The european project PERFECT has developed a computation chain for the simulation of the ageing under neutronic irradiation of the alloys (steel mainly) involved in materials of the nuclear reactors. This chain is made of seven codes, the accuracy of each of them depends on the size of the simulated system. So, the goal of the project PARMAT is to optimize three codes (ab initio, monte-carlo, chemical kinetics) of the chain for the future petaflopic architecture made of some hundreds of thousands of cores like the IBM machine BlueGene in order to reach the sufficient size of the simulated system.

Contact

Guy BENCTEUX
EDF - R&D
+33 (0)1 47 65 30 88
guy.bencteux@edf.fr

PARMAT

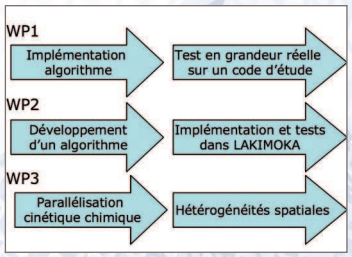
PARallélisation pour la simulation des MATériaux

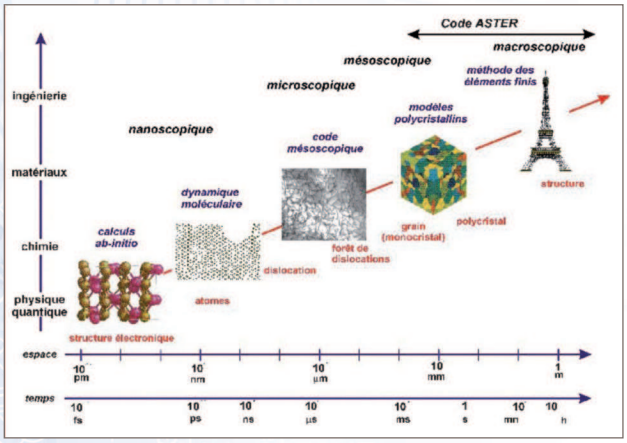
PROJECT PLANS & DELIVERABLES

The projet is divided in three work packages, each of them is dedicated to one code. First, our action on the ab initio solver (developed at EDF) consists in improving the algorithmics for the 3D simulations and illustrating the improvements by some studies in an industrial code as CONQUEST. Secondly, our aim for the EDF monte-carlo code LAKIMOKA is to develop a parallel solver which reveals very efficient for the dedicated application. Finally, we concentrate our efforts on the parallelisation of the solver of the chemical kinetics code MFVISC developed with CEA.

MAJOR PHASES OF THE PROJECT

The main difficulty of the project is to find graduated PhD students with numerical, informatic and physical knowledge. For the moment, one student (two is planned) was found for each code. For the ab initio code, the work on algorithmics is sufficient to investigate the coupling of the EDF solver with the industrial code. A state of art of the algorithms for the parallelization of the computation of one Monte-Carlo trajectory is being done in order to identify the good strategy for our application. A first work on the sequential optimization of MFVISC was done. In the same time, a SSA like stochastic algorithm was proposed. This algorithm is more flexible than the determinist one (MFVISC) and brings to reference computations. So, it allows us to validate the code MFVISC for industrial computations. The code based on the stochastic approach is being developed in order to obtain two codes with the same functionalities. The next step is then to parallelize the determinist and stochastic codes.





STATUS

For each concerned code, the first phase is (or will be soon) completed (sequential optimization, algorithmics improvement, state of art). It remains to add massive parallelism in order to simulate more larger systems than before and show accuracy improvements.

PARTNERS

MAJORS CORPORATIONS — EDF

Coordinator: EDF

Duration: 36 months