$7.0$/Mflops Astrophysical $N$-Body Simulation with Treecode on GRAPE-5

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Abstract

As an entry for the 1999 Gordon Bell price/performance prize, we report an astrophysical $N$-body simulation performed with a treecode on GRAPE-5 (Gravity Pipe 5) system, a special-purpose computer for astrophysical $N$-body simulations. The GRAPE-5 system has 32 pipeline processors specialized for the gravitational force calculation. Other operations, such as tree construction, tree traverse and time integration, are performed on a general purpose workstation. The total cost for the GRAPE-5 system is 40,900 dollars. We performed a cosmological $N$-body simulation with 2.1 million particles, which sustained a performance of 5.92 Gflops averaged over 8.37 hours. The price per performance obtained is 7.0 dollars per Mflops.

1 Introduction

Astrophysical $N$-body simulation is one of the most widely used technique to investigate formation and evolution of astronomical objects, such as galaxies, galaxy clusters and large scale structures of the universe. In such simulations, we calculate gravitational force on each particle from all other particles, and integrate the orbit of each particle according to Newton’s equation of motion. We investigate structural and dynamical properties of the simulated object.

The astrophysical $N$-body simulation has been one of grand challenge problems in computational sciences. In years 1992, 96, 97, and 98, the Gordon Bell prizes were awarded to cosmological $N$-body simulations [1]-[4] and in 1995 the Gordon Bell prize is awarded to $N$-body simulation of a black hole binary in a galaxy [5]. The calculation cost of the astrophysical $N$-body simulation rapidly increases for large $N$, because it is proportional

\[ \text{cost} \propto N^d \]

\[ d \approx 2 \]

\[ \text{for two-body forces} \]
to $N^2$ if we use a straightforward approach. The gravity is a long-range attractive force. A particle feels the forces from all other particles, no matter how far away. We cannot use a cutoff technique which is widely used in MD simulation (e.g. [3]). In order to reduce the calculation costs, various fast algorithms have been developed.

Hierarchical tree algorithm [7] is one of such fast algorithms which reduce the calculation cost from $O(N^2)$ to $O(N \log N)$. In this algorithm, particle are organized in the form of a tree, and each node of the tree represents a group of particles. The force from a distance node is replaced by the force from its center of mass. The Gordon Bell prizes of years 1992, 97 and 98 were awarded to $N$-body simulations with this tree algorithm [1][3][4], which were performed on Intel Touchstone Delta, ASCI-Red, PC cluster, and an Alpha cluster.

We report an astrophysical $N$-body simulation with the tree algorithm on GRAPE-5 (GRAvity PipE) special-purpose computer. GRAPE-5 has dedicated pipelines specialized for the calculation of the gravitational force. It is connected to a host computer, which is a general purpose workstation, and operates as a hardware accelerator for the calculation of the gravitational force. Other operations, such as tree construction, tree traverse and time integration, are performed on the host computer. It has been already demonstrated that the approach using special-purpose machines successfully achieved very high performance in scientific computations, by the Gordon Bell prize simulations of 1995 and 96 [3][2], which were performed on GRAPE-4 [8], and the last Gordon Bell prize simulation [9], which was performed on QCDSP [10].

We performed a cosmological 2.1 million particles simulation using the tree algorithm on GRAPE-5 connected to a COMPAQ AlphaServer DS10. Sustained performance is 5.92 Gflops and price/performance is $7.0/Mflops$. In the rest of this paper, we describe on GRAPE-5 system and the tree algorithm on GRAPE, and report the cost and performance.

2 GRAPE-5 system

We briefly describe architecture of the GRAPE-5 system. More detailed descriptions of the GRAPE-5 system will be given elsewhere [11]. GRAPE-5 is designed to run the tree code with very high speed. Figure 1 summarizes the configuration of the GRAPE-5 system used for the simulation reported in this paper. The GRAPE-5 system consists of 2 processor boards, 2 host interface boards, and a host computer. The processor board performs the force calculation. The host interface board handles the communication between the processor board and the host computer. The host computer performs all other operations. We used COMPAQ AlphaServer DS10 with a 21264/466MHz Alpha processor for the host computer. Figure 2 and figure 3 are photographs of the GRAPE-5 system and GRAPE-5 processor board, respectively.

Each processor board consists of 8 processor chips (G5 chip) and a particle data memory. G5 chip is a custom LSI chip which calculates the gravitational force. Each G5 chip houses 2 pipelines specialized for the force calculation. The particle data memory stores the data of particles which exert the force and supplies them to G5 chip. G5 chip operates at 90MHz and other part of the processor boards operate at 15MHz.

G5 chip is designed for astrophysical $N$-body simulations with the tree algorithm and
Figure 1: Block diagram of the GRAPE-5 system

Figure 2: Photograph of the GRAPE-5 system
calculates a pair-wise force with a relative error of about 0.3%. This might sound rather low, but detailed theoretical analysis [12] and numerical experiment [13] have shown that it is more than enough. The average error of the force in our simulation is around 0.1%, which is dominated by the approximation made in the tree algorithm and not by the accuracy of the hardware. The relative accuracy was practically the same when we performed the same force calculation using standard 64-bit floating point arithmetic.

The theoretical peak speed of the GRAPE-5 system is 109.44 Gflops. Total number of pipeline processors is 32. Each processor pipeline operates 38 operations in a clock cycle, if we use the same counting convention as used in [3][4].

3 Tree algorithm

Our code [14] is based on the Barnes’s modified tree algorithm [15]. The implementation of the modified tree algorithm on GRAPE were discussed in [16]. Using this algorithm, the calculation cost on the host computer is greatly reduced from that of the original algorithm and the forces exerted on multiple particles can be calculated in parallel. In the original algorithm, the interaction list is created for each particle. In the modified tree algorithm, neighboring particles are grouped and one interaction list is shared among the particles in the same group. Forces from particles in the same group is directly calculated.

The modified tree algorithm reduces the calculation cost of the host computer by roughly a factor of \( n_g \), where \( n_g \) is the average number of particles in a group. On the other hand,
the amount of work on GRAPE-5 increases as we increase \( n_g \), since the interaction list becomes longer. There is, therefore, an optimal \( n_g \) at which the total computing time is minimum. The optimal \( n_g \) strongly depends on the ratio of the speed of the host computer and GRAPE. For the present configuration, the optimal \( n_g \) is around 2000.

Note that our modified tree algorithm performs larger number of operations than the tree algorithm on a general purpose computer. When we will estimate the performance in section 5, we will make correction. Note also that the our modified tree algorithm is more accurate than the original tree algorithm for the same accuracy parameter, as shown in [15][17].

4 Cost

The total cost of the GRAPE-5 system is 4.7 M JYE. The GRAPE-5 board is available from a Japanese commercial company for the price of 1.65 M JYE per board. Remaining 1.4 M JYE was spent for the host computer, COMPAQ AlphaServer DS10, including 512 MByte main memory and C++ compiler. The total cost, with the present exchange rate of 1 dollar = 115 JYE, is about 40,900 dollars.

5 Simulation

We report the performance statistics for the astrophysical \( N \)-body simulations with the tree algorithm on GRAPE-5. The performance numbers are based on the wall-clock time obtained from UNIX system timer on the host computer (COMPAQ AlphaServer DS10).

We performed a cosmological \( N \)-body simulation of a sphere of radius 50Mpc (mega parsec) with 2,159,038 particles for 999 timesteps. We assigned the initial position and velocities to particles in a spherical region selected from a discrete realization of density contrast field based on a standard cold dark matter scenario using COSMICS package [18]. A particle represents \( 1.7 \times 10^{10} \) solar masses. We performed the simulation from \( z = 24 \), where \( z \) is redshift, to the present time. Figure 4 shows a snapshot of the simulation.

The total number of the particle-particle interactions is \( 2.90 \times 10^{13} \). This implies that the average length of the interaction list is 13,431. The whole simulation took 30,141 seconds (8.37 hours) including I/O, resulting in the average computing speed of 36.4 Gflops. Here we use the operation count of 38 per interaction.

However, as we described in section 3, our modified tree algorithm performs larger number of operations than the tree algorithm on a general purpose computer. In order to make correction, we estimated the operation count of the original tree algorithm for the same simulation, using five snapshot files and the same accuracy parameter. The estimated number of the interaction is \( 4.69 \times 10^{12} \). The effective sustained speed is \textbf{5.92 Gflops} and the price/performance is \$7.0/Mflops.

References
Figure 4: A snapshot of the simulation at $z = 0$ (present time). Particles in a $45\text{Mpc} \times 45\text{Mpc} \times 2.5\text{Mpc}$ box are plotted.
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