Simplifying FFT-based computational homogenization with automatic differentiation

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Abstract

In the field of solid mechanics, Fast-Fourier Transform (FFT) techniques (1) are extensively employed to solve intricate homogenization problems. However, current FFT-based methods face challenges that limit their applicability to complex mechanical problems. These challenges include the manual implementation of constitutive laws and the use of computationally expensive and complex algorithms to couple microscale mechanisms to macroscale material behavior. Here, we explore the application of automatic differentiation (AD) (2) in the context of an FFT-based framework to address and alleviate these challenges, thereby simplifying computational homogenization.

In this study, we show how AD allows the straightforward computation of stresses and tangent operators directly from the energy density functional, which makes FFT-based methods more accessible for complex hyperelastic materials.We show that AD's ability to perform differentiation across complex tensor manipulations, FFT processes, conditional loops, and Newton-Krylov solvers facilitates the calculation of tangent operators for materials where local stiffness cannot be derived from strain energy density, such as elastoplastic materials, or when an close-form expression does not exist, as in computational homogenization. We apply AD-enhanced FFT-based framework to multiscale problems and show how AD eases the computation of homogenized stiffness tensors, a significant computational bottleneck in multiscale problems.

Our results demonstrate that using AD in conjunction with an FFT-based approach is extremely advantageous. This combination decreases the reliance on explicit expressions of stresses and tangent operators while preserving accuracy and computational efficiency. Moreover, it significantly streamlines the process of computational homogenization for complex solid mechanics problems. (1) H. Moulinec and P. Suquet, A numerical method for computing the overall response of non-linear composites with complex microstructure., Computer Methods in Applied Mechanics and Engineering,157, 1998.
(2) James Bradbury, Roy Frostig, Peter Hawkins, Matthew James Johnson, Chris Leary, Dougal Maclaurin, George Necula, Adam Paszke, Jake VanderPlas, Skye Wanderman-Milne, and Qiao Zhang, JAX: composable transformations of Python+NumPy programs, 2018

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