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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 in predicting the plastic behaviour of crystalline materials. However, it is often the case that 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. 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.

ANISOTROPIC MODEL

The stress field created by a dislocation loop \( (l', t') \) at field point \( x \) is given by Mura’s formula [6]

\[
\sigma(x) = \varepsilon_{ij} \varepsilon_{kl} C_{ijkl} \delta(x - l') \delta(t - t')
\]

(1)

The nodal force \( f_s \) acting at the extremities of a finite dislocation line \((b, t)\) is obtained by integration of the Peach-Koehler force \( (F^P = (\sigma(x) - x \times t) / (2 \pi \rho)) \) over the target line, i.e.

\[
(f_s)_b = \int (\sigma(x) - x \times t) / (2 \pi \rho) dx
\]

where \( N_{ir}=2 \) are linear shape functions. The cost of updating the nodal forces at each time step is quadratic and involves the evaluation of 2 line integrals, therefore it is usually the bottleneck of DD simulations. Moreover, there does not exist an analytic closed form for the anisotropic elastic Green’s function \( G \). Recently Aubry et al. [2] used an integral representation of \( G \) and developed a fast method based on parabolic expansions in order to evaluate the double line integral semi-analytically. On the other hand, past works [5] showed that the anisotropic stress field can be efficiently described using the Stroh axiomatic formalism with (2) the Willis-Steed-Lothe formula for the finite line.

Willis-Steed-Lothe

\[
us_n = \frac{1}{16\pi} \left[ m b C_{ijkl} Q_{ijkl} \right] \left[ \left[ \eta_{ij} \eta_{kl} - (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) / 2 \right] \right] \left[ (b \times t) \cdot \eta_{ij} \right] / (4 \pi \rho)
\]

(2)

where Stroh matrices \( Q \) and \( N \) [5] only depend on \( C_{ijkl} \) and \( r \). They are computed from the eigenvectors of a \( 6 \times 6 \) matrix \( N \) depending on \( (\cos \theta, \sin \theta) \). The notations are recalled fig 1 and the stress field reads

\[
\sigma(x, t, b) = C_{ijkl} \eta_{ij} \eta_{kl} \left[ \frac{(b \times t) \cdot \eta_{ij}}{4 \pi \rho} \right]
\]

In the collinear case \((d = 0)\) the expression is slightly more complicated but can be condensed as follows

\[
us_n (d = 0) = \frac{1}{16 \pi} \left[ m b C_{ijkl} Q_{ijkl} \right] \left[ \left[ \eta_{ij} \eta_{kl} - (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) / 2 \right] \right] \left[ \frac{(b \times t) \cdot \eta_{ij}}{4 \pi \rho} \right]
\]

The singularity in the limit \( r \to 0 \) is currently handled using a simple cutoff parameter like the one defined in [6].

Anisotropy ratio

The degree of anisotropy is quantified by the ratio \( A = 2C_{ijkl}(C_{11} - C_{12}) \). For the BCC \( A = F_i \), this ratio goes from \( A_{BCC} = 2.3 \) to \( A_{L2_1} = 7.1 \).

Spherical harmonic analysis

Stroh matrices only depend on the orientation of the source, i.e. \( X = X(\theta, \phi) \) (see fig 2) hence they can be expanded into spherical harmonics.

\[
X(\theta, \phi) \approx \sum_{l=0}^{\infty} \sum_{m=-l}^{l} X_l^m(\theta, \phi) p_m(\cos \theta) e^{im\phi}
\]

where \( X_l^m \) denote the well known spherical harmonics and

\[
x_l^m = \int_0^{\pi} \int_0^{2\pi} X(\theta, \phi) Y_l^m(\theta, \phi) \sin \theta \sin \phi d\theta d\phi
\]

are the coefficients of the expansion.

Given that Stroh matrices are real the expansion reduces to

\[
X = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} X_l^m(\theta, \phi) p_m(\cos \theta)
\]

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).

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] ScaFFM: software library to simulate large scale n-body interactions using the fast multipole method, developed in l3s team, inria bordeaux.

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