Quantifying uncertainty with stochastic collocation in the kinematic magentohydrodynamic framework

E. Rajbhandari[1,2], N.L. Gibson[1] and C. R. Woodside[2]

[1] Department of Mathematics, Oregon State University

[2] National Energy Technology Laboratory, Albany, OR

E-mail: rajbhane@oregonstate.edu

Abstract. We discuss an efficient numerical method for the uncertain kinematic magnetohydrodynamic system. We include aleatoric uncertainty in the parameters, and then describe a stochastic collocation method to handle this randomness. Numerical demonstrations of this method are discussed. We find that the shape of the parameter distributions affect not only the mean and variance, but also the shape of the solution distributions.

1. Introduction

Magnetohydrodynamics (MHD) is the study of an electrically-conductive medium flowing through a magnetic field [1]. It is a multi-physics problem, governing the behavior of fluid flow, electric fields and currents, magnetic fields, and their interactions. MHD has applications in many different areas of study, such as astrophysics [2], medicine [3] and power generation [1].

These different applications operate under separate conditions, and thus varying assumptions are made on the system. We focus on the power-generation capabilities of MHD, which involves applying a large magnetic field to an electrically conductive plasma, artificially creating an electric field [1]. Following related work to simplify computational complexity [4], we prescribe the fluid-flow, and focus on the electromagnetic behavior of the MHD system. This model is called the kinematic MHD equations, further described in Section 2 and [5].

We are ultimately interested in investigating the feasibility of real-time optimization of an MHD generator. The parameters of the system, including fluid velocity, conductivity, electron mobility, and ion mobility, need to be estimated via observations. This introduces aleatoric uncertainty into the system, as the recovered parameters are then described by probability distributions. Therefore, the optimal design of the generator must consider uncertainty, as each random parameter is governed by some estimated distribution. Related work has investigated the well-posedness of the forward problem under uncertainty [4]. We propose here a non-intrusive approach to quantifying the uncertainty in the forward problem using a numerical model, implemented in COMSOL [13], that has already been validated [5]. This will be incorporated into an optimization under uncertainty problem in future work.

There are many different approaches for dealing with uncertainty in a system in general. Although simplistic for implementation, other methods, such as Monte Carlo, come with a high computational burden [6]. The method we utilize lessens the computational burden both through the choice of points in which we sample the domain, and the way in which we choose to average the solutions. In the following work, we implement an approximation method called *stochastic collocation* (SC) [7]. Utilizing a sparse grid with SC can result in a diminishing of the 'curse of dimensionality' that often affects uncertainty quantification, while maintaining a high degree of accuracy [8], which will allow the utilization of the model in the inverse problem under uncertainty.

We begin by stating the well-posedness of the system under uncertainty. Following, we will go into detail regarding the SC method and the random grid. Finally, we end with a numerical demonstration of the robustness of the method for a variety of different situations, including several complex joint probability distributions of the random variables within the system. These demonstrations will also show that the expected solutions and deterministic solutions vary significantly enough to warrant an approach to optimal design under uncertainty, and that the shape of the solutions' distributions depend on the parameters in the input distributions.

2. Model

For the purposes of this paper, we will not focus on any specific generator model or component, and work in general with the MHD equations. Let the spatial domain be given by $D \subset \mathbb{R}^3$, open with compact closure, and denote the boundary as ∂D. We denote the random space $(\Omega, \mathcal{H}, p)$, where Ω is the set of outcomes, $\mathcal{H}$ is a given sigma algebra of events, and p is some continuous probability measure. As noted in the introduction, we work on the kinematic MHD system, with prescribed fluid-flow, $\mathbf{u}$. We assume that the induced magnetic field is negligible compared to the applied magnetic field [9]. Under the generator model, we then prescribe conductivity, σ, applied magnetic field, $\mathbf{B}$, electron-mobility, μ_e, and ion-mobility, μ_i. We use the standard definition of the l^2 norm of a vector in $\mathbb{R}^3$, as well as the hall parameter and ion-slip parameter, e.g. for $\mathbf{x} \in D,\ \omega \in \Omega$

$$\beta_e(\mathbf{x}, \omega) = \mu_e(\mathbf{x}, \omega)||\mathbf{B}(\mathbf{x})||_{l^2}, \text{ and } \beta_i(\mathbf{x}, \omega) = \mu_e(\mathbf{x}, \omega)\mu_i(\mathbf{x}, \omega)||\mathbf{B}(\mathbf{x})||_{l^2}^2.$$

Finally, we use the conductivity tensor, as defined in [5], given by

$$\underline{\overline{\sigma}}(\mathbf{x}, \omega) = \sigma(\mathbf{x}, \omega) \left(\mathcal{I} - \frac{\beta_e(\mathbf{x}, \omega)}{||\mathbf{B}||_{l^2}} [\mathbf{B}]_\times - \frac{\beta_i(\mathbf{x}, \omega)}{||\mathbf{B}||_{l^2}^2} [\mathbf{B}]_\times^2 \right)^{-1},$$

where $\mathcal{I}$ denotes the identity matrix in $\mathbb{R}^{3\times 3}$ and $[\mathbf{B}]_\times$ is the matrix form of the cross-product. Invertibility of this matrix is guaranteed by the physical restriction $\mu_e, \mu_i > 0$. We now turn to defining the random solution spaces. First, define the random function space

$$L_{2,p}(\Omega) := \left\{ f : \Omega \to \mathbb{R} \;\Big|\; \int_\Omega f^2(\omega)p(\omega)\, d\omega < \infty \right\}, \text{ with norm } ||f||_{L_{2,p}(\Omega)} := \left(\int_\Omega f^2(\omega)p(\omega)\, d\omega \right)^{1/2}.$$

Next, define the deterministic solution spaces for the induced current density, $\mathbf{J}_i$, and the electric potential, $\mathcal{V}$, respectively

$$V(D) := \left\{ \mathbf{f} \in (L^2(D))^3 : \mathbf{f}\cdot\mathbf{n} = -\big(\underline{\overline{\sigma}}(\mathbf{u}\times\mathbf{B})\big)\cdot\mathbf{n} \text{ on } \partial D \right\}, \quad W(D) := W_0^{1,2}(D) = \left\{ f \in H^1(D) : T(f) = 0 \right\},$$

where $\mathbf{n}$ is a vector normal to the boundary and $T(f)$ is the trace of f on D. Finally we define the *random solution space* for $\mathbf{J}_i$ as the tensor product between the deterministic and random function spaces, or

$$\overline{V} := V(D) \times L_{2,p}(\Omega) = \left\{ f : D \times \Omega \to \mathbb{R}^3 \;\Big|\; f(\cdot, y) \in \big(L_{2,p}(\Omega)\big)^3,\ f(\mathbf{x}, \cdot) \in V \right\}.$$

Similarly, define $\overline{W} := W(D) \times L_{2,p}(\Omega)$ for $\mathcal{V}$. We define the norm on $\overline{V}$ as the averaging norm, i.e.

$$||F||_{\overline{V}} = \left(\mathbb{E}\left[||F||_V^2 \right] \right)^{1/2}$$

and define the norm on $\overline{W}$ to be the averaging norm using $||\cdot||_W$. Also define the expected value of a real-valued function to be $\mathbb{E}[f] := \int_\Omega f(\omega)p(\omega)\ d\omega$. With these spaces, the kinematic weak-form MHD equations are given by: find $\mathbf{J}_i \in \overline{V}, \mathcal{V} \in \overline{W}$ that satisfy

$$\mathbb{E}\left[\int_D \underline{\sigma}^{-1}\mathbf{J}\cdot\phi\right] - \mathbb{E}\left[\int_D \nabla\mathcal{V}\cdot\phi\right] = 0\ \forall\phi\in\overline{V}, \tag{1a}$$

$$-\,\mathbb{E}\left[\int_D \mathbf{J}_i\cdot\nabla\psi\right] = \mathbb{E}\left[\int_D \big(\underline{\sigma}(\mathbf{u}\times\mathbf{B})\big)\cdot\nabla\psi\right]\ \forall\psi\in\overline{W}. \tag{1b}$$

We denote the form (1) the *random weak form.* In the following work, to guarantee well-posedness, assume that $\forall\omega\in\Omega$, $\mathbf{u}(\omega), \mathbf{B}$ are in $(L^2(D))^3$ and bounded, and $\sigma(\omega), \beta_e(\omega)$ and $\beta_i(\omega)$ are positive, bounded, and real-valued on D. Then there exist unique solutions, $\mathbf{J}_i, \mathcal{V}$, to (1), that depend continuously on the parameters [4]. With the governing equations defined and well-posedness established, we turn to the focus of this paper, the numerical approximation of the solutions.

3. Polynomial Chaos

As is a standard approach when solving systems numerically, we would like to search for our solutions on some finite-dimensional representation of the solutions spaces. We do so by projecting onto the space of polynomials of random variables. We denote this projection a *polynomial chaos expansion.* However, we require that this polynomial space has finitely-many directions, which leads to the first major assumption required.

3.1. Finite-Dimensional Noise

To implement the SC method, we must first assume there are a finite number of random variables describing the noise [10]. To this end, we assume that the only random variables in the system are the real-valued random parameters μ_e, μ_i, σ, and $\mathbf{u}$. Furthermore, assume each are described by a finite number of independent random variables.

Let Γ be the tensor product of the image of the events under each random variable. Let ρ be the joint independent probability distribution. Then by the Doob-Dynkin's Lemma [11], we have that the solutions $\mathbf{J}_i, \mathcal{V}$ can be described by a finite number of random variables. The numerical problem then equates to approximating $\mathbf{J}_i(\mathbf{x}, y),\ \mathcal{V}(\mathbf{x}, y)$ for $\mathbf{x}\in D,\ y\in\Gamma$. Analogous to the above problem, we attempt to find $\mathbf{J}_i \in V\times L_{2,\rho}(\Gamma),\ \mathcal{V}\in W\times L_{2,\rho}(\Gamma)$ that satisfy

$$\int_D \underline{\sigma}^{-1}\mathbf{J}_i(\mathbf{x},y)\cdot\phi(\mathbf{x},y)\ d\mathbf{x}\ - \int_D \nabla\mathcal{V}(\mathbf{x},y)\cdot\phi(\mathbf{x},y)\ d\mathbf{x}\ = 0 \quad \forall\phi\in V,\ \text{for}\ \rho.a.e.\ y\in\Gamma \tag{2a}$$

$$-\int_D \mathbf{J}_i(\mathbf{x},y)\cdot\nabla\psi(\mathbf{x},y)\ d\mathbf{x}\ = \int_D \underline{\sigma}(\mathbf{x},y)\big(\mathbf{u}(\mathbf{x},y)\times\mathbf{B}(\mathbf{x})\big)\cdot\nabla\psi(\mathbf{x},y)\ d\mathbf{x} \quad \forall\psi\in W,\ \text{for}\ \rho.a.e.\ y\in\Gamma \tag{2b}$$

For notational convenience, we define $\widetilde{V} := V\times L_{2,\rho}(\Gamma)$ and $\widetilde{W} := W\times L_{2,\rho}(\Gamma)$ as the *new* random solution spaces for which we seek a numerical approximation. Note now that this is equivalent to (1), only with the alternative probability space (Γ, H, ρ), where H is the appropriately defined sigma algebra.

We now define the finite-dimensional (FD) random solution subspaces in which we search for our approximate solutions. We begin with the spatial dimension. Define $V_h \subset V$ to be the standard finite element approximation to V, with quadratic polynomials, on some Delauney triangular prism mesh t_h with max side length h. Similarly define $W_h \subset W$, on the same mesh t_h. For the random solution space, define $P_{N_k}(\Gamma_k) \subset L_{2,\rho}(\Gamma_k)$ for $k = 1,\ldots,M$ as the span of all polynomials on Γ_k of degree up to N_k, for $N_k\in\mathbb{N}$. In each direction Γ_k, we choose to

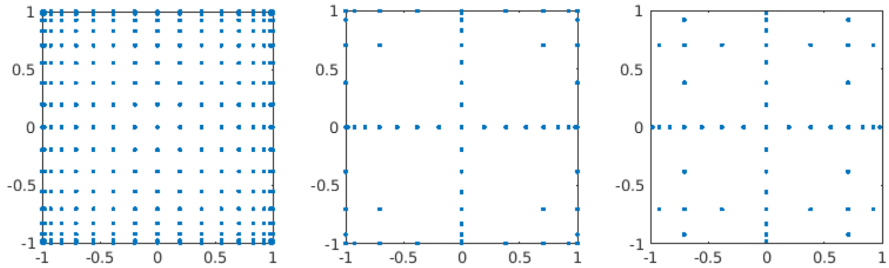

Figure 1: Quadrature grids with level = 5. (From left to right) CC Full: 289 nodes, CC Sparse: 65 nodes, Fejér Sparse: 55 nodes. Constructed using Burkhardt's repository [12].

use the basis of Legendre polynomials $\{r_k^j\}_{j=0}^{N_k}$ [7], which are orthogonal with respect to the uniform density function, e.g., $\int_{\Gamma_k} r_k^j r_k^l \, dy = \delta_{jl}$, where δ_{jl} is the Dirac delta function. Define $N = [N_1, \ldots, N_M]$. Then we approximate our random $L_2(\Gamma)$ space with a tensor product of these polynomial spaces, i.e. $P_N(\Gamma) := \prod_{k=1}^{M} P_{N_k}(\Gamma_k)$. Note that the dimension of P_N is clearly finite. The FD approximation to the random solution spaces are thus given by:

$$\widetilde{V}_{h,N} := V_h \otimes P_N(\Gamma) \text{ and } \widetilde{W}_{h,N} := W_h \otimes P_N(\Gamma).$$

With these spaces, we now describe the SC method in detail, defining the finite-dimensional polynomial chaos expansion.

3.2. Stochastic Collocation Method

We begin the collocation by solving the deterministic equivalent system, for fixed y, to (2). These will then used to build an interpolatant. By solving for fixed y, we treat $\mathbf{J}_i^h$ and $\mathcal{V}^h$ as mappings from Γ to their respective deterministic spaces, i.e. $\mathbf{J}_i^h : \Gamma \to V_h$, $\mathcal{V}^h : \Gamma \to W_h$. We perform the *collocation* by averaging the solutions sampled at the zeros of the polynomial basis of $P_{N_k}(\Gamma_k)$ for each $k = 1, \ldots, M$. By using the Legendre polynomials, we are able to use the Clenshaw-Curtis (CC) or Fejér method of numerical quadrature, which guarantees nesting of the zeros in each random direction [7]. Furthermore, we reduce the number of points, by constructing a Smolyak sparse grid [8]. Although there is not a closed-form method of giving the number of nodes required in each domain, we let $\tilde{N}_k$ denote the total number of points in the Γ_k direction. A more detailed discussion of the construction of such grids can be seen in [8] or [6], while the error analysis for the full-tensor Clenshaw-Curtis grid can be seen in [4]. Figure 1 depicts the difference between a full-tensor and sparse CC and Fejér grid. For the purposes of the grid construction, we assume a uniform max level in each random direction, i.e. an isotropic sparse grid.

With this in mind, we let $y_k^{m_k}$ for $m_k = 1, \ldots, \tilde{N}_k,\ k = 1, \ldots, M$ be the m_k^{th} unique zero in the direction Γ_k. To ease the notation, define $m = [m_1, \ldots, m_M]$ as an array of orders, and define $y_m = [y_1^{m_1}, \ldots, y_M^{m_M}]$, that is, a collection of zeroes in each direction of Γ. As well, define the product of the polynomials of a given order in each direction as $r_m(y) = \prod_{j=1}^{M} r_j^{m_j}$.

Then the polynomial chaos expansions of $\mathbf{J}_i$ and $\mathcal{V}$ are given by

$$\mathbf{J}_i^{h,N}(\mathbf{x}, y) = \sum_{m_1=1}^{\tilde{N}_1} \cdots \sum_{m_M=1}^{\tilde{N}_M} \mathbf{J}_i(\mathbf{x}, y_m) r_m(y), \text{ and } \mathcal{V}_i^{h,N}(\mathbf{x}, y) = \sum_{m_1=1}^{\tilde{N}_1} \cdots \sum_{m_M=1}^{\tilde{N}_M} \mathcal{V}(\mathbf{x}, y_m) r_m(y). \tag{3}$$

Table 1: Distribution parameters for the random parameters. Beta distribution shape parameters recovered from mean and standard deviation, and then translation maps from $[0, 1]$ to the bounded space. Uniform distribution determines the bounds from the given mean and standard deviation.

Parameter	Distribution	Lower Bound	Upper Bound	Mean	Standard Deviation
μ_e	beta	8/6	12/6	10/6	0.5/6
$\mathbf{u}_x$	beta	1200	1800	1700	100
μ_e	uniform	9.13/6	10.86/6	10/6	0.5/6
$\mathbf{u}_x$	uniform	1527	1873	1700	100

Using this interpolation, we arrive at a deterministic form of estimating the expected values of the true solutions. Using Gaussian quadrature to approximate the integral yields

$$\mathbb{E}[\mathbf{J}_i^{h,N}] = \sum_{m_1=1}^{\tilde{N}_1} \dots \sum_{m_M=1}^{\tilde{N}_M} \mathbf{J}_i(\mathbf{x}, y_m)\rho(y_m)w_k^m(y), \text{ and } \mathbb{E}[\mathcal{V}^{h,N}] = \sum_{m_1=1}^{\tilde{N}_1} \dots \sum_{m_M=1}^{\tilde{N}_M} \mathcal{V}(\mathbf{x}, y_m)\rho(y_m)w_k^m(y)$$

where $w_k^m := \prod_{j=1}^{M} w_{k_j}^{m_j}$ and $w_{k_j}^{m_j} := \int_{\Gamma_{k_j}} (r_{k_j}^{m_j})^2 \, dy$, e.g. the weights of the polynomial in each direction. Note that we must include the density functions in the summations as well, to account for the transformation from the given joint density function to a strictly uniform one, which is required to use the CC or Fejér grid.

4. Numerical Experiments

With the collocation method established, and our choice of grid made, we now demonstrate the robustness of the method. For simplicity, we consider only $\mu_e, \mathbf{u}$ as the random parameters in the system. Furthermore, the fluid flow is assumed to be in one direction, $\mathbf{u} = (\mathbf{u}_x, 0, 0)$. We also assume that each is described by a single random variable and are spatially constant. For demonstration purposes, we assume both random variables are described by either a uniform or beta distribution, with a given mean and variance. The distributional choices are described in Table 1.

The results from these numerical experiments can be seen in Figure 2. In these, we examine a 1-D center line of the full 3-D model, running from channel inlet to outlet, of the electric potential $\mathcal{V}$. The random-grid and weights are implemented using Burkhardt's repository [12], while the deterministic solutions are computed with the COMSOL [13] model desribed in [5]. In Figure 2, we see a spatial dependence for the variation of the solution, with higher variances seen at the inlet of the channel. However, despite having the same mean and variance, the shape of the distribution clearly also had an impact on the distribution shape of the solutions, as seen in the right plot of Figure 2. Thus, the shape and variance of the random variables have a significant effect on the variance of the solutions, and inclusion of uncertain parameters within the model is necessary for reliable simulations.

5. Conclusion

In this paper, we explored the numerical propagation of uncertainty within an MHD system. We began by defining the governing equations for our model. We then introduced major assumptions required to implement the SC method, including the FD noise assumption. Next, we described the SC method itself, performing a FD polynomial chaos expansion of the solutions as an interpolation in the random space. We also defined the interpolating points by using the

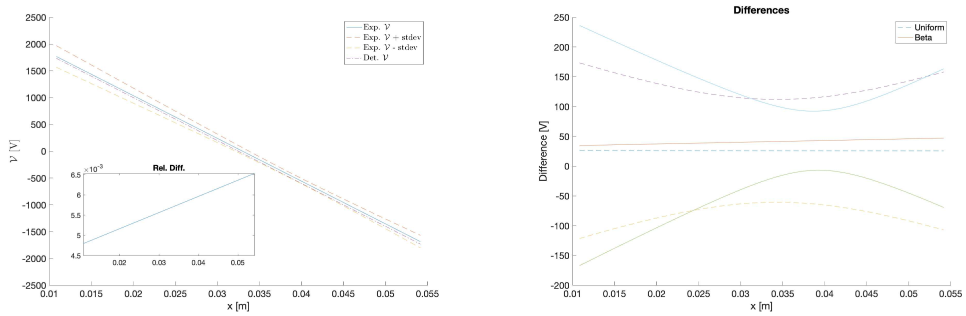

Figure 2: Results from numerical experiments. (Left) beta distributions. Exp. $\mathcal{V}$ is the expected value of $\mathcal{V}$, solved for using the SC method at a level of 5. Det. $\mathcal{V}$ is the deterministic $\mathcal{V}$, solved for with the means of each random parameter. (Inset plot) Relative error defined as the normalized difference between the Exp. $\mathcal{V}$ and Det. $\mathcal{V}$. (Right) Difference between Exp. $\mathcal{V}$ and Det. $\mathcal{V}$, with variances included. Solid line indicates uniform distribution results, dashed line indicates beta distribution results.

zeros of the orthogonal Lagrange basis of the random space, and further reducing the system complexity by utilizing a CC or Fejér sparse grid. Finally, we demonstrated the effectiveness of the SC method with two random variables within the system. It was shown that the inclusion of uncertainty is warranted. The efficiency of the SC method with a sparse grid enables the inverse problem to be considered under uncertainty, and allows for future work involving the optimal design problem of the MHD system.

Acknowledgments

The work was supported by the United States Department of Energy's Crosscutting Research Program, an appointment to the Science Education Programs at the National Energy Technology Laboratory, administered by ORAU through the United States Department of Energy Oak Ridge Institute for Science and Education, and by the National Science Foundation, grant number DMS-2012882.

References

[1] Rosa R 1968 *Magnetohydrodynamic Energy Conversion.* McGraw-Hill
[2] Sutton G and Sherman A 1965 *Engineering Magnetohydrodynamics.* McGraw-Hill series in mechanical engineering. McGraw-Hill
[3] Nacev A, Beni C, Bruno O, and Shapiro B 2011 The behaviors of ferro-magnetic nano-particles in and around blood vessels under applied magnetic fields. In *Journal of Magnetism and Magnetic Materials* **323** 6 651–668
[4] Rajbhandari E, Gibson N, and Woodside C Preprint Stochastic collocation error analysis for the full 3-d magnetohydrodynamic system. In
[5] Rajbhandari E, Gibson N, and Woodside C Preprint Parameter estimation for 3-d magnetohydrodynamics generator. In
[6] Johnson B, Gibson N, and Cotilla-Sanchez E 2021 A coupled Karheunen–Loeve and anisotropic sparse grid interpolation method for the probabilistic load flow problem. In *Electric Power Systems Research*
[7] Smith R 2014 *Uncertainty Quantification: Theory, Implementation, and Applications.* SIAM. ISBN 978-1-611973-21-1
[8] Burkhardt J 2012 The "combining coefficient" for anisotropic sparse grids. In *Interdisciplinary Center of Applied Mathematics And Information Technology*
[9] Bokil V, Gibson N, McGregor D, and Woodside C 2015 Toward estimating current densities in magnetohydrodynamic generators. In *Journal of Physics: Conference Series* **640**
[10] Babuska I, Nobile F, and Tempone R 2007 A stochastic collocation method for elliptic partial differential equations with random input data. In *SIAM Journal on Numerical Analysis* **45**
[11] Oksendal B 2003 Stochastic differential equations. In
[12] Burkhardt J 2021. J. Burkhardt's homepage
[13] Comsol multiphysics v. 5.4