FFT methods for solving the elasto-static and the dislocation transport equations in field dislocation mechanics

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Abstract. The first contribution addresses the critical question of determining accurate local mechanical fields using FFT methods without artificial fluctuations arising from materials and defects induced discontinuities. Precisely, the present contribution introduces a numerical approach based on intrinsic discrete Fourier transforms for the simultaneous treatment of material discontinuities arising from the presence of dislocations and from elastic heterogeneities. To this end, the elasto-static equations of the field dislocation mechanics theory for periodic heterogeneous materials are numerically solved with Fast Fourier Transform (FFT) in the case of dislocations inside or outside elastic heterogeneities. A centered finite difference scheme for differential rules are used for numerically solving the Poisson-type equation in the Fourier space, while centered finite differences on a rotated grid is chosen for the computation of the modified Fourier-Green's operator associated with the Lippmann-Schwinger-type equation. By comparing different methods with analytical solutions for an edge dislocation in a composite material, it is found that the present spectral method is accurate, devoid of any numerical oscillation, and is efficient even for an infinite elastic contrast like a hole embedded in a matrix containing a dislocation. The present FFT method is then used to simulate physical cases such as dislocation dipoles located near the matrix/inclusion interface in a 2D composite material and a dislocation square loop surrounding a hard cubic inclusion in a 3D composite material. In these configurations, the spectral method allows investigating accurately the elastic interactions and image stresses due to dislocation fields in the presence of elastic inhomogeneities.

In a second contribution, a numerical spectral approach is developed to solve in a fast, stable and accurate fashion, the quasi-linear hyperbolic transport equation governing the spatio-temporal evolution of the dislocation density tensor in the mechanics of dislocation fields. The approach relies on using the Fast Fourier Transform algorithm. Low-pass spectral filters are employed to control both the high frequency Gibbs oscillations inherent to the Fourier method and the fast-growing numerical instabilities resulting from the hyperbolic nature of the transport equation. The numerical scheme is validated by comparison with an exact solution in the 1D case corresponding to dislocation dipole annihilation. The expansion and annihilation of dislocation loops in 2D and 3D settings are also produced and compared with finite element approximations. The spectral solutions are shown to be stable, more accurate for low Courant numbers and much less computation time-consuming than the finite element technique based on an explicit Galerkin-least squares scheme.

Keywords: Fast Fourier Transforms, heterogeneities, dislocations, transport equation, spectral filters, heterogeneous media, elastic fields.