**Whole Device Modeling can facilitate validation efforts in boundary physics**

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In a companion white paper submitted to the PMI workshop it is argued that more emphasis and resources should be placed on validation of boundary physics simulations. Here it is argued that many of the requirements for boundary model validation are shared by whole device modeling, so that an increased initiative in the latter would strongly benefit the former. While the focus here is on boundary physics, the arguments should hold for validation efforts in general.

## Motivation

The ReNeW report rightfully identified the plasma boundary and plasma-material interface as major areas of need for future research. Since that time edge physics has received renewed focus on the experimental side, with (for example) significant progress improving the empirical basis for projecting the scrape-off layer heat flux width. In parallel, several advances on the theory and simulation front have been achieved, improving the physics basis for SOL cross-field transport. At present, we are on the verge of new large-scale simulation capability of boundary and PMI physics, with new tools becoming available to model turbulence and transport [1] including full (gyro-) kinetic simulation [2,3,4], as well as surface simulations ranging from molecular dynamics [5] to continuum models targeting device-scales at realistic parameters [6].

These new capabilities hold the promise to dramatically enhance the physics basis for predicting the boundary plasma and PMI characteristics of future devices. However, at present significantly more effort is going towards developing these tools than is going towards validation of existing and new boundary models. As such, the new simulation capabilities carry a strong risk of being under-utilized and un-validated, partly due to a lack of dedicated analysts. It is generally accepted that validation is a necessary element of theory and simulation development and is beneficial not only in guiding further research on the theory side, but also in guiding experimental and diagnostic design to efficiently produce high-impact results. While understaffing is generally a problem, validation efforts in boundary physics are additionally challenged by a) the breadth of physics required for a comprehensive simulation (e.g., ranging from material surface simulation to atomic physics to plasma transport and stability), and b) the coupling between the various processes which makes identifying the weaknesses in an integrated edge simulation difficult.

## Approach

The validation needs in boundary physics would be greatly aided by a strong Whole Device Modeling initiative that included support of general validation efforts as part of its mandate (beyond validation of the WDM itself). This is based on the machinery required for validation having several features in common with that needed for WDM. These include:

1. **Dealing with coupled physics:** This is clearly one of the challenges for whole device modeling, which by its nature attempts to tie together and understand the coupling between disparate physics. General experience in this area would be very valuable for the validation of boundary

physics models, where the degree of coupling is high. As a practical matter, validation of even a limited scope simulation requires quite a bit of coupled physics. For example, performing a simple 2D fluid simulation of edge plasma transport using, e.g., SOLPS or UEDGE, requires an MHD equilibrium to start from, which in turn requires pressure and current profiles and hence involves heating, transport, and current drive. Assuming that a WDM uses a flexible and modular framework, gathering these needed physics as input to the edge model validation would be straightforward, either based on predictive models or experimental data directly.

2. **Uncertainty Quantification:** A natural role of WDM is to perform sensitivity analyses and UQ for the entire system to inform where the high-leverage physics weaknesses may be. This is an area that where increased attention is critical for boundary validation, where the coupled physics and nonlinear interactions make sensitivity analysis vital for quantitative comparisons to experiment. Taking advantage of the UQ machinery that will presumably built in to a WDM would facilitate this type of analysis in boundary physics.
3. **Robustness of simulations:** For WDM to be practical, significant attention will have to be paid to making simulations robust, minimizing code crashes, erroneous results, and active user intervention. Especially for the new, high-performance computing edge physics simulations, making the codes robust would be extremely useful for validation. Ideally analysts should be separated from the code development itself, and so making codes reliable allows users to focus more on being expert in the physics being studied rather than being expert in getting the code to run.

To take advantage of the common set of needs, a WDM initiative should include support of validation efforts beyond validation of the WDM itself, either by funding these activities directly or including a mandate to support validation within other SciDAC or theory projects.

**Impact**

Including general validation support as an aspect of WDM has several broad benefits. In the boundary physics, this will enable more efficient validation by taking some of the more computational responsibilities off the shoulders of analysts, making better use of limited staffing resources. This would also directly or indirectly open up more resources for validation, which is needed and often underfunded. For the WDM initiative, the benefit is partly in simply building a broad user base for the integrated modeling tools being developed, which is necessary for buy-in to a long-term activity. Further, this has the potential to leverage the work outside the WDM, as this would bring simulations being developed elsewhere (e.g., other SciDAC's or theory programs) for use within the WDM itself (once validated, of course).

**References**

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