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NBodyLab Simulation Experiments with GRAPE-6a and MD-GRAPE2 Acceleration

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Abstract. NbodyLab is an astrophysical N-body simulation testbed for student research. It is accessible via a web interface and runs as a backend framework under Linux. NbodyLab can generate data models or perform star catalog lookups, transform input data sets, perform direct summation gravitational force calculations using a variety of integration schemes, and produce analysis and visualization output products. NEMO, a popular stellar dynamics toolbox, is used for some functions. NbodyLab integrators can optionally utilize two types of low-cost desktop supercomputer accelerators, the newly available GRAPE-6a (125 Gflops peak) and the MD-GRAPE2 (64-128 Gflops peak). The initial version of NBodyLab was presented at ADASS 2002. This paper summarizes software enhancements developed subsequently, focusing on GRAPE-6a related enhancements, and gives examples of computational experiments and astrophysical research, including star cluster and solar system studies, that can be conducted with the new testbed functionality.

1. GRAPE Hardware Acceleration

The design objectives and basic functionality of NBodyLab[1] were described in the 2002 ADASS proceedings. Interfaces have been developed for two types of Japanese GRAPE (Gravity Pipeline) desktop supercomputer PCI boards.

Applications using large arrays of GRAPE chips have six times won the annual international Gordon Bell competition for top supercomputer performance. At least two multi-year, well-funded Japanese research programs are developing next-generation GRAPE systems aimed at dominating high-performance astrophysical research and bio-computing. This promising future is further motivation to expose students to GRAPE technology and for researchers and software engineers to gain experience with the capabilities and software interfaces to the current generation of GRAPE's.

NBodyLab development began by developing interfaces to an MD-GRAPE2 accelerator board (Molecular Dynamics - Gravity Pipeline) running at 64 Gflops

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[1] `http://www.nbodylab.com`

peak (128 Gflops peak with optional booster card), handling up to 500K particles for a cost of less than $12K. The MD-GRAPE2 was designed for molecular dynamics (MD) simulations and calculates a general force between all pairs of particles in an N-body particle simulation, supporting Coulomb, van der Waals and user-defined forces. NBodyLab utilizes the MD-GRAPE2 only as a basic Newtonian accelerator for gravitational forces.

In late 2003 the GRAPE-6a, developed at Tokyo University, became available with a PCI interface. Generations of GRAPE chips have been developed specifically for astrophysical research. In their book, GRAPE designers Makino and Taiji describe GRAPE simulations of planetary formation, star clusters, galactic nuclei, galaxy interactions and galaxy formation. (The MD-GRAPE R&D was spun-off into a Japanese research institute and is now aimed at biosciences such protein modeling, headed by Dr. Taiji). A GRAPE-6a board runs at 128 Gflops peak, can handle 64K particles, and costs less than $9K.

GRAPE cards facilitate quick NBodyLab runs by students using a web browser. A 10,000 particle simulation with a stable and accurate integrator takes 10 seconds using the GRAPE-6a; without GRAPE-6a acceleration, the same run takes 10 minutes (10K Plummer sphere; t=0 to 1; Hermite individual time step integrator; 3 GHz P4 host).

2. Integration Schemes

The focus of development of integration options for NBodyLab has been direct integration methods because the GRAPE cards implement direct summation of forces in hardware and direct summation is a straightforward implementation of Newton's Law of Gravitation and easier for undergraduates to understand than, for example, tree algorithms. Hardware-accelerated direct summation is preferable for many classes of astrophysics problems. (An option to use the classic tree algorithm, from NEMO, is available for comparison runs.)

The MD-GRAPE2 force call is simple: *m2_calculate_forces (mu, x, npart, a)* which returns the computed accelerations for each particle. In the initial version of NBodyLab, 1st, 2nd and 4th order (e.g. Runge-Kutta RK4) constant timestep integrators were implemented for the MD-GRAPE2, following basic numerical analysis texts. Astrophysics and MD researchers explained to co-author and developer Vicki Johnson that better schemes were available. The theory, analysis, performance and physical interpretation of numerical integration methods has long been an challenging area of research (see Aarseth).

For example, Prof. Makino, lead designer of the astrophysics GRAPE family, has discussed in personal communications with Johnson some considerations for MD and astrophysics applications: In MD, simulations typically follow the vibration of atoms for very long periods. The typical period of oscillation is on the order of 10 femtoseconds and an MD simulation evolves the system for pico, nano, or microseconds, so energy conservation must be very good. Constant time steps can be used and symplectic (or time-symmetric) integration schemes work well in these cases. By contrast, RK4 gives better accuracy per orbit, but it can cause long-term linear drift of energy. Symplectic schemes do not cause linear drift. For collision-less problems in astrophysics, it is not necessary to follow a large number of orbits. The high accuracy of RK4 is not needed per orbit, so computational speed may be gained by using a 2nd-order symplectic (also known as leapfrog or Verlet) algorithm, which requires less memory to compute. For collisional problems, astrophysical simulations need to use variable and individual timesteps, and leapfrog algorithms do not suffice. High-order schemes are needed, and Hermite has become the method of choice.

The name Hermite is used in numerical analysis to denote a polynomial based on the function and its derivatives. A 4th-order Hermite integrator is implemented by the GRAPE-6a. In the Hermite individual timestep scheme, each particle has its own timestep and integrations proceed as a global time step is incremented by the particle i with the smallest timestep. The positions of all particles at the global time are estimated and the gravitational force on particle i is calculated and its position, velocity, time, timestep, etc. are updated. The 4th-order Hermite scheme is well-proven for accuracy, efficiency, and algorithmic simplicity. The GRAPE-6a hardware performs the expensive calculation of the derivative of acceleration, which is not computed by the MD-GRAPE2.

Prof. Makino provided Interconnect with leapfrog, 4th and 6th order symplectic schemes with constant timestep for incorporation into NBodyLab. Individual and blocked timestep Hermite test codes provided with the GRAPE-6a were adapted to NBodyLab. An interface to a 2nd-order leapfrog method for the GRAPE-6a was developed as well. Versions of all the NBodyLab integration options have been developed for hosts without GRAPE support. Although the MD-GRAPE2 offers software emulation of the hardware (which has its own numerical precision and scaling characteristics), these were not used, in favor of faster direct summation calculated by the PC host processor.

3. Computational Experiments

Undergraduate students not exposed to numerical analysis can be surprised by the results of varying, sometimes only slightly, the parameters or inputs to different integration options. Experiments with small data sets can demonstrate to students the importance of carefully and skeptically interpreting the results of larger n-body simulations, and confirm the value of robust schemes like the Hermite.

NBodyLab's web interface makes it easy to perform a variety of computational physics experiments with different input data sets, transformations, integrators and parameters like softening. The advantages of NBodyLab's newly developed GRAPE-6a support and Hermite options are evident in runs with an n=100 Plummer model – see Makino and Taiji for an analysis of interesting system behaviors that can be studied with this small model.

With the new GRAPE-6a related features, students can achieve better performance, stability and accuracy for studies of small systems, such as binary, triple and binary-binary encounters, and larger stellar dynamics simulations. They can compare conservation of energy, momenta, etc., for GRAPE-6a versus MD-GRAPE accelerated evolutions and use the more computationally expensive Hermite for large numbers of particles or long time scales. Comparisons of individual timestep algorithms with variable blocked timestep or constant fixed-step schemes are now possible.

4. Astrophysical Investigations

Co-author Alper Ates' master's thesis, entitled *N-Body Simulations and HR diagrams of Nearby Stars*, 2004, used NBodyLab with the MD-GRAPE2 to model the geometric evolution of nearby stars and an open star cluster Collinder 70. This research utilized a new NBodyLab tool developed to search Hipparcos and SKY2000 star catalogs, find stars in a user-specified volume, extract values, and convert and scale their units and estimate masses from their luminosity. NBodyLab simulated the geometric evolution of the selected regions. Ates analyzed errors and investigated scaling by simulating two 1 solar mass stars freely falling on each other; the time to reach 1/2 distance and the velocity at that point was calculated classically. Time and velocity values simulated with NBodyLab with RK4 and symplectic integrators were compared with calculated theoretical values. Ates also used NbodyLab to study star clusters, using catalog data, and he compared the simulations to telescope observations he made using Pomona College observatories, as presented in his January 2003 AAS poster. His most recent work concentrates on the Solar System. Recently simulations from Ates' work have been run with the new NBodyLab GRAPE-6a and Hermite options. Small systems studied by Ates using NBodyLab have included:

- *Ursa Major* – Using data obtained from SKY2000 catalog, the well-known 7 members of Big Dipper were modeled. This model was created to check the accuracy of Cartesian coordinate conversion algorithms. An OpenGL 3D visualizer revealed the well-known Big Dipper shape. Since Big Dipper is just 7 members of a larger cluster this work concentrated on positional accuracy, not the time evolution.
- *Star cluster Hyades* – The flatness of the cluster parallel to the galactic plane was observed and convergent motion was successfully simulated.
- *Collinder 70* – Very accurate astrometric data for this cluster is available, but surprisingly no prediction on the future geometric evolution of this cluster had been made. Using the NBodyLab catalog extraction, 46 members of the cluster were retrieved and simulated for 75,000 years and the future shape of the cluster predicted.
- *Solar System* – Since the heliocentric coordinates and mass for each planet are well-known, the study focused on accurate scaling and achieving long term stability and accuracy of the orbits. Software to convert heliocentric coordinates was developed and a scaling scenario designed involving the Sun and the Jupiter, where Jupiter is left free to fall onto Sun and the time it takes to reach half distance and the velocity at that point classically calculated. Once scaling was done the Heliocentric positions of the planets obtained from VSOP routines for any given date were converted into Cartesian units, and the orbital velocities calculated and scaled for the NBodyLab simulation. Resultant orbits show good eccentricities and are stable over 200 years. Hermite schemes generally have lower energy errors for planetary N-body simulations than other NBodyLab integrators, as confirmed with GRAPE-6a runs.
- *Halley's comet* – The simulation shows 76 year periodic orbits. Surprisingly the comet is seem to be approaching from z= 300 to z=270 in 4 revolutions. The fast change in the inclination angle deserves future investigation of errors and calculation of initial conditions.

Pomona College student J. Wertheimer, in his 2003 senior thesis entitled *Tidal Shocking of Globular Clusters*, used NBodyLab with the MD-GRAPE2. He started with a single Plummer sphere to simulate a globular cluster and let it evolve in a constant potential. He imposed a tidal radius to simulate the tidal force from the galaxy. Periodically the cluster was shocked by letting it pass through the disk of a simulated Milky Way derived from GalactICS. Runs took 10-20 hours with RK4. Running this simulation with the GRAPE-6a Hermite option will likely yield interesting differences in energy and radial distributions.

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