

An Efficient Interpolation Based FMM for Dislocation Dynamics Simulations

Based on uniform grids and FFT acceleration.

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PASC 2016, Lausanne, June 9, 2016

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Partially funded by the associate team **FastLA** and the **ANR Cosinus**.

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**)

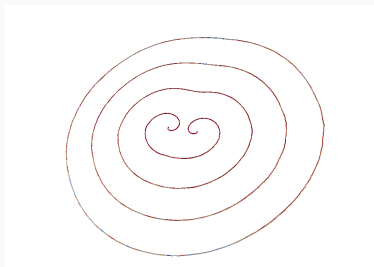


Figure 1: A Frank-Read Source (FRS) simulated in **OptiDis**.

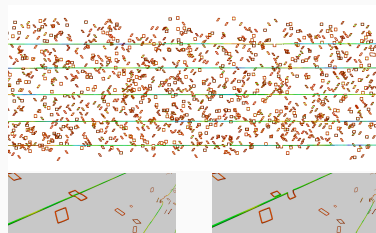
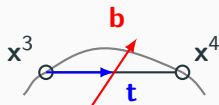


Figure 2: **Top:** Channelling mechanisms in Zr. **Bottom:** An FRS splits a loop.

- Spatial Discretization: Dislocation line \rightarrow **Segments**
- Main loop:
 - Compute Forces** \rightarrow Update Topology \rightarrow Handle Collisions
 - \swarrow Output Statistics \leftarrow Refine Mesh \searrow
- Let $(\mathbf{b}, \mathbf{t}, L)$ characterize a target dislocation line $[\mathbf{x}^3 \mathbf{x}^4]$.



- The **elastic force** acting on \mathbf{x}^4 resulting from stress state σ

$$f_i^4 = \int_0^L \varepsilon_{ijk} \sigma_{jp}(x) b_p t_k \frac{x}{L} dx$$

- The *internal* elastic stress created by the network (\mathcal{C}') equals

$$\sigma_{ij}(\mathbf{x}) = C_{ijkl} \oint_{(\mathcal{C}')} \varepsilon_{lnh} C_{pqmn} G_{kp,q}(|\mathbf{x} - \mathbf{x}'|) b'_m t'_h dx$$

- The *isotropic* elastic Green's function reads as

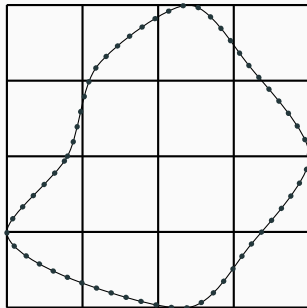
$$G_{ij}(r) = \frac{1}{8\pi\mu} (\delta_{ij} r_{,pp} - \frac{1}{2(1-\nu)} r_{,ij})$$

where (μ, ν) are elastic constants and $r = |\mathbf{x} - \mathbf{x}'|$.

- **Boundary Integral** formulation involving fast decreasing and **long-ranged interactions**

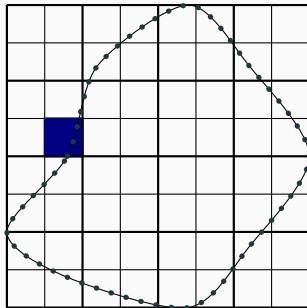
The Fast Multipole Method (FMM)

- Direct computation $\mathcal{O}(n^2)$, where $n = \#segments$
- Alternative: Fast Multipole Method (FMM)
 - **Approx.** n -body interactions in $\mathcal{O}(n)$ ops
 - Hierarchical partitioning (octree)
 - Balance nearfield and farfield



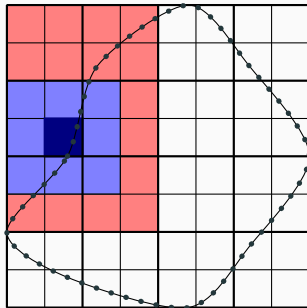
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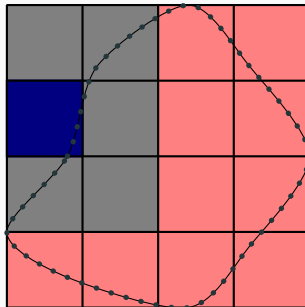
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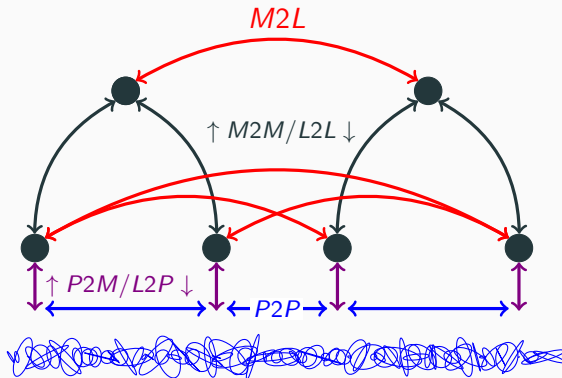


Figure 3: Definition of FMM operators on a 1D tree structure.

Fast Multipole DD (FMDD)

- Nearfield interactions
 - Numerical integration **prohibitiv** as $r \searrow$ [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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Contributions to **OptiDis** code:

- Rely on **ScaIFMM**, an open-source parallel FMM library.
 - Extend physical capabilities
 - Benefit from abstraction and parallelism
- Apply **Black-Box FMM** to DD:
 - Chebyshev polynomials: $\mathcal{O}(p^6)$ 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: $\mathcal{O}(p^3)$ M2L, $\mathcal{O}(p^3 \log p)$ overall

Farfield approximation

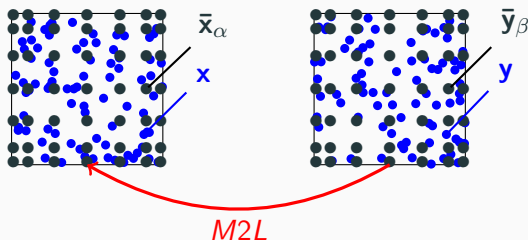
- \mathbf{k} : the interaction kernel

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

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

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

- Chebyshev interp.: Dense MVP $\mathcal{O}(p^6)$



Farfield approximation

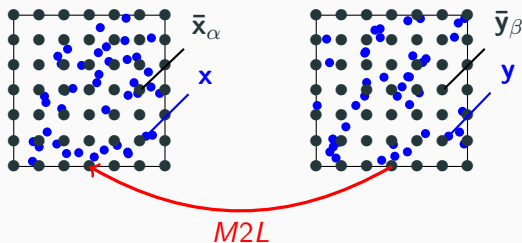
- \mathbf{k} : the interaction kernel

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

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

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

- Lagrange interp.: Circ. Embed. + FFT $\mathcal{O}(p^3 \log p)$



- approximation of the elastic stress field σ

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

where

$$\tilde{\sigma}_{ij}^A(\mathbf{x}) = \sum_{|\alpha| \leq p} S_\alpha(\mathbf{x}) \sum_{|\beta| \leq p} k_{m\beta}^{\alpha\beta} \varepsilon_{jmk} \oint_{(C')} S_\beta(\mathbf{x}') b'_k t'_i dx'$$

$$\tilde{\sigma}_{ij}^B(\mathbf{x}) = \sum_{|\alpha| \leq p} S_\alpha(\mathbf{x}) \sum_{|\beta| \leq p} k_{ijm}^{\alpha\beta} \varepsilon_{nmk} \oint_{(C')} S_\beta(\mathbf{x}') b'_k t'_n dx'$$

- Farfield force approximation (L2P)

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

$$(\tilde{\sigma}_{ij}^A)$$

$$(\tilde{\sigma}_{ij}^B)$$

(P2M) Aggregate segments contributions at interpolation nodes

$$\mathcal{M}_{ik}^\beta = \oint_C S_\beta(\mathbf{y}) b_k dy_i$$

(M2L) Transfer multipole to local expansion

$$\mathcal{L}_{ij}^\alpha = \sum_{|\beta| \leq \ell} R_{,mpp}^{\alpha\beta} \varepsilon_{jmk} \mathcal{M}_{ik}^\beta$$

$$\mathcal{L}_{ij}^\alpha = \sum_{|\beta| \leq \ell} R_{,ijn}^{\alpha\beta} \varepsilon_{nmk} \mathcal{M}_{nk}^\beta$$

(L2P) Accumulate contributions at target points

$$\tilde{\sigma}_{ij}(\mathbf{x}) = \sum_{|\alpha| \leq \ell} S_\alpha(\mathbf{x}) \mathcal{L}_{ij}^\alpha$$

Shifting derivatives: Formulation

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

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

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

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

- Trick** (applies to many BIE formulations)

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

- Thus, the new interpolation formula reads as

$$\tilde{k}_{ijk}(\mathbf{x}, \mathbf{y}) \approx - \sum_{|\alpha| \leq p} S(\bar{\mathbf{x}}_\alpha, \mathbf{x}) \sum_{|\beta| \leq p} k_{ij}(\bar{\mathbf{x}}_\alpha, \bar{\mathbf{y}}_\beta) \nabla_{y_k} S(\bar{\mathbf{y}}_\beta, \mathbf{y})$$

Shifting derivatives: Benefits

- Combine stress and energy farfields

$$E((C)) = -\frac{\mu}{8\pi} \oint_{(C)} b_i dx_i \oint_{(C)} r_{,kk} b'_j dx'_j + \dots$$

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

Approach	\mathcal{O}_t^σ	\mathcal{O}_t^E	$\mathcal{O}_m^{\sigma+E}$
$R_{,ijm}$	45	—	10 + 6
$R_{,ij} \nabla_m$	21	36	6
$(R_{,ij} R_{,pp}) \nabla_m$	12	36	7

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

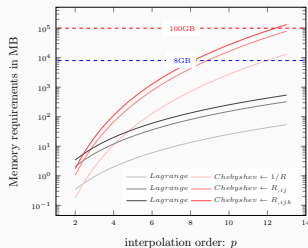


Figure 5: Theoretical memory requirements w.r.t. order p .

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Artificial test cases: density of BCC loops

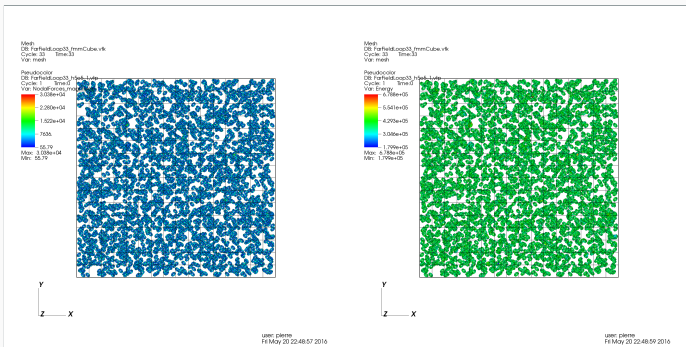


Figure 6: Density of $d = 5e19$ BCC loops with $\mathbf{b} = [111]$, diameter $d = 100$ and $L = 20$. The exact nodal force (left) and segment energy (right) is represented on the dislocation lines for each configuration.

Artificial test cases: 1 BCC loop per leaf

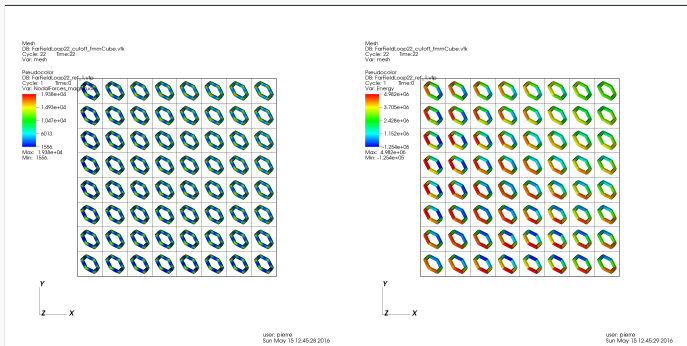


Figure 7: 1 BCC loops per leaf with $\mathbf{b} = [111]$, diameter $d = 500$ and $L = L_{min} + 1 = L_{max} - 1 = 100$. The exact nodal force (left) and segment energy (right) is represented on the dislocation lines for each configuration.

Accuracy: 1 BCC loop per leaf

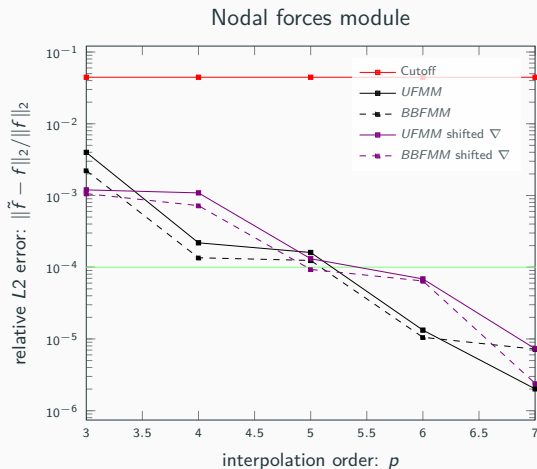


Figure 8: Accuracy of the nodal forces (left) and energy (right) evaluation for different interpolation schemes with respect to the interpolation order.

Running time: 1 BCC loop per leaf

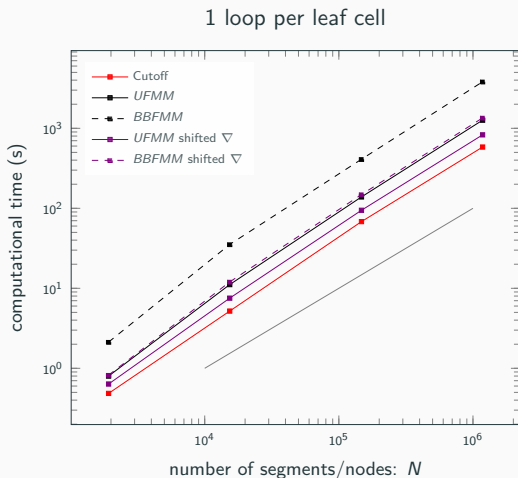


Figure 9: Computational time required by nodal forces and energy evaluation for different interpolation schemes ($p = 5$) w.r.t. # segments.

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Conclusions:

- 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](#)]

Ongoing:

- Linear time generation of Gaussian Random Fields
 - Eric Darve, Amalia Kokkinaki, Peter Kitanidis (Stanford)
 - Fast Multipole accelerated Randomized SVD ($\mathcal{O}(r^2n)$)
 - 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 $1/r$



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