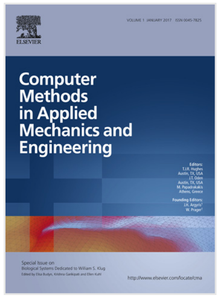
Accepted Manuscript



On domain symmetry and its use in homogenization

Cristian Barbarosie, Daniel A. Tortorelli, Seth Watts

PII: S0045-7825(16)30850-7
DOI: http://dx.doi.org/10.1016/j.cma.2017.01.009
Reference: CMA 11294

To appear in: *Comput. Methods Appl. Mech. Engrg.*

Received date: 1 August 2016
Revised date: 18 November 2016
Accepted date: 4 January 2017

On domain symmetry and its use in homogenization

Cristian Barbarosie[1], Daniel A. Tortorelli *[2], and Seth Watts[2]

[1]Faculty of Sciences, University of Lisbon
[2]Lawrence Livermore National Laboratory

November 18, 2016

Abstract

The present paper focuses on solving partial differential equations in domains exhibiting symmetries and periodic boundary conditions for the purpose of homogenization. We show in a systematic manner how the symmetry can be exploited to significantly reduce the complexity of the problem and the computational burden. This is especially relevant in inverse problems, when one needs to solve the partial differential equation (the primal problem) many times in an optimization algorithm. The main motivation of our study is inverse homogenization used to design architected composite materials with novel properties which are being fabricated at ever increasing rates thanks to recent advances in additive manufacturing. For example, one may optimize the morphology of a two-phase composite unit cell to achieve isotropic homogenized properties with maximal bulk modulus and minimal Poisson ratio. Typically, the isotropy is enforced by applying constraints to the optimization problem. However, in two dimensions, one can alternatively optimize the morphology of an equilateral triangle and then rotate and reflect the triangle to form a space filling D_3 symmetric hexagonal unit cell that necessarily exhibits isotropic homogenized properties. One can further use this D_3 symmetry to reduce the computational expense by performing the "unit strain" periodic boundary condition simulations on the single triangle symmetry sector rather than the six fold larger hexagon. In this paper we use group representation theory to derive the necessary periodic boundary conditions on the symmetry sectors of unit cells. The developments are done in a general setting, and specialized to the two-dimensional dihedral symmetries of the abelian D_2, i.e. orthotropic, square unit cell and nonabelian D_3, i.e. trigonal, hexagon unit cell. We then demonstrate how this theory can be applied by evaluating the homogenized properties of a two-phase planar composite over the triangle symmetry sector of a D_3 symmetric hexagonal unit cell.

Keywords : symmetric domain; finite element method; inverse homogenization

1 Introduction

Group representation theory has frequently been applied to reduce the cost of finite element and boundary element simulations of linear elastic structures that exhibit domain symmetry. However, the theory is seldom applied to reduce the cost of the "unit strain" simulations over morphological symmetric unit cells that are required to evaluate the unit cell's homogenized properties. This is despite the fact that the unit cells of many composite materials exhibit such morphological symmetries. In the following we revisit the group representation theory as it applies to the simulation of linear elastic structures that exhibit domain symmetry and extend the theory to address the periodic boundary condition computations that are required for homogenization.

The number of applications of group theory to boundary-value problems defined on domains (and their corresponding meshes) with symmetry are many. In the numerical approach, group theory is applied to the discretized governing partial differential equations and used to transform the stiffness matrix into one with block diagonal form whereby the single large linear problem is replaced with a series of smaller linear problems. In effect, the solution space $\mathbb{R}^n$ is partitioned into a series of systematically derived complementary

*corresponding author, tortorelli2@llnl.gov