White Paper for Discussion on Uncertainty Quantification
Integrated Simulations for Magnetic Fusion Energy Sciences
Panel Topic E: Beyond interpretive simulations / Uncertainty quantification

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In this document, we discuss issues that arise in simulation of physical systems when some components of models are not known with certainty. We take as an example a model of magnetohydrodynamics (MHD) kinematics in which the fluid velocities are treated as random fields. In addition, we describe some of the computational challenges associated with performing such simulations efficiently. Similar approaches can be applied to more complex plasma models where physical parameters are treated as uncertain.

1. Uncertainty in Models of MHD. The following equations represent a simplified model of the steady-state kinematics of MHD obtained by eliminating the current density and electric field from Maxwell's equations, and assuming that the fluid velocities and pressures governed by the Navier-Stokes equations are specified:

$$\begin{aligned} \nabla \times \left(\frac{\eta}{\mu}\nabla \times \vec{B}\right) - \nabla \times (\vec{u} \times \vec{B}) &= \vec{0}, \\ \nabla \cdot \vec{B} &= 0. \end{aligned} \tag{1}$$

The solution sought is the magnetic induction, $\vec{B}$. One way to explore the simplification implicit in the assumption about fluid variables is to treat the velocity vector $\vec{u}$ as a random field instead of a known quantity. Then we can consider the impact of uncertainty of the velocities by starting with some given choice $\vec{u}_0$ and examining properties of resulting solutions $\vec{B}$ of (1) for (deterministic) $\vec{u} = \vec{u}_0$ and for perturbed values $\vec{u} = \vec{u}_0 + \delta\vec{u}(\omega)$, where $\delta\vec{u}(\omega)$ represents some systematically determined random perturbation.

A representative example of what can happen in this scenario is shown in Figure 1, which shows the effect of incompressible perturbations of velocities on properties of the solution, the magnetic induction, for a two-dimensional model (with several values of variance in the perturbation). These results are taken from [1], which also reports a variety of other similar phenomena. It can be seen that character of the magnetic field is significantly affected by the perturbations, which suggests that fluid vorticity plays a large role in generating magnetic fields, and important effects may be difficult to discern from models that use only mean fluid velocities.

2. Computational Issues. Performing simulations of the type discussed above are computationally very highly demanding. The results shown here were obtained using Monte Carlo simulation, which is straightforward to implement, requiring only repeated sampling of random parameters. However, Monte Carlo methods have some drawbacks. First, as is well known, they are very slow to converge. Moreover, in simulations such as these, finding a sample value entails solving a complex algebraic system of equations. For accurate simulations of three-dimensional models, the combination of slow convergence of Monte Carlo simulation coupled with high cost of sampling may be prohibitive. Thus, there is a need to develop new computational tools for such simulations.

There are two ways to reduce computational costs. One entails development of new computational algorithms for solving models, in this case of MHD [2]. The other is to develop new

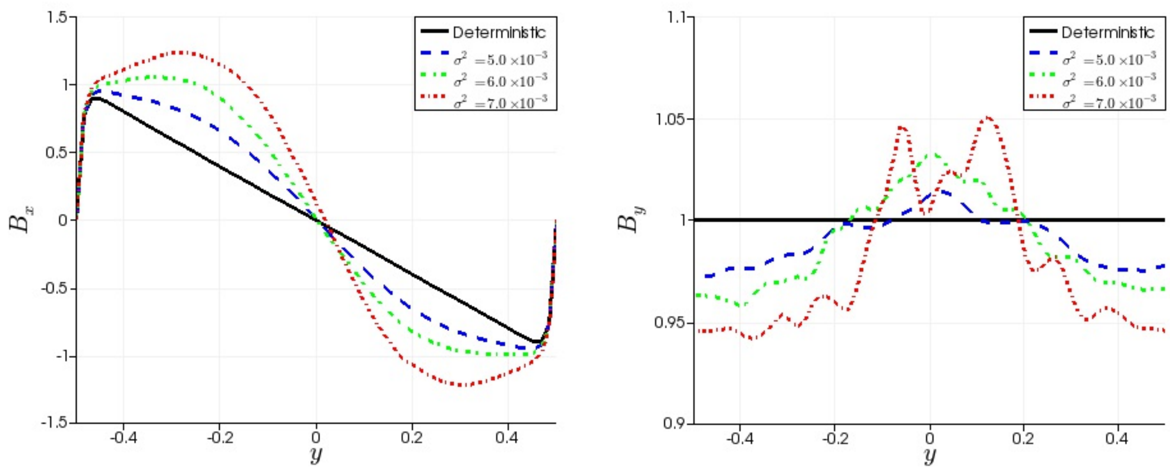

Figure 1: Example profiles of means of components B_x and B_y of solutions $\vec{B}$ of equation (1) determined from randomly perturbed velocities, plotted along one line of the physical domain.

approaches for the statistical component of simulations. Both methodologies are important; here we give a brief statement about ways to address the latter part of the problem.

One way to do this is to use so-called spectral methods to create surrogate solutions that can be sampled cheaply. For example, suppose the desired solution $\vec{B}$ depends on a set of m parameters $\boldsymbol{\xi} \equiv (\xi_1, \ldots, \xi_m)^T$; these might correspond to different but uncertain values of velocities in different parts of the physical domain. Monte Carlo simulation of $\vec{B}(\boldsymbol{\xi})$ would repeatedly sample these parameters and estimate moments of $\vec{B}$ using the sample solutions. An alternative is to evaluate $\vec{B}(\boldsymbol{\xi})$ at a distinguished set of sample values $\boldsymbol{\xi}^{(1)}, \ldots, \boldsymbol{\xi}^{(M)}$ and then to define a surrogate $\vec{B}_{surr}(\boldsymbol{\xi})$ that *interpolates* $\vec{B}(\boldsymbol{\xi})$ at the distinguished points. Thus, sampling of $\vec{B}$ would be replaced by sampling of the surrogate $\vec{B}_{surr}$, which is dramatically cheaper. It has been shown that when the distinguished set is chosen using *sparse grid* algorithms, then in many settings the resulting surrogate represents an accurate approximation, and this is an effective alternative to traditional sampling [3]. These approaches have only been tested in a narrow regime of applications, and it is not certain that this approach avoids the "curse of dimensionality," i.e., whether the number of points M determining the surrogate can be kept small. Rigorous study of new approaches of this type is of critical importance for enabling fast and accurate simulations of physical phenomena such as MHD.

BIBLIOGRAPHY

[1] E. G. Phillips and H. C. Elman. A stochastic approach to uncertainty in the equations of MHD kinematics. *J. Comput. Phys.*, 284:334–350, 2015.

[2] E. G. Phillips, H. C. Elman, E. C. Cyr, J. N. Shadid, and R. P. Pawlowski. A block preconditioner for an exact penalty formulation for stationary MHD. *SIAM J. Sci. Comput.*, 36:B930–B951, 2014.

[3] D. Xiu and J. S. Hesthaven. High-order collocation methods for differential equations with random inputs. *SIAM J. Sci. Comput.*, 27:1118–1139, 2005.