
Computing Virtual DMA Response of Viscoelastic Materials with an Enhanced Composite Voxels Method

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Abstract

Following the recent development of a FFT solver for computing DMA response of viscoelastic composite materials (1), we present several improvements. First, the tool has been transposed in python language using CUDA (Cupy) library for GPU acceleration, secondly and mainly, composite voxels methods (CVs) have been implemented. CVs are voxels crossed by an interface separating two distinct phases and whose effective properties are calculated by a homogenization law. This allows modeling the mechanical behavior of microstructure interfaces that are not perfectly localized between two FFT coordinates. CVs methods introduced by Kabel et al. (2) and developed in `Amitex_fft` code (3) for FFT codes simulating classic mechanical response of materials as a function of time was adapted to our virtual DMA tool, in which storage and loss moduli are computed as a function of frequency and/or temperature.

We present developed preprocessing tools generating microstructures meshed with CVs using 3 methods: subsampling, integration or analytical. These methods have been validated through DMA computed frequency response: 1) considering a 3D Hashin structure (2) (spherical inclusion with a core shell configuration satisfying specific material properties relationship between 3 phases) and compared made with the corresponding analytical solution, and 2) considering a 128^3 digital microstructure made of 17% short glass fibers embedded in a polyamide (PA66) matrix and a composite voxel approach which is compared to the 512^3 same microstructure without composite voxels. The known homogenization laws for composite voxels properties: Voigt, Reuss, or laminate, were tested in the frequency framework. Results reveal significant improvements in accuracy and enable us to work at lower resolutions than conventional FFT DMA simulations.

(1) André, S.; Boisse, J.; Noûs, C. An FFT Solver Used for Virtual Dynamic Mechanical Analysis Experiments: Application to a Glassy/Amorphous System and to a Particulate Composite. *Journal of Theoretical, Computational and Applied Mechanics* 2021.

(2) Kabel, M.; Merkert, D.; Schneider, M. Use of Composite Voxels in FFT-Based Homogenization. *Computer Methods in Applied Mechanics and Engineering* 2015, 294, 168–188.

(3) Charière, R.; Marano, A.; Gélébart, L. Use of Composite Voxels in FFT Based Elastic Simulations of Hollow Glass Microspheres/Polypropylene Composites. *International Journal of Solids and Structures* 2020, 182–183, 1–14.

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