The Computational Requirements of Multi-Scale Gyrokinetic Simulation and Its Impact on Modeling of Tokamak Plasmas

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Background

The existence of a well-developed theory and years of model validation efforts on tokamaks worldwide has dramatically improved our confidence in predicting kinetic profiles of future fusion devices and has established core transport as amongst the most well developed area of tokamak modeling. At the present time, gyrokinetic model validation focuses almost exclusively on comparing ion-scale (long wavelength: $k_\theta\rho_s < 1.0$) simulation with experimental heat fluxes and turbulence measurements. Despite the success of this long wavelength model, electron heat flux predictions that are robustly lower than experiment are not uncommon and "anomalous" transport in the electron channel has remained poorly understood. Such disagreements have generally been swept aside, suggesting that the "missing" electron heat transport can be recovered by resolving short wavelength, electron-scale (short wavelength: $k_\theta\rho_s < 60.0$) turbulence. However, due to the extreme computational requirements associated with coupled ion and electron-scale (multi-scale) gyrokinetic simulation this was not demonstrated. As a result, our understanding of how (and if) ion and electron-scale turbulence couples in current experimental plasma conditions and future reactors remains effectively unknown.

The Need for Multi-Scale Gyrokinetic Simulation

Recent results obtained from full physics, (3 gyrokinetic species, collisions, ExB shear, realistic electron mass, etc.) coupled ion ($k_\theta\rho_s < 1.0$) and electron-scale ($k_\theta\rho_s < 60.0$) simulation demonstrate that electron-scale turbulence can play an important, even dominant role in the core of standard Alcator C-Mod, L-mode plasmas and that significant ion-electron cross-scale coupling exists [1]. In simulation of experimental plasma conditions, coupled interactions between ion and electron-scale turbulence have been observed to increase the simulated electron heat flux by up to a factor of 10 and increase the ion heat flux by a factor of 3 relative to corresponding long wavelength simulation [2]. These results call into question the validity of applying any long wavelength model for the prediction of kinetic profiles of ITER and beyond, as the parameter space where such cross-scale coupling is important is not yet known. In order to address this open question, significant computing resources need to be dedicated to performing, multi-scale gyrokinetic simulations over a wide range of input parameters to both understand the coupling between ion and electron-scale turbulence and to identify regions of parameter space where cross-scale coupling is important. Ultimately, this exercise will allow us to incorporate the relevant physical processes into reduced-models used for the prediction of plasma profiles on ITER and will result in improved confidence and accuracy in these predictions.

Requirements for Multi-Scale Turbulence Simulation

The computational requirements for performing multi-scale gyrokinetic simulation are extreme and until recently were effectively inaccessible. Multi-scale simulations must simultaneously resolve both the ion and electron spatiotemporal scales. Resolving spatial scales spanning over 2-3 orders of magnitude ($k_\theta\rho_s \sim 0.1 - 60.0$) and temporal scales associated with the linear growth rates of short wavelength turbulence (~60x larger than long wavelength turbulence) requires extremely high spatial (grid spacing ~ 60x greater than standard long wavelength simulation) and temporal resolutions. All particle species simulated must be fully gyrokinetic. To make direct comparison with experiment, an impurity species, effects of rotation, ExB shear, and collisions all must generally be included, and all of which increase computational requirements. Attempts to reduce computational demands by artificially reducing the electron mass have failed to produce quantitatively or qualitatively meaningful results in some plasma conditions [3]. To date, 7 simulations meet the requirements outlined above and been quantitatively compared with experiment. These simulations were all performed with the GYRO code [4]. However, in principle ~3 existing gyrokinetic codes should be capable of performing such simulations. Each simulation required approximately 15M CPU hours, while utilizing approximately 17k processors (~37 days on the NERSC Edison supercomputer), making them amongst the most expensive gyrokinetic calculations ever performed. Simulation capabilities and scaling with processors are constantly improving. However, we note that even with approximately a 3-fold linear increase in simulation performance (~ 50k processors), such simulations would require almost 13 days on Edison for completion of a single simulation.

Increase Emphasis on the Computing Paradigm Required for Rigorous Testing of the Multi-Scale Gyrokinetic Model

The computational requirements outlined in the previous section emphasize the need for dedicated computing resources to perform multi-scale gyrokinetic simulation. With current ERCAP allocations on NERSC typically ranging from 10-25M CPU hours, perhaps only a single multi-scale computation could be performed with a year's computing allocation. Single multi-scale simulations are of only limited benefit as they do not allow for any investigation into model sensitivities within experimental uncertainties and therefore provided limited ability to extrapolate to even slightly different conditions. In reality, computing grants in the range of 100M CPU hours are required to perform a relatively rigorous assessment (including a handful of parameter scans) of a **single** plasma condition. Completion of such studies will provide more information on sensitivity of cross-scale turbulence coupling and will allow for a more complete validation of the multi-scale gyrokinetic model by exploring results within experimental uncertainties. Such large computing allocations are only available at NERSC, Argonne, and Oak Ridge through the ALCC and INCITE computing grants. However, emphasis at these computing facilities is generally focused on large, capacity computations that require a majority the site's capabilities, but 24 hours or less for completion. In contrast, a set of parameter scans (bundled to make reach capacity processor counts or individually submitted) composed of large, 17-50k processor jobs, running for longer time periods (as outlined in the previous section), are the only means to provide a rigorous test of the multi-scale gyrokinetic model. Such a paradigm is generally not rewarded by the queue policies or resource allocations (and often frowned upon) at computing facilities. Such policies are in direct conflict with a meaningful comparison of simulation and experiment and ultimately push the field of plasma physics computation in a direction with less emphasis on physics and more emphasis placed on strong linear scaling with processor count, with the physics output seen as secondary. In order to validate the multi-scale gyrokinetic model and assess the importance of cross-scale turbulence coupling, increased emphasis and resources must be dedicated to a computing paradigm geared towards rigorous comparison with experiment and not solely on short, capacity computations.

Impact

The first-principles, multi-scale gyrokinetic calculations discussed in this paper represent perhaps the most complete description of plasma turbulence. However, due to their extreme computational requirements, these simulations will not be applicable for predictive modeling for years to come. The objective of performing these simulations is to assess the relevant physics needed to accurately model experimental heat and particle fluxes, with the ultimate goal of producing a physics-based, reduced model utilized for predictive modeling of tokamak discharges.

[1] N.T Howard, *et. al.* Physics of Plasmas **21**, (2014) 112510

[2] N.T. Howard, *et. al. Cross-Scale Coupling of Ion and Electron-Scale Turbulence in Experimental Tokamak Discharges* – Presented at Transport Task Force Meeting, Salem, MA (2015) – *In preparation for submission to PRL*

[3] N.T Howard *et. al.* Plasma Physics and Controlled Fusion **57** (2015) 065009
[4] J. Candy and R.E. Waltz, Journal of Computational Physics **186** (2003) 545-581