11th World Congress on Computational Mechanics (WCCM XI)
5th European Conference on Computational Mechanics (ECCM V)
6th European Conference on Computational Fluid Dynamics (ECFD VI)
July 20–25, 2014, Barcelona, Spain

LARGE SCALE DISLOCATION DYNAMICS SIMULATIONS

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Key words: *Dislocation Dynamics, Octree, hybrid parallelization, task model*

Dislocation dynamics (DD) is a key framework based on physical principles to study and understand the mechanical behavior of crystalline materials. For instance, in the nuclear field the toughness study of irradiated materials is critical in order to forecast nuclear power plant life. Consequently, there are very active research initiatives that aim at performing large scale and accurate simulations to better understand and master the physics.

However, to use the simulation as a predictive tool, one must be able to perform calculation with one or two more orders of magnitude of dislocation density than current simulations, also including more advanced physics.

In this talk, we will discuss the current and future research activities on the design of our parallel scalable Dislocations Dynamics simulation for large scale problems arising from the study of crystalline material.

Large scale simulation of dislocation dynamics require a lot of different tools. This kind of nodal simulation we implement imply that dislocation lines are discretized by 1D finite element method. As dislocations move in their grain, they expand, shrink, collide and annihilate, which means that we are facing a extremely dynamic n-body problem. To answer this dynamic constraint a cache-conscious data structure managing creation/deletion in a large set of data is used. Moreover, to achieve high performance a domain decomposition and an hierarchical approach are considered. We will present how we use Fast Multipole Method through our open source ScalFMM library to reduce the cost of pairwise force computations and collision detection. Finally, we will present numerical results that illustrate the scalability of our code using hybrid parallelism MPI/OpenMP.