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SYNCHRONOUS PARALLEL KINETIC MONTE CARLO SIMULATION OF AL_3SC PRECIPITATION

Alfredo Moura[1], António Esteves[2(*)]

[1]Institute of Polymers and Composites, University of Minho, Guimarães, Portugal
[2]Computer Science and Technology Center, Informatics Department, University of Minho, Braga, Portugal
[(*)]*Email:* **esteves@di.uminho.pt**

ABSTRACT

The main objective of the present work is to profound the applicability of a synchronous parallel kinetic Monte Carlo (spkMC) algorithm for simulating the nucleation of Al_3Sc precipitates. Parallel processes communication is implemented through Message Passing Interface (MPI). Consequently, the capability of extending time and length scales of atomistic kinetic Monte Carlo (kMC) will be attested. Lastly, we present the results obtained from simulations of nucleation of Al_3Sc precipitates, which include a comparative view between sequential and parallel algorithms.

Keywords: *Al_3Sc precipitation, kMC, MPI, spkMC.*

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 (pkMC) 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 article we propose a synchronous, parallel generalization of the rejection-free n-fold kMC method of Bortz, Kalos, and Lebowitz. We describe the implemented algorithm in detail, discuss its precision and give insight to specific simulation details such as the treatment of boundary conflicts, and we study its potential intrinsic performance. We will validate the implemented method and study its scalability (processor and memory usage) and inter-process communication performance, by solving a well-understood diffusion problem: nucleation of Al_3Sc precipitates.

IMPLEMENTATION, RESULTS AND CONCLUSIONS

The spkMC strategy is based on: a 3D lattice decomposition into sub-domains, further sub-domain division into 2×2×2 sectors, the usage of a checkerboard scheme to avoid boundary conflicts, periodical synchronization among all processes by building a frequency line for

each process events, at the synchronization steps the changes that occurred in the boundary region are communicated to the respective owners.

The simulation results cover comparatively sequential (Fig. 1) versus parallel data over the following simulation outputs: precipitate dimension in terms of radius measure, steady-state nucleation rate, cluster size distribution, and computation time.

The sequential and parallel simulations presented are obtained by simulation runs on the SeARCH cluster, located at the University of Minho.

The outcome of the work undertaken is a set of software applications 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), with and without DBSCAN analysis.

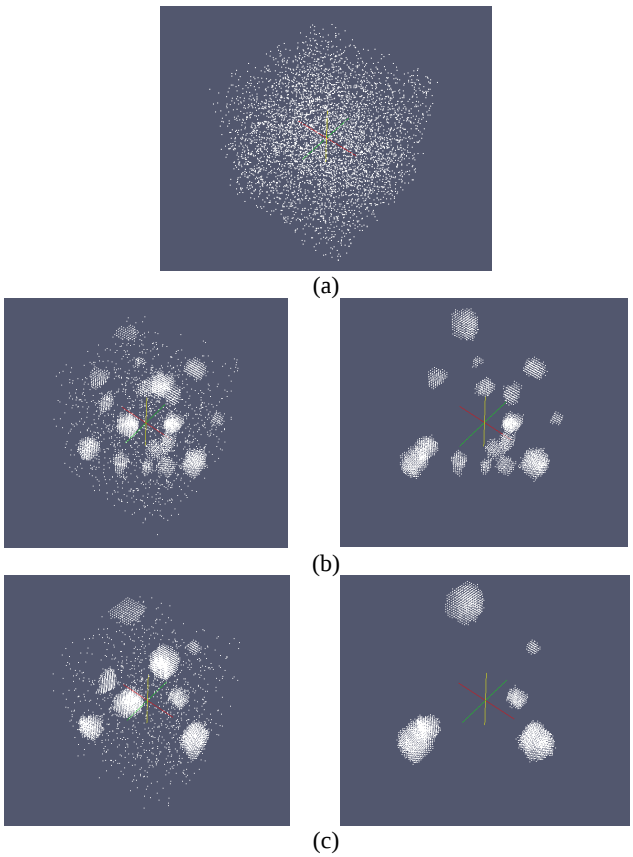

Fig. 1 - Evolution of simulation: (a) initial configuration; (b) t=1.55ms; (c) t=4.945ms (left/right ⇔ before/after applying DBSCAN).

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