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OptiDis: A parallel Fast Multipole Dislocation Dynamics code

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ABSTRACT

Among all the steps involved in DD simulations, the computation of the internal elastic forces and energy are by far the most resources consuming. However, since these are long-ranged and fast decreasing interactions, hierarchically algorithms like the Fast Multipole Method (FMM) are well suited for their fast evaluation. The relatively low accuracy required for the interaction forces between dislocations brought us to develop a more efficient approximation method for the farfield. On the other hand, the nearfield interactions are still evaluated analytically, which required a rather performant implementation (AVX, GPU...).

Regarding parallelism, our code benefits from a hybrid OpenMP/MPI paradigm and a cache-conscious datastructure. Finally, an accurate handling of topological elements intersecting the structure of the octree was considered. The latter feature implied careful modifications of the P2M/L2P operators in order to deal with shared memory model of parallelism.

MODEL

The motion of dislocations is ruled by a prescribed mobility law (e.g. viscous glide) depending on the internal (i.e. created by dislocations themselves) and external (i.e. applied by user) contributions on the nodal forces. The isotropic elastic stress field created by a dislocation loop ($\Gamma^2$) at point $x$ in space is given by Mura’s formula [4]

$$\tau_{ij}(x) = \frac{\mu}{\pi} \left( \frac{1}{r} \right) \left[ (A_{ij}(x) + A_{ji}(x)) + \frac{3}{8} \Omega_{ij} - A_{ij} \Omega_{ij}(x) \right]$$

where $(\mu, \nu)$ are the Lami coefficients and

$$(A_{ij}(x) = \frac{1}{r} R_{ijm}(x,y) \psi_{i,j,m} d\Omega d\nu)$$

and

$$(B_{ij}(x)) = \frac{1}{r} R_{ijm}(x,y) \gamma_{i,j,m} d\Omega d\nu)$$

where $R_{ijm}(x,y)$ are linear shape functions. While the isotropic elastic interaction energy is given by

$$\varepsilon_{ij}(x) = \frac{\mu}{2(r^2 + l^2)} (\delta_{ij} - \frac{l^2}{r^2 + l^2} \delta_{ij})$$

The cost of updating the nodal forces (and the energy) at each time step is quadratic and involves the evaluation of 2 line integrals, therefore it is usually the bottleneck of DD simulations.

A NEW FFT-ACCELERATED FMM

Fast Multipole DD

The idea of the FMM is to balance the computational cost of near and far field interactions by approximating the farfield and rely on a tree structure (see figure 1) to perform all computations. In our case we consider the interaction potential $R(x,y) = (R_{ij}(x,y))_{i,j=1...N}$ and apply the interpolation formula

$$R_k(x,y) = \sum_{j=1}^{N} R_{kj}(x,y) S_j(x,y)$$

where $S_j$ and $y_{j}$ denote sets of interpolation nodes in 2 well separated clusters containing x and y. $S$ denotes a polynomial interpolator (either Lagrange or Chebyshev).

IMPLEMENTATION AND PERFORMANCES

Our experiments 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 implemented is one discipline P2M/L2P routines involving exact integration over segments as well as analytic expressions for nearfield taken from Arsenlis et al [2].

REFERENCES

[1] ScaLAPACK: software library to simulate large scale n-body interactions using the fast multipole method. Implemented by hipacs team, inria bordeaux.


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