PARMAT

PARallélisation pour la simulation des MATériaux

ON GOING PROJECT

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 themdepends on the size of the simulated system. The goal of the project PARMAT is to optimize three codes (*ab initio*, Monte Carlo, chemical kinetics) in the chain in order to prepare for the future petaflopic architecture made of some hundreds of thousands of cores, as prefigured by the IBM BlueGene machine. Then, the size of the simulated system will be satisfying.

TECHNOLOGICAL OR SCIENTIFIC INNOVATIONS

- Modeling how the defects grow in an irradiated material requires huge computational resources. In this project, innovations have been proposed in order to reduce the time needed for simulations and to better exploit the potentialities of the newest supercomputers. All developments have in commons to go towards an increase in the parallelism of the algorithms.
- *Ab initio* computations may take advantage of a new algorithm developed by the project, based on domain decomposition. It has been tested on million-atoms linear alkane molecules and proved efficient up to 1,000 processors. On going works aim at treating more general molecules.
- Mean-field models describe the population of defects as the constituents of an homogeneous reacting mixture. The chemical kinetics that have to be computed involve up to billions species. A new stochastic approach has been proposed to integrate very detailed models for which a deterministic approach would lead to an unreachable number of unknowns.
- Kinetic Monte Carlo computations refine the mean-field computations. They are demanding because the algorithm is intrinsically sequential. A domain decomposition approach is currently tested.

STATUS - MAIN PROJECT OUTCOMES

For each of the concerned codes, 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 larger systems than before and to show accuracy improvements.

CONTACT

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

PARTNERS

Large companies:
EDF

SMEs:
CAPS

Research institutes, universities:
CEA, CNRS, ENPC

PROJECT DATA

Coordinator:
EDF

Call:
ANR

Start date:
January 2007

Duration:
48 months

Global budget (M€):
1.4

Funding (M€):
0.5