Star clusters and black holes in galaxies across cosmic time
Proceedings IAU Symposium No. 312, 2014
Y. Meiron, S. Li, F.-K. Liu & R. Spurzem, eds.

doi:10.1017/S174392131500798X

Acceleration of hybrid MPI parallel NBODY6++ for large *N*-body globular cluster simulations

Long Wang[1], Rainer Spurzem[2,1], Sverre Aarseth[3], Keigo Nitadori[4], Peter Berczik[2], M.B.N. Kouwenhoven[1] and Thorsten Naab[5]

[1]Kavli Institute for Astronomy and Astrophysics, Peking University, Beijing, China
email: long.wang@pku.edu.cn

[2]National Astronomical Observatories and Key Laboratory of Computational Astrophysics, Chinese Academy of Sciences, Beijing, China

[3]Institute of Astronomy, University of Cambridge, Cambridge, UK

[4]RIKEN Advanced Institute for Computational Science, Kobe, Japan

[5]Max-Planck Institut für Astrophysik, Garching, Germany

Abstract. Previous research on globular clusters (GCs) dynamics is mostly based on semi-analytic, Fokker-Planck, Monte-Carlo methods and on direct N-body (NB) simulations. These works have great advantages but also limits since GCs are massive and compact and close encounters and binaries play very important roles in their dynamics. The former three methods make approximations and assumptions, while expensive computing time and number of stars limit the latter method. The current largest direct NB simulation has $\sim$ 500k stars (Heggie 2014). Here, we accelerate the direct NB code NBODY6++ (which extends NBODY6 to supercomputers by using MPI) with new parallel computing technologies (GPU, OpenMP + SSE/AVX). Our aim is to handle large N (up to 10^6) direct NB simulations to obtain better understanding of the dynamical evolution of GCs.

Keywords. methods: numerical, globular clusters: general

1. The features of NBODY6/NBODY6++

Star clusters are dense groups in which the relaxation timescale is short. Thus, the frequent close encounters and binaries play an important role in star cluster dynamics. NBODY6 (Aarseth 2003) is a state-of-the-art direct NB simulation code specifically designed for star clusters. It uses the 4th order Hermite integrator with a block time step and neighbor scheme which improve the integration speed. Kustaanheimo & Stiefel (1965) (KS) and Chain regularization (Mikkola & Aarseth 1993) are used to ensure the highly accurate treatment of close encounter and binaries.

The direct NB simulation is very costly. The cost per relaxation timescale can be $O(N^{10/3}/\ln N)$ (Makino & Hut 1988). Thus parallelization is necessary if we want to simulate large particle system like GCs. We present our new version of NBODY6++GPU by combining the massively parallel multi-node code NBODY6++ (Spurzem 1999 and Hemsendorf *et al.* 2003) with the hybrid parallelization libraries (GPU + OpenMP + AVX/SSE) from NBODY6-GPU (Nitadori & Aarseth 2012). The parallelization structure of NBODY6++GPU is shown in Figure 1. One cycle of integration can be separated to three hierarchical time step blocks: (1) Regular block: particles belong to the current regular time step blocks will obtain forces calculated from all other particles by using GPU acceleration. (2) Irregular block: particles belong to the irregular time step blocks only cumulate forces from their neighbors. AVX/SSE together with OpenMP is used to

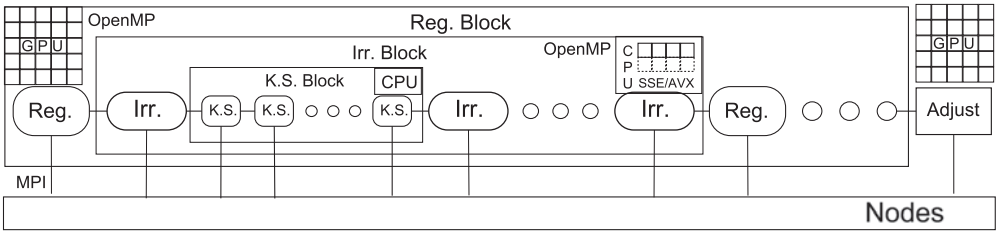

Figure 1. The NBODY6++GPU code parallelization structure. The MPI, GPU, OpenMP and AVX/SSE are used for different components.

accelerate position and velocity prediction and force calculations. (3) KS block: KS pairs will be integrated inside KS time step blocks with MPI parallelization support.

2. Benchmarks and resources

The detailed performance analysis will be published soon (Wang *et al.* 2015 and Huang *et al.* 2015). For 10^6 particles with Plummer (1911) sphere and a Kroupa, Tout & Gilmore (1993) initial mass function (IMF), we get ~ 800 seconds computing time per NB time unit with 8 nodes (160 Intel Ivy Bridge cores (2.8 GHz) and 16 NVIDIA K20X GPU) on the "Hydra" Cluster, Max-Planck-Supercomputing center, Garching. For a realistic globular cluster simulation with one million stars including 5% primordial binaries, King (1966) profile and Kroupa (2001) IMF, the same configuration of hardware results in a stable computing time of ~ 1500 seconds per NB time unit.

Future improvements will speed up the KS regularization performance. With the current NBODY6++GPU we can already handle the million-body GC direct NB simulations. Future developments of hardware with faster bandwidth and latency and optimizations of communication and data management will open the window for simulations of larger system like nuclear star clusters.

The code is free for downloading by two links:

- Subversion: svn co http://silkroad.bao.ac.cn/repos/betanb6
- GitHub: git clone https://github.com/lwang-astro/betanb6pp.git

The user manual is also provided in downloading resource with detailed descriptions of code features, input and outputs.

References

Aarseth S. J., 1963, *MNRAS*, 126, 223
Heggie D. C., 2014, *MNRAS*, 445, 3435
Hemsendorf M., Khalisi E., Omarov C. T., & Spurzem R., 2003, *High Performance Computing in Science and Engineering*. Springer Verlag, 71, 388
Huang, S., Spurzem, R., & Berczik, P. 2015, *RAA*, in press (arXiv:1508.02510)
King I. R., 1966, *AJ*, 71, 64
Kroupa P., Tout C. A., & Gilmore G., 1993, *MNRAS*, 262, 545
Kroupa P., 2001, *MNRAS*, 322, 231
Kustaanheimo P. & Stiefel E., 1965, *J. Reine Angew. Math.*, 218, 204
Makino J. & Hut P., 1988, *ApJS*, 68, 833
Mikkola S. & Aarseth S. J., 1993, *CeMDA*, 57, 439
Nitadori K. & Aarseth S. J., 2012, *MNRAS*, 424, 545
Spurzem R., 1999, *JCoAM*, 109, 407
Plummer H. C., 1911, *MNRAS*, 71, 460
Wang L., Spurzem R., Aarseth S., *et al.* 2015, *MNRAS*, 450, 4070

https://doi.org/10.1017/S174392131500798X Published online by Cambridge University Press