Fast Fourier Transform (FFT)-based models for microstructure/property relationships of polycrystalline materials

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Crystal plasticity (CP) are well-established models, used, e.g., in scale-bridging applications to obtain microstructure-sensitive mechanical response of polycrystalline materials. These models require a proper consideration of the single crystal deformation mechanisms, a representative description of the microstructure, and an appropriate scheme to connect the microstates with the macroscopic response. FFT-based methods, originally proposed by Moulinec and Suquet for composites [1] and extended to polycrystals [2] (our most recent formulation, including non-local large-strain elasto-viscoplasticity reported in [3]) are attractive due to their higher efficiency compared with CP-Finite Elements, and their direct use of voxelized microstructural images. In this talk, we will report recent progress on FFT-based polycrystal plasticity, with emphasis in novel implementations, including strain-gradient plasticity, achieving geometric accuracy working with voxelized images, non-periodic extensions, and dynamic effects. We will show applications of these methods to: micromechanics of nano-metallic laminates, wave propagation in heterogeneous materials, multiscale coupling with Lagrangian hydrocodes, integration with 3-D characterization methods, and use for training and validation of machine-learning methods.

[1] H. Moulinec, P. Suquet, A numerical method for computing the overall response of nonlinear composites with complex microstructure, *Comput. Methods Appl. Mech. Eng.* **157**(1–2), 69–94, 1998. https://doi.org/10.1016/S0045-7825(97)00218-1

[2] R.A. Lebensohn, N-site modelling of a 3D viscoplastic polycrystal using Fast Fourier Transform, *Acta Mater.* **49**(14), 2723–2737, 2001. https://doi.org/10.1016/S1359-6454(01)00172-0

[3] M. Zecevic, R.A. Lebensohn, L. Capolungo, Non-local large-strain FFT-based formulation and its application to interface-dominated plasticity of nanometallic laminates, *J. Mech. Phys. Solids* **173**, 105187, 2023. https://doi.org/10.1016/j.jmps.2022.105187