

NBODY6++GPU: Ready for the gravitational million-body problem

Long Wang^{1,2*}, Rainer Spurzem^{3,4,5,1}, Sverre Aarseth⁶, Keigo Nitadori⁷, Peter Berczik^{3,4,5,8}, M.B.N. Kouwenhoven^{1,2}, Thorsten Naab⁹

¹*Kavli Institute for Astronomy and Astrophysics, Peking University, Yiheyuan Lu 5, Haidian Qu, 100871, Beijing, China*

²*Department of Astronomy, School of Physics, Peking University, Yiheyuan Lu 5, Haidian Qu, 100871, Beijing, China*

³*National Astronomical Observatories and Key Laboratory of Computational Astrophysics, Chinese Academy of Sciences, 20A Datun Rd., Chaoyang District, 100012, Beijing, China*

⁴*Key Laboratory of Frontiers in Theoretical Physics, Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, 100190, China*

⁵*Astronomisches Rechen-Institut, Zentrum für Astronomie, University of Heidelberg, Mönchhofstrasse 12-14, 69120, Heidelberg, Germany*

⁶*Institute of Astronomy, University of Cambridge, Madingley Road, Cambridge CB3 0HA, UK*

⁷*RIKEN Advanced Institute for Computational Science, Kobe, Japan*

⁸*Main Astronomical Observatory, National Academy of Sciences of Ukraine, 27 Akademika Zabolotnoho St., 03680, Kyiv, Ukraine*

⁹*Max-Planck Institut für Astrophysik, Karl-Schwarzschild-Str. 1, D-85741 Garching, Germany*

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ABSTRACT

Accurate direct N -body simulations help to obtain detailed information about the dynamical evolution of star clusters. They also enable comparisons with analytical models and Fokker-Planck or Monte-Carlo methods. NBODY6 is a well-known direct N -body code for star clusters, and NBODY6++ is the extended version designed for large particle number simulations by supercomputers. We present NBODY6++GPU, an optimized version of NBODY6++ with hybrid parallelization methods (MPI, GPU, OpenMP, and AVX/SSE) to accelerate large direct N -body simulations, and in particular to solve the million-body problem. We discuss the new features of the NBODY6++GPU code, benchmarks, as well as the first results from a simulation of a realistic globular cluster initially containing a million particles. For million-body simulations, NBODY6++GPU is 400 – 2000 times faster than NBODY6 with 320 CPU cores and 32 NVIDIA K20X GPUs. With this computing cluster specification, the simulations of million-body globular clusters including 5% primordial binaries require about an hour per half-mass crossing time.

Key words: methods: numerical – globular clusters: general

1 INTRODUCTION

Direct simulations of star clusters have a long history. As algorithms and hardware have improved, larger numbers of stars could be simulated, allowing a more realistic representation of the dynamical evolution of globular star clusters. NBODY6 (Aarseth 2003) is a state-of-the-art direct N -body simulation code specifically designed for star clusters. It uses several algorithms to enhance the computing speed and accuracy, especially for strong interactions that arise from a large fraction of binaries and relatively short relaxation

timescales (≤ 100 Myr for typical open clusters and ≤ 1 Gyr for typical globular clusters) in collisional and dense stellar systems. Here, the terms “collisional” and “dense” are not well defined in the literature. The classical two-body relaxation time, as defined e.g. by Chandrasekhar (1942); Spitzer (1987), describes how important distant gravitational two-body encounters are for the orbital motion of stars. If the relaxation time is very long, a system is denoted as “collisionless” (for example, galactic disks or bulges); the motion of stars is entirely determined by the smooth mean gravitational field of the system. If the relaxation time is short (e.g., shorter than the lifetime of the system) we denote the cluster as “collisional” (e.g., globular and open star clusters,

* E-mail: long.wang@pku.edu.cn

nuclear star clusters). If the stellar density is high enough, close two-body gravitational encounters and stellar collisions may occur. This aspect is crucial when studying “dense” star clusters. In dense and collisional star clusters a correct integration of stellar motions requires pairwise gravitational interactions to be included between many if not all stars in the cluster. This is the situation for which codes such as NBODY6 are designed.

Direct N -body simulation of star clusters can be very time consuming. In a system with N particles, the full force calculation cost of one particle scales with $O(N)$. With individual time steps for each particle, the cost per crossing time (t_{cr}) depends on the number of steps per particle (N_s) which varies with different time step criteria, integration methods and star cluster properties. Makino & Hut (1988) and Makino & Aarseth (1992) found that for the Hermite scheme with a time step criterion based on relative force change (Aarseth 1985), N_s is roughly proportional to $N^{1/3}$ for systems with homogeneous density. Thus, when using individual time steps the total computational cost per crossing time of N particles scales with $O(N^{7/3})$. For systems with a power-law density distribution $\rho \propto r^{-\alpha}$, N_s depends on the power index α . Then the cost per crossing time scales with $O(N^{7/3})$ for $\alpha < 24/11$ and $O(N^{(6-\alpha)/(6-2\alpha)})$ for $\alpha \geq 24/11$ (Makino & Hut 1988). Considering the half-mass relaxation timescale, t_{rh} is proportional to $t_{\text{cr}}N/\ln N$ (Spitzer 1987; Sugimoto et al. 1990), the computational cost per t_{rh} is $O(N^{10/3}/\ln N)$ for homogeneous systems and for power-law systems with $\alpha < 24/11$ and $O(N^{(12-3\alpha)/(6-2\alpha)}/\ln N)$ for $\alpha \geq 24/11$. Thus, an efficient parallelization of a direct N -body code is necessary for large particle numbers.

Sugimoto et al. (1990) discussed the fundamental problem that direct numerical simulations of globular star clusters could not be completed for decades if extrapolating the standard evolution of computational hardware (Moore’s law). They called for the construction of a special-purpose computer GRAPE, which finally was successfully initiated and completed by their team (Makino, Kokubo, & Taiji 1993; Makino & Taiji 1998; Makino et al. 2003). In the following years, graphical processing units (GPU) widely replaced GRAPE (e.g., Harfst et al. 2007; Hennebelle, Audit & Miville-Deschènes 2007; Portegies Zwart, Belleman & Geldof 2007; Belleman, Bédorf & Portegies Zwart 2008; Schive et al. 2008) and much of the GRAPE software could be ported to GPU (Gaburov, Harfst & Portegies Zwart 2009).

Spurzem (1999); Spurzem et al. (2008) and Hemsendorf, Khalisi, Omarov & Spurzem (2003) discussed several different types of hardware for parallelization and extended NBODY6 to NBODY6++ for general parallel supercomputers. Later, Nitadori & Aarseth (2012) developed a GPU-based parallel force calculation for NBODY6. As a result, large N -body simulations ($N \sim 10^5$) became possible on a single desktop computer or workstation with GPU hardware. They also implemented the parallel force calculation based on Streaming SIMD Extensions (SSE) and Advanced Vector Extensions (AVX) for recent CPU architectures. Spurzem et al. (2011); Berczik, Spurzem & Wang (2013) and Berczik et al. (2013) discussed the performance of large N -body simulations with the GPU-accelerated codes ϕ GPU and a provisional version of NBODY6++GPU.

With these parallelization methods, we can now study

star clusters with a number of stars exceeding 10^5 . Hurley & Shara (2012) simulated 200,000 stars including 5000 primordial binaries with initial half-mass radius 4.7 pc using NBODY4 on a GRAPE-6 based computer to investigate core collapse and core oscillation. Later, Sippel & Hurley (2013) studied the multiple stellar-mass black holes in globular clusters by simulating 262,500 stars including 12,500 primordial binaries with initial half-mass radius 6.2 pc using NBODY6-GPU. The current largest direct N -body simulation modeling the globular cluster M4 used one computing node including 12 Intel Xeon X5650 cores (2.66 GHz per core) and 2 NVIDIA TESLA C2050 GPUs with 448 cores each (1.15 GHz per core) with NBODY6-GPU (Heggie 2014). This simulation contained 500,000 stars with 7% binaries and a small half mass radius of 0.58 pc. Nowadays, we can make an effort to reach one million stars by using parallel supercomputers with GPUs.

In this paper, we first introduce the parallel algorithm used by NBODY6-GPU and NBODY6++ in Section 2. Then we describe the new version of NBODY6++GPU with a hybrid parallel method and also the new algorithms that are necessary for large number of particle parallelization in Section 3. Performance tests are carried out in Section 4. In Section 5 we show an application to a globular cluster with one million stars. In Section 6, we discuss the parallelization limit and future development of NBODY6++GPU. Finally, we present our conclusions in Section 7.

2 THE FEATURES OF NBODY6/6++

NBODY6 uses the fourth-order Hermite integration method. Makino (1991) presented a careful analysis of the performance and energy error of the Hermite integrator. He showed that it reduces to the similar asymptotic error behaviour as the standard Aarseth scheme (fourth-order method; see Aarseth 1985) but it has some advantages in the time step choice and data structure.

The hierarchical block time steps method is used together with the Hermite integrator (McMillan 1986; Makino 1991) in NBODY6, which avoids the overheads of particle position and velocity prediction in an individual time step method. In this method, particle time steps are adjusted to quantized values, usually an integer power of 0.5. Then at each time step, active particles (the particles that satisfy the time step criterion) are integrated together.

To speed up the force calculation, NBODY6 uses the Ahmad-Cohen (AC) neighbor scheme (Ahmad & Cohen 1973). The basic idea is to employ a neighbor list for each particle. The integration is separated into two parts: regular force integration for large time steps (regular steps) and irregular force integration for small time steps (irregular steps). The regular force is the summation of the forces from particles outside the neighbor radius and the irregular force accumulates only the neighbor forces. During the irregular step, the regular force and its first order derivative calculated at the last regular step are used for position and velocity prediction. The AC scheme gains efficiency with sequential computing (without parallelization). The speed gained by the AC scheme is roughly proportional to $N^{1/4}$ (Makino & Hut 1988; Makino & Aarseth 1992). However, in parallel computing, this gain is limited by the complexity of

the implementation of this algorithm (see Section 4). Also, the benefit of reducing overheads of particle prediction in the block time step method is strongly limited in the neighbor scheme.

Portegies Zwart & Boekholt (2014) discussed the integration accuracy requirement for self-gravitating systems simulated with direct N -body codes. They found that for three-body systems the integration should have total energy conserved better than 1/10th. Although this accuracy requirement is uncertain when the simulation is extended to large particle number systems, this work indicates the importance of careful integration treatment for direct N -body systems. One important feature of NBODY6 is that it uses the algorithms of Kustaanheimo & Stiefel (1965) (hereafter KS) and chain regularization (Mikkola & Aarseth 1993) to deal with an accurate solution of close encounters, binaries and multiple systems, which play a significant role in star cluster dynamical evolution. These strong interactions require very small time steps during integration and may produce large errors with standard integrators such as the Hermite scheme. Using KS and chain regularization is also the most important feature of NBODY6 for star cluster simulations.

Here, we have briefly introduced the main algorithm used in NBODY6/6++. In the next section we will focus on the parallelization of the codes.

3 PARALLELIZATION OF NBODY6++GPU

3.1 MPI parallelization of NBODY6++

Spurzem (1999) and Hensendorf, Khalisi, Omarov & Spurzem (2003) developed NBODY6++ based on NBODY6 using MPI parallelization with the copy algorithm. Both regular and irregular forces were parallelized. Here different MPI processors calculate different subsets of the active particles. Each MPI processor has the complete particle dataset. Another available parallel algorithm is the ring algorithm which splits the full particle dataset for different MPI processors. It reduces the memory cost in each MPI process. The benefit of the copy algorithm compared to the ring algorithm is that there is no requirement for extra communication of the neighbor particle data which is not in the same MPI process during the irregular force calculation. The disadvantage is the particle number limit due to memory size on the computing node. The MPI communication with the copy algorithm has constant time cost (independent of MPI processor number except for latency). The scaling of the regular force with different MPI processors is very good. Since the regular force dominates the calculation, this results in a good scaling of the total computing time. Dorband, Hensendorf & Merritt (2003) provided a detailed discussion of these communication algorithms. Lippert et al. (1998) and Makino (2002) suggested an efficient communication algorithm (hypersystolic) for extremely large processor numbers.

3.2 Basic NBODY6-GPU implementation

After the GPU computing (CUDA) became popular, the shared memory parallel NBODY6-GPU code was developed

for workstation and desktop computers (Nitadori & Aarseth 2012). The OpenMP, GPU (CUDA) and AVX/SSE parallel methods are used to make the code as fast as possible. However, NBODY6-GPU can only be used in a single node (no massively parallel MPI implementation) so the number of particles is limited for a reasonable simulation time.

3.2.1 Regular force and potential (GPU)

The GPU library of Nitadori & Aarseth (2012) is used for calculating the regular force, which dominates the direct integration, and potential energy calculation. The cost for regular force calculation per particle scales with $O(N)$ and for potential energy calculation scales with $O(N^2)$. The performance of GPU force calculation is very good since the pure force calculation is easy to parallelize. GPUs also help to accumulate the neighbor list very efficiently during the regular force calculation.

3.2.2 Prediction and irregular force (AVX/SSE)

When GPU accelerates the regular force very efficiently, the irregular force becomes expensive. However, this part is hard to parallelize on GPUs due to the complexity of the AC neighbor scheme. Thus, Nitadori & Aarseth (2012) developed the AVX/SSE and OpenMP parallel library for neighbor particle prediction and irregular force calculation. AVX/SSE is an instruction set for CPUs developed in recent years, which supports vector calculation in the specific cache. The advantage of AVX/SSE with OpenMP is that there is no extra memory copy compared to GPU. For both AVX/SSE and GPU libraries, the data needs to be copied once for changing data structure to obtain computing efficiency. This is because that NBODY6 has a very long development history, thus to completely change the data structure to be consistent with AVX/SSE and GPU libraries is very time consuming. But for GPU, there is extra data copy from the host memory on the mother board to the device memory on GPU. Besides, since the neighbor force calculation is not efficient for the distributed memory parallel method (with MPI parallelization; see discussion below), this kind of shared memory parallel method is more efficient.

3.3 Code improvements in NBODY6++GPU

In this subsection we describe our new implementations in NBODY6++GPU.

The GPU acceleration, especially of the long-range (regular) gravitational forces, is very efficient so this part does not dominate the computational time any more, as we show below. Secondly, the AVX/SSE implementation accelerates prediction and neighbor (irregular) forces, which is the next most time consuming part of the code.

We have combined the GPU and AVX/SSE acceleration, which was done for a single node in NBODY6-GPU, with the MPI parallelized NBODY6++ designed for multi-node computing clusters for the new version NBODY6++GPU. This work requires additional efforts to keep the code consistent (see below). In addition, we have

worked on remaining bottlenecks, such as time step scheduling and stellar evolution, which become important for million bodies because the usual computationally intensive tasks have been accelerated very effectively by GPU and AVX/SSE.

3.3.1 New algorithm of selecting active particles for block time steps

For the block time step method, active particles should be selected at every time step. It is very expensive to search all particles for the active ones, especially for the irregular force calculation. In this case, for one block time step the cost of selecting active particles scales with $O(N)$ while the irregular force calculation cost scale with $O(N_i \langle N_b \rangle)$. If $N \gg N_i \langle N_b \rangle$, the former can be more expensive. When the simulation reaches millions of particles, the block time step levels can be quite deep (the smallest time step can reach $0.5^{20} - 0.5^{22}$) and the deep blocks with few particles and small time steps can easily satisfy this condition. One may consider to use a temporary list to save particles with small time steps and only search all particles at some selected time interval from the temporary list each time step. However, this method is still expensive where there are many particles with small time steps (such as the wide binaries that are not KS regularized). Indeed, we find that the time of selecting active particles can be much larger than the irregular integration time, even with this temporary list algorithm for one million particles including 5% primordial binaries. Another reason that forces us to deal with this issue is that the active particles selection is very difficult to parallelize efficiently (the cost is almost independent of processor numbers) and would be prohibitive for a million-body simulation. Thus, we propose a better algorithm that uses a time step sorting list (hereafter sorting list algorithm; see Figures 1 and 2). Zhong (2014) implemented a similar algorithm for ϕ -GRAPE+GPU and evaluated its performance. The basic idea is that when we have the index list sorted by particle time step from smallest to largest, and the indicators of each boundary offset $I_{\text{off}}(i)$ between the block of the same step particles (the largest particle index with step 0.5^i), we only need to find the correct offset at each block time step by using the algorithm shown in Figure 1 to select active particles (shown as black squares in Figure 2). After integration, we adjust the sorted list by sorting the active particles' new time steps. The specific sorting method for this adjustment can be optimized to $O(N_i)$ if we ignore the stability of sorting (stability means no exchange of the order for the particles with same steps) and assume that many active particles keep the same step as before or have small time step changes.

3.3.2 The initialization

The initialization of a simulation in NBODY6 is relatively expensive. We improve it with MPI, GPU and OpenMP parallelization and a better algorithm. The initial model for million-body simulations is very important and needs to be carefully tested. This improvement is very useful for fast testing of the initial models with large particle numbers, especially for a large number of primordial binaries.

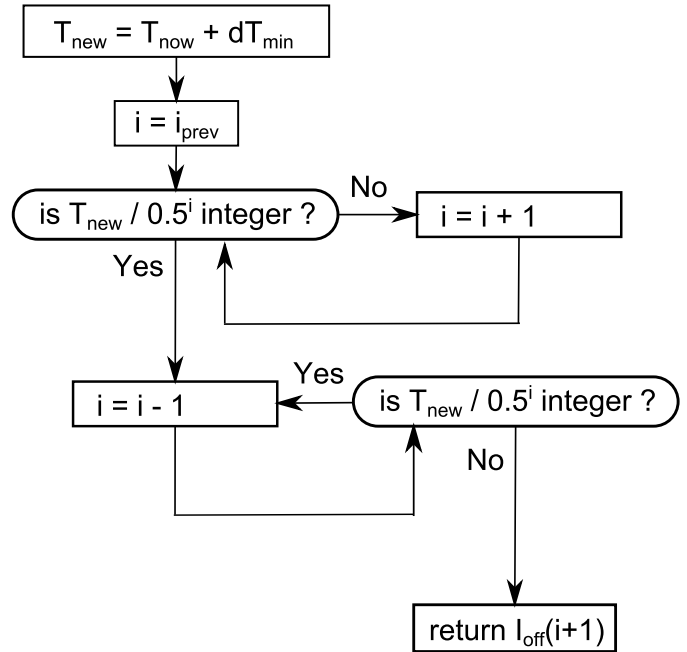


Figure 1. The flow chart for obtaining the correct offset in the sorting list algorithm. T_{new} is the time after next integration. T_{now} is current time. dT_{min} is the current smallest time step (the time step of the first particle in sorting list). i_{prev} is the previous offset.

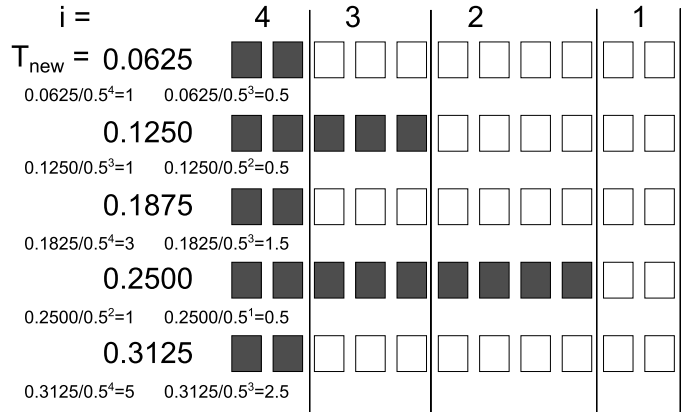


Figure 2. Diagrammatic sketch of sorting list algorithm for selecting active particles. The time step of each particle block is 0.5^i separated by boundary indicators $I_{\text{off}}(i)$ (vertical lines). The integration advances vertically in the chart. Active particles are shown as black squares.

The initialization of NBODY6 can be divided into four parts:

- (i) reading or generating masses, positions, velocities and stellar evolution parameters of all stars;
- (ii) scaling all parameters into N -body units (the N -body units¹ are defined in Heggie & Mathieu 1986);

¹ It has been suggested to name the N -body time unit to honour M. Hénon as Hénon time unit (D.C. Heggie, private communication)

(iii) initialization of forces, neighbor lists and time steps of all stars;

(iv) initialization of primordial KS binaries.

In the second part of the initialization, the total potential energy of the system is needed and costs $O(N^2)$. Actually, NBODY6-GPU does this calculation twice for scaling purpose in the case of an external tidal field. The GPU is used in NBODY6-GPU to speed up this part and it is very efficient. Our new improvements are for the third and fourth parts. In the traditional NBODY6-GPU version forces and neighbor lists are initialized separately without parallelization. NBODY6++ parallelizes the scaling and initialization of the force parts, but only through MPI. For million-body simulations this is very slow and requires hours to be finished. We improved it by using GPU based force and neighbor list calculations (the same as for the regular force calculation). The fourth part is very costly with more than 5% primordial KS binaries in the traditional NBODY6-GPU (several hours). During initialization of KS binaries, the force and its three derivatives (Hermite scheme) need to be renewed for center-of-mass particles. All neighbor lists that contain KS binary component indices also need to be replaced by the center-of-mass particle indices. The cost is approximately $O(N\langle N_b \rangle N_{KS})$ where N_{KS} is the number of primordial KS binaries. We find a much simpler way to initialize KS binaries (cost scales with $O(N_{KS})$) by just switching the order of the third and fourth parts: initialize KS binaries first without recalculating forces, their derivatives and neighbor lists (only the KS transformation is needed) and then do the third process with the new center-of-mass particles data generated by former process instead of each binary component in the old way. In this case there is no need to update the forces and neighbor lists.

3.3.3 Position and velocity prediction

During the force calculation, the predicted positions and velocities are used to calculate the force and its first derivative for the Hermite integrator. In principle, we can avoid prediction of the same particles with the AC neighbor scheme and block time steps. However, in practice we need to search all neighbors of each active particle and the search itself is computationally expensive. Thus, it does not save much time to avoid neighbor prediction overlap and it is much simpler to predict all neighbors and do the force calculation within one loop. The disadvantage of this method is that it costs more when the average neighbor number $\langle N_b \rangle$ multiplied by the active particle number N_i is larger than the total particle number N , compared to all the particle predictions with a non-AC scheme block time step. One solution is to try predicting all particles once instead of predicting each neighbor when $\langle N_b \rangle N_i > N$. But the mixture of predicting only neighbors and predicting all particles increases the complexity of code. We therefore use only neighbor prediction in the code.

However, there is a major complication for the parallel neighbor prediction in NBODY6++GPU, which does not exist in NBODY6-GPU. Since we use AVX/SSE and GPU and the code is mixed with CUDA, C++ and Fortran 77 programming language, the AVX/SSE and GPU libraries keep the individual copies of particle datasets. Thus, the predictions of particles have overlaps and are usually inconsistent

for different copies distributed on MPI processors. Due to the complexity of NBODY6/6++ (e.g., using predicted positions for regularization) this leads to problems of synchronization later on, such as differences of time steps for the same particle on different processors. The safest but very costly way is to always predict all particles at every irregular integration step, which is the case in the older versions of NBODY6++. To solve this problem, much effort has been made to ensure that every particle is predicted to the current time before it is used in stellar evolution, KS and hierarchical regularization, because these parts are not parallelized and should have the same computing results on every MPI processor.

3.3.4 Stellar evolution and neighbor force correction

The neighbor scheme also leads to performance losses for the calculation of stellar evolution. When a star experiences mass loss, other stars feel a smaller force. In the neighbor scheme, the regular force is predicted from the value calculated at the last regular time step, thus if particles outside the neighbor radius experience mass loss between the previous and next regular time steps, the regular force will be inconsistent after that. The correction for the regular force should be done for all particles which have the mass loss particle outside their neighbor radius. To avoid a large value of the third and fourth derivatives of the force, the irregular force also needs to be updated if the mass loss particle is inside the neighbor radius. When mass loss is frequent, the calculation performance will be reduced significantly. We currently use OpenMP to speed up the force correction, but it cannot completely solve this issue since the force correction with cost of $O(N)$ per particle cannot be avoided.

3.4 Hybrid MPI parallelization

Based on the above parallel methods, we develop a new version of NBODY6++GPU to include hybrid parallel procedures. The parallel structure of NBODY6++GPU is shown in Figure 3. In computer clusters, each computing node uses one MPI process. Each MPI process opens multiple threads via OpenMP for the irregular force calculation. GPUs inside one node are controlled by OpenMP threads. Each GPU has a similar particle dataset size for regular force and potential energy calculation. GPUs of different nodes are isolated without communication. Thus all GPUs in the same node together access the complete particle dataset. The best code configuration is to use multiple CPU cores (such as 8 – 16 cores) and several GPUs (such as 1 – 4 GPUs with a few thousand cores) per node, and choose node numbers based on the total number of particles.

4 PERFORMANCE TEST

4.1 Pure MPI and hybrid MPI

Figure 4 shows significant improvement of NBODY6++GPU by using hybrid MPI including GPU, as compared to the pure MPI case. We see that the GPU gives about 33 times faster regular force integration. This is to be expected since GPU is designed for large parallelization

Table 1. The definitions of abbreviations for all figures

| Abbreviation | Definition |
|--------------|---|
| Reg. | Regular integration (force) and neighbor list determination |
| Irr. | Irregular integration (force, prediction (AVX/SSE version) and correction) |
| Pred. | Neighbor (Non-AVX/SSE version) and all particles (for regular force) prediction |
| Init.B | Initialization of active particle list for block time step |
| Move | Particle data copy prepared for MPI communication |
| Comm.I. | MPI communication for irregular integration |
| Comm.R. | MPI communication for receiving integration |
| Send.I. | Particle data copy for AVX/SSE irregular force calculation |
| Send.R. | Particle data copy for GPU regular force calculation |
| Adjust | Energy checking, adjustment of parameters and data results |
| KS | KS regularization calculation (binary and hierarchical systems) |
| Barr. | MPI communication barrier waiting time due to the imbalance and network traffic between different nodes |

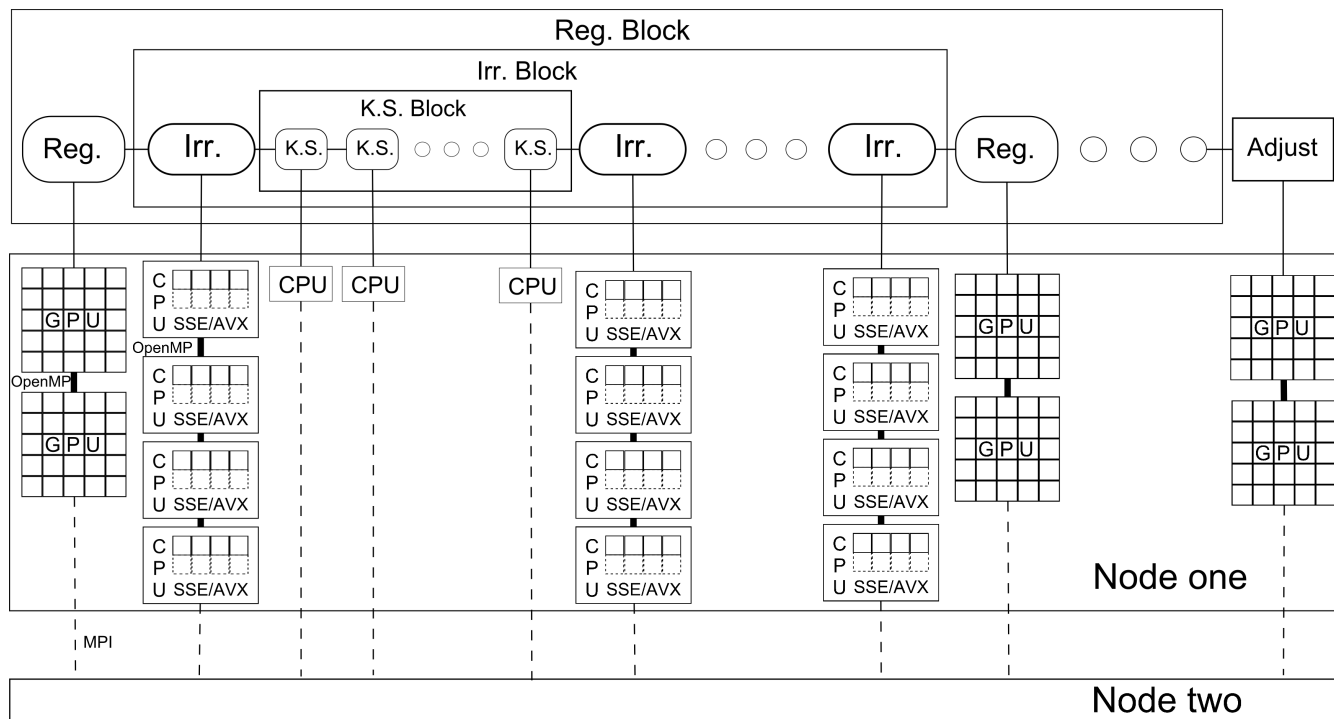


Figure 3. NBODY6++GPU code structure. It shows one cycle of simulation. Based on the time steps, the integration can be divided into three hierarchical parts (see Table 1): KS calculation (KS), irregular integration (Irr.) and regular integration (Reg.). The KS has smallest time step distribution. Thus, between two nearest Irr. block time steps there are several KS steps. Similarly, between two Reg. block time steps there are several Irr. time steps. After several Reg. time steps there is one “Adjust” (see Table 1). Inside one node, Reg. and Adjust are parallelized by multiple GPUs and Irr. is parallelized by AVX/SSE with OpenMP. MPI parallelization are done for all 4 parts between different nodes.

by using many computing cores and large memory bandwidth within one card. Using AVX/SSE with OpenMP gives about 3 times faster irregular integration including predictions. OpenMP reduces the MPI communication cost by a factor of 5 – 10. The individual MPI communication process is not directly sped up by OpenMP. When we use MPI parallelization together with OpenMP method, inside one node the irregular and regular force calculations are done by multiple threads with OpenMP instead of MPI parallelization, thus we can set a larger block particle number threshold for MPI parallelization by a factor of the OpenMP thread number and reduce the total MPI

communication frequency. This then results in shorter total MPI communication time.

4.2 Scaling with different particle numbers and processors

The scaling with different particle numbers and processors demonstrate the possibility of using large computing resources for simulations. We test hybrid parallel NBODY6++GPU scaling with different node numbers N_{node} (1, 2, 4, 8 and 16; up to 320 CPU cores and about 80k GPU cores) and different particle numbers (16k, 32k, 64k, 128k, 256k and 1024k) on the “Hydra” cluster of the

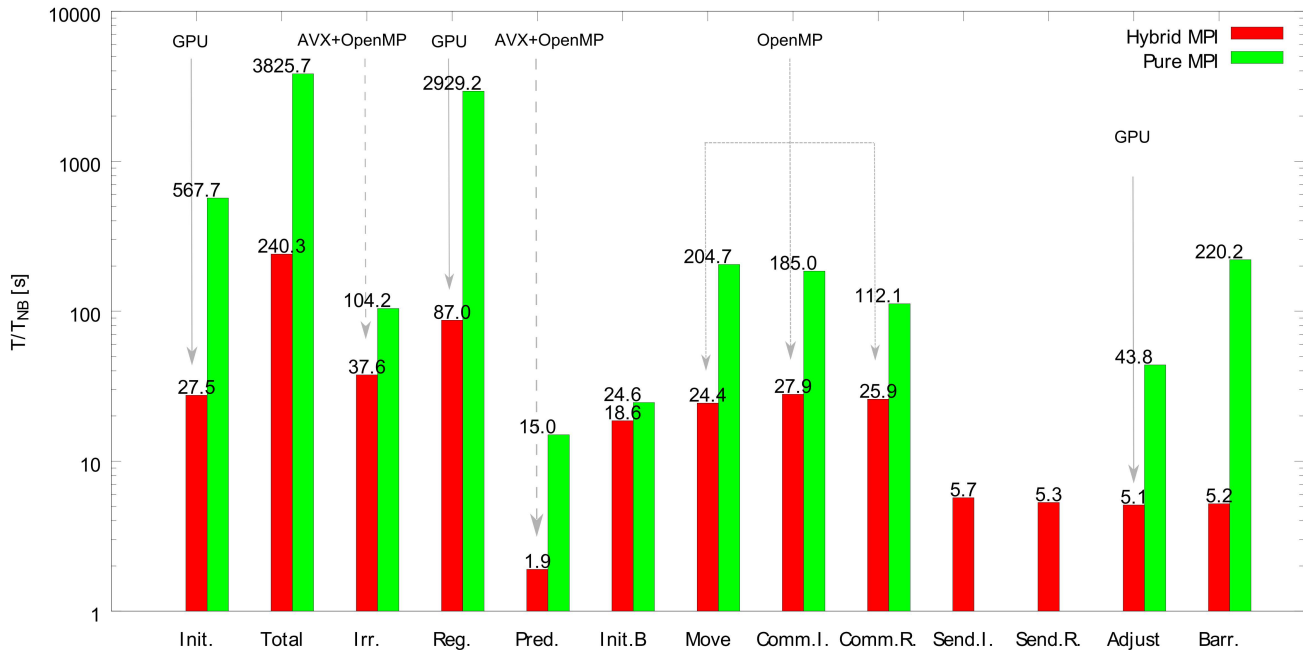


Figure 4. Comparison of performance between pure MPI and hybrid MPI (GPU + AVX/SSE + OpenMP + MPI) on the “Kepler” cluster at ARL, Heidelberg University. The test uses 256k particles with a Plummer model, IMF from Kroupa (2001) with mass range $0.08 - 100M_{\odot}$. The hybrid MPI test uses 4 nodes and each node includes 32 Intel Xeon E5-2650 cores (2.00 GHz per core) and 4 NVIDIA K20m with 2496 cores each (706 MHz per core). The pure MPI test uses the same configuration of nodes and CPU cores. The label “Total” means total time cost for 1 N -body unit and “Init.” denotes the initialization time of the simulations.

Max-Planck Supercomputing Centre (RZG) Germany. Each node is completely controlled (no other tasks on the node) and has two NVIDIA K20X with 2688 cores each (732 MHz per core) and 20 Intel Ivy Bridge cores (2.8 GHz per core). The total computing time for one N -body time unit $T_{\text{tot}}/T_{\text{NB}}$ is shown in Figure 5. The irregular and regular force integration computing time (T_{irr} and T_{reg}) are shown in Figure 6. All these three times are the averaged computing times of the first two N -body time units of each simulation. We test two basic initial models. One has no primordial binaries and another has 5% binaries. Both use a Plummer sphere (Plummer 1911) and initial mass function (IMF) from Kroupa, Tout & Gilmore (1993) with mass range $0.08 - 20M_{\odot}$ and no stellar evolution.

In the non-binary case, the scaling with different N_{node} for the total time is not ideal because of the communication cost. Here the speed-up saturates at about 8–16 nodes depending on the particle number. But if we consider the number of cores per node (20 CPU cores and 5376 GPU cores), the scaling with cores is excellent, since with 16 nodes 320 CPU cores and 86016 GPU cores are used. With one node, the performance of NBODY6++GPU is similar to that of NBODY6-GPU. Nitadori & Aarseth (2012) showed that NBODY6-GPU gives about 100 times speed-up compared to the sequential NBODY6 with two NVIDIA GeForce GTX 560 Ti with 384 cores each (822 MHz per core) and 4 Intel i7-2600K cores (3.40 GHz per core). On the “Hydra” cluster node, the speed-up can reach 100–500 depending on the particle number. Thus, with 16 nodes for one million particles, we can reach a factor of 400–2000 speed-up compared to the sequential NBODY6. Besides, the absolute time cost is very good, especially for the million-body case, the

total time is about 800 s for $N_{\text{node}} = 16$. For the ϕ GPU code tested in the “Laohu” cluster with 32 NVIDIA K20 GPU, one million particles take about 1500 s. Although we cannot compare the two codes directly with different computing cluster specifications, with the similar GPU type and number NBODY6++GPU can reach better performance. CPU cores are ignored here because the time fractions on the CPU for these two codes are very different: ϕ GPU spends about 90% computing time on the GPU while NBODY6++GPU has much less time fraction (Section 4.3). In the case with 5% primordial binaries, the scaling is not as good as for the case with no binaries due to the KS calculation. We discuss this issue in more detail in Section 6.

The regular and irregular integration times in Figure 6 are close to ideal for million-body simulations. It means that when ignoring MPI communications, the MPI parallelization speeds up regular and irregular calculation excellently for large number of particles. For small particle numbers ($< 10^5$) the scalings of both regular and irregular integrations depart from the ideal parallel limit. The reason is that the number of operations on each node (for regular integration is on GPU) is small. Thus, the cost of internal memory accessing and modification during integration, which cannot be scaled with computing cores or nodes, dominates the time.

4.3 Time fraction for different parts

We show the fraction of time spent on different parts of NBODY6++GPU in Figure 7. In the model without binaries, MPI communication and data moving consumes about

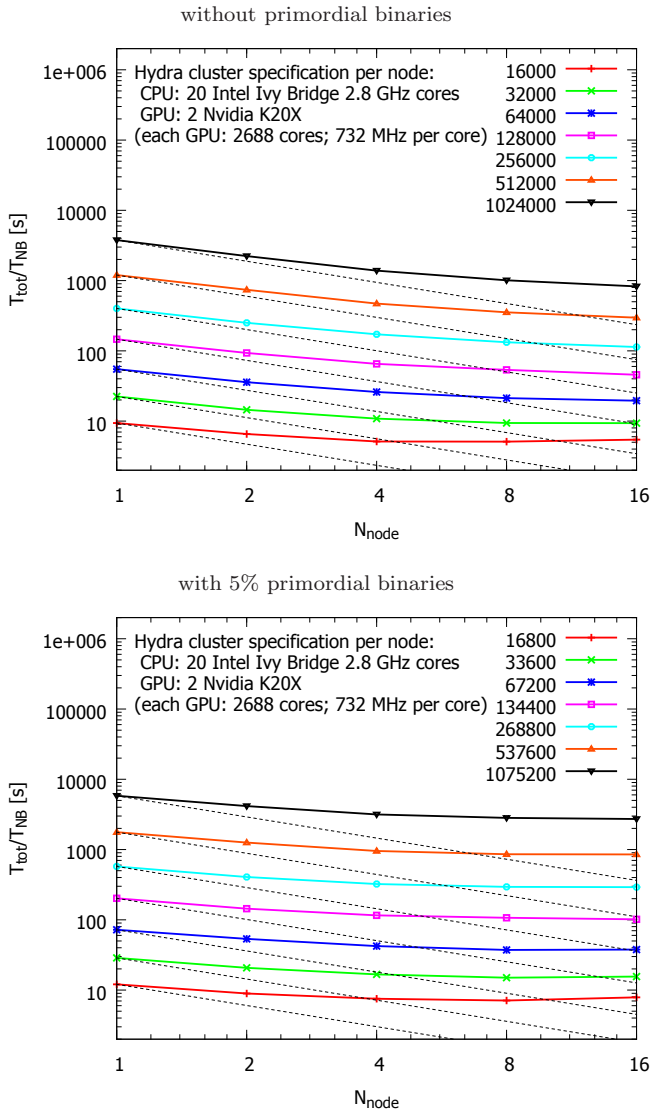


Figure 5. Performance of NBODY6++GPU with hybrid MPI on the “Hydra” cluster as the function of node number N_{node} . $T_{\text{tot}}/T_{\text{NB}}$ shows the computing time cost per N -body time unit. The configurations of each node are indicated in the panels. The dashed line shows the ideal parallel limit with zero communication cost. Different colors represent different particle numbers.

half of the total time in the case of 1024k particles with $N_{\text{node}} = 16$ and 128k particles with $N_{\text{node}} = 8$, which means the scaling reaches the MPI parallelization speed-up break-even point. For the 1024k particles with 5% binaries, the KS takes about half of the calculation time when $N_{\text{node}} \geq 8$. Thus, the KS procedures become the performance bottleneck.

4.4 Sorting list algorithm for selecting active particles

In Figure 8, we compare the performance of the sorting list algorithm and temporary list algorithm described in Section 3.3.1. The star cluster in our test simulation is modelled as a King sphere (King 1966) with $W_0 = 6$ using 1024k stars,

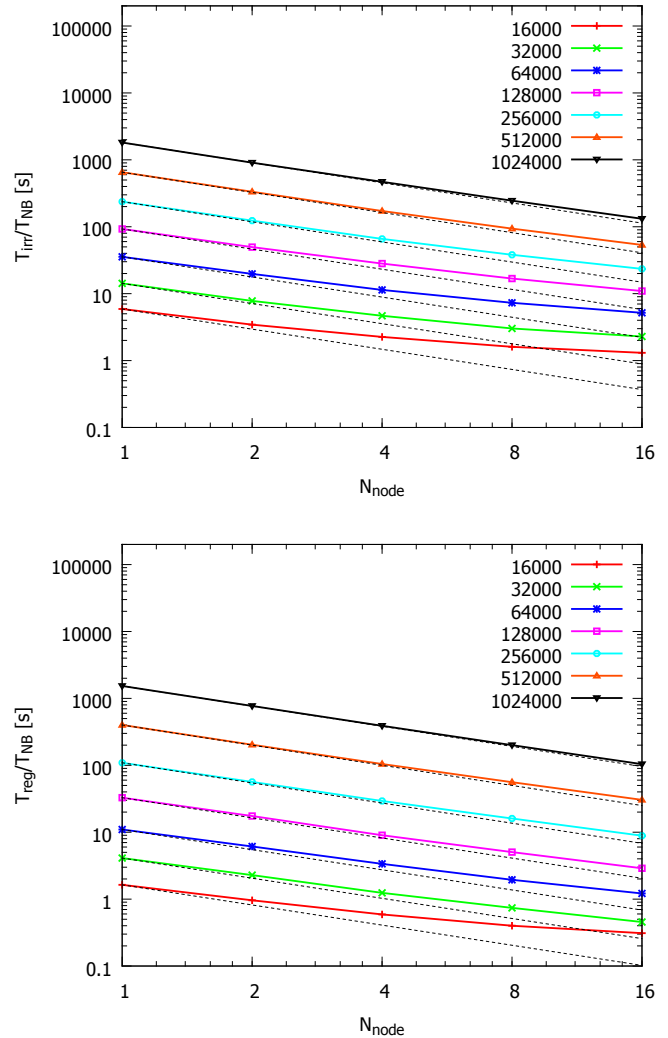


Figure 6. Performance of regular and irregular integration on the “Hydra” cluster as the function of N_{node} . Here the same node configurations and line types as in Figure 5 are used. $T_{\text{irr}}/T_{\text{NB}}$ and $T_{\text{reg}}/T_{\text{NB}}$ shows the irregular and regular integration computing time cost per N -body time unit respectively.

5% of primordial binaries and 8 nodes with the same node configuration as in Figure 5. To indicate that the sorting is very fast, the time of pure sorting part in this algorithm is also shown. We can see the sorting list algorithm is about 5 times faster than temporary list algorithm.

The time fraction of active particle selection with the new algorithm is shown as yellow part (Init.B.) in Figure 7. We can see Init.B. costs more for simulations with a larger number of particles. Even with this new method, it is close to irregular integration cost for the one million particles case ($\sim 7\%$).

5 APPLICATION

The main task for NBODY6++GPU is to simulate large star clusters. For a typical globular cluster, the total mass is $10^5 - 10^6 M_{\odot}$, thus the total number of particles is of the

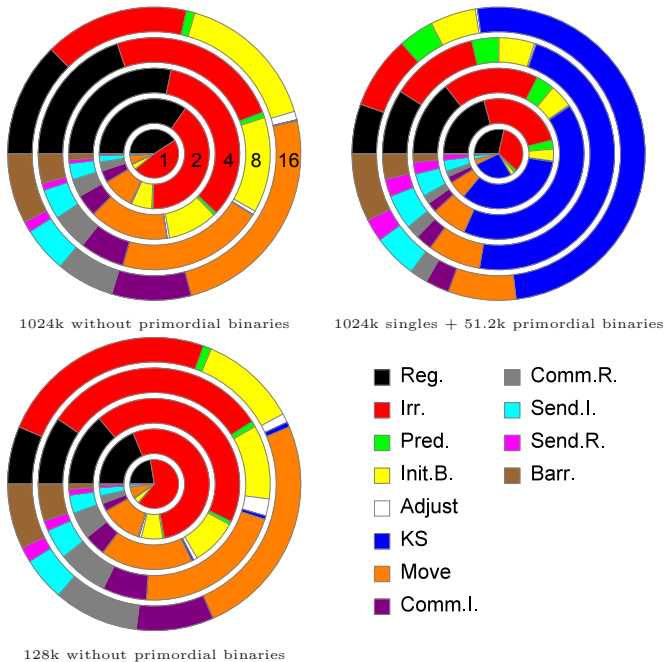


Figure 7. Pie charts showing the same test as Figure 5 but time fraction of different components in Hybrid MPI parallel NBODY6++. In each chart different rings show different N_{node} . From inside to outside rings, N_{node} are 1, 2, 4, 8 and 16. The two pie charts on the left show the model without primordial binaries and the pie chart on the right shows the model with 5% binaries. The models in top two pie charts include 1024k particles (singles + binaries) and the model in the pie chart at the bottom include 128k single particles. An explanation of the legends is provided in Table 1

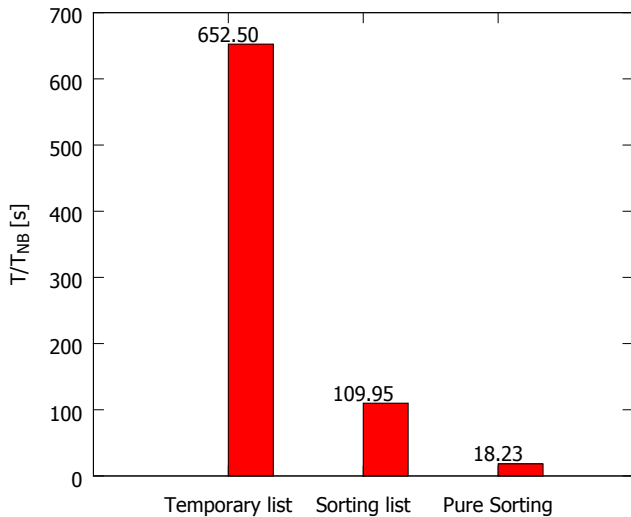


Figure 8. Comparison of performance between the sorting list algorithm and the temporary list algorithm. The “Pure Sorting” means the time cost of sorting part in sorting list algorithm.

order 10^6 . The typical age is about 12 Gyr. In our 1M stars with 5% primordial binary globular cluster model (the same as shown in Figure 8), we choose the parameters similar to NGC 4372 (Harris 1996). The initial half-mass radius is 7.5 pc and the tidal radius is 89.2 pc with a circular orbit around a point-mass galactic potential. One N -body time unit corresponds to 0.622 Myr. The computing time and number of particles are shown in Figure 9.

Initially, the computing time per N -body time unit was about 3000 s and this increased when several small time step particles formed. Later, we carried out several adjustments, then the simulation sped up and became about 1500 s. The number of particles only decreased slightly during 4500 N -body time units, but the computing speed actually increased at a later stage. The reason for the early slow speed was the two unsuitable criteria for triggering or terminating the two-body KS regularization. The first is the separation criterion R_{cl} and the second is the time step criterion Δt_{cl} . If the auto-adjustment of R_{cl} and Δt_{cl} are used, they are determined following Aarseth (2003)

$$R_{\text{cl}} = \frac{4R_{\text{h}}}{N(\rho_{\text{d}}/\rho_{\text{h}})^{1/3}},$$

$$\Delta t_{\text{cl}} \simeq 0.04 \left(\frac{\eta_{\text{I}}}{0.02} \right)^{1/2} \left(\frac{R_{\text{cl}}^3}{\langle m \rangle} \right)^{1/2}, \quad (1)$$

where $\rho_{\text{d}}/\rho_{\text{h}}$ is the central density contrast, η_{I} is the standard irregular time step coefficient and $\langle m \rangle$ is average mass. The factor $4R_{\text{h}}/N$ is the impact parameter for a 90 degree deflection in a two-body encounter. The auto-adjustment results in $R_{\text{cl}} = 1.4 \times 10^{-6}$ and $\Delta t_{\text{cl}} = 6.8 \times 10^{-8}$ N -body units at the beginning of this simulation. But these values are too small and many wide binaries including some unperturbed binaries are not regularized. Thus we switched off auto-adjustment and used $R_{\text{cl}} = 5.0 \times 10^{-6}$ and $\Delta t_{\text{cl}} \leq 2.0 \times 10^{-7}$ before about 2800 time units. We found that the R_{cl} and Δt_{cl} parameters were still too small, thus we enlarged R_{cl} to 1.0×10^{-5} and Δt_{cl} to 5.0×10^{-7} . Then the computing sped up after 2800 time units. The small parameters from auto-adjustment is because Eq. 1 is originally designed for small number of particles ($N = 10^2 - 10^3$). For the million-body simulation, the central density is usually high and $\rho_{\text{d}}/\rho_{\text{h}}$ is large. The criterion from Eq. 1 is only suitable for the central region of the cluster but too small for the outer region. There were several jumps in the computing time after the auto-restart with reduced time steps. These happened when a large energy error appeared due to specific events, such as difficult triple systems or the sudden change of force caused by large mass loss or premature perturbation of the neighbor sphere (such as neutron stars with high kick velocities). After we restore the normal time step parameters the computing time was again reduced.

There are also a few more models currently in progress and we will report in detail about the results from these simulations in a future publication.

6 DISCUSSION

While standard Hermite codes report a high efficiency using up to 700,000 cores on hundreds if not thousands of GPUs (Berczik, Spurzem & Wang 2013; Berczik et al. 2013), we find that our performance saturates at about

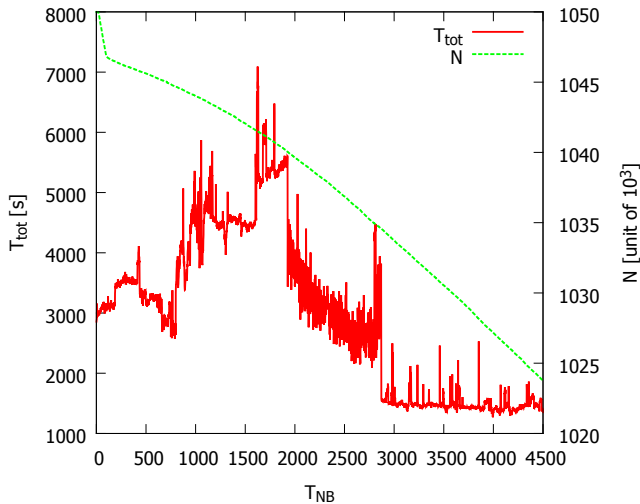


Figure 9. The evolution of the computing time per N -body time unit and the number of particles for the 1M globular cluster simulation as function of N -body time.

86,000 GPU cores and 320 CPU cores. This is not surprising, because NBODY6 and NBODY6++ are inherently more efficient than standard Hermite codes (less operations for the same physical result). A more detailed scaling analysis of NBODY6++GPU will be published separately (Huang et al., private communication).

As discussed in sections 4.2 and 4.3, the data movement and MPI communications become the bottleneck when the node number N_{node} is large since they have constant cost and the KS integration dominates the calculation when there are many primordial binaries. For the data copying and communication limit, a better communication algorithm (such as non-blocking communication as suggested by Dorband, Hemsendorf & Merritt (2003), which we will probably work on in the future), a higher network bandwidth between nodes and faster memory access are required.

In the common computer architecture today, the pure calculation operations for CPU is about two orders of magnitude faster than to access data from the host memory. For the non-shared memory parallelization like MPI, if the data communication consumption is larger than the calculation, the parallelization cannot improve the performance and sometimes even reduces the speed. Table 2 compares the calculation and communication costs for the regular force, the irregular force and the KS perturbation calculations. The ratio of calculation cost to communication cost, R_c , for the regular force is proportional to the full particle number N . Thus, the GPU and MPI parallelization for the regular force gives a very good scaling. For the irregular force, R_c is proportional to the average neighbor number. When there are many neighbors, the MPI parallelization is good. For typical star cluster simulations, the neighbor number N_b is a few hundred, thus it is acceptable. In NBODY6++GPU, the data movement and MPI communication is significant for the irregular force (Figure 7). For KS perturbation calculation, R_c is proportional to the average perturber number N_p , which is usually quite small (less than 100). Thus, MPI parallelization for KS can be inefficient. The reason for the

Table 2. Estimation of calculation and communication cost

| Cost | Regular force | Irregular force | KS perturbation |
|---------------|---------------|------------------------------|------------------------------|
| Calculation | $O(N_i N)$ | $O(N_i \langle N_b \rangle)$ | $O(N_i \langle N_p \rangle)$ |
| Communication | $O(N_i)$ | $O(N_i)$ | $O(N_i)$ |

* N_i : Active particle number

* N : Full particle number

* $\langle N_b \rangle$: Average neighbor number

* $\langle N_p \rangle$: Average perturber number for KS

small N_p is that usually in star cluster simulations, a large fraction of the KS binaries is unperturbed with $N_p = 0$, and perturbed KS binaries also tend to have small N_p (otherwise they would be terminated or transformed to hierarchical systems). Therefore, to get good performance of KS parallelization, the unperturbed and perturbed KS parts should be treated separately, since unperturbed KS only needs few operations and should avoid communication when parallelized (shared memory parallelization such as OpenMP or MPI-3). We are working on this and will show our KS parallelization method and benchmarks in a future publication. There is also another effort to parallelize KS with block time steps (Nitadori 2014, private communication).

We also find that the KS initialization and termination can be costly when there are wide binaries that frequently switch between KS and Hermite solutions. As discussed in Section 3.3.2, during the KS initialization and termination, the force and its first three derivatives need to be renewed for center-of-mass particles or two components (cost of $O(N)$) and the neighbor list of every particle and perturber list of KS pairs should be updated with new particle index (cost of $O(N \langle N_b \rangle)$). The regular part can be improved by using existing values instead of a direct calculation. The latter can be improved by using a reverse neighbor list for fast searching which particle has the KS pair as its neighbors. However, this requires large memory cost and coding effort.

When testing the code performance in computer clusters, we usually use the empty nodes where no other tasks are performed simultaneously. But for the applications, whether we can use scheduling whole nodes depends on the task management system in the clusters. Some clusters, such as “Laohu” at NAOC and “Milkyway” at the Jülich Computing center, only allow very few CPU cores for GPU tasks (1 – 2 CPU cores per GPU) and all other CPU cores in the same nodes are reserved for pure CPU tasks. NBODY6++GPU is not suitable for these kinds of clusters since it relies on heavy calculation on CPU (irregular and KS integration, data movements; see Figure 7). Moreover, in the shared nodes, different tasks compete with each other for network bandwidth, CPU loading and host memory. This sometimes results in a serious load imbalance: The MPI barrier time (Table 1) covers almost half of the total computing time. The only solution is to use computing clusters in which GPU nodes can be fully occupied by one GPU task each time.

Both NBODY6 and NBODY6++ have been developed over a long time. The codes have become more and more complicated which makes it difficult for beginners. Therefore, we also present documentation for the new version of NBODY6++GPU. The document includes a detailed

description of all input parameters and output data and will be updated with more details and new implementations. We also show several important differences between NBODY6++GPU and NBODY6-GPU in the Appendix.

The future improvements of the codes and hardware may lead to simulating even larger particle numbers, e.g., for nuclear star clusters using more GPU nodes appears feasible. The key to keep total wall clock times reasonable will be further optimization of communication and data management, especially for particles with very small time steps near a central black hole. Also, bandwidth and latency of communication hardware may help to gain one more order of magnitude, but not to reach the Exaflop/s regime. For the latter, hybrid codes seem more appropriate, which treat a large number of particles in the outskirts self-consistently, but not with full N^2 accuracy of the force computation (see, for recent examples, e.g., Meiron et al. 2014; Karl, Aarseth, Naab & Haehnelt 2015).

7 CONCLUSIONS

Direct numerical simulations of star clusters contribute significantly to the theoretical understanding of star cluster dynamics. Due to hardware and software limits, direct N -body simulations of real globular clusters with large number of particles have been a major challenge for many years. Sugimoto et al. (1990) pointed out that direct numerical simulations of globular star clusters could not be completed for the next decades unless there are breakthroughs in parallel computing which violate Moore’s law. After that, many efforts were made to reach this goal by using specially designed acceleration hardware (GRAPE and GPU).

In this paper, we present NBODY6++GPU. It combines for the first time the massively parallel multi-node code (MPI parallelized) NBODY6++ (Spurzem 1999; Hemsendorf, Khalisi, Omarov & Spurzem 2003) with the GPU and AVX/SSE acceleration on each node, using the libraries of Nitadori & Aarseth (2012). We discuss the performance tests (Figure 4, 5, 6 and 7) and new algorithms (Figure 1, 2 and 8) to accelerate the NBODY6++GPU. For the non-binary case, the overall scaling is good up to 16 nodes (320 CPU cores and 32 NVIDIA K20x GPUs including 86016 GPU cores) with a speed up of 400 up to 2000 depending on the particle numbers. The speed up is mainly achieved by the usage of GPUs to accelerate the long-range (regular) gravitational forces, which gives about 33 times faster force calculation (Figure 4). The AVX/SSE increase the speed of prediction of positions and velocities and neighbor (irregular) forces by a factor of 3. We also worked on the consistency of the code when combining several parallel methods together to ensure the stability. When GPU and AVX/SSE accelerate the force calculation very efficiently, other parts become bottlenecks of performance, such as time step scheduling and stellar evolution. We designed new algorithms to improve these parts.

We have demonstrated how NBODY6++GPU can simulate a realistic globular cluster with one million particles, stellar evolution and 5% primordial binaries for several Gyr (one half-mass crossing time requiring about an hour computational time; see Figure 9). A few more models are currently in progress and we will report the detailed results of

these simulations in future publications. With our final code version, which is publicly available², we can claim to have finally reached the goal of Sugimoto’s “dream” of 1990. A million-body cluster can be simulated for about 20 crossing times in one day on 320 cores with 32 GPUs. In the future, with the faster bandwidth and latency of hardware as well as optimizations of communication and data management, even larger system like the nuclear star clusters may be simulated by direct N -body codes.

The previous paragraphs show that our contribution to this would be impossible without the achievements of our predecessors and collaborators; in particular the current dominance of GPU hardware has been assisted by the development of GRAPE software over the last few decades which finally could be ported to GPU without fundamental problems.

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² We use Subversion and Github to manage NBODY6++GPU. The beta version can be downloaded by commands “svn co <http://silkroad.bao.ac.cn/repos/betanb6>” or “git clone <https://github.com/lwang-astro/betanb6pp.git>”

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Table A1. Differences between NBODY6++ and NBODY6

| | Subroutine | NBODY6++ | NBODY6 |
|----------------------------------|---|--|--|
| Installation | | Use configure script (see GPU Autoconf software ¹) | Use Makefile |
| Parallelization | | Can enable/disable features among MPI, GPU, OpenMP and AVX/SSE, except AVX/SSE requires OpenMP enabled | Use GPU, OpenMP and AVX/SSE together or OpenMP with AVX/SSE (only OpenMP or GPU with OpenMP are not supported) |
| Data files | | Rename most of output data files, change contents of some files and describe all data in a manual | Describe in a document |
| Basic data initialization | | Support different reading data format (see the manual for option KZ(22)) | Support N -body and astronomical unit data format |
| Primordial binary initialization | binpop.[f/F] | Support period distribution (Kroupa 1995) | Support modified period distribution with maximum semi-major axis 1000 AU and minimum period 1 day |
| Neighbor criterion | regcor_gpu.f gpucor.f | Adjust neighbor number to input parameter <code>MNBOPT</code> | Adjust neighbor number based on density contrast |
| Stellar evolution | kick.[f/F] | Use Maxwellian distribution of neutron star kick velocity with velocity dispersion 265 km/s (one dimension; Hobbs et al. 2005) | Use Maxwellian distribution of kick velocity with velocity dispersion $2 \times \text{VSTAR}$ (velocity scaling factor) and maximum kick velocity $10 \times \text{VSTAR}$ |
| | hrdiag.f kick.[f/F] | Use mass fall back for black hole kick (increase the remnant mass and reduce kick velocity; Belczynski, Kalogera & Bulik 2002) | Use black hole mass based on Eldridge & Tout (2004) (may add Belczynski, Kalogera & Bulik 2002 kick method in the future) |
| | brake4.f | – | Support gravitational radiation analytical orbit shrinkage |
| | intgrt.[f/F] intgrt_omp.f mdot.[f/F] | Apply mass loss only during regular step for thread-safety Only apply force correction when large mass loss happens (less accuracy but much faster) | Apply mass loss with minimum time step 100 years Calculate new force and its derivatives for large mass loss |
| Galactic tidal force | xtrnlf.f fbulge.f | Support point-mass + disk + halo + Plummer model | Support point-mass + disk + halo + bulge + Plummer model |

¹ <http://www.gnu.org/software/autoconf/>

APPENDIX A: DIFFERENCES BETWEEN NBODY6++ AND NBODY6

There are several differences with NBODY6 . Table A lists some of the most important. The manual in the NBODY6++GPU code directory gives more details.