect to the mean field. His computations use the heuristic model for poloidal flow damping electron drag, together with resonant perturbations to excite tearing. The energy transfer analysis is being applied to the different phases of evolution, which are the fast initial pulse, slow growth, and fast growth. He finds that the n=2 and n=3 modes are driven linearly during the slow phase, while the n=1 has significant linear and nonlinear drive until it becomes neoclassically unstable in the fast phase.

Hankyu Lee gave an update on his implementation of general moment equations to model parallel transport. The moment equations are derived from the DKE. The non-Maxwellian moments in NIMROD are presently computed at the same time levels as flow velocity. He has compared the general-moment computations for parallel heat-flux, parallel drag, and electron parallel viscosity with those from Braginskii, and at high collisionality, the time-dependent results from the general moment equations evolve to those from Braginskii.

Sina Taheri implemented the dynamic neutral model in NIMROD and is investigating numerical practicalities and efficiencies. The semi-implicit advance for the charged and neutral species flow-velocity equations are coupled through nonlinear iteration. Atomic processes are highly nonlinear, but they are described by ODEs. Taheri has implemented two numerical approaches: one uses Crank-Nicolson with the full evolution of a given field, such as the continuity equation for neutral species, and the other uses Strang splitting of the atomic terms. The unsplit method uses iteration, unlike the split method. Taheri compared different sources of error in 0D test cases. A property of the split method is that there is a Δt-dependent error, even in steady conditions, as demonstrated in 1D tests.

Session on May 6

Omar Lopez has been simulating sawtoothing behavior in CTH plasmas and examining magnetic evolution with the benefit of a new topological diagnostic. The new diagnostic is a fixed-point search in NIMFL and is used to find *x*- and *o*-points. Lopez first demonstrated these searches on standard Kadomtsev reconnection in a tokamak configuration. He then showed that the behavior with external transform is similar, where sawtoothing occurs through symmetry-preserving islands, but is similar to the tokamak case in the emergence of new *x*- and *o*-points, followed by island growth that ends with the merger of the *x*-point and the original *o*-point.

Andrew Spencer summarized his work on numerical integration for the "field" terms of the linearized Coulomb collision operator for the continuum DKE implementation. The challenge is the $|\boldsymbol{v}-\boldsymbol{v}'|^{-1}$ singularity in the integrand. He compared the cylindrical- and spherical-coordinate (in $\mathbf{v}$) versions and noted that the elliptic integrals of the former has been addressed in the astrophysics literature by a regularization method. This method can also be applied for the spherical form, which is better when considering speed integration. Spencer splits the speed integration into three segments, due to the extreme variations and oscillations of its integrand.

Scott Kruger gave a short tutorial on theoretical numerical analysis and noted the textbook by Atkinson and Han as a good reference. Theoretical numerical analysis is based on functional analysis, which makes derivations as general as possible. PDEs are considered mappings from one space to another, and numerical consistency and stability are related to the continuity and coercivity of a given formulation. Many problems of interest, e.g. MHD with large dimensionless parameters, are saddle-point problems, and "stabilization" methods, such as least-squares and discontinuous Petrov-Galerkin have been developed to achieve coercive formulations.

Nan Ding of LBL is one of the CTTS SciDAC collaborators, and she presented her work on multi-GPU development for the triangular solve of SuperLU_DIST. The motivation is the limited memory that is available within individual GPUs. Software for direct GPU-initiated communication (NVSHMEM) is now available and makes multi-GPU implementations possible. She summarized the strategy of parallel triangular solves, which is related to directed acyclic graphs to optimize parallelization. To understand and optimize multi-GPU performance, she has developed a critical-path performance model, and she has applied the model to a representative NIMROD double-precision complex matrix.

Yang Liu is also a SciDAC collaborator from LBL, and he gave a presentation on autotuning NIMROD using the GPTune (Gaussian Process) software. The scientific challenge is the large space of parameters, e.g. SuperLU_DIST's supernode size parameters and NIMROD's block decomposition, and deciding which tests to run to best model performance, particularly when each test is expensive. This decision-making is what GPTune does. For NIMROD, Liu has found that 1) using CrayMPICH and libsci is more stable and faster than OpenMPI and MKL, 2) smaller supernode sizes are better, and 3) tuning with multi-time-step runs is helpful but overhead is large.

Jake King gave a preview of his IAEA presentation on validating NIMROD simulations of QH-mode operation in DIII-D. He noted that MHD computations start from fits of experiments, where the macroscopic dynamics have relaxed the profiles. Thus, he increases the pedestal gradient of fitted equilibria to excite non-axisymmetric MHD activity. Results from different profiles are compared with experimental density and temperature profiles. King emphasized that comparison of fluctuation spectra is sensitive to the inference of rotation profiles. This motivates direct modeling of rotation, including ion orbit-loss torque and interaction with neutrals.

Joseph Jepson completed his benchmarking study of axisymmetric poloidal flow damping with the continuum DKE model in NIMROD. The computation finds the steady-state poloidal flow coefficient, and there are two approaches to solving the system. The "DK4D" approach, named after Brendan Lyon's work, solves the DKE twice: once with the poloidal flow drive and then with the temperature-gradient drive. The Ramos approach solves a simplified Chapman-Enskog-like equation. Jepson showed numerical convergence information on a large aspect-ratio case and on a small aspect-ratio NSTX case. He is now applying the model to the NTM case being considered by Eric Howell.

Jeong-Young Ji presented his study of applying the moment approach to the Boltzmann collision operator, which is motivated by RE kinetics and other situations with large relative particle motion, where large-$\Delta\boldsymbol{v}$ scattering events lead to important effects. Ji described the functional form of the moments and how one can compute them. He also plotted different moments as relative speed is varied for different values of $\ln \Lambda$ and made comparison with the Landau operator to show where it is necessary to use the Boltzmann operator.

Gavin Held gave a presentation on his study of applying the DKE computation in NIMROD to the RE vortex in phase space. The vortex results from the balance of parallel-**E** drive in competition with collisional scattering and synchrotron radiation. He found that it is necessary to pack the mesh in pitch-angle in order to have a stable computation. He finds that collision coefficients agree well with those from Guo, et al. The NIMROD computation runs long enough such that the vortex develops, but it eventually runs into problems with the distribution function becoming negative at points in phase space.

Carl Sovinec gave an update on the formulation and implementation of NIMSTELL. He described different possible approaches to impose a gauge condition with the *H*(curl) space being used for vector potential. Results from 1D cylindrical eigenmode computations show that imposing the Coulomb gauge via a damping term is better than via dissipation and that using a smaller polynomial degree for flow-velocity allows convergence on local interchange from the stable side. Sovinec also described what differs from NIMROD when programming diagonal-in-Fourier operators for preconditioning.