An Artificial Neural Network based Solution Scheme to periodic Homogenization

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Artificial neural networks (ANNs) have aroused research’s and industry’s interest due to their excellent approximation properties and are broadly used nowadays in the field of machine learning. In the present contribution, ANNs are used for finding solutions of periodic homogenization problems. The construction of ANN-based trial functions that satisfy the given boundary conditions on the microscale allows for the unconstrained optimization of a global energy potential. Goal of the present approach is a memory efficient solution scheme as ANNs are known to fit complicated functions with a relatively small number of internal parameters. The method is tested for a three-dimensional example using a global trial function and is qualitatively compared to a fast Fourier transform (FFT) based simulation.

1 Homogenization Framework

Computational homogenization is concerned with the prediction of material behavior based on microstructural effects. In general, the difference of length scales of the microstructure, which influences the material’s effective properties, and of the macroscopic problem at hand is of several orders of magnitude. Therefore, one usually chooses a representative volume element (RVE) $B$ of size $|B|$, which governs a statistically representative region in terms of its microstructure. In the present contribution, we consider the homogenization of electrostatic problems. Having a suitable RVE at hand, the global electrostatic potential appears as

$$\Pi(\phi) = \int_B \Psi(E) \, dV + \int_{\partial B_0} q \phi \, dA \quad \text{and} \quad \phi = \phi^* \text{ on } \partial B_0,$$

where $\phi$ denotes the scalar electric potential, $\Psi(E)$ is a constitutive electric energy density in terms of the electric field vector $E = -\nabla \phi$, $\partial B_0$ and $\partial B_0^*$ denote boundaries along with electric charges $q$ and electric potential $\phi^*$ as prescribed. In line with the assumption of length-scale separation and first-order homogenization, we decompose the electric field vector

$$E = \bar{E} - \nabla \tilde{\phi} \quad \text{with} \quad \bar{E} = \frac{1}{|B|} \int_B E \, dV$$

into a constant macroscopic contribution $\bar{E}$ and the gradient of the fluctuative scalar electric potential $\tilde{\phi}$. Finally, an optimization of the global microscopic potential (1) needs to be performed under appropriate boundary conditions. The celebrated Hill-Mandel macrohomogeneity condition [1] gives an integral relationship between the macroscopic and the microscopic energy potential. It is satisfied by the periodic boundary conditions

$$\tilde{\phi}(x^+) = \tilde{\phi}(x^-) \quad \text{and} \quad \frac{\partial \Psi}{\partial E} \cdot N(x^+) = -\frac{\partial \Psi}{\partial E} \cdot N(x^-) \text{ on } \partial B.$$

2 Optimization Principle

When optimizing the global energy potential (1), we need to constrain our approximation function to be periodic according to the boundary conditions (3). We thus follow the idea of LAGARIS ET AL. [2] who proposed the construction of a trial function

$$\tilde{\phi}_n(x, p) = A_0(x) + A_1(x)N_1(x, p_1) + A_2(x)N_2(x, p_2) + ... + A_n(x)N_n(x, p_n),$$

using artificial neural networks $N_i(x, p_i)$ with the coordinate $x$ as input and weights and biases $p_i$. Here, $A_i$ are multiplicative functions ensuring that the periodic boundary conditions are fulfilled a priori [3]. This procedure allows for an unconstrained optimization of the global potential

$$\Pi = \sup_{p} \frac{1}{|B|} \Pi(p),$$

now with respect to the weights and biases $p_i$. 

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3 Numerical Examples

We now test the robustness of the method for a three-dimensional cubic RVE of unit length \( l = 1 \) with a spherical inclusion of radius \( r_0 = 0.178l \). We then optimize the normalized global potential

\[
\Pi = \sup_p \frac{1}{|\mathcal{B}|} \Pi(p) = \sup_p \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} -\frac{1}{2} \kappa \mathbf{E}_t \cdot \mathbf{E}_t \, dV \quad \text{with} \quad \mathbf{E}_t = \mathbf{E} - \nabla \tilde{\phi}_t,
\]

where the material parameter is set to \( \kappa = 1 \) in the matrix and \( \kappa = 10 \) in the inclusion. The RVE is loaded with a macroscopic field of \( \mathbf{E}_1 = 1, \mathbf{E}_2 = 0, \mathbf{E}_3 = 0 \). The global trial function appears as

\[
\tilde{\phi}_t(x, p) = A_1 N_1(x, p_1) + A_2 N_x(x_1, x_2, p_{x12}) + A_3 N_x(x_1, x_3, p_{x13}) + A_4 N_x(x_2, x_3, p_{x23}) + A_5 N_x(x_1, p_{x1}) + A_6 N_x(x_2, p_{x2}) + A_7 N_x(x_3, p_{x3}),
\]

where periodicity is fulfilled by choosing the following multiplicative functions.

\[
A_1 = x_1(1 - x_1) x_2(1 - x_2) x_3(1 - x_3), \quad A_5 = x_1(1 - x_1), \\
A_2 = x_1(1 - x_1) x_2(1 - x_2), \quad A_6 = x_2(1 - x_2), \\
A_3 = x_1(1 - x_1) x_3(1 - x_3), \quad A_7 = x_3(1 - x_3), \\
A_4 = x_2(1 - x_2) x_3(1 - x_3).
\]

For the numerical integration, we employ \( 43 \times 43 \times 43 \) equidistant integration points. The ANN \( N_1 \) is a two-layer perceptron with 8 neurons in each layer. All other ANNs are single layer perceptrons, having 4 neurons along each edge ANN and 5 neurons along each surface ANN. The softplus function is chosen as activation function in the neurons. Figure 1 shows the contour plots for the electric field component \( E_1 \). One can see a good agreement with the FFT-based simulation.

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