Project Team INRIA : **HiePACS**

Author of the post-doctoral research subject : O. Coulaud
Title of the post-doctoral research subject :
An efficient fast multipole method for dislocation interactions

Scientific priorities :
Modeling, Simulation and Optimization of Complex Dynamic Systems

Scientific Research context :

Dislocation modeling is a practical tool in the development of semiconducting devices. Areas of application include calculation of single dislocation behavior in transistors and memory cells and investigation of dislocation nucleation at stress concentrators.

The interaction between dislocations is long ranged and anisotropic, leading to severe computational challenges for large-scale simulations. The introduction of hierarchical methods based on an octree structure has dramatically reduced the amount of computation needed to simulate those systems for a given error tolerance. The Fast Multipole Method (FMM) developed for gravitational potentials in astrophysics and for electrostatic (coulombic) potentials in molecular simulations, solves this N-body problem for any given precision with O(N) runtime complexity against $O(N^2)$ for the direct computation.

Post-doctoral researcher work description :

In references [1,2], is presented an extension of the fast-multipole method of Greengard and Rokhlin to the case of the long-range interactions between parallel edges (in arbitrary orientations) and screw dislocations. Moreover, the best way to exploit the internal parallelism and the cache hierarchy inside a processor is to consider a matrix formulation of the problem and to use the standard BLAS routines in the implementation of the FMM operators. The goal of this work is first to understand the extension of the method to dislocations and then to propose a matrix formulation of the multipole to local operator. Finally, this approach will be integrated and validated in our parallel Fast Multipole code [3].

Required Knowledge and background :

The successful development of the scientific work described above requires a strong background in applied mathematics (to design/adapt numerical schemes) and in computer science (to perform an efficient parallel implementation); therefore a PhD in computational sciences (applied maths and/or computer science) would be ideal.

Former experiences in parallel code development (MPI, muti-threading) and a good knowledge in parallel algorithms is a requirement. A strong interest in large numerical simulation would surely be an additional asset.

References :

[1] R. Le Sar, J. M. Rickman. Multipole expansion of dislocation interactions: Application to discrete dislocations. PHYSICAL REVIEW B, VOLUME 65, 144110.

[2] H.Y. Wang and R. LeSar, O(N) algorithm for dislocation dynamics Philos. Mag. A 71, 149, 1995.

[3] O. Coulaud, P. Fortin, J. Roman. High performance BLAS formulation of the multipole-to-local operator in the Fast Multipole Method. Journal of Computational Physics 227, 3 (2008) 1836-1862.

Keywords : Fast Multipole Method, pairwise interaction, linear algebra, large scale parallel simulation.
Duration : 12 months