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A model order reduction technique for FFT-based microstructure simulation using a geometrically adapted reduced set of frequencies

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The FFT-based method introduced by Moulinec and Suquet [9] serves as an alternative for the classical finite element based simulation of periodic microstructures. This simulation approach makes use of fast Fourier transforms (FFT) as well as fixed-point iterations to solve the microscopic boundary value problem which is captured by the Lippmann-Schwinger equation. Kochmann et al. [5] introduced a model order reduction technique using a reduced set of frequencies to decrease the computational effort of solving the Lippmann-Schwinger equation in Fourier space. This earlier proposed method is based on a fixed sampling pattern, which determines the reduced set of frequencies. Instead of the fixed sampling pattern, we propose to use a geometrically adapted choice of frequencies, which corresponds to the representation of phases within the considered microstructure.

1 Reduced FFT-based microstructure simulation

The FE-FFT-based two-scale method may be used to capture the overall material behavior as well as microstructural material changes [7, 10]. The method utilizes the finite element (FE) method to solve the macroscopic boundary value problem (BVP) and the fast Fourier transform (FFT)-based method [9] to solve the microscopic BVP. Although the FFT-based method already serves as an efficient alternative to the classical FEM in the context of periodic microstructures, the development of model order reduction (MOR) techniques is advisable for the two-scale simulation of complex structures in reasonable computation times. An efficient two-scale simulation approach is presented in [2, 5] based on a coarsely discretized microstructure. This results in a required post-processing step to generate highly resolved microstructural results. Other, FFT-based MOR techniques utilize canonical polyadic decomposition (CDP) [11] or proper orthogonal decomposition (POD) [1] to generate more accurate results. The MOR technique, which is used in the present paper, is adapted to the spectral character of the FFT-based simulation approach and uses a reduced set of frequencies to solve the Lippmann-Schinger equation [8] in Fourier space [6].

2 A geometrically adapted reduced set of frequencies

The accuracy of the MOR technique using a reduced set of frequencies depends on the number of considered frequencies, but also on their choice. Since the choice of frequencies does not influence the efficiency of the method, we propose to use a geometrically adapted sampling pattern [3] instead of the earlier introduced fixed sampling pattern [6]. Doing that, a characteristic function is defined to be 1 within the inclusions and 0 within the matrix material to capture the microstructural

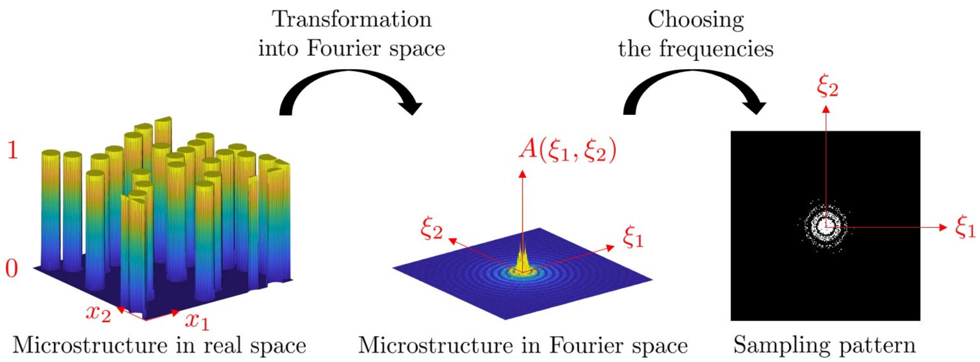

Fig. 1: Procedure for creating the geometrically adapted sampling pattern. Left: Microstructure in real space with coordinates x_1 and x_2, center: Required frequencies ξ_1 and ξ_2 with associated amplitude $A(\xi_1, \xi_2)$ for mapping the microstructure in Fourier space and right: Resulting geometrically adapted sampling pattern.

phase distribution. This function is transferred into Fourier space and the reduced set of frequencies is defined to consist of the frequencies with the highest amplitudes (see Fig. 1). The resulting reduced set of frequencies is subsequently used to

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decrease the computational effort of solving the Lippmann-Schwinger equation in Fourier space in terms of the basic fixed-point scheme.

3 Numerical example

In the linear elastic case, the resulting microstructural strain field is strongly related to the present phase distribution. This results in a very good performance of the geometrically adapted sampling pattern [3].

Nevertheless, also for the non-linear case, such an adapted sampling patter performs much better than the fixed sampling pattern, see Fig. 2. Here, the resulting microstructural stress field in x-direction for the geometrically adapted sampling pattern is compared to the results of the fixed sampling pattern and the reference solution (computed with the full set of frequencies). In addition, the difference of the reduced simulations compared to the reference solution is plotted in the bottom row. It can be seen, that the geometrically adapted sampling pattern leads to significantly better results compared to the fixed sampling pattern.

Independent of the definition of the reduced set of frequencies, the computational time is reduced by about 80 % using the proposed MOR technique.

In order to further improve the accuracy of the reduced simulation, the sampling pattern may also be defined based on the current strain field [4]. In that case, the sampling pattern needs to be updated after each load step.

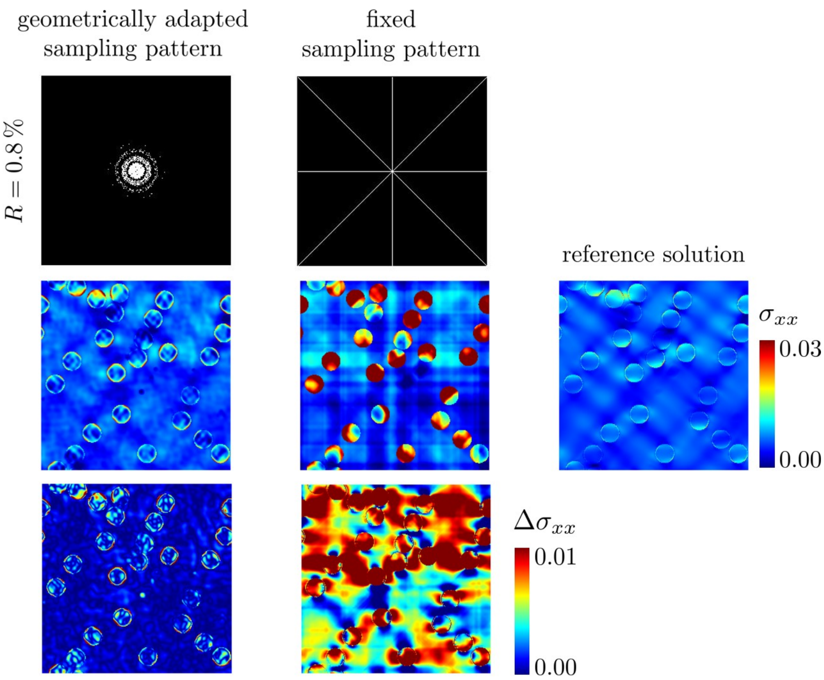

Fig. 2: Comparison of the computed stress in x-direction based on the geometrically adapted and fixed sampling pattern. Top: Sampling patterns, center: Results from the reduced simulation and reference solution (computed with the full frequency set) and bottom: Errors in the reduced simulations.

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