AN INFORMATION-THEORETIC MULTISCALE FRAMEWORK WITH APPLICATIONS TO POLYCRYSTALLINE MATERIALS

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Abstract

We considered the feasibility of utilizing High Dimensional Model Representation (HDMR) technique in the stochastic space to represent the model output as a finite hierarchical correlated function expansion in terms of the stochastic inputs starting from lower-order to higher-order component functions. HDMR is efficient at capturing the high-dimensional input-output relationship such that the behavior for many physical systems can be modeled only by the first few lower-order terms. An adaptive version of HDMR is developed to automatically detect the important dimensions and construct higher-order terms only as a function of the important dimensions. In this work, we also incorporate the newly developed adaptive sparse grid collocation (ASGC) method into HDMR to solve the resulting sub-problems. The efficiency of the proposed method is examined by comparing with Monte Carlo (MC) simulation.

Finally, we developed a unique data-driven strategy to encode the limited information on initial texture in deformation processes and represent it in a finite-dimensional framework. We have developed the ability to produce the probabilistic distribution of the macro-scale properties of the material subjected to a specific process induced by the uncertainty in initial texture.

1 Status of effort

We have made a significant progress in the third and last year of our project and built on our earlier success. Some key achievements in this year (not all reviewed in this report) are given below:

- Development of a non-linear model reduction strategy to construct stochastic input models of meso-scale topology variations based on limited data (emphasis on polycrystalline materials).

- Development of an adaptive hierarchical sparse grid collocation algorithm for stochastic partial differential equations.

- Development of a stochastic multiscale paradigm to address simultaneously the effects of randomness and multiscale nature of physical systems.

- Development of a stochastic optimization technique for robust design of deformation processes of polycrystalline metals.
- Development of a surrogate stochastic model for accelerating multiscale estimation in Bayesian inference approaches.
- Development of a maximum entropy approach for predicting macroscopic property variability induced by uncertainty in initial microstructure in deformation processes.
- Development of an HDMR framework for representing the input/output relation of complex systems in high-dimensions.

We will next briefly review only the last two items with additional details available in the relevant references.

1.1 An adaptive high dimensional stochastic model representation technique for the solution of stochastic partial differential equations

HDMR represents a function in high-dimensions in the following form:

$$f(\mathbf{Y}) = f_0 + \sum_{i=1}^{N} f_i(Y_i) + \sum_{1 \le i_1 < i_2 \le N} f_{i_1 i_2}(Y_{i_1}, Y_{i_2}) + \cdots + \sum_{1 \le i_1 < \cdots < i_s \le N} f_{i_1 \cdots i_s}(Y_{i_1}, \ldots, Y_{i_s}) + \cdots + f_{12\cdots N}(Y_1, \ldots, Y_N)$$

Here f_0 is the zeroth-order component function which is a constant denoting the mean effect. The first-order component function $f_i(Y_i)$ is a univariate function which represents individual contributions to the output f(Y). It is noted that $f_i(Y_i)$ is general a nonlinear function. The second-order component function $f_{i_1 i_2}(Y_{i_1}, Y_{i_2})$ is a bivariate function which describes the interactive effects of variables Yi1 and Yi2 acting together upon the output f(Y). The higher-order terms reflect the cooperative effects of increasing number of input variables acting together to impact f. The last term gives gives any residual dependence of all input variables cooperatively locked together to affect the output f(Y). Once all the component functions are suitably determined, then the HDMR can be used as a computationally efficient reduced-order model for evaluating the output. This is the same idea as the stochastic collocation method where we also obtain an approximate representation of f(Y).

In this work, the CUT-HDMR is adopted to construct the response surface of the stochastic solution. With this method, a reference point $\bar{\mathbf{Y}} = \left(\bar{Y}_1, \bar{Y}_2, \ldots, \bar{Y}_N\right)$ is introduced. The component functions of CUT-HDMR are explicitly given as follows

$$f_0 = f(\bar{Y}), \quad f_i(Y_i) = f(\mathbf{Y})|_{\mathbf{Y}=\bar{\mathbf{Y}}\setminus Y_i} - f_0$$

$$f_{ij}(Y_i, Y_j) = f(\mathbf{Y})|_{\mathbf{Y}=\bar{\mathbf{Y}}\setminus (Y_i,Y_j)} - f_i(Y_i) - f_j(Y_j) - f_0, \quad \ldots$$

The basic conjecture underlying HDMR is that the component functions arising in typical physical problems will not likely exhibit high-order cooperativity among the input variables such that the significant terms in the HDMR expansion are only those of low order. Therefore, it is expected that the HDMR expansion will converge very fast. For most well-defined physical systems, the first- and second-order expansion terms are expected to have most of the impact upon the output and the contribution of higher-order terms would be insignificant. However, the importance of higher-order terms in HDMR is problem-dependent. The exact effect in stochastic space from the input variability is unclear and this will be one of the focus points in this paper.

We have considered two issues related to adaptivity. At first the component functions are computed using the adaptive sparse grid collocation method (ASGC) [2]. The error in ASGC is controlled by the user based on the values of the hierarchical surpluses and hierarchical basis functions. The second level of adaptivity is to decide on the fly which component functions to compute. Note that for high-dimensional problems even the computation of all two-body terms is computationally very expensive. Rigorous error estimates have been derived and preliminary results are reported in [1]. In this work, we examined flow in random heterogeneous media and have reported examples of up to 500 random dimensions (note this is the highest stochastic dimension problem that is currently reported in the literature based on a non Monte Carlo based approaches).

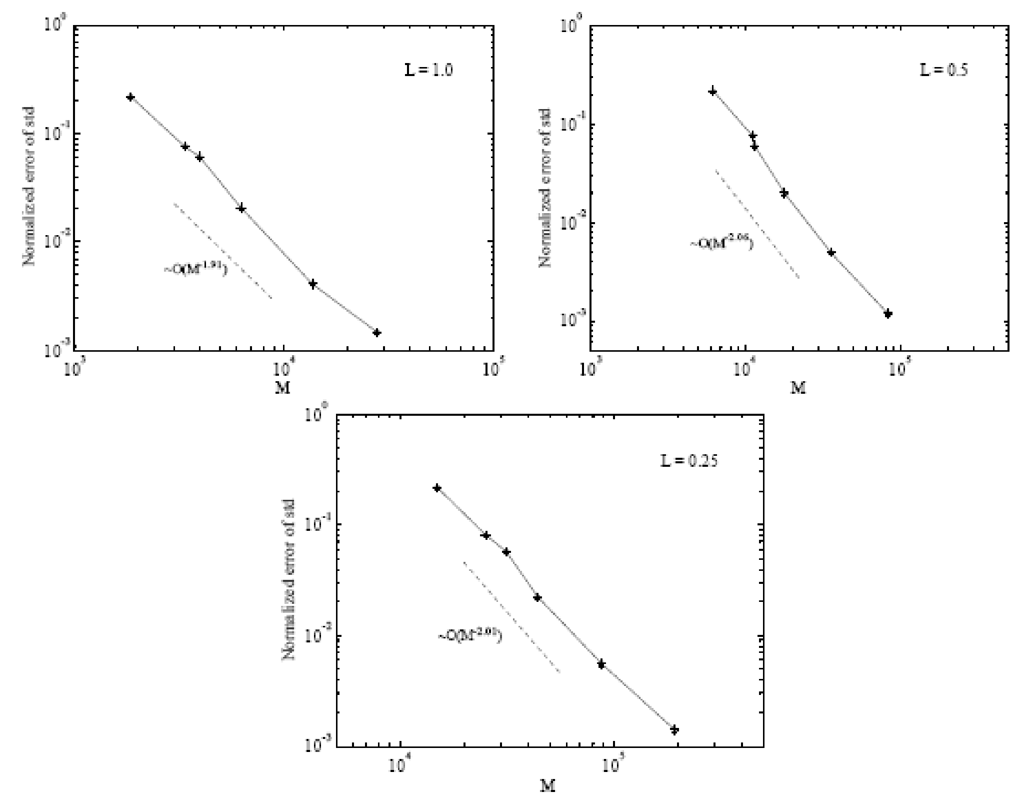

Figure 1. Convergence of the L_2 normalized errors of the standard deviation of the v

velocity-component for different correlation lengths, where $\sigma^2 = 1.0$ and $\theta_1 = 10^{-4}$versus the total number of collocation points. The problem here refers to flow(squared domain) in random media using an exponential kernel for the log-permeability (with high variability defined by $\sigma^2 = 1.0$) . The convergence plot here indeed exhibits algebraic rate. The parameter θ_1 is used to control the adaptive selection of the critical dimensions.

1.6 Predicting property variability of polycrystals induced by microstructural uncertainty: A maximum entropy approach [3]

The quantification and propagation of uncertainty in process conditions and initial microstructure on the final product properties in a deformation process were investigated. The stochastic deformation problem was modeled using the sparse grid collocation approach. The ability of the method in estimating the statistics of the macro-scale microstructure-sensitive properties and constructing the convex hull of these properties is shown through examples featuring randomness in initial texture and process parameters. A data-driven model reduction methodology together with a maximum entropy approach is used for representing randomness in initial texture in Rodrigues space. Comparisons are made with the results obtained from the Monte-Carlo method. In modeling the texture evolution, the random initial texture was represented as a random field. The available information on initial microstructure provided as a set of x-ray diffraction images is rarely enough to completely define the aforementioned random field. In this situation, one needs to resort to the maximum entropy approach in which the random field is constructed such that the entropy of the information it conveys is maximized. The method used in this work is fairly general and as the known information on the microstructure increases it can be easily incorporated in approximating the random field.

A stochastic framework is presented for obtaining the convex hull of properties obtained from a material subjected to uncertain process parameters and initial texture. This can be important for providing us with the means to quantify how well process conditions and microstructure need to be known to attain desired properties but also to identify risks (e.g. failure probabilities) affiliated with critical values of the material properties. To the best of our knowledge this is the first time these concepts have been explored in the analysis and design of polycrystalline materials. See Figures 2 and 3 for two particular results obtained from this work.

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References

[1] X Ma and N. Zabaras, An efficient high-dimensional stochastic model representation technique for the solution of stochastic PDEs, J. Comput. Physics, submitted.

[2] X. Ma and N. Zabaras, "An adaptive hierarchical sparse grid collocation algorithm for the solution of stochastic differential equations", Journal of Computational Physics, Vol. 228, pp. 3084-3113, 2009.
[3] B. Kouchmeshky and N. Zabaras, “The effect of multiple sources of uncertainty on the convex hull of material properties”, Acta Materialia, submitted.
[4] B. Ganapathysubramanian and N. Zabaras, "A non-linear dimension reduction methodology for generating data-driven stochastic input models", Journal of Computational Physics, Vol. 227, pp. 6612-6637, 2008.
[5] B. Ganapathysubramanian and N. Zabaras, "A seamless approach towards stochastic modeling: Sparse grid collocation and data driven input models", Finite Elements in Analysis and Design, Vol. 44, Issue 5, pp. 298-320, 2008.
[6] B. Ganapathysubramanian and N. Zabaras, "A stochastic multiscale framework for modeling flow through heterogeneous porous media", Journal of Computational Physics, Vol. 228, pp. 591-618, 2009.
[7] N. Zabaras and B. Ganapathysubramanian, "A scalable framework for the solution of stochastic inverse problems using a sparse grid collocation approach", Journal of Computational Physics, Vol. 227, pp. 4697-4735, 2008.
[8] V. Sundararaghavan and N. Zabaras, “A multilength scale continuum sensitivity analysis for the control of texture-dependent properties in deformation processing”, International Journal of Plasticity, Vol. 24, pp. 1581-1605, 2008.
[9] X. Ma and N. Zabaras, “An efficient Bayesian inference approach to inverse problems based on adaptive sparse grid collocation method”, Inverse Problems (Institute of Physics), Vol. 25, 035013 (27pp), 2009.

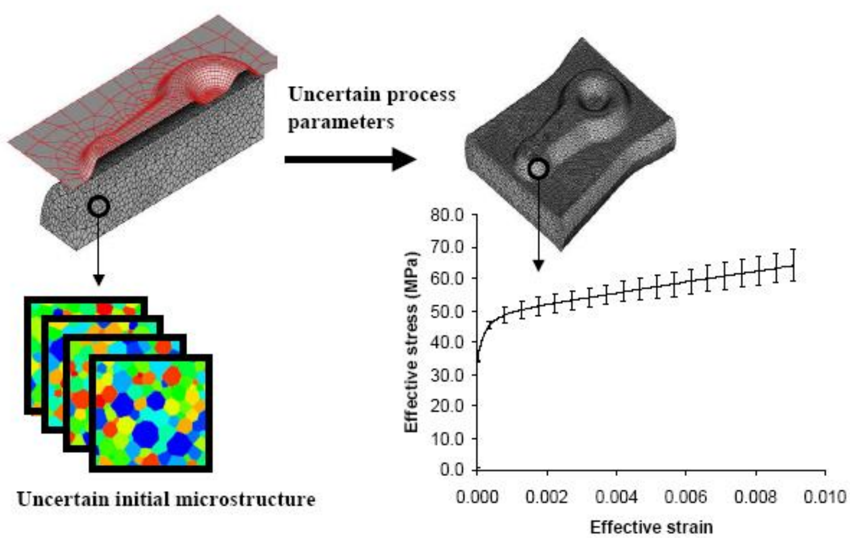

Figure 2: Schematic view of the effects of uncertainty in initial texture on the final material properties. The error bars on the effective stress/strain response at a material point shown are due to the uncertainty in initial texture and variability in processing. (bottom).While these calculations are at a material point of a polycrystal, they pave the way for computing the property variability in a workpiece during processing induced from lack of information on the microstructure of the initial workpiece.

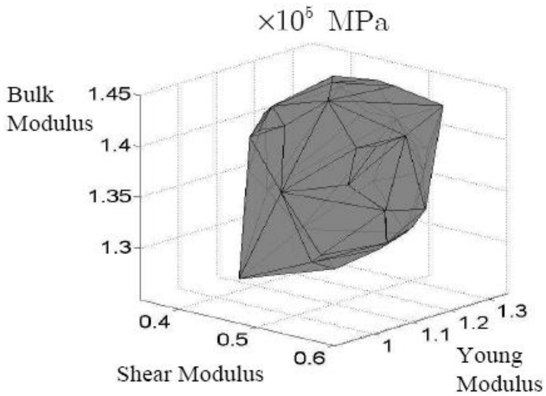

Figure 3: The convex hull of Bulk modulus, shear modulus and Young modules for an FCC polycrystal obtainable in tension for random initial texture (uncertainty driven by data). Extremal properties can be indentified together with the affiliated probabilities. These unique ideas are very important not only for design under uncertainty but also for failure prediction from extremal scenarios.

Personnel Supported During Duration of Grant

N. Zabaras (PI), X. Ma, B. Ganapathysubramanian (now Assistant Professor, ISU, Ames, Iowa), B. Kouchmeshky and K. Mathew (GRAs supported in part) Affiliation: Cornell University.

Publications

As listed in the references

AFRL Point of Contact

This work is being communicated with the group of Dr. J. Simmons, AFRL/MLLM.

New Discoveries

(a) Develop an HDMR framework to address the high-dimensionality of stochastic PDE systems, (b) Non-linear reduced order model that could capture correlations in non-linear spaces and efficiently represent/process information of complex structures, (c) developed a hierarchical adaptive sparse-grid collocation scheme that captures the crucial stochastic dimensions and thus solve problems which were earlier infeasible, (d) developed a variational stochastic multiscale framework for material systems, (e) developed a non-intrusive (collocation) framework for design of complex systems under uncertainty and applied it to the design of deformation processes of polycrystalline materials, (f) used the adaptive sparse grid collocation solver as a surrogate model for accelerating multiscale Bayesian inference approaches and finally (g) developed a maximum entropy based framework for predicting the effects of uncertainty in initial texture on macroscopic property variability in deformation processes of polycrystalline materials.