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A framework for data-driven analysis of materials under uncertainty: countering the curse of dimensionality

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Abstract

A new data-driven computational framework is developed to assist in the design and modeling of new material systems. The proposed framework integrates three general steps: 1) design of experiments, where the input variables describing material geometry (microstructure), phase properties and external conditions are sampled; 2) efficient computational analyses of each design sample, leading to the creation of a material response database; and 3) machine learning applied to this database to obtain a new design or response model.

In addition, the authors address the longstanding challenge of developing a data-driven approach applicable to problems that involve unacceptable computational expense when solved by standard analysis methods – e.g. finite element analysis of representative volume elements involving plasticity and damage. In these cases the framework includes the recently developed "self-consistent clustering analysis" method in order to build large databases suitable for machine learning. The authors believe that this will open new avenues to finding innovative materials with new capabilities in an era of high-throughput computing ("big-data").

Keywords: design of experiments, reduced order model, self-consistent clustering analysis, machine learning and data mining, plasticity

1. Introduction

Structural and materials design is a highly iterative process where one seeks an optimal design for chosen quantities of interest. Even the simplest structures and materials are composed by multiple building blocks that can be combined in a large number of possibilities. These building blocks together with the range of boundary conditions applied to the material/structure can lead to drastically different optimal designs.

For the particular case of material systems design, the high-dimensionality of the engineering design space is particularly striking when considering the overwhelming amount of possible combinations that lead to different materials. Meyers *et al.* [1] examined the extraordinary diversity in biological materials that are often composed of weak constituents assembled in complex structures with radically different macroscopic mechanical properties. Jang *et al.* [2] designed three-dimensional hollow ceramic nanostructures inspired by the observation of biological structures with hierarchical arrangements of basic structural elements. Wang et al. [3] explored the design of elastic beam elements attached to an elastomeric core matrix to obtain a metamaterial with intriguing acoustic properties. Other examples can be encountered in investigations on the influence of nano- and micro-reinforcements on the behavior of elastomers [4, 5, 6], polymeric foams [7], metal matrix composites [8], and the effect of fiber hybridization in polymer matrix composites [9, 10].

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