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Parallelization comparison and optimization of a scale-bridging framework to model Cottrell atmospheres

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ABSTRACT

Low carbon steels undergo strain aging when heat treated, which causes an increased yield strength that can be observed macroscopically. Such strengthening mechanism is driven by atomistic scale processes, i.e., solute segregation of carbon (C) or nitrogen interstitial atoms. Due to its low solubility, alloying elements can diffuse to defects (e.g., dislocations) and form the so-called Cottrell atmospheres. Consequently, the mobility of defects is strongly reduced because of the interaction with solutes, and higher stresses are needed to unpin them from the Cottrell atmosphere. As C segregation and atomistic motion take place at separate timescales, Classical Molecular Dynamics (MD) and Metropolis Monte Carlo (MC) are coupled in a unified framework to capture collective effects with underlying slow dynamics. The number of degrees of freedom and the need for large computational resources in this simulation requires the choice of an optimal parallelization technique for the MC part of such multi-scale simulations using an unbiased sampling of the configuration space. In the present work, two different parallel approaches for the MC routine applied to the simulation of Cottrell atmospheres are implemented and compared: (i) a manager-worker speculative scheme and (ii) a distributed manager-worker over a cell-based domain decomposition approach augmented by an efficient load balancing scheme. The parallel performance of different Fe-C containing defects with several millions of atoms is analyzed, and also the possible optimization of the efficiency of the MC solute segregation process is evaluated regarding energy minimization.

1. Introduction

Formability is an exciting material property that determines the scope of application of engineering materials and this property depends on the ability of the material to deform plastically. In this aspect, dislocation mobility is strongly related to the plastic deformation behavior of crystalline metallic materials, and the accumulation of solute atoms in the vicinity of defects can lead to solid-solution strengthening. The light elements in the solid solution interact with the stress field introduced by a given dislocation and distribute around its core, forming the so-called Cottrell atmosphere [1], and thereby restricting the dislocation mobility during the plastic deformation. This mechanism was first observed and postulated by Cottrell and Bilby [2] as a static strain aging in ferritic steels. Much research has been directed towards the experimental and numerical understanding of the solute-dislocation interactions, and in some cases, it has been possible to find direct correlations to macroscopically observed material properties. In the case of bake hardened steels, which are specially used for manufacturing automobile components because of their excellent dent resistance [3], an increase in the yield strength is attributed to the interaction of carbon Cottrell atmospheres with dislocations.

In particular, the formation of carbon (C) Cottrell atmospheres in defect iron (Fe) structures is considered as a process composed of rare events, i.e., a C atom oscillates at a local minimum for a long time until it overcomes an energy barrier to find a new local minimum in the potential energy landscape. Based on the experimentally computed diffusion coefficients, the C diffusion in ferritic steels spans in a time frame between seconds to hours [4] depending on the operating conditions (e.g., temperature or solute concentration). On the one hand, atomistic simulation approaches like Classical Molecular Dynamics (MD) are well suited for this simulation, but the integration of Newton's equations of motion at each time step [5] has a feasible timescale of only a few nanoseconds. On the other hand, Monte Carlo provides an alternative approach which is independent of underlying time scales.

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Therefore, Classical MD and Metropolis [6] Monte Carlo (MC) are here coupled using virtual atoms to overcome the timescale limitation. Each virtual atom is defined as a placeholder, that is, a site in the system which may potentially be suitable to place a C atom: consequently, the number of virtual atoms in a system depends strongly on the crystal structure [7]. Considering this scope, two different parallelization approaches applied for the MC simulation in the coupling scheme are compared for different scenarios according to its performance and statistical efficiency, so that the prediction capabilities of the underlying physics and the computational performance of these algorithms is evaluated. Both parallel approaches are based on the manager-worker scheme: the first approach is a general manager-worker based on a speculative scheme developed by the authors [7] and the second approach is newly proposed scheme with a distributed manager-worker that uses domain decomposition combined with a load balancing routine. The main contributions of the paper are (1) the description of the design and implementation of the distributed manager-worker, (2) it's comparative analysis with the previous general manager-worker algorithm on different ferritic systems with defects, and (3) the study of further statistical optimization possibilities for the MC procedure based on system energy data.

The rest of the work is organized as follows. Section 2 describes previous advances in parallel MC methods. Section 3 presents background information about the parallel simulation problem and describes the two parallel algorithms used in this work, with the particular focus on the distributed approach. Section 4 shows the performance comparison of the parallel algorithms for different simulations of single crystalline metallic materials with defects. Finally, Section 5 summarizes the main outcome of the work and gives an outlook for the future work.

2. Related work

Many previous parallelization strategies for MC algorithms [8–13] have generally been inspired by different short-range techniques used for MD since many years [14–16], and they have been proposed based on several factors: geometry, task, algorithm, and target hardware architectures. Geometry parallelization is based on independent regions and suitable for applications where the inter-atomic interactions are particularly short-ranged, like for embedded-atom method (EAM) [17] potentials. A farm parallelism approach is used in work by Jones et al. [9], where a manager process performs the actual trial moves and the energy of a trial configuration is computed in parallel by worker processes. However, this approach by Jones et al. requires sequential equilibration, therefore limiting its application to large systems. In case of event parallelism, a large simulation is broken into smaller blocks of equal length executed concurrently on all workers and manager. It is particularly useful for computing the average quantities where the order of summation does not play any role. Nevertheless, this is not suitable for the simulation of solute segregation, because each trial conformation should account for chemical and mechanical changes in the environment to mimic a sequential approach. Esselink et al. [10] devised another MC algorithm showing a chain molecule as an example, in which many trial conformations are constructed in parallel and conformation with the highest probability is chosen: nevertheless, this algorithm is most suitable for applications with very low acceptance of trial moves.

More recent implementations of parallel MC have been accomplished using a domain decomposition scheme. One simple and interesting approach by Uhlherr et al. [18] obtained relevant results for the simulation of large polymer chains: here the system was split into active and inactive regions, therefore ensuring complete independence between parallel trial move executions. However, considering its application for C segregation in deformed steel, executing independent sequences of individual trial moves might cause C to be trapped in local minima (active regions), and thus preventing them from finding global minima. Sadigh et al. [13] proposed a scalable parallel MC algorithm for variance constrained semi-grand canonical ensembles with spatial domain decomposition, where the MC sample selection is performed using non-interacting moving cubes (*sampling volume*) concurrently on all processes. This approach presents interesting features regarding parallelism, but it is not effective for modeling solute segregation in the system with a fixed background concentration of solutes. One main reason is that the acceptance rate tends to decline or decay for the structural minimization problems, and also solute particles might get redistributed to a specific set of processes causing a serious load balancing issue. Another parallel MC implementation for different statistical ensembles has been done by Yamakov et al. [19] for the simulation of the swap, and displacement trial moves similarly to a serial MC algorithm. Here the domain decomposition strategy is extended from the work of Sadigh et al. so that each domain has independent sampling zones and is defined using a link cell mesh for effectively identifying the neighbor particles within the prescribed interaction range. This work states the difficulty in the parallelization for canonical ensembles with swap trial moves, as well as the non-availability of an efficient algorithm to perform random swap trial moves in parallel.

In general, previous parallelization strategies are often advantageous, although limited because of the trade-off between the acceptance rate and quality of sampling, therefore being problem-specific. In this sense, the present work provides more insight on the performance of the parallel MC approach for modeling the interstitial solute segregation, and also discussing the design decisions to reduce the execution time and exploit computational resources efficiently without systematically affecting the simulation. As it is difficult to hand pick any existing parallel approach for this particular application of Cottrell atmospheres modeling, because of several challenges with the different system requirements and fluctuating acceptance rate, a new scalable parallel scheme called 'distributed manager-worker'is presented, and it is compared in performance with an earlier developed scheme, referred to as 'general manager-worker'and implemented by the same authors [7].

3. Parallel implementations

The target simulations in this work are performed on ferritic (α-Fe, with bcc crystal structure) defect systems that consist of three types of atoms: Fe, C, and, virtual atoms. The Metropolis MC algorithm is implemented and executed in four main steps:

- Choose a random C atom (i.e., 'target') and a random virtual atom (i.e., 'sample') from the current system configuration.
- Perform a swap trial move between target and sample atoms by interchanging their positions.
- Compute the energy of the new configuration following the trial move.
- Evaluate the acceptance criterion by testing if the new configuration achieves lower energy than the initial configuration.

In general, the trial moves of Metropolis MC are performed sequentially because of its dependency on the previous configuration, and therefore the parallelization of the MC routine needs to adapt to this fact. In this aspect, the use of swap trial moves has been selected in order to facilitate an energy minimization by C redistribution in the simulated system, but this choice may be modified (e.g., using trial moves to insert/delete a C atom, or swapping many C atoms) without affecting the applicability or scalability of the algorithms presented in this work. The management protocols of the parallel executions are independent of the selected trial move type.

First principle studies inform that a C atom prefers an octahedral site inside the bcc-Fe host matrix. Such introduced C atom creates a tetragonal lattice distortion in the ferritic host matrix and therefore exerts tension on the two first nearest neighbors and compression on