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The explicit jump discretization with Lippmann-Schwinger solvers for thermal computational homogenization problems

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We present a Lippmann-Schwinger equation for the explicit jump discretization of thermal computational homogenization. Our solution scheme is based on the fast Fourier transform and thus fast and memory-efficient. We reformulate the explicit jump discretization using harmonically averaged thermal conductivities and obtain a symmetric positive definite system. Thus, a Lippmann-Schwinger formulation is possible. In contrast to Fourier and finite difference based discretization methods the explicit jump discretization does not exhibit ringing and checkerboarding artifacts.

1 Introduction

A conductivity tensor field $A : \mathrm{Y} \to \mathrm{Sym}(d)$ on a rectangular box $\mathrm{Y} \subseteq \mathbb{R}^d$, $d = (2, 3)$ and a macroscopic temperature gradient $\bar{\xi}$ are given. We further assume the conductivity tensor to be isotropic $A = \kappa\,\mathrm{Id}$ with $\kappa : \mathrm{Y} \to \mathbb{R}$ piecewise constant. We seek a periodic temperature field $\vartheta : \mathrm{Y} \to \mathbb{R}$ solving the corrector equation

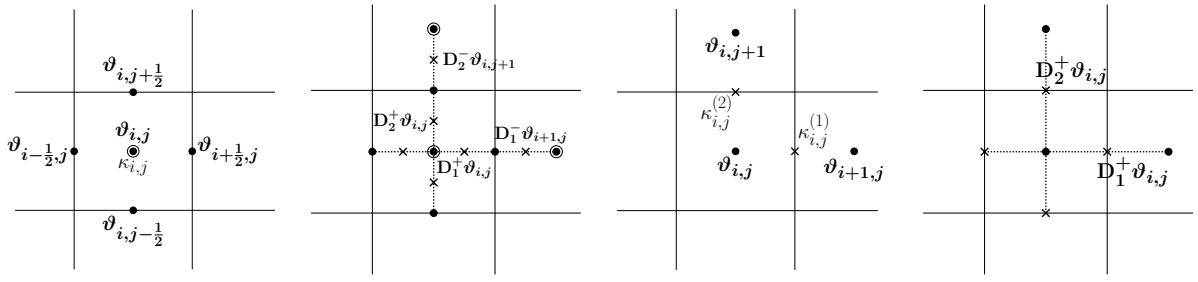
$$\operatorname{div} A(\bar{\xi} + \nabla\vartheta) = 0\,. \tag{1}$$

Besides the continuous and symmetric formulation of the corrector equation as a partial differential equation presented in Eq. (1) it is also possible to formulate the problem of heat conduction into a continuous but non-symmetric boundary integral equation. Wiegmann and Zemitis used a discrete version of this boundary integral formulation for the Explicit Jump Immersed Interface Method (EJIIM) [1]. Local solution fields computed with this method are free of artifacts and robust convergence in the presence of pores is observed. However, since the resulting equations of this formulation are non-symmetric they are solved using BiCGSTAB. For our purposes we prefer to use the conjugate gradient method (CG) due to the superior storage footprint. Thus, we want to reformulate the explicit jump discretization into a symmetric and positive definite system which enables us to use CG while retaining to positive features of explicit jump.

2 The explicit jump discretization

2.1 Setup

For simplicity we show our formulation of the explicit jump discretization in 2D. However, our numerical implementation and experiments are performed in 3D. The explicit jump discretization is a finite volume discretization. In its original formulation it features temperatures in the center $\vartheta_{i,j}$ and on the interfaces $\vartheta_{i+1,j}, \vartheta_{i,j+1}$ of each pixel, cf. Fig 1(a). The gradients are computed as forward differences between adjacent center and interface temperatures, cf. Fig. 1(b). We condense the interface temperatures consistenly, cf. appendix of [2], which requires introducing a harmonically averaged thermal conductivity tensor $A^*_{i,j} = \operatorname{diag}\left(\frac{2}{1/\kappa_{i+1,j}+1/\kappa_{i,j}}, \frac{2}{1/\kappa_{i,j+1}+1/\kappa_{i,j}}\right)$ at the pixel interfaces, cf. Fig. 1(c). Notice that we assumed the thermal conductivities of the constituents to be isotropic yet $A^*_{i,j}$ is in general othotropic.



(a) temperatures, orig. EJ **(b)** gradients, orig. EJ **(c)** temperatures, cond. EJ **(d)** gradients, cond. EJ

Fig. 1: Location of temperatures and gradients in the original an the condensed explicit jump (EJ) discretization

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2.2 Variational formulation and Lippmann-Schwinger equation

Using the condensed stencil presented in Figs. 1(c) and 1(d) we can formulate a positive and quadratic energy

$$\mathcal{E}(\vartheta) = \frac{1}{2N^2} \sum_{i,j=0}^{N-1} \left(\bar{\xi} + \nabla^+\vartheta\right)_{i,j} \cdot A^*_{i,j} \left(\bar{\xi} + \nabla^+\vartheta\right)_{i,j} \quad \text{with} \quad \nabla^+\vartheta = \begin{bmatrix} D_1^+\vartheta \\ D_2^+\vartheta \end{bmatrix} \equiv \begin{bmatrix} (\vartheta_{i+1,j} - \vartheta_{i,j})/h \\ (\vartheta_{i,j+1} - \vartheta_{i,j})/h \end{bmatrix} . \quad (2)$$

The critical point of $\mathcal{E}(\vartheta)$

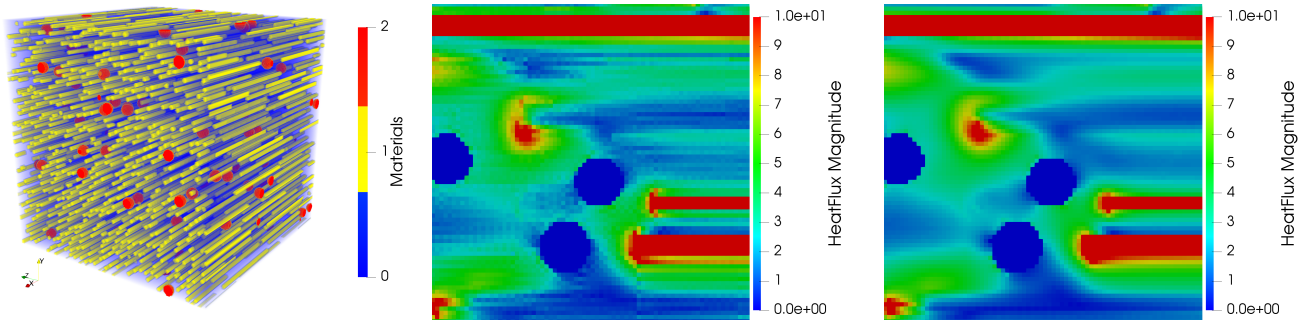
$$\operatorname{div}^- A^* \left(\bar{\xi} + \nabla^+\vartheta\right) = 0 \quad (3)$$

is the discrete version of the corrector equation of heat conduction Eq. (1). The operator div^- is the discrete backward divergence which is associated to the forward gradient operator ∇^+. This resulting equation is symmetric and positive definite and admits using CG. After introducing the reference conductivity $A_0 = \kappa_0 \,\mathrm{Id}$ and the associated Green's functions G_0 and Γ_0 the Lippmann-Schwinger formulation of Eq. (3) reads

$$\xi + \Gamma_0(A^* - A_0)\xi = \bar{\xi} \quad \text{with} \quad G_0 = \frac{1}{\kappa_0}\left(\operatorname{div}^-\nabla^+\right)^{-1} \quad \text{and} \quad \Gamma_0 = \nabla^+ G_0 \operatorname{div}^- . \quad (4)$$

A similar equation, albeit without harmonically averaged conductivity tensor A^*, has been established by Willot et al. [4].

3 Numerical experiments



(a) Microstructure **(b)** Fourier discretization [3] **(c)** Explicit jump discretization [2]

Fig. 2: Volume image of microstructure and heat flux for two different discretizations, magnified section of 80^2 pixels

We demonstrate our formulation of the explicit jump discretization for a generated microstructure of size 256^3. The structure comprises three materials: matrix (conductivity $\kappa = 1\ \frac{\mathrm{W}}{\mathrm{mK}}$), fibers ($\kappa = 1000\ \frac{\mathrm{W}}{\mathrm{mK}}$) and spherical inclusions ($\kappa = 0\ \frac{\mathrm{W}}{\mathrm{mK}}$), c.f. Fig. 2(a). The unidirectional fibers as well as the macroscopic temperature gradient are aligned in x direction. We solve the problem using CG with a convergence tolerance of 10^{-6}. Comparing the two heat flux fields in Figs. 2(b) and 2(c) reveals that the explicit jump discretization yields smooth solution fields even in the presence of pores and large material contrast.

4 Summary and conclusion

We transferred the explicit jump discretization into a symmetric and positive definite formulation which enabled using CG. Positive features of the explicit jump discretization, such as smooth solution fields, are retained. Integration into existing FFT-based solvers is ensured. This discretization can potentially be applied to non-local damage problems.

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