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Multiscale modeling using goal-oriented adaptivity and numerical homogenization. Part I: Mathematical formulation and numerical results

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ABSTRACT

This paper is the first in this series to develop a numerical homogenization method for heterogeneous media and integrate it with goal-oriented finite element mesh adaptivity. We describe the physical application, Step and Flash Imprint Lithography, in brief and present the mathematical ideas and numerical verification. The method requires the Moore–Penrose pseudoinverse of element stiffness matrices. Algorithms for efficiently computing the pseudoinverse of sparse matrices will be presented in the second paper.

The purpose of numerical homogenization is to reduce the number of degrees of freedom, find locally optimal effective material properties, and perform goal-oriented mesh refinement. Traditionally, a finite element mesh is designed after obtaining material properties in different regions. The mesh has to resolve material discontinuities and rapid variations in the solution. In our approach, however, we generate a sequence of coarse meshes (possibly 1-irregular), and homogenize material properties on each coarse mesh element using a locally posed constrained convex quadratic optimization problem. This upscaling is done using the Moore–Penrose pseudoinverse of the linearized fine-scale element stiffness matrices, and a material-independent interpolation operator.

Numerical verification is done using a two dimensional conductivity problem with known analytical limit. Finally, we present results for two and three dimensional geometries. The results show that this method uses orders of magnitude fewer degrees of freedom to give fast and approximate solutions of the original fine-scale problem.

1. Introduction

Step and Flash Imprint Lithography (SFIL) is an imprint lithography process designed to transfer circuit patterns to fabricate microchips in low-pressure and room-temperature environments [1–3]. Photopolymerization is the main process to create polymeric patterns on a substrate. It is accompanied by densification which affects the shape of imprinted features [4].

In this research, we are interested in the post-polymerization step of the SFIL process. The object of interest is a heterogeneous glassy polymeric structure created on an organic polymer layer which in turn is on a silicon substrate. The structure is modeled as monomers interacting with pair-potentials with neighbors in a lattice. An equilibrium configuration is found by minimizing the energy of the lattice. Numerical solution of such a molecular statics fine-scale base model is computationally very expensive due to the problem size, which is on the order of millions of degrees of freedom (DOFs). Rapid variation in material properties, ill-conditioning, nonlinearity, and non-convexity make this problem even more challenging to solve.

Typical dimensions of the patterns in the structure are much larger than individual molecules, but the discreteness plays an important role in modeling of such objects. In the context of SFIL, an approach for coupling of discrete polymer elasticity models with continuum hyperelasticity models has been presented in [5,6].

Our objective is to approximate a nonlinear base model of the polymeric structure (based on molecular statics) by local numerical homogenization of fine-scale material properties and use goal-oriented adaptivity to change the models spatially. Before presenting the local numerical homogenization method, we give a brief review and background of multiscale methods and mesh adaptivity.

1.1. Multiscale methods and numerical homogenization

The desire to capture fundamental or more accurate small-scale models into large-scale models has given rise to the field of multiscale methods [7]. Such methods find the approximate solution on a coarse mesh but use the fine mesh to construct the relevant

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information. The numerical techniques allow us to avoid the assumption of periodicity that is typically used in the analytical techniques of homogenization.

Hughes et al. use concepts of variational multiscale and residual-free bubbles to resolve the fine-scales [8,9]. Engquist et al. use wavelet basis to compute effective homogenized operators and use truncation for a sparse approximation [10,11]. Hou et al. compute operator-dependent basis functions by solving local auxiliary problems [12]. For two-phase flow in porous media, a numerical upscaling technique based on the assumption that net flux between coarse elements occurs only on the coarse-scale has been introduced by Arbogast [13]. In [14], Knapek introduced operator-dependent interpolation in the context of multigrid methods. Feyel and Chaboche do a micromacro analysis to compute solutions of multiscale problems without using closed-form macroscopic constitutive equations [15].

Voigt [16] and Reuss [17] were pioneers in analyzing effective elastic properties of heterogeneous continuum materials. However, both made completely different assumptions in simplifying the heterogeneity. Voigt assumed a uniform strain field which led to an averaging of the elasticity tensor. Reuss assumed a uniform stress field instead which resulted in an averaging of the compliance tensor (inverse of the elasticity tensor). Both are imperfect assumptions. Voigt's assumption results in statically inadmissible stress fields and Reuss's assumption leads to kinematically inadmissible strain fields [18]. Our method cannot be classified as being one of these two methods, but it closer to the Reuss's assumption. We linearly transform the inverse of the fine scale element stiffness matrix to compute the inverse of the coarse scale element stiffness matrix. The inverse of the coarse scale element stiffness matrix is then inverted to assemble the coarse global system. However, we always maintain the kinematic constraints because the degrees of freedom are consistent across adjacent elements.

1.2. Mesh adaptivity and error estimation

Critical to the accuracy, reliability and mesh adaptivity in finite element methods is existence of good *a posteriori* error estimates. Such estimates not only provide confidence in the solution on the current mesh but also indicate elements to be refined further for an automatic refinement strategy. Use of effective automatic refinement algorithms is essential to obtain an accurate solution of problems in complex domains.

Many researchers have contributed to the vast field of *a posteriori* error estimation and mesh refinement. For a comprehensive introduction and analysis of various methods, we refer to the monographs by Babuška and Strouboulis [19] and by Oden and Ainsworth [20].

For many applications, interest is restricted to part of the full domain or a goal represented by a functional of the solution. Usually, in the context of linear problems, the goal is a bounded linear functional on the Hilbert space containing the solution. Many algorithms have been developed for optimizing the mesh for reducing the error in a given quantity of interest rather than in some energy norm. Such algorithms provide the basis for the so-called goal-oriented adaptivity. The main tool behind such algorithms is characterization of the error in the goal in terms of the solution of the adjoint problem (which is driven by the goal). Amongst others, this approach was taken by Becker and Rannacher [21] and Oden and Prudhomme [22].

1.3. Overview of this work

We develop and implement a framework for numerical homogenization and goal-oriented adaptivity for nonlinear lattice elasticity problems. It is developed with the polymer base model of SFIL in mind, but is quite general and can be applied to continuum problems with a given fine mesh that sufficiently resolves the fine-scale material properties.

The main research contribution lies in mathematical development and efficient software implementation of local numerical homogenization. Mathematical details of the application area (SFIL) are presented in this paper. Numerical verification and detailed results are also shown. Algorithms for efficiently computing the Moore–Penrose pseudoinverse of sparse matrices, which form the core of homogenization, will be the topic of the second one [23].

We describe the SFIL process and its modeling in Section 2. In Section 3, we present the local numerical homogenization method. A coarse mesh is selected first and homogenization is done on each individual element of the mesh. On each element, the homogenization method works with the Moore–Penrose pseudoinverse of the element stiffness matrix to produce pseudoinverse of the local homogenized stiffness matrix as the output. The homogenized stiffness matrices can be assembled in the usual manner and the resulting system solved to compute the coarse-scale solution. The work extends the existing goal-oriented *h*-refinement strategy [24] to numerical homogenization where coarse-scale and fine-scale operators are different. The adjoint solutions on coarse and fine meshes provide a basis of automatic goal-oriented adaptivity. This gives rise to 1-irregular meshes with hanging nodes. These are handled using the constrained approximation techniques [25,26].

In Section 4, the homogenization method is verified using a 2-D chessboard conductivity problem in with a known homogenized limit [27]. The results provide evidence of the accuracy, robustness in presence of nonlinearities and mesh adaptivity. The adjoint solutions on coarse and fine meshes provide a basis of automatic goal-oriented adaptivity [24]. This gives rise to 1-irregular meshes with hanging nodes. These are handled using the constrained approximation techniques [25]. We present the details for 2-D and 3-D geometries in Section 7.

2. Description and modeling of Step and Flash Imprint Lithography

Step and Flash Imprint Lithography (SFIL) is a viable low-cost alternative to existing lithography techniques. This technique was initially developed by the Willson Research Group at The University of Texas at Austin in the late 1990s [2]. It is designed for fabricating microchips in low-pressure and room-temperature environments [1–3]. It has enabled imprinting of features smaller than 20 nm (nm). Moreover, it has the inherent resolution necessary to define sub-10 nm geometries [28]. Roughly speaking, a template contains "negative" of the desired pattern. If liquid were to be trapped inside these negative features and polymerized, on removal of the template, we would obtain a polymer with the "positive" pattern. Fig. 1 shows the basic idea behind the process and the resulting geometry. This section describes the process and the model of elasticity of polymeric lattices created in SFIL. Parameter estimation for bond potentials is discussed in [29]. The lattice elasticity model is described in detail in [5,6].

2.1. Description of the SFIL process

Multiple separate processes have to be carried out to complete the pattern transfer. To create a pattern layer, an organic polymer layer (transfer layer) is spin-coated on a silicon substrate. A low viscosity, photopolymerizable, organosilicon solution (etch barrier) is then distributed on the wafer. A transparent template, which has patterned relief structures, is placed over the coated silicon substrate. This displaces the etch barrier solution which gets trapped