AN INFORMATION-THEORETIC MULTISCALE FRAMEWORK WITH APPLICATIONS TO POLYCRYSTAL MATERIALS

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Abstract

Modeling of uncertainty propagation in multi-scale models of deformation is extremely complex considering the nonlinear coupled phenomena that need to be accounted for. The ongoing work addresses key mathematical and computational issues related to robust control of microstructure-sensitive properties in deformation applications. Our research accomplishments for this year include development of new mathematical models based on adaptive collocation methods and spectral polynomial chaos for modeling propagation of uncertainties in material processes. We have developed a novel methodology to incorporate mesoscale topological uncertainties using a non-linear data-driven model reduction technique. This framework- which constructs stochastic input models of the topological variability based on limited information- seamlessly allows for accessing the effects of microstructural variability on the reliability of macro-scale systems. We have developed the first fully decoupled stochastic variational multiscale simulator based on the seamless coupling of proven deterministic multiscale models and adaptive stochastic collocation based algorithms. We have developed the first fully decoupled stochastic optimization framework. This framework is based on stochastic sensitivities that are computed in a decoupled manner, significantly enhancing the computational efficiency of the optimization procedure. This framework coupled with the non-linear data-driven stochastic input model generation framework is a powerful tool in the design and control of microstructural properties in the presence of multi-length scale uncertainties.

1 Status of effort

Substantial progress has been made in the achievement of the project objectives within the first year of this project. Key developments for the first year are listed below:

- Development of an adaptive stochastic collocation framework to access the effects of uncertainty propagation.
- Development of a non-linear data-driven methodology to construct stochastic input models of meso-scale topology variations based on limited data.
- Development of a fully decoupled stochastic multiscale framework.
- Development of a stochastic optimization framework using sparse grid collocation techniques.

Particular contributions are briefly summarized below with more details given in the provided references.

1.1 Adaptive framework for analysis of stochastic PDEs [1,3]

We have developed two methodologies based on a collocation approach for solving stochastic PDEs. The first algorithm is based on a finite element representation of the support space of random variables. This approach, called Non-Intrusive Stochastic Galerkin (NISG) method, was presented in [1]. The technique can be directly applied to deterministic software with minimal effort for computing the complete PDF of the stochastic process. NISG approach involves FEM discretization of the random support space and piecewise continuous interpolation of the PDF over the support space with deterministic function evaluations at integration points. For the large deformation problems considered with varying levels of randomness in the input and boundary conditions, the NISG method was found to provide highly accurate estimates of the statistical quantities of interest within a fraction of the time required using existing Monte Carlo methods. The developed scheme for discretization of the stochastic support space closely follows the FEM discretization of spatial domains in various applications and inherits all its properties. The h and p convergence characteristics of the discretized domain are identical to the case of spatial finite elements.

When a tensor product rule is used to interpolate the variables in stochastic space, the number of realizations required to build the interpolation scheme increases as power of the number of random dimensions. We recently developed a methodology using the Smolyak algorithm to build sparse grid interpolants in large dimensional space [3]. The Smolyak algorithm provides a way to construct interpolation functions based on a minimal number of points in multi-dimensional space. Using this method, interpolation schemes can be constructed with orders of magnitude reduction in the number of sampled points to give the same level of approximation (up to a logarithmic factor) as interpolation on a uniform grid. An extension of the collocation approach to include adaptive refinement in important stochastic dimensions is utilized to further reduce the numerical effort necessary for simulation. This dimension dependant adaptivity is incorporated by automatically detecting the underlying structure (i.e. additive, nearly-additive, anisotropic, discontinuous) of the stochastic solution. We were able to show the significant computational gains of the developed methodology over other conventional uncertainty representation schemes in our recent paper [3]. This methodology has been shown to accurately capture equilibrium shifts and efficiently scale to a large number of stochastic dimensions. This work further provides a road map to convert any deterministic code to include the effects of input uncertainty in a non-intrusive manner utilizing the adaptive sparse grid collocation method.

1.2 Data-driven methodology to construct stochastic input models of meso-scale topological/property variations [2, 6]

Stochastic analysis of heterogeneous media provides information of significance only if realistic input models of the property variations are used. The thermal and elastic properties of polycrystals are highly anisotropic and heterogeneous, depending on the local orientation of the crystals as well as the nature of the grain boundaries separating the crystals. Knowledge of the topology/property variation of 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. Our recent paper [6] proposes a framework to construct such input stochastic models using a data-driven strategy. Given only some statistical information about the property distribution (like two-point correlation functions and size distribution functions), the framework constructs a reduced-order stochastic representation of the property variation. This problem of constructing low-dimensional stochastic representations of property variation is analogous to the problem of manifold learning and parametric fitting of hyper-surfaces encountered in image processing and psychology. A non-linear dimension reduction strategy is utilized to map the space of viable property variations to a low-dimensional region. Ideas from differential geometry are used to show that the space is a compact manifold embedded in a high-dimensional input space. An isometric mapping from this high-dimensional space to a low-dimensional, compact, connected set is constructed. This mapping serves as an accurate, low-dimensional, data-driven representation of the property variation. Asymptotic convergence of the representation of the property variation in the mesoscale using this low-dimensional descriptor is shown [6]. The framework is shown to work exceedingly well in constructing models of various property variations. The reduced-order model of property variation is subsequently used as an input in the solution of stochastic PDEs that describe the evolution of dependant variables (like temperature, stress, velocity). Fig. 1 shows a brief schematic of the developed methodology- starting from an image of the microstructure, a reduced order stochastic input model of the topological variation is constructed.

The basic model reduction ideas envisioned in this work are not limited to generation of viable stochastic input models of property variations. This framework has direct applicability to problems where working in high-dimensional spaces is computationally intractable, for instance, in visualization of property evolution, extracting process-property maps in low-dimensional spaces, among others. 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.

1.3 Decoupled stochastic multiscale framework based on collocation strategies [4]

The design and control frameworks envisioned in this proposed work must satisfactorily deal with some important issues related with the multi-length scale property/phenomena arising in the analysis of polycrystalline materials coupled with the corresponding uncertainties at each scale. Conventional analysis treat each of these twin issues—(i) the multi-scale nature of property and process interaction, and (ii) the effect of uncertainties in each scale of analysis arising from limited information and aleatory effects – separately without considering the corresponding (possibly essential) interacting effects.

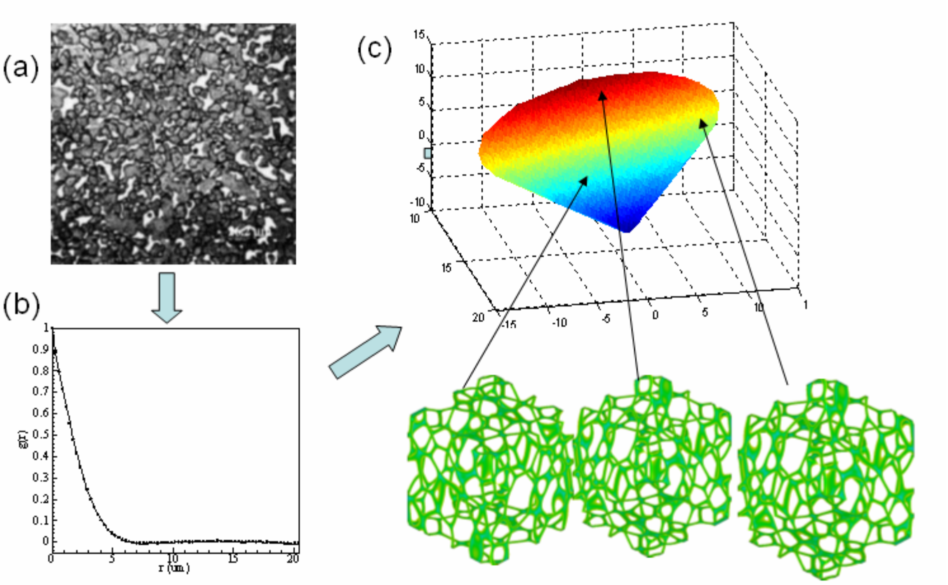

Fig. 1 (a) Experimental image of microstructure (b) Statistics extraction and reconstruction of multiple plausible 3D microstructures (c) The reduced order stochastic model of the topological variability. Each point represents a unique microstructure.

We recently developed a highly efficient stochastic multiscale framework for solving the twin issues raised above [4]. A decoupled scheme is used to tackle the problems of stochasticity and multi-length scale variations in properties. A sparse-grid collocation strategy is utilized to reduce the solution of the stochastic PDE to a set of deterministic problems. A variational multiscale method with explicit subgrid modeling is used to solve these deterministic problems. The proposed methodology seamlessly ties together three distinct aspects of realistic modeling of complex systems, namely (i) a general methodology for generating data driven models of material and topological variations for use as stochastic inputs, (ii) a general decoupled methodology for accessing the effect of these input uncertainties on the complex system, and (iii) a multi-scale methodology for upscaling the effects of fine scale features of the system. This is the first time that a robust methodology has been developed that seamlessly merges all these various aspects of analyses: from developing a data-driven model for generating inputs to a stochastic (multiscale) framework with an ultimate goal obtaining the probability distribution of the physical fields that arise from the randomness of the topology and properties of the underlying medium. The other attractive feature of this framework is the ability to seamlessly mesh with any deterministic multiscale framework, thus opening up potentially huge areas of significant analysis. Fig. 2 illustrates the use of the developed framework in accessing the variability in the thermal evolution of a heterogeneous media due to the uncertainties in the underlying microstructure.

1.4 Stochastic optimization framework using sparse grid collocation techniques [7]

In previous developments, we have reported formulations for stochastic optimization of metal forming processes based on the continuum stochastic sensitivity method (CSSM). The CSSM is an extension of our continuum sensitivity method (CSM) in the context of

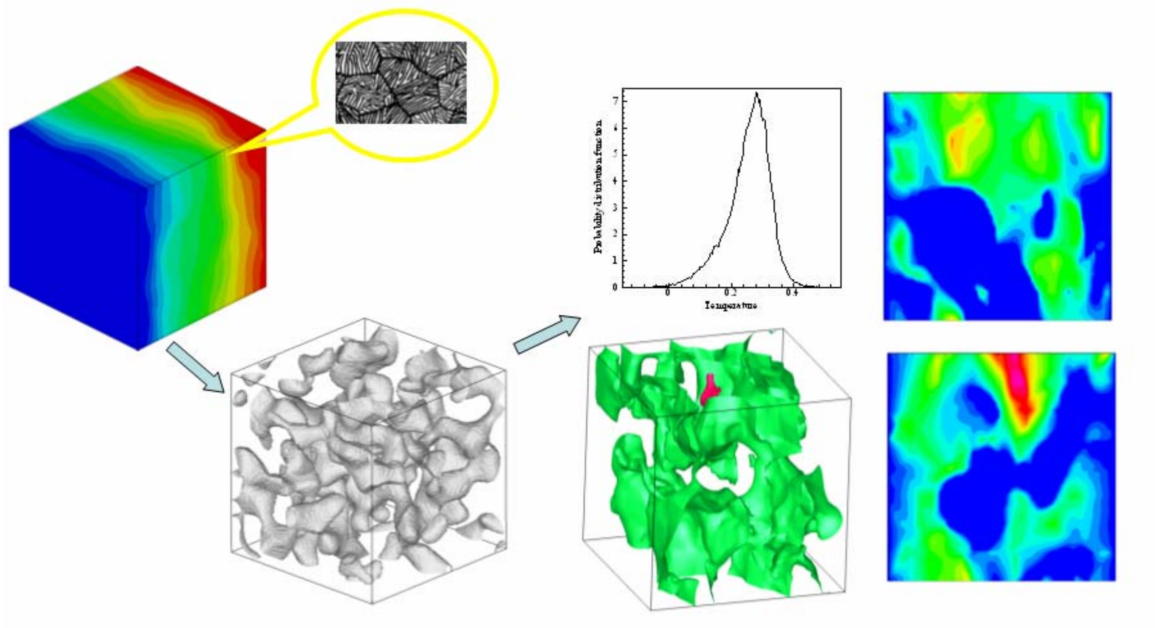

Fig. 2 Stochastic multiscale framework: In the first step the stochastic problems is reduced to the solution of multiple deterministic problems. Each deterministic problem is solved using a multiscale framework. The figure on the right plots the resulting distribution (higher moments) of the field variable due to meso-scale uncertainties.

deterministic deformation processes. The objective of the stochastic optimization scheme is to undertake (robust) process design in the presence of uncertainty. The design variables are allowed to be random functions. In the context of stochastic processes, the sensitivity of a random field is defined as the change in the PDF of the field variable as a result of infinitesimal perturbations to the PDF of the random design variables. 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 [7]. This framework is based on the efficient computation of the stochastic sensitivity using parallel sparse grid collocation schemes. The gradients with respect to collocated values of the design variables are defined using appropriate stochastic sensitivity problems. The implementation requires minimum intrusion into existing deterministic solvers and it is thus applicable to a variety of problems. We are currently applying this framework for the efficient stochastic optimization of metal forming processes.

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References

[1] S. Acharjee and N. Zabaras, "A non-intrusive stochastic Galerkin approach for modeling uncertainty propagation in deformation processes", Computers and Structures Vol. 85, Issues 5-6, pp. 244-254, 2007.

[2] S. Sankaran and N. Zabaras, "Computing property variability of polycrystals induced by grain size and orientation uncertainties", Acta Materialia, Vol. 55, Issue 7, pp. 2279-2290, 2007.

[3] B. Ganapathysubramanian and N. Zabaras, "Sparse grid collocation methods for stochastic natural convection problems", Journal of Computational Physics, Vol. 225, pp. 652-685, 2007.

[4] B. Ganapathysubramanian and N. Zabaras, "Modelling diffusion in random heterogeneous media: Data-driven models, stochastic collocation and the variational multi-scale method", Journal of Computational Physics, in press

[5] N. Zabaras and S. Sankaran, "An information-theoretic approach to stochastic materials modeling", IEEE Computing in Science and Engineering (CiSE), special issue of "Stochastic Modeling of Complex Systems", pp. 50-59, 2007.

[6] B. Ganapathysubramanian and N. Zabaras, "A non-linear dimension reduction methodology for generating data-driven stochastic input models", J. Comp. Physics, submitted.

[7] N. Zabaras, S. Sankaran and B. Ganapathysubramanian, "An efficient approach to stochastic sensitivity analysis using a sparse grid collocation scheme", J. Comp. Physics, in preparation.

Personnel Supported During Duration of Grant

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Publications

As listed in the references.

Honors & Awards Received

ASME Fellow—awarded 2006

AFRL Point of Contact

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

Transitions

While no immediate commercialization plans are in place for the developed computational mathematics technologies, we strongly believe that their transition to immediate needs of AFRL and industrial partners is forthcoming.

New Discoveries

(a) A novel model reduction strategy to incorporate meso-scale uncertainties was developed. (b) The first fully decoupled stochastic multiscale framework was developed (c) A highly efficient stochastic optimization framework is under current development.