Abstract

The effect of diverse sources of uncertainties and the intrinsically multi-scale nature of real-world physical systems poses a considerable challenge to analyze such systems. Such phenomena are particularly critical in material systems wherein microstructural variability and randomness at lower scales have a significant impact on the behavior of the system. Towards this goal, some of our accomplishments over the last year include the development of an adaptive sparse grid collocation technique for multiscale systems, development of a stochastic variational multiscale framework and developing tools for robust design for deformation processes. In our adaptive hierarchical sparse-grid framework, we developed a technique that constructs the stochastic collocation points based on the function being represented, thus avoiding the computational overhead associated with superfluous collocation points. We derived a multiscale stochastic framework that can resolve the stochastic and multiscale components of a system simultaneously. A stochastic analogue of the mixed multiscale finite element technique using concepts from adaptive sparse grid collocation was employed for the same. We have also developed a methodology to incorporate topological uncertainties in microstructures using a non-linear data-driven model reduction technique. This framework seamlessly allows for accessing the effects of microstructural variability on the reliability of macro-scale systems. In addition, we recently applied the adaptive sparse-grid collocation scheme for the design of general processes under uncertainty including the robust design of deformation processes of polycrystalline materials.

1 Status of effort

We have made a significant progress in the second year of our project and built on our success in the first year. Some key achievements in this year 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.
- 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.

Some of our contributions are summarized below while additional details are available in the relevant references.

Figure 1: The figure depicts the standard deviation of temperature profile across a random composite microstructure due to its topological uncertainty. A temperature gradient is applied across the left and right end of the microstructure. The figure shows (a) standard deviation contours within the microstructure (b) standard deviation isosurfaces (c) temperature pdf at a point and (d-f) standard deviation slices

1.1 Data-driven methodology to construct stochastic input models of meso-scale topological/property variations [1]

The importance of performing stochastic analysis on heterogeneous media necessitates the development of realistic input models of the microstructural features. The thermal, mechanical and chemical behavior of microstructures is highly anisotropic and heterogeneous, depending on the randomness of features of importance. For instance, orientation of the crystals as well as the nature of the grain boundaries represents sources of randomness in polycrystalline materials. Knowledge of the topology/property variation of say, a polycrystalline material is usually known only in a statistical (or averaged) sense (in terms of say, grain size distribution and the texture map). To provide reliable failure criteria for critical applications involving such materials, it becomes imperative to access this variability in properties, quantify it and predict its effect on the performance of the system. In a recent paper [1], we have developed a framework for reduced-order stochastic representation of the property variation. Ideas from differential geometry are used to show that the space is a compact manifold embedded in a high-dimensional input space. The main advantage of this work lies in the efficiency in which complex models can be represented using the non-linear model-reduction technique. While traditional linear model reduction techniques can capture only linear correlations in the microstructural data, the technique we developed can perform significantly better. For the
Ag-W composite microstructure shown in Fig.1, the non-linear model reduction technique required just nine dimensions for representation whereas the linear model reduction required around 70 dimensions to represent the same. Furthermore, the generation of a low-dimensional surrogate space has major ramifications in the optimizing of properties-processes and structures, making complicated operations like searching, contouring and sorting computationally much more feasible.

Figure 2: The figure shows (2.1) representation of a line singularity function using the adaptive sparse grid collocation scheme and (2.2) the u- and v-velocity profiles for the Rayleigh-Bernard instability problem[3] using the adaptive sparse grid collocation scheme (top) and its comparison with the corresponding Monte-Carlo solutions.

1.2 Hierarchical adaptive framework for analysis of stochastic PDEs [2][3]

In the first year of our grant, we had come up with a stochastic collocation technique for analysis of stochastic PDEs that approximates the solution in the stochastic space using Lagrange polynomial interpolation[2]. The collocation method requires only repetitive calls to an existing deterministic solver similar to the Monte Carlo method and performed better than pre-existing spectral techniques when the number of random dimensions is high. However, both the SSFEM (stochastic spectral finite elements) and sparse grid collocation methods utilize global polynomials in the stochastic space. In the presence of steep gradients or finite discontinuities in the stochastic space, these methods converge very slowly or even fail to converge. Recently[3], we developed an adaptive sparse grid collocation strategy using piecewise multi-linear hierarchical basis functions wherein the concept of hierarchical surplus is used as an error indicator to detect regions of discontinuities in the stochastic space. The basic idea in this methodology is to efficiently capture only the important stochastic dimensions which are usually far lesser than the actual number of random dimensions. We found that utilizing this method, we could tackle very high stochastic dimensional problems (Ref.[3] wherein we have depicted its application on a 75-dimensional problem). Figure 2 shows some of our recent work in this area.
1.3 Decoupled stochastic multiscale framework [4]

Extending on our adaptive sparse grid collocation technique, we developed a stochastic variational multiscale formulation to incorporate uncertainties in multiscale material systems. In this scheme, a stochastic analogue to the mixed multiscale finite element framework is used to formulate the physical stochastic multiscale process. For the effective resolution of the multiscale problem, the solution was split using an additive decomposition into its coarse scale and fine scale parts. We employ the local conservation assumption through which we convert the global sub-grid problem into a set of local sub-grid problems. This is the first time that a multiscale variational technique has been applied for stochastic PDEs.

In [4], we applied this framework to analyze flow through random heterogeneous media when only limited statistics about the permeability variation are given. Linear and non-linear model reduction techniques are used to convert the limited information available about the permeability variation into a viable stochastic input model. An adaptive sparse grid collocation strategy is used to efficiently solve the resulting stochastic partial differential equations. However, our mathematical developments in this context are very generic in nature and can be easily extended to other applications. Fig. 3 shows the effect of uncertainty in multiscale permeability on the flow through the porous medium.

![Figure 3: The figure shows data-driven modeling employed to compute the effect of localized uncertainty in multiscale permeability.](image)

1.4 Robust design of polycrystalline materials [5][6]

In our earlier works [6], we have reported formulations for design of metal forming processes using the continuum sensitivity method (CSM). Recently, we have extended this technique to perform design in the presence of uncertainties using a stochastic optimization scheme. The design variables are allowed to be random functions and the sensitivities of the PDF of a field variable due to infinitesimal perturbations to the PDF of the random design variables are computed. The task of optimizing a complex process becomes increasingly complicated in the presence of multiscale uncertainties arising either as boundary conditions or variations in material properties. We have recently developed a novel collocation based decoupled stochastic optimization scheme that
significantly reduces the computational effort necessary to perform such complex control and optimization problems [5]. This framework is based on the efficient computation of the stochastic sensitivity using parallel sparse grid collocation schemes.

In large deformation manufacturing processes such as forging, it is necessary to ensure that the quality of the final product is good as well as the cost involved in the production of the product is minimized. A number of diverse sources of uncertainties such as friction coefficient, forging velocity and initial preform shape might affect the quality of the final product. Further, these processes are governed by constrained stochastic partial differential equations. The objective (quality of the final product) is to minimize flash (material wastage) and to maximize the fill of the die under the uncertain conditions that the deformation process is subject to. Fig. 4 illustrates the robust design technique applied to a forging process due to uncertainties in forging velocity.

![Figure 4](image)

**Figure 4:** The figure depicts robust design of a forging process to obtain better quality product (minimizing flash and underfill) under uncertain forging velocity. Fig. (a) shows the reduction of the mean objective function using the stochastic optimization scheme. Fig. (b) shows the final shape of workpiece at the left tail of the forging velocity (0.09 mm/s), (c) shows the final shape at the right tail of the forging velocity (0.11 mm/s) and (d) shows the final mean shape of the workpiece.

**Acknowledgment/Disclaimer**

This work was sponsored by the Air Force Office of Scientific Research, USAF, under grant/contract number FA9550-07-1-0139. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of the Air Force Office of Scientific Research or the U.S. Government.
References


Personnel Supported During Duration of Grant

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Publications
As listed in the references

Honors & Awards Received

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

Transitions

New Discoveries
(a) Non-linear reduced order model that could capture correlations in non-linear spaces and efficiently represent/process information of complex structures, (b) developed a hierarchical adaptive sparse-grid collocation scheme that captures the crucial stochastic dimensions and thus solve problems which were earlier infeasible, (c) developed a variational stochastic multiscale framework for material systems and (d) 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.