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A framework for FFT-based homogenization on anisotropic lattices

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ABSTRACT

In order to take structural anisotropies of a given composite and different shapes of its unit cell into account, we generalize the basic scheme in homogenization by Moulinec and Suquet to arbitrary sampling lattices and tilings of the d-dimensional Euclidean space. We employ a Fourier transform for these lattices by introducing the corresponding set of sample points, the so called pattern, and its frequency set, the generating set. The pattern and the generating set represent the anisotropy of both the shape of the unit cell and the chosen preferences in certain sampling directions. In several cases, this Fourier transform is of lower dimension than the space itself. For the so called rank-1-lattices it reduces to a one-dimensional Fourier transform having the same leading coefficient as the fastest Fourier transform implementation available. We illustrate the results using the generalized basic scheme on an anisotropic laminate and on a generalized ellipsoidal Hashin structure. For both we give an analytical solution to the elasticity problem, in two- and three dimensions, respectively. We then illustrate the possibilities of choosing a pattern. Compared to classical grids this introduces both a reduction of computation time and a reduced error of the numerical method. It also allows for anisotropic subsampling, i.e. choosing a sub lattice of a pixel or voxel grid based on anisotropy information of the material at hand.

1. Introduction

Modern materials are often composites consisting of multiple components which are designed to obtain overall properties like high durability, flexibility, or stiffness. These inhomogeneities are usually small in comparison to the overall structure of the material or tool. Therefore, it is computationally beneficial and sometimes even necessary to replace the inhomogeneous material by a homogeneous one, having the same macroscopic properties. This process is called homogenization.

The underlying assumption is that the microstructure is represented by a reference volume that can be repeated periodically to generate the geometry. While many of these microstructures show macroscopically isotropic behavior, there are also composites that have one or multiple predominant directions.

The classical approach to solve the equations of linear elasticity with periodic boundary conditions is to use finite element or finite difference methods such as multi scale finite element methods [1,2] or local homogenization [3,4]. On representative volume elements, the gradient-enhanced method [5] and the asymptotic homogenization approach [6,7] are used to solve the partial differential equation. When dealing with data on very large regular meshes, e.g. with computer

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tomography images, the matrix-free method proposed by Moulinec and Suquet [8,9] performs better than finite element methods [10]. This algorithm is called the basic scheme and has evoked many enhancements and modifications. Amongst them, there are different discretization methods of the differential operator [11–13], adaptions to composites with infinite contrast, e.g. porous media [13,14], incorporation of additional information about the geometry [15], and the solution of homogenization problems of higher order [16].

These variants of the method of Moulinec and Suquet have in common that they are formulated on regular tensor product grids, i.e. they make use of the commonly known multidimensional fast Fourier transform (FFT). In some cases it is not possible to rotate the representative volume element without violating the periodicity condition of the microstructure and then a change of the discretization grid can be used to adapt the mesh to the geometry.

Galipeau and Castañeda [17,18], for example, construct a periodic laminate structure of elastomers where each of the two phases consists of aligned elongated particles of a magnetic material. In this material, the two phases differ in orientation and do not face into the direction of lamination, nor orthogonal to it. Lahellec, et al. [19] consider a multi-particle problem where they have an evolving computational grid. The basis vectors of this grid depend on the macroscopic velocity of a Newtonian fluid and they hint that the grid for the FFT does not have to be a rectangular one without elaborating this point. In both cases it might be beneficial to consider a more general sampling, i.e. sampling on anisotropic lattices.

Besides the theory of a discrete Fourier transform (DFT) on abelian groups, also known as generalized Fourier transform [20], the DFT has also been generalized to arbitrary sampling lattices, e.g. in order to derive periodic wavelets [21,22] and a corresponding fast Fourier and fast wavelet transform [23]. The computational complexity on these lattices stays the same as on the usual rectangular or pixel grid.

Furthermore, using the theory of rank-1-lattices, Kämmerer et al. [24,25] and Potts and Volkmer [26] derive several adaptive schemes to approximate both a certain set of frequencies and a set of sampling points and derive approximation errors for functions of certain smoothness. This includes a constructive derivation of the vector that generates the lattice. For these special lattices, the Fourier transform even in high-dimensional space reduces to a one-dimensional Fourier transform, hence reducing both the organization of the sampled data and the computational cost for the FFT. The theory of rank-1-lattices therefore allows for directly taking known anisotropic properties of a function into account and thereby reduces the necessary number of sample values or measurements by adapting the lattice. Furthermore, it decreases the computational cost or data organization overhead due to the reduction from a high-dimensional FFT to a one-dimensional transform.

In this paper we generalize the basic scheme by Moulinec and Suquet to arbitrary anisotropic periodic lattices. This introduces the possibility to prefer directions other than the coordinate axes in the reference volume and hence in the solution. This allows for aligning the basis functions with the dominant orientations of the geometry and for controlling the refinement in these directions. This generalization of the basic scheme to arbitrary anisotropic sampling lattices introduces the form of the grid as an algorithmic parameter without additional computational costs. For a special set of rank-1-lattices, after sampling in a high-dimensional space, the computation of the fast Fourier transform even reduces to a one-dimensional FFT. Therefore, additionally to the new possibility of choosing directions of preference, one can also choose such special lattices to reduce the computational efforts.

The remainder of the paper is organized as follows. In Section 2 we establish the preliminaries regarding the parametrization, properties of anisotropic lattices, and their patterns on the unit cube. Further, we introduce the FFT on such patterns, where the usual tensor product grid is a special case. Exemplary for a homogenization problem we introduce the periodic equations of quasi-static elasticity in Section 3 and generalize the basic scheme. Based on this we explain the difference between making a coordinate transformation and choosing a lattice adapted to the geometry of the lattice. In Section 4 we generalize two known geometries to an anisotropic setting: the laminate structure and the Hashin structure that serves as the main analytical example for this work. Both are anisotropic structures using isotropic material laws that provide an analytic solution for the strain field and the effective matrix. This allows us to study effect of the pattern orientation on the solution and the effective properties in Section 5. Section 6 concludes the paper with a short outlook.

2. Preliminaries

Throughout this paper we will employ the following notation: The symbols $a \in \mathbb{C}$, $\mathbf{a} \in \mathbb{C}^d$ and $\mathbf{A} \in \mathbb{C}^{d\times d}$ denote scalars, vectors, and matrices, respectively. The only exception from this are f, g, h, which are reserved for functions. We denote the inner product of two vectors by $\mathbf{a}^{\mathrm{T}}\mathbf{b} := \sum_i a_i b_i$ and reserve the symbol $\langle \cdot, \cdot \rangle$ for inner products of two functions or two generalized sequences, respectively. For a complex number $a = b + \mathrm{i}c$, $b, c \in \mathbb{R}$, we denote the complex conjugate by $\overline{a} := b - \mathrm{i}c$.

Usually, we are concerned with d-dimensional data, where $d = 2, 3$, but the theory is written in arbitrary dimensions. Sets are denoted by capital case calligraphic letters, e.g. $\mathcal{P}(\cdot)$ or $\mathcal{G}(\cdot)$ and the same for the Fourier transform $\mathcal{F}(\cdot)$; all of these might depend on a scalar n or matrix $\mathbf{M}$, given in brackets. We denote second-order tensors by small Greek letters as λ, ε with entries λ_{ij} are indexed by scalars i, j. We denote fourth-order tensors by capital calligraphic letters, where $\mathcal{C}$ is the most prominent one. Finally, constants like Euler's number e or the imaginary unit i, i.e. $\mathrm{i}^2 = -1$, are set upright.

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