Non-intrusive Reduced Order Modeling: Interpolating Parameterized Simulation Results

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Abstract

As the power and availability of computers has increased, the profile of simulation in scientific and engineering endeavors has risen. Computer simulations that model complex physical phenomena now regularly aid in decision-making and design processes. However, the complexity and computational cost of the codes often renders them impractical for design and uncertainty studies, where many runs at different input parameter values are necessary to compute statistics of interest. In such cases, one may employ *reduced order models* (ROMs) as a surrogate to the high fidelity simulation. The goal of the ROM is to accurately reproduce the gross features of the high fidelity model with significantly less computational effort. Typically, the ROM is constructed using a projection method on a relatively small set of high fidelity runs; variants of this idea include Galerkin projection methods with a reduced basis (computed with the proper orthogonal decomposition of a matrix of snapshots) or interpolation methods (e.g., stochastic collocation or Gaussian process models).

In this work, we present a reduced order modeling technique that combines the ease of implementation of the non-intrusive interpolation methods with the dimension reduction of the proper orthogonal decomposition. It is naturally applicable to nonlinear and time-dependent physical models, which cause problems for the Galerkin projection methods. From the singular value decomposition (SVD) of a matrix of parameter snapshots – where each column of the matrix contains the spatially varying time history of the physical field of interest – we obtain orthonormal basis vectors for the time/space domain and a sampling of unknown basis functions for the parameter domain. By using any standard interpolation method on the parameter basis functions (e.g., piecewise polynomial interpolation or radial basis functions), we construct a parameterized ROM for the time/space varying field of interest, which experience shows is computable with three orders of magnitude reduction in computational cost. The structured oscillations of the right singular vectors – which tend to become more oscillatory as the index increases – yield a metric for a truncated approximation; the negelected terms provide a time/space varying predictability measure[1] for the ROM. The predictability measure can be used as an importance sampling distribution for refining the ROM with more high fidelity runs.

To tackle the challenge of computing the SVD on a parameter snapshot matrix – which may contain terabytes of data – we employ a communication-avoiding tall, skinny QR factorization implemented on a MapReduce cluster. This approach leverages the scalable, fault-tolerant computing technologies of MapReduce – developed at Google for massive data queries – to construct the components of the ROM. The ROM is used to perform parameter studies such as uncertainty quantification, sensitivity analysis, and design optimization. We refer to this approach as *simulation informatics.*

We present the details of the method and demostrate its effectiveness on a large-scale, nonlinear, unsteady heat conduction model with uncertain material properties.

[1]This measure is similar to the prediction variance in Gaussian process models.