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OptiDis: Toward fast anisotropic DD based on Stroh formalism.

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ABSTRACT

Dislocation Dynamics (DD) simulations in the hypothesis of isotropic elasticity have proved great reliability to predict the plastic behaviour of crystalline materials. However it is often the case at high temperature (for instance in irradiated BCC iron) that the structural properties of a material will be better described using full anisotropic treatment of the elastic interaction between dislocations.

The computation of the internal elastic forces is by far the most resource consuming step in DD simulations, which is even more true for anisotropic elasticity in the absence of explicit Green’s function.

L. Dupuy, J. Soulacioux and M. Fidel showed that the approaches summarized in Yin [3] can be accelerated using spherical harmonics expansions of the Stroh matrices. This feature was implemented in the DD code OptiDis in order to power the anisotropic forces computation. Here we recall the formalism and we discuss optimizations, performances as well as motivations for future developments.

IMPLEMENTATION AND PERFORMANCES

Our experimentsations were performed on the core program OptiDis whose data structure relies heavily on the open source ScalFMM library [1]. The latter also provides the generic Fast Multipole algorithms. OptiDis is a parallel version of NumbDis, it implements almost all functionalities of NumbDis while providing a hybrid OpenMP/MPI paradigm and a cache-conscious data structure.

ONGOING & PERSPECTIVES

Ongoing
• Optimized expansion for hexagonal crystallographs
• Perspectives
• Implementation of the farfield (either iso- or anisotropic)
• Efficient analytic integration of the expansion over the target segments
• Derivation of a consistent non-singular theory for the Stroh approach

REFERENCES

1: ScalFMM: software library to simulate large scale n-body interactions using the fast multipole method, developed by the hipacc team, inria bordeaux

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