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A Numerical Method for Computing the Response of Periodic Structures with Arbitrary Stiffness Distribution

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A method based on Fourier series is presented, which allows to calculate the local stress-strain response of a periodic structure subjected to an applied (spatial average) strain field. The periodicity allows the reduction of the problem to that of a Representative Volume Element (R.V.E.), which can be solved by transferring it into Fourier space. - First, a review of Fourier series as a particular method of solving the set of differential equations is given. Second, the solution operator is calculated in Fourier space. Third, a related problem is studied, in which the material is homogeneous and fourth, the solution for the problem with arbitrary stiffness distribution is presented as well as the algorithm for the numerical calculation of the desired fields. Finally, example problems are studied, and the results are compared to those obtained by the method of Discrete Fourier Transforms (Müller, 1996).

1 Fourier Coefficients/Fourier Expansion of Function and Derivatives

Let the wave number vector $\boldsymbol{k} = (k_1, k_2, k_3) \in \mathbb{Z}^3$ and f be a periodic function (i.e., any of the given or desired fields) with period 1 in each orthogonal direction of space α_i. The Fourier series expansion $f(\boldsymbol{\alpha})$ and the Fourier coefficients $\hat{f}(\boldsymbol{k})$ of a piecewise continuously differentiable function f are given by

$$\begin{aligned} f(\boldsymbol{\alpha}) &= \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \sum_{k_3=-\infty}^{\infty} \hat{f}(k_1,k_2,k_3) e^{\mathrm{i}2\pi(k_1\alpha_1+k_2\alpha_2+k_3\alpha_3)} = \sum_{\boldsymbol{k}=-\boldsymbol{\infty}}^{\boldsymbol{\infty}} \hat{f}(\boldsymbol{k}) e^{\mathrm{i}2\pi\boldsymbol{k}\cdot\boldsymbol{\alpha}} =: \mathcal{F}^{-1}\{\hat{f}(\boldsymbol{k})\}, \\ \hat{f}(\boldsymbol{k}) &= \int_{\alpha_1=0}^{1} \mathrm{d}\alpha_1 \int_{\alpha_2=0}^{1} \mathrm{d}\alpha_2 \int_{\alpha_3=0}^{1} \mathrm{d}\alpha_3 f(\alpha_1,\alpha_2,\alpha_3) e^{-\mathrm{i}2\pi(k_1\alpha_1+k_2\alpha_2+k_3\alpha_3)} =: \mathcal{F}\{f(\boldsymbol{\alpha})\}. \end{aligned} \tag{1}$$

The Fourier coefficients can be calculated approximately by the following formula, in which α_i is substituted by $\frac{\beta_i}{N_i}$, and N_i is the discretization in each direction of space.[1] The approximation is useful only for $|k_i| \leq \frac{N_i}{2}$ (Nyquist critical frequency):

$$\hat{f}(\boldsymbol{k}) \approx \frac{1}{N_1 N_2 N_3} \sum_{\beta_1=0}^{N_1-1} \sum_{\beta_2=0}^{N_2-1} \sum_{\beta_3=0}^{N_3-1} f(\frac{\beta_1}{N_1}, \frac{\beta_2}{N_2}, \frac{\beta_3}{N_3}) e^{-\mathrm{i}2\pi(k_1\frac{\beta_1}{N_1}+k_2\frac{\beta_2}{N_2}+k_3\frac{\beta_3}{N_3})}. \tag{2}$$

Using these coefficients, the function itself is approximated by the finite series

$$f(\boldsymbol{\alpha}) \approx \sum_{k_1=-\frac{N_1}{2}+1}^{\frac{N_1}{2}} \sum_{k_2=-\frac{N_2}{2}+1}^{\frac{N_2}{2}} \sum_{k_3=-\frac{N_3}{2}+1}^{\frac{N_3}{2}} \hat{f}(k_1,k_2,k_3) e^{\mathrm{i}2\pi(k_1\alpha_1+k_2\alpha_2+k_3\alpha_3)}. \tag{3}$$

Note that the last approximation can be evaluated at every point in space described by α_i, and not only at discrete points. Note also that Formula (2) and Formula (3) evaluated at $\alpha_i = \frac{\beta_i}{N_i}$ represent the discrete forward and backward Fourier transform.

If f is a) continuous and b) piecewise continuously differentiable in the R.V.E. domain $[0,1]^3$, the Fourier series

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[1] Each N_i should be a power of 2 to exploit the advantages of Fast Fourier Transform (see Press et al. (1996)).

of its derivatives with respect to the spatial coordinates $x_i = \alpha_i 2\pi L_{\underline{i}}$ are [2]:

$$\frac{\partial f}{\partial x_j} = \sum_{\boldsymbol{k}=-\infty}^{\infty} \frac{\mathrm{i}}{L_{\underline{j}}} k_j \hat{f}(\boldsymbol{k}) e^{\mathrm{i}k_p \frac{x_p}{L_{\underline{p}}}}, \tag{4}$$

$$\frac{\partial f^2}{\partial x_j \partial x_l} = \sum_{\boldsymbol{k}=-\infty}^{\infty} -\frac{1}{L_{\underline{j}} L_{\underline{l}}} k_j k_l \hat{f}(\boldsymbol{k}) e^{\mathrm{i}k_p \frac{x_p}{L_{\underline{p}}}} \quad . \tag{5}$$

2 Discussion and Solution of the Problem

In this section the response of a periodic structure with periodic boundary conditions and arbitrary stiffness distribution is studied. Let the strain ε consist of a fluctuation term $\tilde{\varepsilon}$ with spatial average zero and a constant term (the strain average) ε_0, so that $\varepsilon = \tilde{\varepsilon} + \varepsilon_0$. Consequently, the total displacement u consists of $u = \tilde{u} + u_0$. We assume a linear relationship between strains ε and stresses σ defined by the material tensor C (Hooke's law). Moreover we use small deformation theory. A spatial average strain $< \varepsilon >$ is defined by

$$\begin{aligned} < \varepsilon > &= \frac{1}{2\pi(L_1 + L_2 + L_3)} \int_{x_1=0}^{2\pi L_1} \int_{x_2=0}^{2\pi L_2} \int_{x_3=0}^{2\pi L_3} \varepsilon \; \mathrm{d}x_3 \mathrm{d}x_2 \mathrm{d}x_1 \\ &= \int_{\alpha_1=0}^{1} \int_{\alpha_2=0}^{1} \int_{\alpha_3=0}^{1} \varepsilon \; \mathrm{d}\alpha_3 \mathrm{d}\alpha_2 \mathrm{d}\alpha_1 = \hat{\varepsilon}(\boldsymbol{0}). \end{aligned} \tag{6}$$

The aim is to calculate the local strain and stress field inside of an R.V.E. with a given arbitrary stiffness distribution and a given average strain. [3]

2.1 The Basic Problem, Introduction and Calculation of the Solution Operator Γ

Consider the basic problem of an elastically homogeneous R.V.E. (the material tensor C^0 is constant in $\boldsymbol{x}$) subjected to a stress field $\tau(\boldsymbol{x})$. The following set of equations plus boundary conditions resulting from the periodicity of the problem describe the problem. The unknown is the fluctuation strain field $\tilde{\varepsilon}(\boldsymbol{x})$:

$$\left.\begin{aligned} &< \tilde{\varepsilon} >= 0 \\ &\tilde{\varepsilon} = \frac{1}{2}(\nabla \tilde{u} + \tilde{u} \nabla) \\ &\nabla \cdot (C^0 \cdot\cdot \, \tilde{\varepsilon}) = \nabla \cdot \tau \end{aligned}\right\} \tag{7}$$

Let Γ be an operator so that

$$\tilde{\varepsilon} = \Gamma \tau \quad \Leftrightarrow \quad \tilde{\varepsilon} \text{ solves (7)} . \tag{8}$$

Note that Γ projects divergence-free (and in particular constant) fields to zero.

In order to explicitly calculate Γ in Fourier space, we combine the second and third Equation of (7) to yield:

$$C^0_{ijkl} \frac{\partial^2 \tilde{u}_k}{\partial x_j \partial x_l} = \frac{\partial \tau_{ji}}{\partial x_j}. \tag{9}$$

By using (4) and (5) we find that:

$$-C^0_{ijkl} \sum_{\boldsymbol{k}=-\infty}^{\infty} \frac{1}{L_{\underline{j}} L_{\underline{l}}} k_j k_l \hat{\tilde{u}}_k(\boldsymbol{k}) e^{\mathrm{i}k_p \frac{x_p}{L_{\underline{p}}}} = \sum_{\boldsymbol{k}=-\infty}^{\infty} \frac{\mathrm{i}}{L_{\underline{j}}} k_j \hat{\tau}_{ji}(\boldsymbol{k}) e^{\mathrm{i}k_p \frac{x_p}{L_{\underline{p}}}}. \tag{10}$$

By using the orthogonality conditions we find $\forall \boldsymbol{k} \setminus \boldsymbol{0}$:

$$-C^0_{ijkl} \frac{1}{L_{\underline{j}} L_{\underline{l}}} k_j k_l \hat{\tilde{u}}_k = \frac{\mathrm{i}}{L_{\underline{j}}} k_j \hat{\tau}_{ji} \qquad \Leftrightarrow \qquad \hat{\tilde{u}}_l \; = B_{lop} \hat{\tau}_{po} \tag{11}$$

[2] The introduction of spatial coordinates x_i allows to map the unit lenght problem on a problem with R.V.E. dimensions $2\pi L_1 \times 2\pi L_2 \times 2\pi L_3$. The underlined index i denotes that no summation is carried out.

[3] For further reading see also Eyre and Milton (1999) and Moulinec and Suquet (1998).

with $B_{lop} = M_{lo}^{-1} \frac{\mathrm{i}}{L_{\underline{p}}} k_p$ and $M_{ik} = -C^0_{ijkl} \frac{1}{L_{\underline{j}} L_{\underline{l}}} k_j k_l$ known a priori. Hence we obtain

$$\begin{aligned} \tilde{\varepsilon}_{lm}(\boldsymbol{x}) = \frac{1}{2}\Big(\frac{\partial \tilde{u}_l}{\partial x_m} + \frac{\partial \tilde{u}_m}{\partial x_l}\Big) = \sum_{\boldsymbol{k}=-\infty}^{\infty} \frac{1}{2}\Big(\frac{\mathrm{i}}{L_{\underline{m}}} k_m \hat{\tilde{u}}_l + \frac{\mathrm{i}}{L_{\underline{l}}} k_l \hat{\tilde{u}}_m\Big) e^{\mathrm{i}k_p \frac{x_p}{L_{\underline{p}}}} = \\ \sum_{\boldsymbol{k}=-\infty}^{\infty} \frac{1}{2}\Big(\frac{\mathrm{i}}{L_{\underline{m}}} k_m B_{lop} + \frac{\mathrm{i}}{L_{\underline{l}}} k_l B_{mop}\Big) \hat{\tau}_{po} e^{\mathrm{i}k_p \frac{x_p}{L_{\underline{p}}}} = \sum_{\boldsymbol{k}=-\infty}^{\infty} \hat{\Gamma}_{lmop} \hat{\tau}_{po} e^{\mathrm{i}k_q \frac{x_q}{L_{\underline{q}}}}. \end{aligned} \tag{12}$$

The Fourier coefficients of the unknown $\tilde{\varepsilon}$ can therefore explicitly be calculated from:

$$\hat{\tilde{\varepsilon}}_{lm}(\boldsymbol{k}) = \hat{\Gamma}_{lmop}(\boldsymbol{k}) \hat{\tau}_{po}(\boldsymbol{k}) \qquad \text{with} \qquad \hat{\Gamma}_{lmop} = \frac{1}{2}\Big(\frac{\mathrm{i}}{L_{\underline{m}}} k_m B_{lop} + \frac{\mathrm{i}}{L_{\underline{l}}} k_l B_{mop}\Big). \tag{13}$$

For $\boldsymbol{k} = \boldsymbol{0}$ we set $\hat{\tilde{\varepsilon}}_{lm}(\boldsymbol{0}) = 0$. This is necessary to satisfy the first equation in (7). Note that according to (6) and (1) we have $\hat{\tilde{\varepsilon}}(\boldsymbol{0}) =< \tilde{\varepsilon} >$. Due to this, the fact that $\hat{\Gamma}$ cannot be evaluated at $\boldsymbol{k} = \boldsymbol{0}$ does not give cause for a problem.

2.2 The Related Problem with Spatially Constant Stiffness C^0 and Non-vanishing Strain Average ε_0

Consider the related problem, in which the stiffness of the R.V.E. is constant in $\boldsymbol{x}$ (elastically homogeneous material as in the previous basic problem). Additionally, assume a non-vanishing strain average and a given stress field τ:

$$\left.\begin{array}{l} < \varepsilon >= \varepsilon_0 \\ \varepsilon = \frac{1}{2}(\nabla u + u\nabla) \qquad \Leftrightarrow \qquad \tilde{\varepsilon} + \varepsilon_0 = \frac{1}{2}(\nabla \tilde{u} + \tilde{u}\nabla) + \frac{1}{2}(\nabla u_0 + u_0 \nabla) \\ \nabla \cdot (C^0 \cdot\cdot \varepsilon) = \nabla \cdot \tau \end{array}\right\} \tag{14}$$

The solution of this problem is $\varepsilon = \Gamma\tau + \varepsilon_0$ (use (7) and (8) to verify).

2.3 The Problem with Spatially Varying Stiffness $C(\boldsymbol{x})$

Now consider the following problem, in which the stiffness of the R.V.E. is defined by $C = C(\boldsymbol{x})$. Assume a non-vanishing strain average within the R.V.E. as in the previous related problem. The following equations describe the problem:

$$\left.\begin{array}{rcl} & & < \varepsilon >= \varepsilon_0 \\ & & \varepsilon = \frac{1}{2}(\nabla u + u\nabla) \\ \nabla \cdot (C(\boldsymbol{x}) \cdot\cdot \varepsilon) = 0 & \Leftrightarrow & \nabla \cdot (C^0 \cdot\cdot \varepsilon) = \nabla \cdot \big(\delta C \cdot\cdot \varepsilon\big) \end{array}\right\} \tag{15}$$

with $\delta C = C^0 - C$.

The solution of (15) is known from the related problem (see Subsection 2.2). We introduce the operators

$$\begin{aligned} A_{\delta C} &: \text{arg} \to \Gamma \delta C \cdot\cdot \text{arg}, \\ A_{C^0} &: \text{arg} \to \Gamma C^0 \cdot\cdot \text{arg}, \\ A_C &: \text{arg} \to \Gamma C \cdot\cdot \text{arg}. \end{aligned} \tag{16}$$

ε must then satisfy the following integral equation, which can be solved on terms of a series (Neumann expansion):

$$\begin{aligned} & \varepsilon = A_{\delta C}\varepsilon + \varepsilon_0 \\ \Leftrightarrow \qquad & (id - A_{\delta C})\varepsilon = \varepsilon_0 \\ \Leftrightarrow \qquad & \varepsilon = (id + A_{\delta C} + A_{\delta C}^2 + ...)\varepsilon_0 = \varepsilon_0 + A_{\delta C}(id + A_{\delta C} + ...)\varepsilon_0 \end{aligned} \tag{17}$$

$(id + A_{\delta C} + A_{\delta C}^2 + ...)$ converges against $(id - A_{\delta C})^{-1}$ if $||A_{\delta C}|| < 1$. The series can be truncated after the $(m-1)$'st addend (and yield ε^{m-1}) or after the m'th addend (and yield ε^{m}). The relation between ε^{m} and ε^{m-1} is given through the *recursion* formula:

$$\left.\begin{aligned} \varepsilon^m &= \varepsilon_0 + A_{\delta C}\varepsilon^{m-1} = \varepsilon_0 + A_{C^0}\varepsilon^{m-1} - A_C\varepsilon^{m-1} = \\ &\varepsilon_0 + \Gamma C^0 \cdot\cdot\, \varepsilon^{m-1} - \Gamma C \cdot\cdot\, \varepsilon^{m-1} = \\ &\varepsilon^{m-1} - \Gamma C \cdot\cdot\, \varepsilon^{m-1} = \varepsilon^{m-1} - \Gamma\sigma^{m-1} \qquad \text{with } \sigma = C \cdot\cdot\, \varepsilon. \end{aligned}\right\} \tag{18}$$

In the previous formula we made use of $\varepsilon^{m-1} = \varepsilon_0 + \Gamma C^0 \cdot\cdot\, \varepsilon^{m-1}$. This equation is true, because the left and the right hand side of this equation solve the following problem:

$$\left.\begin{aligned} &< \varepsilon >= \varepsilon_0 \\ &\varepsilon = \frac{1}{2}(\nabla u + u\nabla) \\ &\nabla \cdot (C^0 \cdot\cdot\, \varepsilon) = \nabla \cdot (C^0 \cdot\cdot\, \varepsilon^{m-1}) \end{aligned}\right\} \tag{19}$$

Since Γ is explicitly known in Fourier space according to Equation (13), the solution for (15) be obtained iteratively using the following algorithm:

$$\left.\begin{aligned} &\text{Set} \quad \varepsilon^0 = \varepsilon_0, \quad \sigma^0 = C \cdot\cdot\, \varepsilon^0, \quad \hat{\varepsilon}^0 = \mathcal{F}\{\varepsilon^0\}, \quad m = 1, \quad \text{iterate:} \\ &\cdot\ \hat{\sigma}^{m-1} = \mathcal{F}\{\sigma^{m-1}\} \\ &\cdot\ \text{Stop, if } \frac{\sqrt{< ||k \cdot \hat{\sigma}||^2 >}}{||\hat{\sigma}(\mathbf{0})||} < \text{tolerance, else} \\ &\cdot\ \hat{\varepsilon}^m = \hat{\varepsilon}^{m-1} - \hat{\Gamma} \cdot\cdot\, \hat{\sigma}^{m-1} \quad \forall \boldsymbol{k} \setminus \mathbf{0} \quad \text{else} \quad \hat{\varepsilon}^m = \varepsilon_0 \\ &\cdot\ \varepsilon^m = \mathcal{F}^{-1}\{\hat{\varepsilon}^m\}, \quad \sigma^m = C \cdot\cdot\, \varepsilon^m \\ &\cdot\ m = m + 1 \end{aligned}\right\} \tag{20}$$

Note that the algorithm is valid for the continuous case.

3 Examples

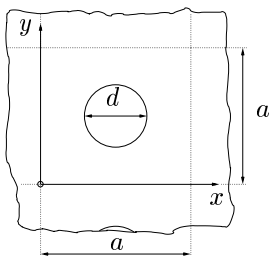
The following examples have been calculated for discretizations described by N_i. Formula (2) and Formula (3) have been used for the forward and backward transform in the method presented here.

3.1 First Example for the Basic Problem: Eigenstrains within a Circular Domain in an Elastically Homogeneous Material

An elastically homogeneous isotropic R.V.E. ($E = 1000, \nu = 0$, i.e., plain strain) is subjected to eigenstrains $\varepsilon^*_{11} = \varepsilon^*_{22} = 1$ within a circular domain of diameter $d = \frac{2}{5}a$ and to zero eigenstrains elsewhere. Consequently, inside of the domain we put:

$$\left.\begin{aligned} \tau_{ji} &= C^0_{ij11}\varepsilon^*_{11} + C^0_{ij22}\varepsilon^*_{22} \\ \Rightarrow \tau_{11} &= \tau_{22} = C^0_{1111} \end{aligned}\right\} \tag{21}$$

and we set all other components of τ equal to zero inside of the domain. Outside of the domain all components of τ are set to zero.



The total strain $\tilde{\varepsilon}_{11}$ is calculated with the method of Müller (1996) as well as with the method presented here (basic problem). The method of Müller (1996) uses the Discrete Fourier Transform (D.F.T.) and approximates difference quotients by finite difference schemes. It provides no information in between the gridpoints, because no shape functions for fields are assumed. In contrast to this, the method presented here provides *continuous* information for all fields.

Errors in the method presented here result from the truncation of the Fourier series, the approximation of the Fourier coefficients with Riemannian sums (discrete Fourier Transform) and from Equations (4) and (5) not being applicable due to the fact, that τ is not continuous in this example. The following figures show results computed for $N_1 = N_2 = 64$:

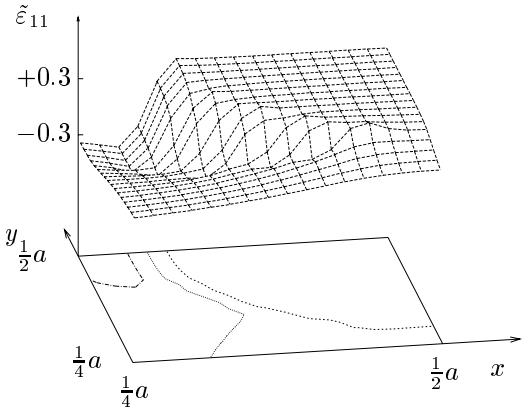


Figure 1: Discrete values for $\tilde{\varepsilon}_{11}$ computed with the method of Müller (1996)

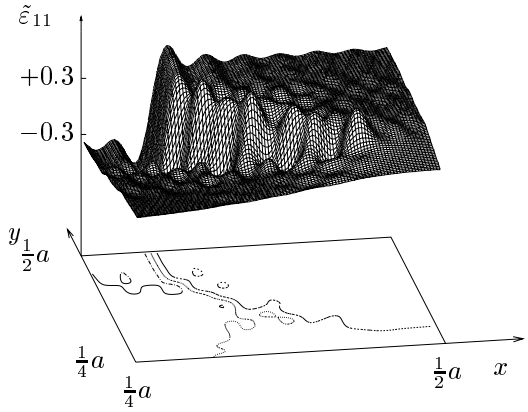


Figure 2: Continuous $\tilde{\varepsilon}_{11}$ distribution computed with the method presented in this paper

3.2 Second Example for the Basic Problem: Sine Eigenstrains in an Elastically Homogeneous Material

Reconsider the homogeneous isotropic plain strain R.V.E. (dimensions $a \times a \times 1$) from the previous example. Now the eigenstrains are prescribed as $\varepsilon^*_{11}(x,y) = \varepsilon^*_{22}(x,y) = \sin\frac{2\pi x}{a}\sin\frac{2\pi y}{a}$. τ is therefore given by:

$$\tau_{11}(x,y) = \tau_{22}(x,y) = C^0_{1111}\sin\frac{2\pi x}{a}\sin\frac{2\pi y}{a}.$$

Only four Fourier coefficients of τ are (independent of the choice of N_i) distinct from zero, namely those for $\boldsymbol{k} = (-1,-1,0), (-1,1,0), (1,-1,0)$ and $(1,1,0)$.

The method presented here yields the exact solution (see Figure (4)). In contrast to this, the solution of Müller (1996) is a more or less accurate approximation to the exact solution (see Figure (3)).

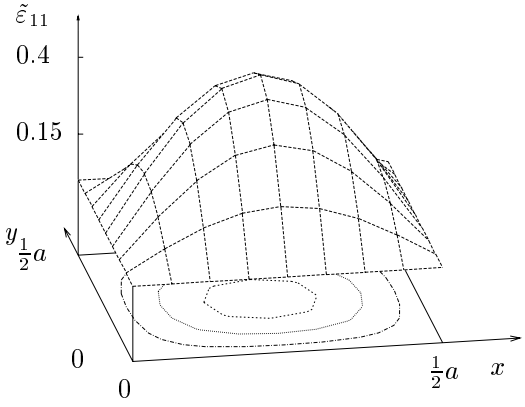


Figure 3: $\tilde{\varepsilon}_{11}$ computed with the method of Müller (1996) ($N_1 = N_2 = 16$)

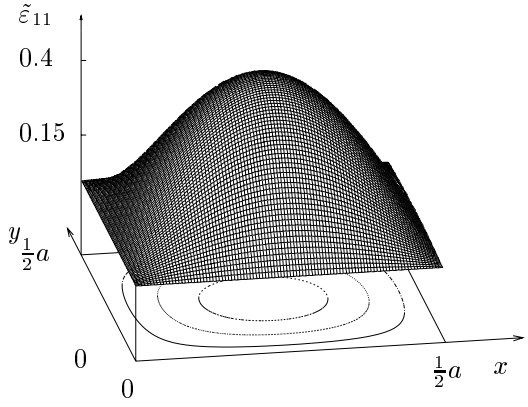


Figure 4: Exact solution for $\tilde{\varepsilon}_{11}$ from the method presented in this paper ($N_1 = N_2 = 4$)

3.2.1 Comparison of the Results from Both Methods

In order to assess the accuracy of the D.F.T. results of Müller (1996), we compute

$$e = \frac{\sum(\tilde{\varepsilon}^{\text{exact}}_{11} - \tilde{\varepsilon}^{\text{D.F.T.}}_{11})^2}{(N_1 \times N_2)^{\text{D.F.T.}}} \qquad (22)$$

where the summation is carried out w.r.t. all gridpoints used for the D.F.T. caculations. The decrease of this error with increasing number of discretization points for the method of Müller (1996) $(N_1 \times N_2)^{\text{D.F.T.}}$ is shown in Figure 5.

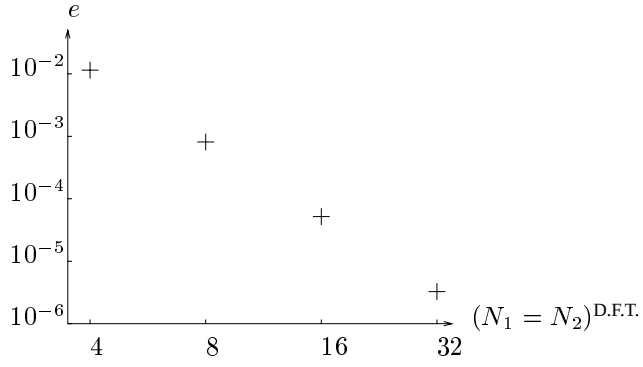


Figure 5: Deviation between D.F.T. results (Müller (1996)) and exact solution from the method presented here

4 Conclusions and Outlook

A method based on Fourier series has been presented, which allows calculating the local stress-strain response of a periodic structure subjected to an applied field. Results have been presented for two case studies (homogeneous and isotropic material was used for both cases), for which the solution operator Γ was explicitly given in Fourier space. The same operator is used for problems with arbitrary stiffness distribution.

The method presented here provides continuous information for all fields. The quality of the solution (from the method presented here) is strongly dependent on the given field τ.

As it was pointed out in Brown et al. (2003) the convergence of the Neumann approach used for predicting the local stress-strain response in the case of different stiffnesses of inclusions and matrices depends strongly on the stiffness contrast and on the data used for C^0. Similar effects can be expected in the case of Fourier series as mentioned in the work of Eyre and Milton (1999). A detailed investigation of this problem will be presented in a later paper.

References

Brown, C. M.; Dreyer, W.; Müller, W. H.: The convergence of a dft-algorithm for solution of stress/strain problems in composite mechanics. *ASME Journal of Engineering Materials and Technology, 125 (2003), pp. 27-37*.

Eyre, D. J.; Milton, G. W.: A fast numerical scheme for computing the response of composites using grid refinement. *Eur. Phys. J. AP 6, 41-47*.

Moulinec, H.; Suquet, P.: A numerical method for computing the overall response of nonlinear composites with complex microstructure. *Comput. Methods Appl. Mech. Engrg. 157 pp. 69-94.*

Müller, W. H.: Mathematical versus experimental stress analysis of inhomogeneities in solids. *J. Phys. IV 6 C1-139-C1-148*.

Press, W. H.; Teukolsky, S. A.; Vetterling, W. T.; Flannery, B. P.: *Numerical Recipes in Fortran 77.*. Press Syndicate of the University of Cambridge, ISBN 0 521 43064 X (1996).

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