SPECIAL-PURPOSE COMPUTERS FOR CLASSICAL PARTICLE SIMULATIONS

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Abstract. We have developed parallel special-purpose computer systems for classical particle simulations, GRAPE. GRAPE is an accelerator for calculations of two-body central forces such as gravitational, Coulomb, or Van der Waals forces. The GRAPE-4 system for astrophysical N-body simulations achieved teraflops speed first in the world. Such high-performance was achieved by the very-long-pipeline architecture and the broadcast memory architecture. The possibility of programmable semi-general-purpose computers for particle simulations is also discussed.

1. Introduction

Classical particle simulation is the very important method to study astrophysical objects such as galaxies and globular clusters, condensed matter physics, protein structures, vortex dynamics, and so on. In many simulations, almost all computational time is spent in calculating long-range forces such as gravitational or Coulomb forces, since the number of interactions between particles is proportional to the square of the number of particles. Thus, they require huge computing resources to simulate realistic systems. We have developed special purpose computer systems GRAPE (GRAvity PipE) to accelerate astrophysical N-body simulations and molecular dynamics simulations(Sugimoto et al., 1990; Ebisuzaki et al., 1993). Among them, GRAPE-4 became the first teraflops computer in the world (Taiji et al., 1994a; Taiji et al., 1995).

GRAPE calculates only two-body central forces. The host workstation, which is connected to GRAPE, performs other operations like integrations. The GRAPE systems have very long pipelines specialized for the calcula-
tions of gravitational interactions. These pipelines perform a few tens of arithmetic operations per cycle. The calculation of long range forces dominates computational time, which costs $O(N^2)$. On the other hand, both the calculation in a host and the communication between a host and a GRAPE system cost $O(N)$. Therefore, commercial workstations can satisfy the requirements for the communication speed as well as for the calculation speed, although the calculation speed of GRAPE exceeds teraflops.

What is special for these particle simulations? There are two basic styles to describe physical systems. One is the method using "force and particle", and the other uses "field and mesh". In field and mesh style, The physical space is divided by mesh and the physical quantities on the mesh points are calculated. The field equation is given by partial differential equation, thus the interaction between mesh points is local. This style of description is suitable for distributed memory massive parallel processors since the communication is essentially local.

In force and particle style, the motions of (pseudo) particles are simulated by calculating forces between particles. The force on a particle is obtained by gathering a pairwise force from each particle. Especially for long-range force, we have to sum up all pairwise interactions. Thus, the force calculation is the most time-consuming in classical particle simulations. Because one particle interacts with many other particles, the positions and other information on the particle is necessary for force calculation on all other particles. Thus, if we calculate the forces at many locations in parallel, the same information on the particle can be commonly used. Therefore, many processor units can share common inputs from a memory unit. This architecture makes the parallelization quite easy. It is one of the most important advantage of special-purpose computers for particle simulations. We will discuss details in the later section.

There are many mixed style of these two approaches like the Particle-Particle Particle-Mesh (PPPM) method (Hockney and Eastwood, 1988), or the fast multipole method (FMM) (Greengard and Rokhlin, 1987). There also exists the tree algorithm (Barnes and Hut, 1986) which uses superparticles. These algorithm reduce the cost of force calculations to $O(N \log N)$ or $O(N)$. In all these methods the neighbor forces should be calculated directly, therefore we can use GRAPE to accelerate these algorithms. For example, Makino implemented a tree algorithm (Makino, 1991b) and Brieu et al. implemented the PPPM algorithm on GRAPE-3 (Brieu et al., 1995).

In this paper, firstly we describe on the GRAPE-4 system as an example of GRAPE systems in section 2. In section 3 we discuss why the GRAPE systems can have high-performance at low cost. Next, we briefly describe the MD-GRAPE system. Finally, we discuss the possibility of semi-general-purpose computers for particle simulations in section 5.