Next Steps in Whole Device Modeling.

D L Green*[1], D B Batchelor[1], J M Canik[1], W R Elwasif[1], D E Bernholdt[1], N Bertelli[2], C Holland[3], J M Park[1]
[1] ORNL, [2] PPPL, [3] UCSD
*Corresponding Author : greendl1@ornl.gov
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Summary

- **Motivation :** The number of researchers wanting to do integrated modeling at some level, with the models we have now, is significant. However, many integration workflows are prevented by a lack of component code modularity, robustness, or availability.
- **Approach & Impact :** By (**1**) employing a common framework to facilitate modularity, (**2**) funding the various non-physics activities required to achieve robust component codes, and (**3**) incentivising code availability via funding opportunities, we assert that significant research that would otherwise go undone can be enabled within acceptable levels of funding.

Motivation : In proposing a path forward for whole-device-modeling we consider who are the end users, what opportunities exist from their perspective, and at a practical level, what the needs of the code developers might be to make progress on these opportunities. Beyond the standard list of whole device modeling use cases (e.g., designing new experimental scenarios, discharge optimization, etc), here we list a few examples that highlight near term needs, in that they could be done now except for some non-physics reason.

Unraveling how coupled physics models interact, e.g., performing a 2-D fluid simulation of edge plasma transport requires an initial MHD equilibrium, which in turn requires pressure and current profiles and hence involves heating, transport, and current drive. At present, gathering these needed physics as input is not straightforward. Being able to select from modularly available predictive models, or even experimental data directly, as components would enable the isolation of the impact of each model, and therefore aid in understanding how the models interact.

Rigorous identification of weakness in present models - UQ & Validation, e.g., beyond single time slice and "representative" - i.e., hand picked by the code developer - single case validation. Such rigorous validation and uncertainty quantification (UQ) - required for a robust and predictive whole device model - requires that available models be robust enough to test for some range of parameters, and a statistical ensemble of sanitized experimental data to be compared with. Timely rigorous validation may also require models be made available to external validators / analysts, rather than squeezing the developer to run their code for every case.

Systems design, e.g., device design point identification at medium-fidelity (beyond the 0-point models used now), high-fidelity investigation of specific design points such as how neutrons pass through realistic engineering structures, or cost / risk type studies of various reactor concepts. Such studies could utilize a hierarchy of model fidelities, i.e., with the computers and high performance computing enabled frameworks for integration available now, design studies beyond the 0-point spreadsheet models are possible - we just don't have a robust set of validated models beyond the 0-point fidelity.

Approach : A functional whole-device-model would be useful now, with the physics models we have now. However, there are practical requirements that the component codes be modular, robust, usable, and available. By consolidating, and de-institutionalizing available capabilities, there is an opportunity to improve understanding and provide a persistent target for integration of future codes that may eventually enable a true high fidelity whole device model. Going forward we propose the following measures.

1. Employ a common (existing) framework to facilitate modularity and extensibility : For any integrated or whole device model to be useful for a range of use cases it has to be modular, i.e., be able to interchange models of varying physics, fidelity, or compute capacity without doing any coding. Useful modularity implies open to the community for anyone to submit their model, which in turn means a set of open standards and a framework that facilitates the construction of various workflows and communication of its component models. The fusion community has several such "frameworks / workflow managers" in various states of usefulness in regards to modularity and future extensibility. We expect that focusing the communities integration efforts on one, or some merger of logically complementary frameworks that best provide these capabilities, will result in an increased capability and subsequent expansion of it's user base.

2. Fund user support, code developer support time & software engineering : Here we recognize / admit that the suite of existing physics codes that would compose any whole device or integrated model in the near term are too fragile - especially legacy components. Physics code developers focus on the physics - and correctly so. However, to make progress on a whole device model composed of community contributed codes, there is much in the way of non-physics that could help. i.e.,

I. <u>Fund integrated modeling experts to support end users</u> - obvious.
II. <u>Fund code developer time</u> - to do what is required for integration.
III. <u>Fund implementation of software engineering best practices</u> - to be clear, this is not computer science, e.g., build systems, regression testing, code maintenance, etc.

3. Use funding opportunities as incentives to contribute : The development of a whole device model, or creation of any production predictive capability is really a product development effort. This is in contrast to discovery science / fundamental research. While the product may be used for discovery science, it itself is an implementation of existing or provided (say from the SciDAC institutes) components and technologies. Unsolved problems are the domain of base-theory and the SciDAC institutes where high risk physics exploration is encouraged. In contrast, a production whole device modeling effort should be incremental via continual addition of ever improving, rigorously validated models for the various parts of the problem. So, if a production whole device model is to be a real goal, we expect that a <u>persistent</u> integration effort that focuses on the production predictive capability running in parallel to the <u>transient</u> discovery SciDAC institutes is an appropriate programmatic model, i.e., don't keep re-inventing the integration wheel every 5 years.

While de-institutionalizing the integration effort by setting standards will enable everyone to contribute, we expect it will require crafting funding opportunities to provide incentive to move groups towards actually contributing. Not that this is the only way, but perhaps one metric of the next round of SciDACs could be the production of reduced models based on their large compute scale investigations, or delivering codes that are "component-available" within the community framework, for the reasons of facilitating comparisons with reduced models, or benchmarking.

Impact : The proposed steps are valuable now, but will be more valuable ten years from now.