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Parallel Simulation of Ceramic Grain Growth on the Platform of MPI

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Abstract. A computation method for parallel simulations of ceramic grain growth at an atomic scale in a PC cluster is proposed, by combining the Message Passing Interface (MPI) with the serial simulation of grain growth. A parallel platform is constructed for the simulation of grain growth with program modules of grain assignments, grain growth, data exchanges and boundary settlements, which are coded with Microsoft Visual C++ 6.0 and MPICH. Quantitative results show that the computing speed of parallel simulations with this platform is obviously increased compared with that of serial simulations. Such a computing mode of grain growth is in good agreement with practical situations of ceramic grain growth.

Introduction

It is of importance to speed up the computing process and to improve the realistic degree for computer simulations of ceramic grain growth at an atomic scale. Although the images simulated by the serial algorithm are basically in agreement with the practical microstructure of ceramics [1-2], the speed of serial simulations is so slow that it is almost impossible to achieve a level of millions of atoms for a grain in actual ceramics. In addition, there is a difference between the modes of serial simulations and practical situations of grain growth, as in practice all of ceramic grains grow simultaneously instead of sequentially. In this paper, a platform for parallel simulations at an atomic scale in a PC cluster is constructed based on the MPI and the serial simulation of ceramic grain growth.

Parallel Computation Method for Simulating Ceramic Grain Growth

MPI, the most popular platform for parallel programming [3], provides not only a self-contained communication library, but also a highly efficient and reliable run-time environment for parallel programs. Moreover, parallel programs with the MPI can be easily transplanted and extended.

There are mainly three parts for MPI programs, including initialization, application entity and finalization, in which the application entity contains calculation control modules and communications in processes. Two basic design patterns of MPI programs, master-slave and all-to-all patterns, can be implemented in a Single Program Multiple Data (SPMD) model. In the process of executing SPMD program, the program runs in different processors, in which memory spaces are independent and the communication is easily implemented by calling MPI functions. Moreover, each process gets an exclusive ID (rank), numbered from 0 at the beginning of running an MPI program.

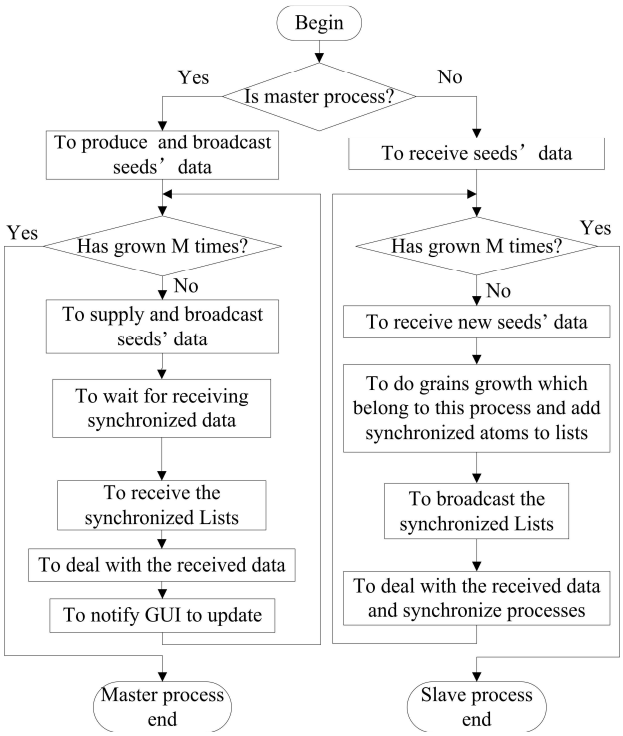

Fig. 1 Flow chart of parallel simulation

Table 1 Initial parameters of simulation

Initial seed number	Seed activation coefficient	Sintering temperature [^{o}C]	Atomic radius [nm]
25	0.1	1300	0.5

Table 2 Comparison of data between parallel and serial simulations

Growth times	Parallel simulation		Serial simulation	
	Total number of atoms	Time [second]	Total number of atoms	Time [second]
50	45742	872	44455	675
100	51447	1925	50293	2595
200	53020	3945	52057	6529
400	54292	7763	53739	15021
600	54698	11571	55438	24553
800	55092	15470	55565	35370
1000	55728	19344	55992	47948
1200	58020	23246	57923	62750

Parallel flow of simulations. In our work, the serial computation method of simulations [1] is adopted and paralleled to an MPI program. A flow of parallel computing (Fig. 1) is proposed for the simulation of ceramic grain growth at an atomic scale in a PC cluster as follows. As the experimental result of the serial algorithm is basically in agreement with the microstructure of ceramics, the serial algorithm is utilized for the parallel simulation to keep the consistency in maximum between parallel and serial simulations in algorithms of grain growth. Meanwhile, attentions are paid to deal with grain assignments, data structure of communications, data exchanges in processes and boundary dealing in designing parallel programs.

Results and Discussion

Comparison of speeds between the parallel simulation and the serial simulation. A parallel simulation environment is constructed with MPICH windows v1.2.5 and 3 PCs. The experiments of parallel and serial simulations are completed with the same initial parameters respectively (Table 1), and the data of simulation experiments are shown in Table 2.

With the experimental results of simulation (Table 2), it is confirmed that the total number of atoms in the parallel simulation and the serial simulation is similar. After growth times exceed 400, the total number of atoms is nearly kept at a stable level.

However, the evolution of grain growth is enhanced with parallel computing and a PC cluster, which can be seen in Fig. 2. It is demonstrated that the time for the parallel simulation is much shorter than that for the serial simulation at the middle and late stages of growth. To evaluate the performance of parallel computing, speedup ratio (Sp) and parallel efficiency (fp) are employed, which are described by Eq. 1 and Eq. 2.

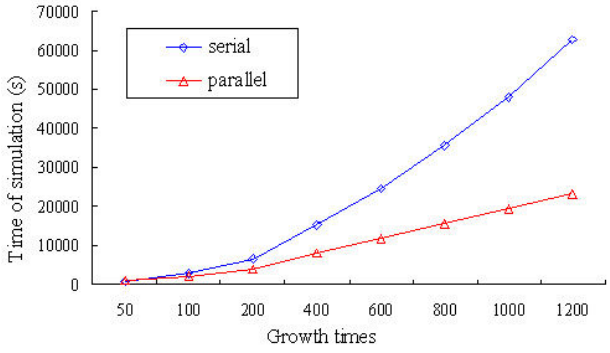

Fig. 2 Comparison of the speeds between parallel and serial simulations

$$Sp = Ts/Tp \quad (1)$$

$$fp = Sp/p \quad (2)$$

where p is the number of nodes, Tp is the time in a PC cluster and Ts is the time in a single PC. Here, the value of Sp describes the ratio of time spent for the calculation by using a single process to that by using multiple processes, and fp represents the utilization factor of computer resource in parallel computing.

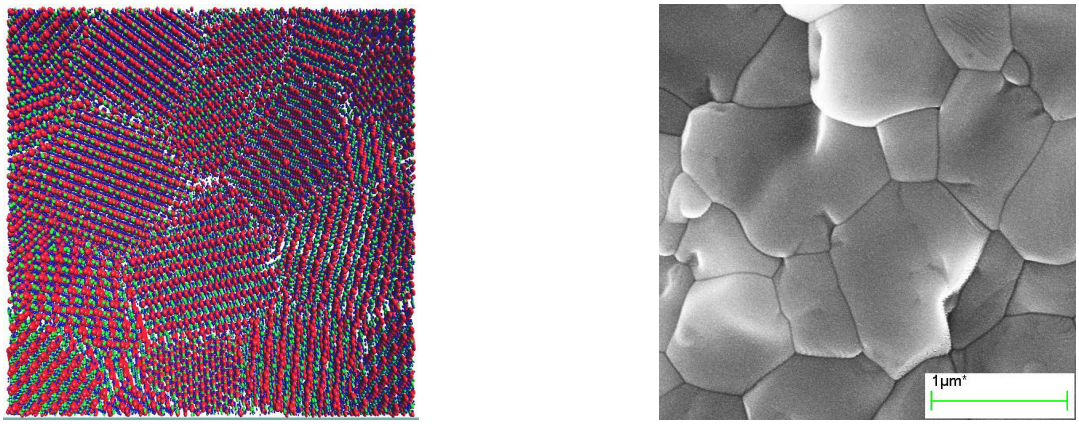

Fig. 3 The image of parallel simulation (left) and the micrograph of the actual ceramic (right)

At the late stage of growth, the curves of simulation time vs. growth times for both the parallel simulation and the serial simulation almost increase linearly. So the relationship between Tp and Ts at this period can be estimated as follows:

$$Tp=Ts/(P*fp) \quad (P>2) \tag{3}$$

where P is the number of PCs, and the value of fp is kept between 0.8 and 0.9. Thus, with an increasing number of PCs, the evolution of grain growth is greatly accelerated and the time for the parallel simulation is significantly reduced.

Comparison between images of the parallel simulation and the actual micrograph of ceramic. The image of the parallel simulation, with the initial parameters shown in Table 1, is displayed on the left in Fig. 3. The micrograph of the actual ceramic is illustrated on the right of Fig. 3. There are a few similar resemblances between the simulated image and the micrograph of the actual ceramic. For example, the common boundaries of three grains are formed nearly as 120°.

Conclusions

Based on the MPI and the serial simulation of ceramic grain growth, a computation method for parallel simulations of ceramic grain growth at an atomic scale in a PC cluster is proposed. Several modules for grain assignments, grain growth, data exchanges and boundary dealing are designed and analyzed, and the parallel simulation of grains growth was successfully implemented. Quantitative experimental results show that the simulation speed is obviously enhanced and a high efficiency of simulation is obtained by using of the parallel computation method. Moreover, it is shown that the simulating image is quite similar to the micrograph of the actual ceramic.

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