

REDUCED ORDER MULTISCALE MODELING  
OF NONLINEAR PROCESSES  
IN HETEROGENEOUS MATERIALS

Abstract

by

Satyaki Bhattacharjee

Predicting effective material properties of nonlinear heterogeneous materials from the knowledge of its micro-structure through numerical modeling and computational homogenization (CH) has many applications in engineering design. Direct numerical modeling (DNM) using finite element method (FEM) is capable of predicting material behavior accurately. Unfortunately, DNM and/or CH are computationally expensive methods. To address the computational complexity issue, many researchers have focused on reduced order modeling. However, most of the available schemes are only suited for linear and moderately nonlinear behavior in 2D setting. Moreover, these techniques do not preserve local micro-scale fields in localization processes and cannot accommodate generic loading conditions.

Addressing these shortcomings, this doctoral work presents a robust reduced order modeling technique for heterogeneous materials with nonlinear hyper-elastic constitutive behavior in a finite strain setting. The model is not only capable of predicting homogenized (overall) material properties, but also recovers the micro-fields (i.e., the local deformation gradients) with acceptable accuracy. In the present work, a novel manifold based reduced order model has been developed for nonlinear hyperelastic materials utilizing advanced machine learning techniques. This data-driven model can perform well in comparison with traditional CH.

Proposed technique extracts the pattern in the solution manifold, which consists of an ordered set of micro-scale deformation fields. Each point on the manifold represents data obtained from a detailed parallel finite element simulation of a representative micro-structure. Since essential micro-fields are invariant of macro-rotations, the parameter space is created based on the macro-scale stretch tensor, which is parameterized by three principal stretches and three rotation parameters which represent the corresponding principal directions. This parametrization leads to a 6-dimensional loading space. Also a novel pattern/physics based sampling strategy has been introduced to construct a representative solution manifold with a few number of simulations. This graph-based technique essentially explores the rotational (principal direction) sensitivity (in terms of an approximate diameter of the submanifold) of the principal stretch vector with a few number of FE solutions and guides to achieve a representative HD manifold by eliminating the redundant expensive simulations. In this work, a global dimension reduction technique, Isomap, is used to understand the underlying pattern of the submanifolds. Isomap returns a reduced low-dimensional Euclidean space which approximately unfolds the HD manifold by preserving the geodesic distances. Next, a map between the reduced space and the macroscopic loading conditions has been established using a Neural Network. Finally, the micro-scale deformation field is obtained through a nonparametric regression model by exploiting the concept of reproducing kernel Hilbert space (RKHS).

This novel reduced order model is able to predict the macro-scale as well as micro-scale deformation field for any unknown loading condition without any expensive simulation. Furthermore, this model potentially can accelerate the traditional CH by providing an initial solution vector.