Available online at www.sciencedirect.com
SCIENCE DIRECT®
ELSEVIER
Computational Materials Science 32 (2005) 387–391
COMPUTATIONAL MATERIALS SCIENCE
www.elsevier.com/locate/commatsci

Fourier series for computing the response of periodic structures with arbitrary stiffness distribution

Sven Kaßbohm [a,*], Wolfgang H. Müller [a], Robert Feßler [b]

[a] Institut für Mechanik der TU Berlin, Fachgebiet Kontinuumsmechanik und Materialtheorie, Einsteinufer 5, D-10587, Berlin, Germany
[b] Fraunhofer-Institut für Techno- und Wirtschaftsmathematik (ITWM) Gottlieb-Daimler-Str., Geb. 49, D-67663 Kaiserslautern, Germany

Abstract

A method based on Fourier series is presented, which allows to calculate the local stress–strain response of a three-dimensional periodic structure subjected to a spatial average of strain. The periodicity allows the reduction of the problem to that of a Representative Volume Element (RVE). The solution operator (which can easily be calculated in Fourier space) is defined for a simplified problem, and it is shown that this operator may also be used for the original problem. In order to illustrate the use of this procedure, an example problem is presented. A global error is defined and calculated for the example problem.

PACS: 62.20.−x; 62.20.Dc; 02.30.Jr; 02.30.Nw; 61.66.Dk
Keywords: Composites; Numerical; Periodic; Fourier series

1. Introduction

We focus on the numerical solution of

$$\langle \varepsilon \rangle = \varepsilon_0, \quad \nabla \cdot (C\varepsilon) = 0, \tag{1}$$

defined in a three-dimensional rectangular domain (the RVE). The tensor ε_0 is defined as the strain field average $\langle \varepsilon \rangle$. C is the material stiffness tensor field, and periodic boundary conditions are applied.

From all possible fields ε only those are taken into consideration, for which ε is derived from a displacement field u, so that $\varepsilon = \frac{1}{2}(\nabla u + u\nabla) = \mathrm{sym}(\mathrm{grad}\, u)$ holds. We use Fourier series to solve the problem as done in [2,4–6]. The desired local strain field (and a resulting local stress field $\sigma = C\varepsilon$) may be used for homogenization techniques, for which periodic boundary conditions show several advantages as shown in [3].

* Corresponding author. Tel.: +49 30 314 25025; fax: +49 30 314 24747.
E-mail address: sven.kassbohm@tu-berlin.de (S. Kaßbohm).

0927-0256/$ - see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.commatsci.2004.09.028

2. Fourier coefficients/Fourier expansion of function and derivatives

Let $k = \langle k_1, k_2, k_3\rangle$ be the wave number vector, and let f be a periodic function (i.e., any of the given or desired fields) with period $2\pi L_i$ in each orthogonal direction of space x_i ($i = 1,2,3$). The Fourier coefficients $\hat{f}(k)$ and the Fourier series expansion of a smooth [1] function f are given by:

$$\hat{f}(k) = \int_{\alpha_1=0}^{1} \mathrm{d}\alpha_1 \int_{\alpha_2=0}^{1} \mathrm{d}\alpha_2 \int_{\alpha_3=0}^{1} \mathrm{d}\alpha_3 f(\alpha) \mathrm{e}^{-\mathrm{i}2\pi k\cdot\alpha} = \mathbb{F}\{f\},$$

$$f(\alpha) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \sum_{k_3=-\infty}^{\infty} \hat{f}(k) \mathrm{e}^{\mathrm{i}2\pi k\cdot\alpha} = \mathbb{F}^{-1}\{\hat{f}\}$$

with the vector $\alpha = \frac{1}{2\pi}\langle x_1/L_1, x_2/L_2, x_3/L_3\rangle$.

The Fourier series of the derivatives of the field with respect to the spatial coordinates x_i are:

$$\frac{\partial f}{\partial x_j} = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \sum_{k_3=-\infty}^{\infty} \frac{\mathrm{i}}{L_{\underline{j}}} k_j \hat{f}(k) \mathrm{e}^{\mathrm{i}2\pi k\cdot\alpha},$$

$$\frac{\partial f^2}{\partial x_j \partial x_l} = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \sum_{k_3=-\infty}^{\infty} -\frac{1}{L_{\underline{j}} L_{\underline{l}}} k_j k_l \hat{f}(k) \mathrm{e}^{\mathrm{i}2\pi k\cdot\alpha}.$$

The Discrete Fourier Transform (DFT), with which the Fourier coefficients can be calculated approximately, is defined as follows:

$$\hat{f}_k = \frac{1}{N_1 N_2 N_3} \sum_{n_1=0}^{N_1-1} \sum_{n_2=0}^{N_2-1} \sum_{n_3=0}^{N_3-1} f_n \mathrm{e}^{-\mathrm{i}2\pi k\cdot\alpha_n} \approx \hat{f}(k)$$

with $\alpha_n = \langle n_1/N_1, n_2/N_2, n_3/N_3\rangle$ and $f_n = f(\alpha_n)$.

The discretization in each direction of space is defined by *odd* numbers $N_i = 2m_i + 1$ (with $m_i \in \mathbb{N}$) and the approximation is only useful for $| k_i | \leqslant \frac{N_i - 1}{2}$ (Nyquist critical frequency). The Inverse Discrete Fourier Transform (IDFT) is defined by:

$$f_n = \sum_{k_1=0}^{N_1-1} \sum_{k_2=0}^{N_2-1} \sum_{k_3=0}^{N_3-1} \hat{f}_k \mathrm{e}^{+\mathrm{i}2\pi k\cdot\alpha_n}.$$

Once the solution of a set of differential equations has been calculated in Fourier space, the IDFT is performed resulting in *discrete* values f_n, which may be *interpolated* by the trigonometric polynomial:

$$\mathrm{int} f_n = \sum_{k_1=-m_1}^{m_1} \sum_{k_2=-m_2}^{m_2} \sum_{k_3=-m_3}^{m_3} \hat{f}_k \mathrm{e}^{\mathrm{i}2\pi k\cdot\alpha}. \tag{2}$$

3. Problem solution

3.1. The basic problem

Consider the following problem for a fluctuation field $\tilde{\varepsilon}$ with a given constant tensor C^0 and with a given field τ valid in the RVE with periodic boundary conditions:

$$\langle\tilde{\varepsilon}\rangle = 0, \quad \nabla\cdot(C^0\tilde{\varepsilon}) = \nabla\cdot\tau. \tag{3}$$

In order to find a function $\tilde{\varepsilon} = \mathrm{sym}(\mathrm{grad}\ \tilde{u})$ we define the solution operator Γ by

$$\tilde{\varepsilon} = \Gamma\tau \quad \Longleftrightarrow \quad \tilde{\varepsilon}\ \text{solves (3)}. \tag{4}$$

Note that Γ projects divergence-free (and in particular constant) fields to zero. If we consider that $C^0_{ijkm} = C^0_{jikm}$ and $C^0_{ijkm} = C^0_{ijmk}$, Γ can easily be calculated in Fourier space (see [4]), and the solution of (3) can be written as:

$$\hat{\tilde{\varepsilon}}_{lm} = \widehat{\Gamma}_{lmop}\hat{\tau}_{po} \quad \forall k \neq 0 \quad \text{and} \quad \langle\tilde{\varepsilon}\rangle = \hat{\tilde{\varepsilon}}(0) = 0. \tag{5}$$

3.2. The extended problem

Now consider the extended problem defined in the same domain:

$$\langle\varepsilon\rangle = \varepsilon_0, \quad \nabla\cdot(C^0\varepsilon) = \nabla\cdot\tau \tag{6}$$

with $\varepsilon = \varepsilon_0 + \tilde{\varepsilon} = \mathrm{sym}(\mathrm{grad}(\nabla\cdot\varepsilon_0 + \tilde{u}))$. It can be seen, that $\varepsilon = \Gamma\tau + \varepsilon_0$ is the solution of this problem, so that

$$\hat{\varepsilon}_{lm} = \widehat{\Gamma}_{lmop}\hat{\tau}_{po} \quad \forall k \neq 0 \quad \text{and} \quad \langle\varepsilon\rangle = \hat{\varepsilon}(0) = \varepsilon_0. \tag{7}$$

[1] The convergence of the series is discussed in [1].