An Efficient Interpolation Based FMM for Dislocation Dynamics Simulations

Based on uniform grids and FFT acceleration.

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Dislocation Dynamics (DD)
  Isotropic DD Simulations
  Fast Multipole Formulations

A new efficient Fast Multipole DD
  An interpolation based fast summation
  Fast Multipole summation scheme
  Shifting derivatives

Numerical Benchmarks
  Artificial test cases
  Accuracy & Running Time

Conclusions & Perspectives
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DD Simulations

- Dislocations: **line defects** induced by radiations...
- Simulating **elastic interactions** in massive ensembles of dislocations in order to
  - study strain hardening,
  - better understand crystal plasticity.
- Clear band channels in Zr alloys, Laurent Dupuy (CEA)

**Figure 1:** A Frank-Read Source (FRS) simulated in **OptiDis**.

**Figure 2:** Top: Channeling mechanisms in Zr. Bottom: An FRS splits a loop.
DD simulations

- Spatial Discretization: Dislocation line → **Segments**
- Main loop:
  
  **Compute Forces** → Update Topology → Handle Collisions

  \[ \text{Output Statistics} \leftarrow \text{Refine Mesh} \downarrow \]

- Let \((b, t, L)\) characterize a target dislocation line \([x^3 x^4]\).

- The **elastic force** acting on \(x^4\) resulting from stress state \(\sigma\)

\[
f_i^4 = \int_0^L \varepsilon_{ijk} \sigma_{jp}(x) b_p t_k \frac{x}{L} dx
\]
• The *internal* elastic stress created by the network \((C')\) equals

\[
\sigma_{ij}(x) = C_{ijkl} \int_{(C')} \varepsilon_{lnh} C_{pqmn} G_{kp,q}(|x - x'|) b'_m t'_h dx
\]

• The *isotropic* elastic Green’s function reads as

\[
G_{ij}(r) = \frac{1}{8\pi\mu} \left( \delta_{ij} r_{,pp} - \frac{1}{2(1 - \nu)} r_{,ij} \right)
\]

where \((\mu, \nu)\) are elastic constants and \(r = |x - x'|\).

• **Boundary Integral** formulation involving fast decreasing and long-ranged interactions
The Fast Multipole Method (FMM)

- Direct computation $\mathcal{O}(n^2)$, where $n = \#\text{segments}$
- Alternative: Fast Multipole Method (FMM)
  - Approx. $n$-body interactions in $\mathcal{O}(n)$ ops
  - Hierarchical partitionning (octree)
  - Balance nearfield and farfield
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Figure 3: Definition of FMM operators on a 1D tree structure.
Fast Multipole DD (FMDD)

- Nearfield interactions
  - Numerical integration **prohibitiv** as $r \downarrow$ [Arsenlis et al., 2007]
  - **Analytical formulae** via non-singular theory [Cai et al., 2006]
    \[
    r_a = \sqrt{r^2 + a^2}
    \]

- Farfield interactions (existing schemes)
  - Taylor expansions [Arsenlis et al., 2007]
  - Spherical Harmonics [Zhao et al., 2010] ...
  - **Kernel specific** and **slow convergence** (w.r.t. # modes)
  - **Alternative:** interpolation based FMM
    - **Kernel independent**
    - Black-Box FMM [Fong and Darve, 2009]
    - Optimizations, *e.g.*, compression [Messner et al., 2012]
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A new efficient Fast Multipole DD

Contributions to OptiDis code:

- Rely on ScalFMM, an open-source parallel FMM library.
  - Extend physical capabilities
  - Benefit from abstraction and parallelism
- Apply Black-Box FMM to DD:
  - Chebyshev polynomials: $O(p^6)$ M2L and overall
  - Exact integration over segment
  - Extend bounding box
- However, no compression allowed
  - $k$ is neither symmetric, nor homogeneous.
  - $k$ has high dimension (10 with sym.)
- Implement faster scheme: UFMM
  - Lagrange interpolation
  - FFT acceleration: $O(p^3)$ M2L, $O(p^3 \log p)$ overall
Farfield approximation

- $k$: the interaction kernel

$$k_{ijk}(x, y) = r_{ijk}$$

- $\tilde{k}$: the order-$p$ interpolant of $k$

$$\tilde{k}(x, y) = \sum_{|\alpha| \leq p} S(\bar{x}_\alpha, x) \sum_{|\beta| \leq p} k(\bar{x}_\alpha, \bar{y}_\beta) S(\bar{y}_\beta, y)$$

- Chebyshev interp.: Dense MVP $O(p^6)$
Farfield approximation

- **k**: the interaction kernel

\[ k_{ijk}(x, y) = r_{ijk} \]

- **\( \tilde{k} \)**: the order-\( p \) interpolant of **k**

\[ \tilde{k}(x, y) = \sum_{|\alpha| \leq p} S(\bar{x}_\alpha, x) \mathcal{F}^{-1} \left[ \mathcal{F}(k(\bar{x}_\alpha, 0)) : \mathcal{F}(S(\bar{y}_\beta, y)) \right] \]

- Lagrange interp.: Circ. Embed. + FFT \( O(p^3 \log p) \)
Farfield approximation

- approximation of the elastic stress field $\sigma$

$$\sigma_{ij}(x) \approx \frac{\mu}{8\pi} (\tilde{\sigma}_{ij}^A(x) + \tilde{\sigma}_{ji}^A(x) + \frac{2}{1-\nu} (\tilde{\sigma}_{ij}^B - \delta_{ij}\tilde{\sigma}_{pp})(x))$$

where

$$\tilde{\sigma}_{ij}^A(x) = \sum_{|\alpha| \leq p} S_\alpha(x) \sum_{|\beta| \leq p} k_{\alpha\beta}^{mp} \varepsilon_{jm} \int_{(C')} S_\beta(x') b_k t_i dx'$$

$$\tilde{\sigma}_{ij}^B(x) = \sum_{|\alpha| \leq p} S_\alpha(x) \sum_{|\beta| \leq p} k_{ij\beta}^{nm} \varepsilon_{nm} \int_{(C')} S_\beta(x') b_k t'_n dx'$$

- Farfield force approximation (L2P)

$$\tilde{f}_i^4 = \int_0^L \tilde{\sigma}_{ij}(x) b_p t_k \frac{x}{L} dx, \forall i \in \{1, 2, 3\}$$
FM summation scheme

\[(\tilde{\sigma}^A_{ij}) \quad (\tilde{\sigma}^B_{ij})\]

**P2M** Aggregate segments contributions at interpolation nodes

\[\mathcal{M}^\beta_{ik} = \int_{C} S_\beta(y) b_k dy_i\]

**M2L** Transfer multipole to local expansion

\[\mathcal{L}^\alpha_{ij} = \sum_{|\beta| \leq \ell} R^{\alpha\beta}_{,mp}\varepsilon_{jmk}\mathcal{M}^\beta_{ik}\]

\[\mathcal{L}^\alpha_{ij} = \sum_{|\beta| \leq \ell} R^{\alpha\beta}_{ijn}\varepsilon_{nmk}\mathcal{M}^\beta_{nk}\]

**L2P** Accumulate contributions at target points

\[\tilde{\sigma}_{ij}(x) = \sum_{|\alpha| \leq \ell} S_\alpha(x) \mathcal{L}^\alpha_{ij}\]
Shifting derivatives: Formulation

• Let us consider the **lower dimensionnal** kernel

\[ k_{ij}(x, y) = r_{,ij} = \nabla_{x_i} \nabla_{x_j} r \]

• \( \tilde{k} \): the order-\( p \) interpolant of \( k \)

\[ \tilde{k}(x, y) = \sum_{|\alpha| \leq p} \sum_{|\beta| \leq p} k(\bar{x}_\alpha, \bar{y}_\beta) S(\bar{y}_\beta, y) \]

• **Trick** (applies to many BIE formulations)

\[ \tilde{k}_{ijk}(x, y) \approx \nabla_{x_k} \tilde{k}_{ij}(x, y) = -\nabla_{y_k} \tilde{k}_{ij}(x, y) \]

• Thus, the new interpolation formula reads as

\[ \tilde{k}_{ijk}(x, y) \approx - \sum_{|\alpha| \leq p} \sum_{|\beta| \leq p} k_{ij}(\bar{x}_\alpha, \bar{y}_\beta) \nabla_{y_k} S(\bar{y}_\beta, y) \]
Shifting derivatives: Benefits

- Combine stress and energy farfields
  \[
  E((C)) = -\frac{\mu}{8\pi} \oint_{(C)} b_i dx_i \oint_{(C)} r_{kk} b'_j dx'_j + \ldots
  \]

- Theoretical memory requirements at M2L step:
  - Black-Box FMM $O(p^6)$
  - Uniform FMM $O((2p - 1)^3)$

<table>
<thead>
<tr>
<th>Approach</th>
<th>$O^{\sigma}_t$</th>
<th>$O^E_t$</th>
<th>$O^{\sigma+E}_m$</th>
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<tr>
<td>$R,ijm$</td>
<td>45</td>
<td>-</td>
<td>10 + 6</td>
</tr>
<tr>
<td>$R,ij\nabla_m$</td>
<td>21</td>
<td>36</td>
<td>6</td>
</tr>
<tr>
<td>$(R,ij</td>
<td>R,pp)\nabla_m$</td>
<td>12</td>
<td>36</td>
</tr>
</tbody>
</table>

**Figure 4:** Relative cost (t: time, m: memory) of various approaches.

**Figure 5:** Theoretical memory requirements w.r.t. order $p$. 
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Artificial test cases: density of BCC loops

**Figure 6:** Density of $d = 5e19$ BCC loops with $b = [111]$, diameter $d = 100$ and $L = 20$. The exact nodal force (left) and segment energy (right) is represented on the dislocation lines for each configuration.
Artificial test cases: 1 BCC loop per leaf

Figure 7: 1 BCC loops per leaf with $b = [111]$, diameter $d = 500$ and $L = L_{min} + 1 = L_{max} - 1 = 100$. The exact nodal force (left) and segment energy (right) is represented on the dislocation lines for each configuration.
Accuracy: 1 BCC loop per leaf

Figure 8: Accuracy of the nodal forces (left) and energy (right) evaluation for different interpolation schemes with respect to the interpolation order.
Figure 9: Computational time required by nodal forces and energy evaluation for different interpolation schemes ($p = 5$) w.r.t. # segments.
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Conclusions & Perspectives:

Conclusions:

- Efficient $\mathcal{O}(n)$ scheme for force & energy computation
- low computational cost: $\mathcal{O}(p^3)$ with $p \approx 5$
- low memory footprint: $\mathcal{O}(p^3)$
- Optimized: shifted derivative, homogeneity...
- Cache Aware Data Structure (Etcheverry’s thesis)

Perspectives:

- Extend to anisotropic case [Aubry and Arsenlis, 2013]
Related Works

Ongoing:

- Linear time generation of Gaussian Random Fields
  - Eric Darve, Amalia Kokkinaki, Peter Kitanidis (Stanford)
  - Fast Multipole accelerated Randomized SVD ($O(r^2 n)$)
  - Obs. perturbation in Ensemble KF
  - Poster Session CSM08 “FMR: Fast randomized algorithms for covariance matrix computations.”

- Multipolar interactions for advanced MD simulations
  - Benjamin Stamm, Etienne Polack (Paris VI)
  - high dimensionnal interaction tensors
  - arbitrary-order partial derivatives of $1/r$

A non-singular continuum theory of dislocations. 

The black-box fast multipole method. 
*Journal of Computational Physics, 228*(23):8712–8725.

Messner, M., Bramas, B., Coulaud, O., and Darve, E. (2012).  
Optimized m2l kernels for the chebyshev interpolation based fast multipole method.  