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PARALLELIZATION OF KINETIC MONTE CARLO ALGORITHM TO SIMULATE AL$_3$SC PRECIPITATION

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Abstract

INTRODUCTION

It is truthfully proven that kinetic Monte Carlo (kMC) is an extremely powerful method to simulate the time evolution of Markovian processes. kMC relies on the a priori knowledge of a given set of transition rates characterizing the simulated processes, which are assumed to obey Poisson statistics. Because of its versatility, ease of implementation, and wide range of applications, kMC has been the object of a significant parallelization effort in order to take advantage of existing and upcoming peta- and hexa-scale computing capabilities. However, the difficulty of parallelizing kMC lies in the intrinsic time discreticity underlying event driven simulations, which are sequential in character, and do not lend themselves to trivial parallel implementations. The ultimate validity test for any parallel kMC algorithm is that it solves the same master equation as the sequential method rigorously. This does not necessarily imply that both approaches give the same sequence of events, but that, on average, both give the same kinetic evolution resulting in the same statistical distributions as a function of time [E. Martínez et al 2011].

In this paper we propose a synchronous, parallel generalization of the rejection-free n-fold kMC method of Bortz, Kalos, and Lebowitz. We describe the designed spkMC algorithm in detail, giving some insight to specific simulation details such as the treatment of boundary conflicts, the replication of vacancies, and the communication model. We will validate the algorithm to determine its overall performance, precision, scalability (processor and memory usage), and inter-process communication performance, by solving a well-understood diffusion problem: nucleation of Al$_3$Sc precipitates.

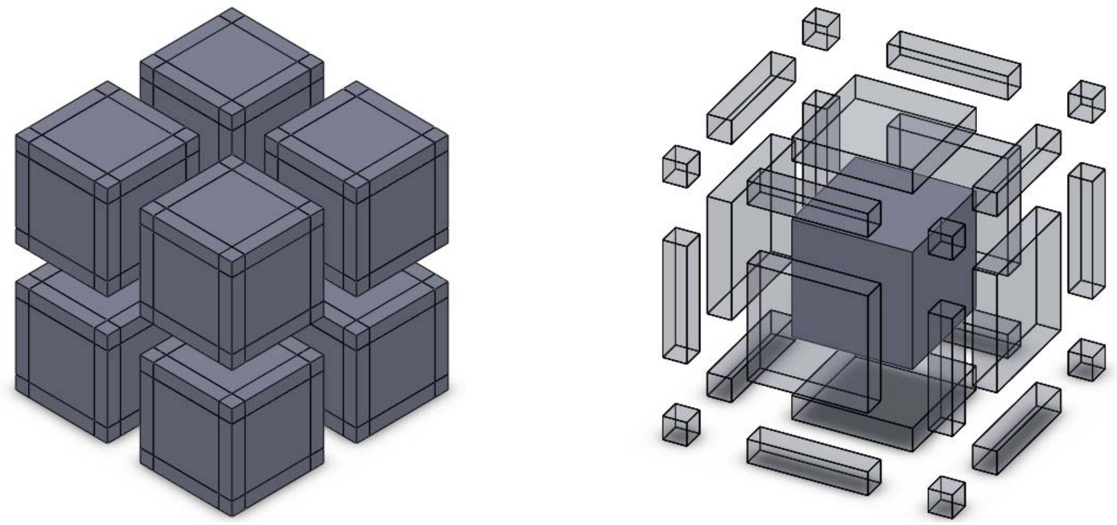
IMPLEMENTATION, RESULTS AND CONCLUSIONS

The spkMC strategy is based on: a 3D lattice is decomposed in a 3D grid of subdomains (Fig. 1), each subdomain is further divided in 2×2×2 sectors, with these 8 sectors it will be implemented a checkerboard scheme that avoids boundary conflicts and simplifies kMC parallelization, a periodic synchronization among processes through a frequency line for each process events, at the synchronization points (end of a sprint) the changes that occurred in the boundary and ghost regions are communicated to the neighbour processes.

The simulation results include a comparison between sequential kMC (Fig. 2) and parallel (spkMC) algorithms, in terms of performance and precision, precipitates dimension in terms of radius measure, steady-state nucleation rate, and cluster size distribution.

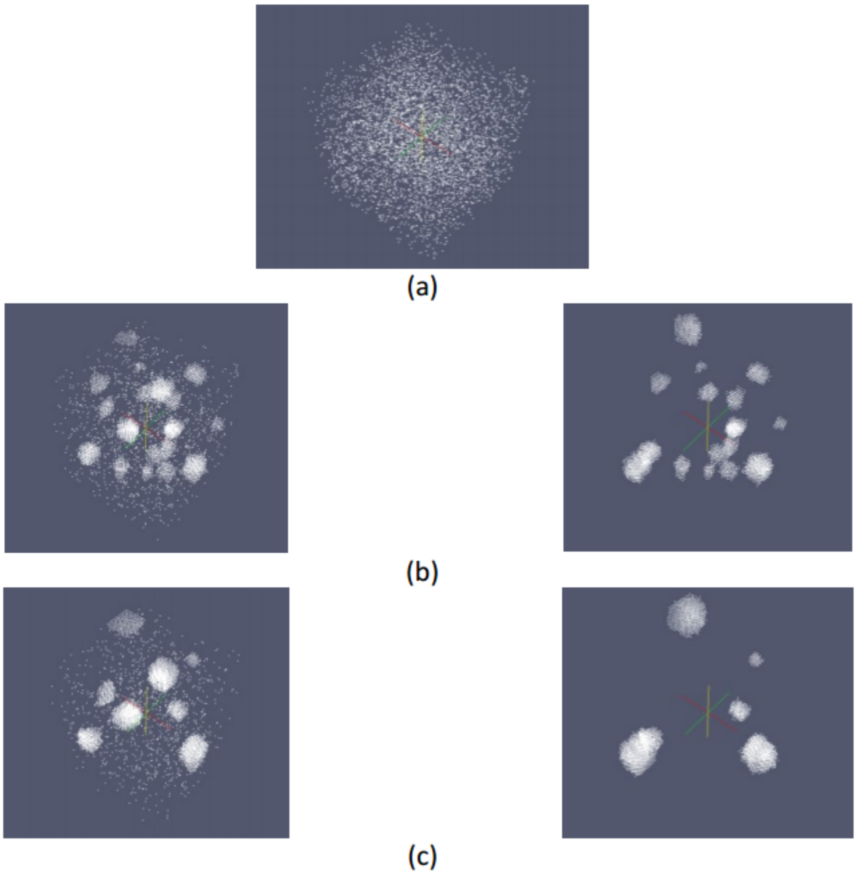
The sequential and parallel simulations were run on the SeARCH cluster, located at the University of Minho.

The outcome of the work undertaken is a set of software applications written in C, that allows us (i) to perform Monte Carlo (MC) simulations with and without MPI, (ii) to analyze the results using the Density Based Spatial Clustering of Applications with Noise (DBSCAN) technique [M. Ester et al 1996], and (iii) to compare the simulation results with the classical nucleation theory. Practical results obtained with these applications are (i) reports about the simulation, the analysis of clusters and precipitates with DBSCAN algorithm, and the application of the classical nucleation theory; (ii) files for 3D visualization of the simulation, at various stages over time, before and after applying DBSCAN to clean unclustered atoms.



(a) (b)

Fig. 1 – Domain decomposition in parallel implementation: (a) a 3D lattice decomposed in 8 subdomains; (b) an individual subdomain and the 26 parts that make up its boundary region.



(a)

(b)

(c)

Fig. 2 - Evolution of simulation: (a) initial configuration; (b) t=1.55ms; (c) t=4.945ms (left/right ⬄ before/after applying DBSCAN).

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