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Numerical strategy for model correction using physical constraints

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ABSTRACT

In this paper we present a strategy for correcting model deficiency using observational data. We first present the model correction in a general form, involving both external correction and internal correction. The model correction problem is then parameterized and casted into an optimization problem, from which the parameters are determined. More importantly, we discuss the incorporation of physical constraints from the underlying physical problem. Several representative examples are presented, where the physical constraints take very different forms. Numerical tests demonstrate that the physics constrained model correction is an effective way to address model-form uncertainty.

1. Introduction

The field of uncertainty quantification (UQ) has undergone rapid developments in the last decade. While tremendous progresses have been made in the quantification of parametric uncertainty, much less has been accomplished in the front of model-form uncertainty. One of the primary goals of model-form uncertainty analysis is to quantify the deficiency of the simulation models, as it is widely accepted that all models are approximations to the physical truth. To this end, the approach developed by Kennedy and O'Hagan [8] has found its use in a variety of applications. See, for example, [1,4,5,11,13], and the references therein. In this approach, the simulation model is corrected by adding a discrepancy term. Then, both the simulation model and the discrepancy term are parameterized by Gaussian processes. The hyper-parameters in the Gaussian processes are then estimated using Bayesian inference based on observational data. While effective in many cases, the explicit introduction of the additive discrepancy term often destroys certain important physical properties of the underlying problem, which are often built into the simulation model via tremendous effort. This undesirable side effect has been recognized in the literature, and efforts have been made to mitigate it, for example, via constrained prior construction in the Bayesian inference [2]. Another approach to preserve the physical properties of the model is to directly embed the model discrepancy in the model, as opposed to treating it as an external additive term. This was proposed in [12], where random parameters are introduced inside the model to allow one to tune the model using data. The random variables are then parameterized by polynomial chaos expansion [3,14] and Bayesian inference is then employed to estimate the expansion coefficients.

In this paper, we first frame the model correction problem in a general manner, using model discrepancy terms both external and internal to the model. More importantly, we discuss a means of explicitly incorporating the physical constraints that the underlying problem should satisfy. This is vital to the corrected model, as it is intended to be an improved model to the underlying physical phenomenon. Upon parameterizing the model correction terms, our model correction problem

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is formulated as an optimization problem, where the distance between the corrected model predictions and observation data is minimized. The physical constraints are also parameterized and then incorporated in the optimization problem as constraints. This results in the core contribution of this paper — the method of physics constrained model correction (PCMC). A general discussion about the physical constraints is difficult, as they can take vastly different forms depending on the underlying physical problems. Instead, we then proceed to use several representative examples to illustrate the effects of the physical constraints. The examples include a diffusion problem with imperfect modeling of the diffusivity and boundary conditions, a mechanical system with conservation of energy, a differential equation model with missing boundary layer transition, and a two-dimensional Navier–Stokes equations model with incompressibility constraint. Using extensive numerical tests, we demonstrate that the PCMC is an effective method to produce improved model predictions and performs better than the unconstrained model correction (UMC) which does not enforce the important physical constraints. We remark that by "better" we merely refer to the fact that PCMC is able to directly incorporate the physical constraints, if desired, into the prediction. Ultimately, the quality of a model should be judged by its predictability and how it compares against the ground truth. Just because one model incorporates certain physical constraints does not necessarily imply it has better predictability. How to judge the predictability of a model is, however, not the scope of this paper. Here we focus exclusively on the numerical implementations of the incorporation of the physical constraints, if one deems their incorporation necessary. Whether and how the incorporation of the physical constraints improves the model prediction is a problem dependent issue and should be decided prior to the model correction procedure.

This paper is organized as follows. In Section 2 we discuss the general forms of model correction. These include external model correction, internal model correction, and mixed model correction using both external and internal corrections. The physics constrained model correction (PCMC) is then presented in Section 3. Several representative examples of the physical constraints are discussed in Section 4. Then, in Section 5, we present extensive numerical tests for these representative systems and demonstrate the effectiveness of the PCMC framework.

2. Model correction

Throughout this paper, we use $M(x; p(x))$ to denote the simulation model. Here $x \in D$ is the coordinate in a physical domain, and $p(x)$ represents an important process embedded in the model. For example, it can be the diffusivity field of a diffusion model. For notational convenience, we do not include the time variable. This is done without loss of generality, as the incorporation of time is straightforward by introducing $(x, t) \in D \times [0, T]$ for some $T > 0$. Our numerical examples shall include a time dependent problem to demonstrate the applicability to time domain. We also restrict ourselves to the discussion of deterministic models.

We denote y^t the "true" (and unknown) output of the underlying physical system, and let

$$d = y^t + e, \tag{2.1}$$

be the observation data with noise e. Let $y = M(x; p)$ be the model output, we seek to construct a *corrected model* $\hat{M}$ such that it is a better approximation of the truth y^t. While there may exist a variety of ways to introduce model corrections, here we focus on the approaches that can be broadly classified as *external correction* and *internal correction*.

2.1. External model correction

In external model correction, we seek to introduce the correction terms outside the simulation model M. The most obvious approach is of additive type, that is,

$$\hat{M} = M(x; p) + \delta(x), \tag{2.2}$$

where $\delta(x)$ is the correction term, and $\hat{M}$ stands for the corrected model. This is the most widely used model correction form. For example, the well known Kennedy–O'Hagan method [8] takes this form.

One may also consider a multiplicative correction and seek

$$\hat{M} = \delta(x) M(x; p). \tag{2.3}$$

Obviously, the two can be combined into a more general form of external correction.

$$\hat{M} = \delta_m(x) M(x; p) + \delta_a(x), \tag{2.4}$$

where δ_m stands for the multiplicative correction factor and δ_a for the additive correction term.

2.2. Internal model correction

In internal model correction, we seek to "correct" the important internal modeling process $p(x)$, in order to improve the model prediction. The similar correction form used in the external correction, (2.4), can now be employed to the internal