Parallelized Simulation of Molecular Dynamics with a Special-Purpose Computer: MDGRAPE-2

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1 Introduction

Molecular dynamics (MD) simulation is a very useful technique for studying the structure and dynamics of biologically important molecules such as proteins and DNA/RNA. In MD simulations, each atom is treated as a classical particle. By MD simulation, we can treat the motion of molecules very precisely. However, we need high performance computational resources for the MD simulation of complex biomolecules. To overcome this difficulty, we have developed the special-purpose computer, MDGRAPE-2 [1] with high speed and accuracy. The most time consumed in the MD simulation is the calculation of non-bonded forces, i.e. Coulomb and van der Waals forces. The special-purpose computer MDGRAPE-2 accelerates the calculation of non-bonded forces. The calculation except of non-bonded forces is done by the host computer which is general-purpose computer. We have ported one of the most famous MD program packages for biomolecules, AMBER 6.0 [2] for using it on the MDGRAPE-2 board. In the previous work, we could perform the parallel calculation of the modified AMBER 6.0 by using several MDGRAPE-2 boards. However, the only calculation of the non-bonded forces was parallelized and the other parts were not parallelized with this parallel implementation. The simulation with more than 50,000 particles could be accelerated efficiently, but it is not effective for the smaller systems. The reason is that the calculation of host computer is not parallelized. Therefore, we have ported the MPI source code of AMBER 6.0 for using several MDGRAPE-2 boards. By this implementation, most of calculation are parallelized and this scheme is more effective for the system within 50,000 particles than the previous scheme.
2 Parallel Computation

In parallel implementation of AMBER 6.0 by using several MDGRAPE-2 boards, there are two methods. One is that the calculation of non-bonded forces is only parallelized (Fig. 1(a)), and the other is that most of calculation are parallelized (Fig. 1(b)). In Fig. 1, the system A consists of one CPU in host computer and several MDGRAPE-2 boards. The system B consists of several CPUs and MDGRAPE-2 boards.

3 Results

In this parallel computation, we used Intel Pentium 4 2.5GHz, Gigabit ethernet, and Red Hat Linux 8.0. Figure 2 shows the estimated speed-up of two systems against the number of particles and the standard of this speed-up is the simulation time of one MDGRAPE-2 board in the system B. In the system A, the simulation with less than 50,000 particles is not effective in comparison with the system B. The reason is that the only CPU must communicate to several MDGRAPE-2 boards and this communication time among one CPU and several MDGRAPE-2 boards is bottleneck. In the system B, each CPU communicates one MDGRAPE-2 board in the non-bonded calculation. New parallel implementation by the system B works effectively in the smaller systems within 50,000 particles.

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References
