A Modular Approach to First-Principles Whole-Device Integrated Simulations

Primary topic: C, Cross-cutting: B, D, F

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I agree with many of the other white papers on whole-device modelling and core and edge simulations that will be submitted by others, including the ones by Hawryluk et al., Snyder et al., and Jenko et al. Here I aim to complement those by discussing some key goals and strategies for a whole-device integrated simulation initiative. The overall motivation of an integrated simulation initiative and several applications for it are described in [WP-Hammett-1]. I discussed various aspects of whole-device modelling in more detail in a white paper to the 2014 FESAC Strategy panel [Hammett14].

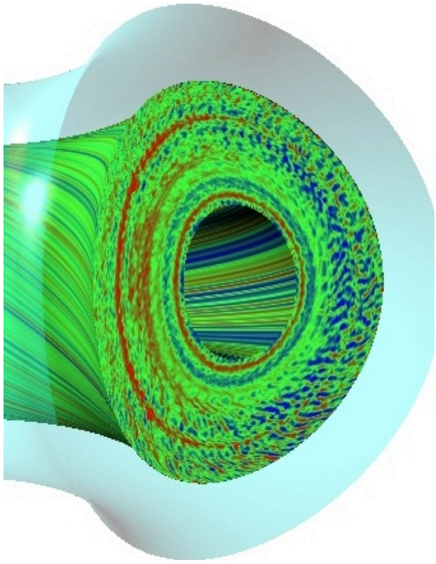

Fig. 1: Example of turbulent density fluctuations calculated by the kind of comprehensive gyrokinetic turbulence simulations that are fairly successful in the core region of tokamaks. (Candy & Waltz, GA.)

Over the past 15 years, comprehensive gyrokinetic turbulence simulations (such as GYRO, GENE, and GS2) have been developed that can simulate the core region of tokamaks fairly well and are being widely used in physics studies and compared with experiments. These codes calculate the particle distribution function $F(\boldsymbol{x}, v_{\|}, \mu, t)$ in 5-D phase space (the fast gyro motion has been rigorously averaged out) and thus the small-scale turbulence driven by drift-type microinstabilities (Fig. 1).

These are computationally intensive simulations that involve 5D dynamics at the 10^{-5} s time scale, and ultimately we want to simulate tokamak plasmas for hundreds of seconds. In order to handle this computationally challenging problem, techniques have been developed that enable a 1D transport code to solve on the long time scale for the macroscopic profiles (like the flux-surface averaged density and temperature), while periodically calling the short-time-scale 5D microscopic gyrokinetic codes for a first-principles calculation of the turbulent fluxes. (This is an example of a multiscale or scale-bridging technique, various types of which are discussed in the recent [Exascale-Math-2014] report.) The general feasibility of this coupling has been demonstrated by the TRINITY code [Barnes08, Barnes10] with GS2 and GENE, and by the TGYRO code with GYRO [Candy09]. (These are simplified transport codes that use source terms calculated by TRANSP or ONETWO interpretive runs, but they still demonstrate the approach.) An example of such calculations compared with the JET experiment is in Fig. 2. While these gyrokinetic codes work well in the main core region of many tokamak experiments, new gyrokinetic codes are needed to be able to handle all of the additional complexities of the edge region, so the simulation in Fig. 2 used the measured profiles at r/a=0.8 as a boundary condition.

A key to making large time steps feasible on the macro-scale is the usage of implicit coupling techniques [Jardin08, Barnes08, Barnes10, Candy09, Peterson11], using calculations of the Jacobian and nonlinear solvers to handle strong nonlinearities in the flux-gradient relation for tokamak turbulence, which makes it even more stiff than normal diffusion problems. Any methods to further accelerate the convergence of the implicit iterations would be useful, perhaps by interpolating in the high dimensional parameter space of a database of recent gyrokinetic simulations.

Reduced (1D) transport models are also being developed that allow for much faster simulations, such as the TGLF transport model (which is based on quasilinear gyrofluid theory with mixing length

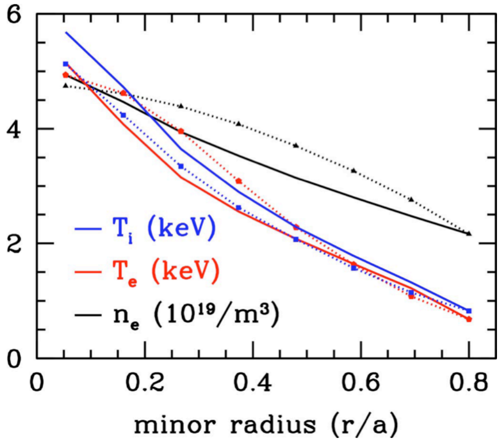

Fig. 2: Measured profiles (dotted lines) in a JET L-mode plasma compared with predictions (solid lines) by the Trinity+GS2 code, using measured boundary conditions at r/a=0.8. This demonstrates the feasibility of direct coupling of a short-time 5D microscopic gyrokinetic turbulence code with a 1D macroscopic transport code to predict the long time profiles. [Barnes10]

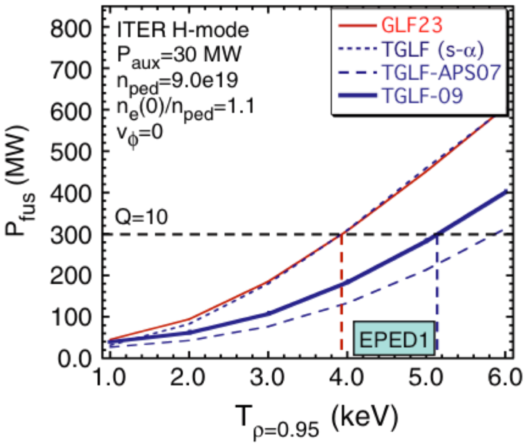

Fig. 3. Gyrokinetic-based predictions of fusion power in ITER as a function of the assumed pedestal temperature (the curves correspond to different assumptions about the gyrokinetic model, but all show a strong dependence on the pedestal temperature). Significant work is needed to develop gyrokinetic codes that can handle the edge region to predict the pedestal temperature and answer other important questions. [Kinsey11]

saturation estimates and is fit to a database of full gyrokinetic simulations). One can use reduced models for a large number of parameter scans, and then use full gyrokinetic codes just for some of the most important cases. Fig 3 shows the fusion power predicted for ITER by gyrokinetic-based reduced transport models, as a function of the assumed pedestal temperature. This strong sensitivity of the core temperature profiles, and thus the fusion power, to the assumed pedestal temperature near the plasma edge is one of the reasons why there is high priority need to develop first-principles gyrokinetic simulations that can handle the plasma boundary region (discussed more in [WP-Hammett-3]). There is some promising initial work on edge simulations exploring various algorithms, but a major initiative will help greatly accelerate progress on this long-standing challenge. Implicit coupling with an edge gyrokinetic code will be more complicated than it was for core gyrokinetics, because of non-local effects like turbulence spreading and intermediate time-scale events like ELMs, but it seems this should be solvable with the various tools available in the applied math bag of tricks.

An integrated simulation code needs to have a modular framework with the flexibility of using different modules for different applications. It should be able to use reduced models to generate results very quickly, and yet also be able to check the most important cases by calling full 5-D nonlinear gyrokinetic codes in the back end that use exascale computers. An important strategy is to work incrementally, building on existing or near-term components, and developing the capability of carrying out some kinds of comparisons with experiments at an early stage. The project can then continue to improve and expand modules in the code over time, with a continual cycle of testing. (There is great value in reusing parts of existing codes. TRANSP has over 2 million lines of code, much of which is for sources and sinks, including a sophisticated Monte Carlo calculation of neutral beam injection.)

I propose that two main initial goals of an integrated simulation initiative would be to (1) accelerate the development of gyrokinetic codes that can simulate the edge region, and (2) couple a top-level, long-time-scale, transport-solver framework with these core and edge gyrokinetic codes to provide a complete predictive capability for MHD-quiescent plasmas. This top-level framework could call extended-MHD codes periodically to check the stability of the plasma and see if disruption boundaries can be avoided. As the capabilities of the various modules grow and are demonstrated in a range of tests, some of this functionally can be expanded or perhaps even incorporated into a more comprehensive back-end gyrokinetic simulation.

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