OptiDis: Toward fast anisotropic dislocation dynamics based on Stroh formalism

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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 resources consuming step in DD simulations, which is even more true for anisotropic elasticity in the absence of explicit Green's function.

L. Dupuy, J. Soulacroix and M. Fivel showed that the approaches summarized in Yin [6] 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.

**SPEHERICAL HARMONIC ANALYSIS**

Stroh matrices only depend on the orientation of the source, i.e. \( X = X(\hat{\mathbf{r}}/|\mathbf{r}|) \) (see fig 2) hence they can be expanded into spherical harmonics.

\[
X(\hat{\mathbf{r}}/|\mathbf{r}|) \approx \sum_{|\mathbf{m}|,|s|} x_m^s Y_m^s(\theta, \phi) \sin \theta d\theta d\phi
\]

where \( Y_m^s \) denotes the well known spherical harmonics and

\[
x_m^s = \int_0^{2\pi} \int_0^\pi X(\hat{\mathbf{r}}/|\mathbf{r}|, \theta, \phi) \cos \theta d\theta d\phi
\]

are the coefficients of the expansion.

Given that Stroh matrices are real the expansion reduces to

\[
X = \sum_{|\mathbf{m}|,|s|} x_m^s Y_m^s(\theta, \phi)
\]

On the other hand depending on the symmetries of \( X \) in \( \theta \) or \( \phi \) some coefficients of the expansions are known to be null (potentially a lot). Once implemented these simplifications lead to a significant acceleration of the method (see fig 4).

**IMPLEMENTATION AND PERFORMANCES**

Our experimentations 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 Muplone algorithms. OptiDis is a parallel version of NumoDis, it implements almost all functionalities of NumoDis while providing a hybrid OpenMP/MPI paradigm and a cache-conscious data structure.

**ONGOING & PERSPECTIVES**

Ongoing
- Optimized expansion for hexagonal crystallography

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 biopics team, inria bordeaux.


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