Towards a truly predictive capability: Ab initio models for the plasma boundary

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While there remain many unanswered physics questions regarding the plasma core, an important new frontier of *ab initio* simulations is undoubtedly a comprehensive description of the plasma boundary. As is widely recognized, many key open issues in fusion research – from the L-H transition and pedestal physics to ELM suppression and plasma-wall interactions – are part of this theme. Moreover, the physical properties of the pedestal determine the overall quality of magnetic confinement to a large degree.

Needless to say that in light of the enormous complexities involved here, a large-scale and long-term effort is called for. Our present understanding in this area is much less developed than for the core, and with respect to certain aspects, we are still at the stage of hunters and gatherers. In order to achieve a truly predictive capability for the boundary region, a significant amount of resources must be provided to sustain a healthy variety of complementary projects, focused on different numerical approaches and/or physics aspects.

Here, a two-fold approach to this Grand Challenge is proposed:

1. Develop efficient new gyrokinetic edge codes and subject them to rigorous V&V
2. Use and extend exisiting gyrokinetic codes for edge-specific applications

1. DEVELOPMENT OF NEW GYROKINETIC EDGE CODES. There are several gyrokinetic efforts ongoing (such as the XGC1 particle-in-cell code, the COGENT finite-volume code, and the Gkeyll discontinuous Galerkin code) that are exploring various numerical algorithms for handling the additional complexities of the edge plasma. The edge is a computationally very challenging region, with a wide range of space and time scales, multiple closely coupled physics processes, and particular challenges such as the need to handle magnetic fluctuations as well as electrostatic fluctuations near the beta limit with kinetic electrons. Even when codes are developed that can handle all of the important physics, there will be ongoing work to subject them to rigorous verification and validation (V&V) and bring down the computational cost of these very expensive simulations. These edge codes are described in other whitepapers. Here, we focus on some ways in which well-established core gyrokinetic codes like GENE (http://genecode.org) can be applied to the edge region.

2. APPLICATION OF EXISTING GYROKINETIC CODES TO THE NEAR-EDGE REGION. Over the last several years, existing gyrokinetic codes (originally developed for the core) like GENE, GS2, GYRO, or GEM have also been applied to the near-edge region. These studies have led to some interesting new insights, including the following:

- **L-MODE NEAR-EDGE TRANSPORT.** The experimentally inferred heat transport levels in the near-edge region of L-mode plasmas in the DIII-D and ASDEX Upgrade devices have been successfully reproduced with GENE simulations out to about r/a=0.9 [1,2]. At the same time, it could be confirmed that turbulent fluctuations at long wavelengths (in the transport dominating region) retain many of their linear properties (like real frequencies and cross phases), such that a quasilinear approach should, in principle, be possible [1]. This would require the development of suitable formulas for the saturation level, however. If and under which conditions more nonlinear and/or nonlocal effects come into play, is an open research question which is important to address, since any future attempt to describe an L-H transition self-consistently needs to be built on the capability to describe outer core L-mode plasmas, even quite close to the separatrix.

- **H-MODE PEDESTAL TRANSPORT.** With the help of linear GS2 simulations, it could be demonstrated that microtearing modes can be expected to play an important role near the top of the edge pedestal in H-mode discharges [3,4]. More detailed information has been obtained via linear and nonlinear GENE simulations. For example, the inter-ELM pedestal profile evolution for an ASDEX Upgrade discharge has been studied [5]. Here, density gradient driven trapped electron modes are the dominant pedestal instability during the early density-buildup phase. Nonlinear simulations produce particle transport levels consistent with experimental expectations. Later inter-ELM phases seem to be simultaneously constrained by turbulence driven by kinetic ballooning modes and electron temperature gradient modes [5,6] (see also [7-10]). Also, the radially nonlocal version of GENE has been applied successfully to near-edge plasmas in TCV and ASDEX Upgrade [6] (see also [11]), recovering flux levels which are roughly consistent with experimental measurements. In a related study of TCV plasmas with internal transport barriers, a pioneering multi-scale study was undertaken, covering, for the first time, a scale range from the system size down to the electron gyroradius, again pointing to the multiscale nature of internal and edge transport barriers [12].

- **CODE EXTENSIONS AND LINKS TO APPLIED MATH.** As far as GENE is concerned, to enable such edge-specific investigations, several algorithmic modifications have been implemented, including:
  - Shifted-metric approach, to capture strong distortions of the turbulent fluctuations in the field-line-following direction induced by large (local) magnetic shear [13]
  - Runge–Kutta–Chebychev time-stepping schemes, to efficiently treat high-collisionality regimes [14]
  - Novel, fast eigenvalue solvers for the identification of edge microinstabilities driving the turbulence, in close collaboration with the SLEPc Team [15-17]
  - Inclusion and careful benchmarking of neoclassical effects [18]

  In addition to that, there are several ongoing and planned code extensions which require strong links to applied math:
  - Adapted phase space grids, to account for large variations in the plasma parameters across the H-mode pedestal; this allows for a significant reduction in computational cost
  - Development of a version of GENE for non-axisymmetric magnetic geometries, e.g., to study turbulence in the presence of external magnetic perturbations (for ELM suppression)
  - Extension of GENE to full-f and sheath boundary conditions, to be able to deal with open field line regions
  - Novel algorithmic techniques to increase the resilience for runs on future machines with millions of cores

  These plans and activities offer many opportunities for interdisciplinary collaborative efforts. Many lessons learned in this context are likely to be beneficial for the development and optimization of new edge gyrokinetic codes, in particular those using grid-based methods. Most importantly, such code extensions enable new kinds of investigations of near-edge plasmas, allow to explore key aspects of pedestal and L-H transition physics, and provide important guidance for the developments of new edge gyrokinetic codes.

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