The Need for Computational Centers that Validate Using Small Experiments

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Purpose of white paper. This white paper is to ask the workshop to support the concept of centers that works with many small experiments for validation of the center's codes and for computational support of the experiments. The Plasma Science and Innovation Center (PSI-Center) is such a center. As an example, the PSI-Center will be described for this white paper.

The Problem: practical, predictive models of plasma behavior. Nonlinear macroscopic modeling is an important component of the mainline MFE theory program. It is applicable to magnetic island evolution, sawteeth, edge localized modes (ELMs), resonant magnetic perturbations (RMP), and disruptions in the tokamak configuration. Among the set of initial 'science drivers' considered for the Fusion Simulation Program (FSP) (http://www.pppl.gov/fsp), macroscopic modeling is a critical component for disruptions, wave-particle interaction, pedestal stability, and self-organization. It will also contribute to understanding core transport in conditions where magnetic islands impact confinement. PSI-Center's application of the same macroscopic modeling tools to a broad range of Concept Exploration (CE) experiments (small well-focused fusion research experiments) will provide validation information over a broader range of conditions. This will provide confidence that the tools have predictive capability beyond a limited range of parameters. In addition, our enhancement of kinetic and neutral modeling capabilities will directly contribute to mainline modeling needs for pedestal stability and disruption, where macroscopic dynamics involve neutrals and plasma across a range of temperature. The PSI-Center is also attacking the basic plasma science problems of sheath boundary conditions.

Advantages to using smaller experiments. We use smaller experiments to calibrate and test the ability of computer codes to model specific phenomena. **This is a very exciting area of research because state of the art codes and computers have now reached the capabilities to make quantitative modeling of these whole experiments possible**. The PSI-Center is needed to provide the resources for the required attention to details in experimental data, and in code development to make this happen. We concentrate on CE experiments for two reasons. First, unlike the mainline fusion concept experiments, many smaller experiments have as their primary effect phenomena that are secondary in larger, hotter machines. For example, the Hall effect is very important in imposed dynamo current drive experiments. Self-organization is essential in spheromak formation and helicity injection ST startup experiments. Flow is dominant in flow stabilized Z-pinches. Charge exchange and other neutral particle effects can dominate small experiments. Using physically accurate boundary conditions is essential for steady-inductive-helicity-injection experiments. Thus, there are advantages to using smaller experiments to calibrate codes that are designed to handle edge effects in larger hotter experiments. Second, the cooler smaller experiments have smaller Lundquist numbers (S) making it practical to run fluid-based codes at actual experimental values for quantitative validation.

Validation Metrics and Uncertainty Quantification. The PSI-Center is using biorthogonal decomposition (BOD or BD)[1] as an impartial validation[2,3] assessment tool. The value of the method is that the dominant spatial and temporal structures of the data are found mathematically. This greatly facilitates a quantitative validation assessment with uncertainties also quantified. The method is an efficient, simple way to include large amounts of data by maximizing the benefit of high speed computing. We are developing methodologies and metrics based on BDs including error propagation for uncertainty quantification.[4]

Why the PSI-Center is needed. Figure 1 shows our long-term vision of using computational predictability to lead to improved parameters for the supported concepts. The goal is to develop predictability of the whole experiment for a good fraction of the time of the discharge for many present experiments. The codes need to be user friendly enough to be used as engineering design tools so that detailed designs of future experiments can be computationally tested before they are built. This is a difficult long term goal that needs a significant level of effort. The first step is accurately predicting present experiments from breakdown to well beyond the best performing part of the discharge. The second step will be using the predictability to design modifications for present experiments that improve performance. Finally, when the confidence is sufficient the next level experiments will be designed and computationally "ran" as they are being designed. Data from the new experiments, after they are built, will then be used to improve the physics for better predictability at the improved parameters, making them ready to be used in designing the next advancement. All the while, advances in computer hardware and algorithms will make the codes faster, more accurate, and more user-friendly. In this way PSI-Center will help all of the collaborating experiments achieve their goals, as CE research evolves, while developing computational predictability that will be valuable to the entire plasma physics community.

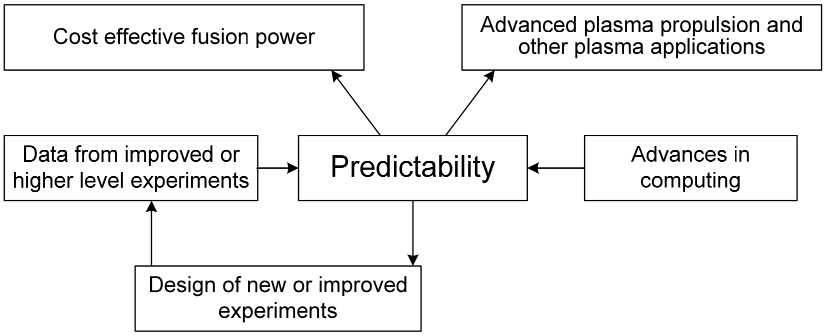

Figure 1: ***Schematic illustrating the contribution of PSI-Center towards the goal of cost effective fusion power.***

This knowledge-led approach supported by the rapid advances in computing technology, and the tokamak plasma and technology knowledge base, may lead to a very cost effective configuration optimization.

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[1] T. Dudok de Wit, A.-L. Pecquet, J.-C. Vallet, and R. Lima. "The biorthogonal decomposition as a tool for investigating fluctuations in plasmas", *Physics of Plasmas*, **1**(10):3288–3300, 1994

[2] M. Greenwald, "Tutorial: Verification and validation for magnetic fusion", Phys. Plasmas **17**, 058101, 2010

[3] C. J. Roy and W. L. Oberkampf, "A comprehensive framework for verification, validation, and uncertainty quantification in scientific computing", Computer Methods in Applied Mechanics and Engineering, Volume **200**, Issues 25–28, 15 June 2011, Pages 2131–2144

[4] B S Victor, C Akcay, C J Hansen, T R Jarboe, B A Nelson and K D Morgan, "Development of validation metrics using biorthogonal decomposition for the comparison of magnetic field measurements", Plasma Phys. Control. Fusion, **57,** 045010, 2015.