OptiDis: Toward fast anisotropic dislocation dynamics based on Stroh formalism
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OptiDis: Toward fast anisotropic DD based on Stroh formalism.

**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. Souloumiac and M. Fidel 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.

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**ANISOTROPIC MODEL**

The stress field created by a dislocation loop \((N, l')\) at field point \(x\) is given by Mura’s formula [6]\
\[
\sigma(x) = \text{const} \sum_{n, s} \int_{S} \frac{d^n}{d^n} \frac{\delta(x - x')}{2\pi r} \frac{1}{r} \frac{d^s}{d^s} \phi(n, s, x') dx'\
\]
where \(N = 1, 2\) 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 \(G\), developed a fast method based in order to parametric expansions in order to evaluate the double line integral semi-analytically. On the other hand, past works [6] showed that the anisotropic stress field can be efficiently described using the Stroh axiometric formalism with (2) the Willis-Steeds-Lothe formula for the line.

**Willis-Steeds-Lothe**

\[
\sigma_m = \frac{1}{4\pi} \sum_{s, n} h C_{mns} \int_{S} \frac{d^n}{d^n} \frac{d^s}{d^s} \phi(n, s, x') dx'\
\]
where Stroh matrices \(Q\) and \(N\) [5] only depend on \(C_{mns}\) and \(\tau\). They are computed from the eigenvectors of a \(6 \times 6\) matrix \(\mathbf{N}\) depending on \(\theta\) and \(\phi\) where \((\hat{d}, \hat{n}) = a \hat{C}_{mns} \hat{h}\). The notations are recalled fig 1 and the stress field reads\n
\[
\sigma_{m}(x, n, s, t, b) = C_{mns} \phi_{n}(x, t, b)
\]

In the collinear case \((\vartheta = 0)\) the expression is slightly more complicated and can be condensed as follows\n
\[
\sigma_{m}(x, s, t, b) = \sum_{n} C_{mns} \phi_{n}(x, t, b)
\]

The singularity in the limit \(\tau \to 0\) 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 \(A = 2C_{12}(C_{11} - C_{12})\). For the BCC \(\alpha = -F_{i}\), this ratio goes from \(A_{\alpha} = 2.3\) to \(A_{\alpha} = 7.1\).

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**IMPLEMENTATION AND PERFORMANCES**

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

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**REFERENCES**

[1] ScaLAPACK: software library to simulate large scale n-body interactions using the fast multiple method.
[6] Jie Yin, David M Barnett, and Wei Cai. Efficient computation of forces on dislocation segment s in \(120^\circ\) micro-crack simulations and increasing tree depth (left). An example of defects distribution and a propagating Frank-Read source (right).

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**ONGOING & PERSPECTIVES**

- Ongoing
- Optimized expansion for hexagonal crystallographies
- 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

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**TABLE 1:**

<table>
<thead>
<tr>
<th>Angle (°)</th>
<th>Computed error (°)</th>
<th>Relative error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.125</td>
<td>1.25</td>
</tr>
<tr>
<td>5</td>
<td>0.025</td>
<td>0.25</td>
</tr>
<tr>
<td>10</td>
<td>0.005</td>
<td>0.05</td>
</tr>
</tbody>
</table>

**FIGURE 2:** Sphasonic matrix components at \(T = 25°C\) for \(\theta \in [0, \pi]\) and \(\phi \in [0, 2\pi]\).

**FIGURE 3:** Accuracy of the expansion for various temperatures.

**FIGURE 4:** Theoretical number of flops involved in self force evaluation (left) and relative computational cost for \(\approx 1000\) segments based on CPU time (right).

**FIGURE 5:** Isotropic near- and farfield computational time balancing for a uniform distribution of dislocation loops and increasing tree depth (left). An example of defects distribution and a propagating Frank-Read source (right).