

Adapting NBODY4 with a GRAPE-6a Supercomputer for Web Access, Using NBodyLab

Vicki Johnson

Interconnect Technologies Corporation, POB 788, Claremont, CA 91711, USA, vlj@interconnect.com

Sverre Aarseth

Institute of Astronomy, University of Cambridge, Cambridge, CB3 0HA, England, sverre@ast.cam.ac.uk

Abstract. A demonstration site has been developed by the authors that enables researchers and students to experiment with the capabilities and performance of NBODY4 running on a GRAPE-6a over the web.

NBODY4 is a sophisticated open-source N -body code for high accuracy simulations of dense stellar systems (Aarseth 2003). In 2004, NBODY4 was successfully tested with a GRAPE-6a, yielding an unprecedented low-cost tool for astrophysical research.

The GRAPE-6a is a supercomputer card developed by astrophysicists to accelerate high accuracy N -body simulations with a cluster or a desktop PC (Fukushige et al. 2005, Makino & Taiji 1998). The GRAPE-6a card became commercially available in 2004, runs at 125 Gflops peak, has a standard PCI interface and costs less than \$10,000.

Researchers running the widely used NBODY6 (which does not require GRAPE hardware) can compare their own PC or laptop performance with simulations run on www.NbodyLab.org. Such comparisons may help justify acquisition of a GRAPE-6a. For workgroups such as university physics or astronomy departments, the demonstration site may be replicated or serve as a model for a shared computing resource. The site was constructed using an NBodyLab server-side framework.

NBodyLab¹, as described in ADASS Proceedings (Johnson et al. 2002, Johnson & Ates 2004) is a testbed framework intended to help students and researchers experiment with N -body simulation codes and GRAPE-family hardware using a convenient web interface.

In the past two years, NBodyLab capabilities have improved, upgrading from an MD-GRAPE2 to the new GRAPE-6a, and now relying on the Hermite scheme instead of RK4, leapfrog and symplectic integrators. Earlier NBodyLab versions performed an N -body simulation with a sequence of separate tools: model generators, a variety of numerical integrators for the N -body evolution, and tools for basic diagnostics and graphical displays. However, the numerical integration was augmented by only rudimentary system energy checks. Many

¹<http://www.nbodylab.org>

of the end-to-end simulation characteristics such as consistent scaling were not addressed. More sophisticated capabilities were needed to improve the realism of simulations.

NBODY4 fully meets those needs, handling close encounters and hard binaries, escapers, mass loss and external forces, and employs several advanced regularization techniques for high accuracy. Designed as a large integrated package (approx. 40,000 lines of code) with over 70 run parameters, NBODY4 ensures consistent scaling, analysis and results. NBODY4 has been refined and tested for over 10 years with GRAPE-family hardware at several installations, and much of the code base is shared with the state-of-the-art, widely used NBODY6 (which employs an efficient neighbor scheme rather than just one force polynomial).

The review paper (Aarseth 1999) and the comprehensive book *Gravitational N-Body Simulations* (Aarseth 2003) presented the NBODYx software suite to a broader scientific community. When the GRAPE-6a became commercially available and the library was adapted to support FORTRAN by Fukushige et al. (2004), NBODY4 became an ideal candidate for a low-cost public demonstration and educational site.

1. Demonstration of NBODY4 Capabilities

An online introduction to running NBODY4 covers topics such as parameter selection, suggested simulations, astrophysical and N -body units, integration methods and the relationship of NBODY4 to NBODY6. For the NBodyLab interactive web presentation, default parameters were selected that are suitable for short demonstration runs, and some parameters were limited by the NBodyLab interface, such as permitted CPU time (currently 20 minutes) and N (15,000 particles). Native runs of NBODY4 are driven by an ASCII parameter input file. Two styles of web presentation were developed for the input parameters: (1) for users familiar with NBODYx-type codes, the concise “classic“ presentation of all parameters, documented on a separate reference web page; and (2) for first-time users, an expository presentation of a subset of parameters:

The screenshot shows the NBODY4 web interface. On the left, there is a text area containing an ASCII input file with the following content:

```

1 10.0 0
1000 1 5 50000 1
0.02 2.0 10.0 100.0 2.0D-05 1.0 0.5
0 0 1 0 1 0 5 0 0 0
0 0 0 1 1 1 0 0 3 0
1 0 2 0 1 0 0 0 0 2
0 0 0 0 0 0 1 0 0 0
1.0E-05 1.0D-04 0.2 1.0 1.0E-06 0.001
2.3 10.0 0.2 0 0.02 0 2.0
0.5 0 0 0

```

Below the text area is a "Browse..." button. To the right of the text area, there are two dropdown menus: "Time scale for diagnostic plots" set to "t (N-body units)" and "Axes length for N-body plots, or 'autoscale'" set to "autoscale". A "Start the simulation" button is at the bottom left.

On the right side of the interface, there is a form for generating an input model. The "Use NBODY4 to generate an input model" dropdown is set to "two Plummer models in orbit". Below this, there is a text input for "N: number of members in first (or single) model" with the value "1000".

Under the heading "For two Plummer models in orbit:", there are four input fields:

- APO: separation, value: 6.0
- ECC: eccentricity of two-body orbit, value: .5
- N2: second Plummer model size, value: 500
- SCALE: second Plummer model scale factor, value: .5

Under the heading "For massive perturber and a planetesimal disk:", there are four input fields:

- APO: separation between the perturber and the Sun, value: 6.0
- ECC: eccentricity of two-body orbit, value: 1.1
- DMIN: minimum distance of approach (periastron), value: 3
- SCALE: perturber mass scale factor (=1 for Msun), value: .5

For scientifically and visually interesting demonstrations, NBODY4 can optionally generate uniform and isotropic models or Plummer models, two Plummer models in orbit, or an external massive perturber passing a thin planetesimal disk. For more realistic star cluster simulations, a population of primordial bi-

naries may be included. Users can also employ their own initial conditions. An ASCII data file containing mass, position and velocity for each member can be uploaded using the standard browser upload facility. The data may be scaled to the standard total energy and velocity magnitudes adjusted by a dimensionless input parameter, or the input data set may be left unscaled.

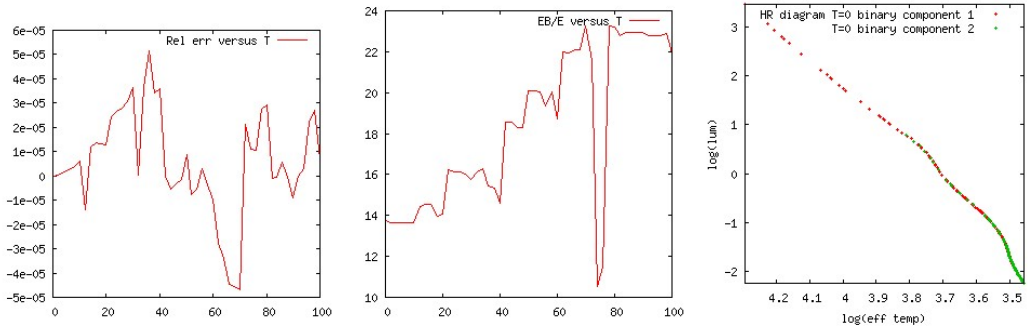
When NBODY4 runs natively, it produces comprehensive output as the run progresses. For the web interface, a subset of the output is presented as progress indicators, and the user is given the choice to halt the run manually. The extensive NBODY4 output file is available through a link from the main simulation result page:

```

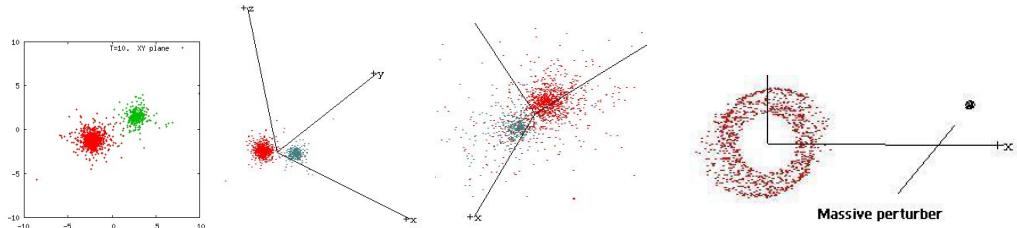
T = 10.0 N = 1000 ES = 0 NH = 0 MM = 0 NS = 1000 NSTEPS = 1521518
RUN = 1 N# = 6 CPU = 0.2 DMIN = 6.9E-05 3.9E-04 AMIN = 1.0E+02 RMAX = 0.0
<R> RTIDE RDENS RC NC MC RHOD RHOM UN NPT RCM VCM AZ
#1 0.73 12.0 0.11 0.242 48 0.107 5.8 31.4 0 0 0.000 0.0000 -0.0210
#2 7389 39 34 NKSPEP NPRECT NKSMOD NTRY NTRIP NQUAD NCHAIN
#4 22 0 0 0 0 0 0 0 28.50 0.0 0.0 0.0 0.0 0
Elapsed real time (secs): 11
Carefully review the parameter assignments and results in the full NBODY4 run output
END RUN TIME = 10.0 CPUTOT = 0.2 mins ERRTOT = 0.000000
    
```

At the completion of the run, diagnostic plots are produced, including

- Number of integration steps (direct integration and regularized pairs).
- Relative energy error summed with signed main output.
- Half-mass radius.
- Closest two-body separation (first is all-time and 2nd is since last time).
- Cluster membership N (in case of escape removal).
- Final sum of all energy errors (i.e. relative and absolute).
- Total energy (should be constant except for escape removal).
- Energy in binaries (relative to total energy).
- Core radius (size of high-density region).
- Density and velocity as a function of average radii in increasing shells.
- Eccentricity and energy dispersion of planetesimal disk.
- HR evolution diagrams for single stars and binary components.



The N -body model evolution is displayed in planar and 3D graphical views. The evolution can be viewed using a 3D animation Java applet that includes rotation, zoom and frame controls.



All data produced by NBODY4, and ancillary files generated for plotting, are made available by NBodyLab and can be saved via the browser for further analysis or plotting.

2. Demonstration of GRAPE Hardware Acceleration

Fukushige et al. (2004) document an $N=16,000$ run with NBODY4+GRAPE-6a that achieved 53 Gflops, or around 40% of the theoretical peak speed of the GRAPE-6a. Fukushige's run for a star cluster simulation lasted 10 days. Some studies using NBODY4 with a GRAPE run for weeks to produce results of a realistic simulation.

Timing comparisons of NBODY4 and NBODY6 running on the demonstration site host (2.8 MHz P4), show that NBODY4+GRAPE-6a yields approximately a 10x performance improvement for dataset sizes appropriate for NBodyLab web demonstrations:

Run times in seconds, single Plummer evolution, $T=0$ to $T=2$

Number of particles	1000	2000	5000	10,000	15,000	20,000	25,000
NBODY4+Grape6a	2	6	24	75	154	260	394
NBODY6	6	21	138	630	1464	2660	4320

3. Modifications Needed for the Back-End NBodyLab Framework

The GRAPE-6a utilities distributed with NBODY4, and the sample codes and libraries provided with the GRAPE-6a, queue requests for the GRAPE-6a because it is assumed that the user is running on a personal workstation. In server mode, alternative handling of GRAPE-6a contention and queueing were implemented to avoid browser time-outs. While running under the HTTP server, the GRAPE-6a library sometimes produced errors that caused NBODY4 to hang, and the GRAPE resource lock was not released; this behavior appears to have been resolved by stderr redirection.

A key principle of the NBodyLab approach is to minimize modifications of the simulation source code, to avoid introducing numerical or scientific errors. There was some concern initially that such a large and complex code as NBODY4 might not be easily adapted using NBodyLab techniques, especially since it is written in FORTRAN, a language rarely used for server-side web applications.

However, NBODY4 is a well-organized code whose logic paths and I/O are clearly delineated, so modifications proved straight-forward. NBODY4 already had several needed features that are OS dependent, such as a parameter to limit CPU time and an OS independent technique to enable a user to halt calculations gracefully. Several challenges presented themselves. On a demonstration site, there is always the risk that inconsistent or untried input parameters might cause anomalous looping or NaN's in NBODY4, and adequate accuracy can not always be guaranteed. CPU time can vary not only due to different N but also from one simulation to another because similar initial conditions may lead to a surprisingly large dispersion in the results, especially as regards the chaotic formation and evolution of energetic binaries. Timings tests for different simulation options were made to estimate sufficiently small progress display intervals to maintain browser connections. A planned future scheduler to run jobs for registered users during idle periods will circumvent some of the unique challenges of supporting interactive web access.

4. Conclusions and Acknowledgments

NBODY4 in combination with the GRAPE-6a is affordable and will help enlarge the community of N -body researchers. The demonstration site is intended to hasten that process, by helping scientists, students and educators see for themselves the the scientific capabilities of NBODY4 and the performance benefits of the GRAPE-6a.

We thank Jun Makino of Tokyo University who generously loaned GRAPE-6a hardware for NBodyLab development and demonstrations.

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