Progress and Challenges in Plasma Boundary Simulations: Opportunities for Improved Algorithms

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In other white papers we discuss the overall motivation for developing integrated simulations to improve fusion reactor designs [WP-Hammett-1], and an incremental modular framework approach for bringing together various pieces needed for first-principles whole-device integrated simulations [WP-Hammett-2]. While many of the pieces exist, one of the biggest remaining challenges is developing simulations that can handle the complex boundary region, the subject of this white paper. This is particularly important because the overall core confinement and thus the predicted fusion gain Q depend sensitively on the assumed pedestal parameters [WP-Hammett-2]. Important questions that edge simulations could study include: What are the conditions required to achieve a transport barrier that suppresses turbulence and how high is the resulting pedestal? Can ELMs be suppressed without degrading performance too much? Why is the Scrape-Off-Layer (SOL) width observed to be so narrow, and can it be broadened to help handle the power? Can advanced divertor concepts, perhaps with continuous vapor shielding, handle the extreme power densities at reactor scales? How much can lithium walls help improve performance?

Gyrokinetic codes like GYRO, GENE, and GS2 have been quite successful in simulating the core region of tokamaks [WP-Hammett-2], but they use algorithms and formulations that are highly optimized for the plasma core region (such as spectral methods and small-amplitude fluctuation assumptions) and would need major modification to handle the additional computational complexities of the boundary region (the pedestal and scrape-off-layer region, i.e., $r/a > \sim 0.9$). These computational / mathematical challenges include the need to handle the change in magnetic topology between closed and open field lines, strong plasma-wall interactions, large amplitude fluctuations (necessitating a full F formulation), and magnetic fluctuations near the beta limit. (Large fluctuations observed in the edge of experiments are long wavelength compared to the gyroradius and so are still low frequency compared to the gyrofrequency.) For example, spectral algorithms can have difficulties with negative density overshoots when there are large fluctuations. These are hard problems, but progress is being made, and there are recent advances in applied-math/computational research that may significantly help, such as discontinuous Galerkin (DG) algorithms and efficient implicit solvers. The success of core gyrokinetic simulations gives us encouragement that a significant initiative should be able to develop codes that fully simulate the edge as well, and thus enable integrated simulations of the whole device. Existing core codes provide valuable benchmarks, and can also be used for important physics studies near the plasma edge (inside the last closed flux surface) [see WP-Jenko-2], or can perhaps be extended even further.

There are 3 efforts exploring different algorithms to handle the computational challenges of the edge region: the XGC PIC code, the COGENT Finite Volume code, and the Gkeyll Discontinuous Galerkin code. In this white paper we focus on the Gkeyll DG code (being developed primarily by Hakim, Shi, and Hammett at PPPL). Before discussing these approaches more, we emphasize that it is crucial to have multiple codes, particularly for these very difficult problems, because they provide invaluable cross-checks against each other. Verification tests and manufactured solutions are helpful, but are often practical only in certain simplified limits. There can be subtle convergence issues in chaotic problems on the long time scale where one is interested in the statistics of the solution, and different algorithms can have tradeoffs in representing various features of the solution. The excellent progress in core gyrokinetic turbulence simulations over the past 15 years has been made in part because of the existence of multiple independent groups.

The XGC project is the largest effort, and at present is the only gyrokinetic code capable of simulating turbulence across the separatrix, handling open and closed field lines simultaneously. It is producing encouraging initial electrostatic results [Ku], with features similar to the particular experiment it simulated. This is an example of extreme-scale computing, using 131k processors and 8k GPUs on the Cray XK-7 at ORNL for a total of 6M processor hours.

Good progress is being made in edge simulations, but we do not yet have a code that can handle all of the key physics that is important in the boundary plasma region, and a major partnership initiative between physicists, applied mathematicians, and computational scientists could greatly accelerate progress. One of the challenges is the inclusion of magnetic fluctuations with kinetic electrons, which is more difficult in the plasma boundary region, which can be near MHD stability limits. Magnetic fluctuations with kinetic electrons have been a challenge in gyrokinetic PIC codes because of the Ampere cancellation problem (two large terms need to offset each other with high accuracy [Candy03, Chen03, Mishchenko14]), though the recent work of [Mishchenko14] looks like an interesting possible solution, perhaps in combination with ideas about basis functions and consistent discretization.

Core continuum gyrokinetic codes (like GENE, GYRO, and GS2) have usually been fairly successful in including magnetic fluctuations (perhaps cancellations are easier to preserve because the particle distribution function is on the same spatial grid as the fields, unlike randomly positioned particles in a PIC code). One of the reasons we are pursuing a DG approach in Gkeyll (in addition to other attractive properties of DG mentioned below) is that it appears to be able to handle Ampere cancellations accurately like other continuum algorithms (once we identified certain important basis function constraints). Gkeyll is relatively new compared to XGC and COGENT and still in an early stage of development, but it has carried out a number of SOL tests in 1D and simplified turbulence tests for problems of increasing dimensionality [Shi15, Hakim15]. More work remains, and it is just now beginning tests in the full 3x-2v of gyrokinetics (in simplified geometry at first).

DG has been a hot topic in the applied math and computational fluid dynamics communities in the past 15 years, and combines certain attractive features of finite-volume and finite-element methods, such as the higher-order accuracy of finite-elements with the locality of finite-volume methods, which makes it easier to parallelize and to implement limiters (which are important to avoid negative density overshoots in the edge region). We developed new versions of DG that conserve energy exactly for Hamiltonian problems even with upwind fluxes (building on work by C.-W. Shu et al.). Another DG feature is the flexibility to use efficient Maxwellian-weighted non-polynomial basis functions. These are an analog of the higher-order Gaussian integration methods used in core gyrokinetic codes, which help them have good convergence with just ~16 $v_{\|}$ and ~8 $v_{\perp}$ grid points [Candy06]. (Resolution needs are highly problem dependent, but are found to be modest for low-frequency tokamak microturbulence, which is driven by macroscopic density and pressure gradients). The moderate collision frequency of the boundary region also helps reduce the velocity resolution requirements. One might someday consider a combination of algorithms, such as a PIC algorithm for ions and a continuum DG algorithm for electrons to handle magnetic fluctuations. Because of their regular data-access patterns and ability to parallelize over the large number of points in the 5D gyrokinetic phase space, grid-based continuum codes can parallelize well to a large number of processors, as demonstrated by GENE, which has shown excellent scaling to ~260,000 cores. Collaborations with computer scientists and applied mathematicians can help extend these codes to future exascale platforms.

While we believe it is feasible to develop comprehensive edge simulations, much work remains to fully implement them, understand them in various parameter regimes, and test them in comparison with experiments. There is also a great need for a range of simulation codes with differing levels of complexity and speed, because it just isn't practical to run the most expensive exascale simulations for all of the applications we need to do. So there is value in having 3D fluid edge turbulence codes as well as theory-based reduced 1D & 2D transport models (that can be fit to full gyrokinetic simulations) that allow much quicker simulations. Reduced models are particularly challenging in the edge region because of the need to handle non-local turbulence spreading and sub-critical or nonlinearly-sustained turbulence not well described by quasilinear models.

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