

Natural description of non-periodic boundary conditions in the context of Fast Fourier Transform (FFT)-based approach: parallel implementation in *AMITEX_FFTP*

Yaovi Armand AMOUZOU-ADOUN¹; Lionel GÉLÉBART¹; Cédric FLAGEUL²; Yushan WANG³

¹ Université Paris-Saclay, CEA, SRMA, Gif-sur-Yvette, 91191, France

² Curiosity Group, Pprime Institute, CNRS - University of Poitiers - ENSMA, France

³ Université Paris-Saclay, UVSQ, CNRS, CEA, Maison de la Simulation, 91191, Gif-sur-Yvette, France

ABSTRACT

Developed in the context of numerical homogenization following the pioneer work of Moulinec and Suquet [1], Fast Fourier Transform (FFT)-based approach is intrinsically limited to periodic boundary conditions (BCs). The present work aims to overcome the periodic loading limitation. This approach is implemented in the massively parallel (MPI) Fortran solver *AMITEX_FFTP* [2], with the objective of investigating the (non-)linear mechanical simulations on heterogeneous unit-cells.

We present a natural description of non-periodic BCs (Dirichlet and Neumann types) leveraging the Discrete Trigonometric Transforms (DTT) [3, 4]. To solve mechanical problems, a simple and versatile iterative displacement-based fixed-point algorithm with Anderson's convergence acceleration procedure is discussed. We introduce various pre-conditioners and finite difference schemes allowing to compute the Green's operators. In this regard, the recently proposed tetrahedron-based discretization scheme [5] is compared to the hexahedral-based finite difference scheme in the context of non-periodic BCs. The current progresses help to close the gap between finite element and FFT-based approaches while preserving the latter method's numerical performance. Several examples of boundary value problems are discussed to demonstrate the ability of the proposed approach to simulate desired structures. Fig. 1 shows an encouraging example of experiment-inspired torsion-bending test of a single crystal.

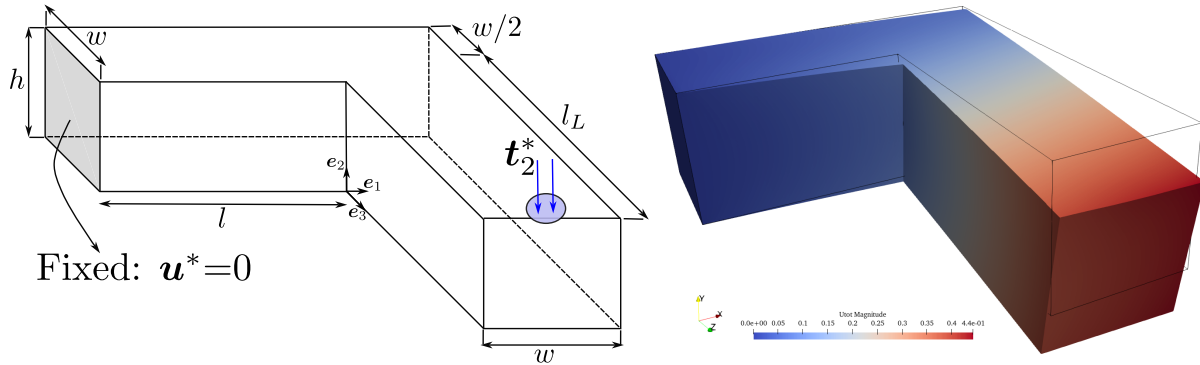


Figure 1: Torsion-bending of a single crystal.

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