

NBodyLab: A Testbed for Undergraduates Utilizing a Web Interface to NEMO and MD-GRAPE2 Hardware

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Abstract. An N-body simulation testbed called NBodyLab was developed at Pomona College as a teaching tool for undergraduates. The testbed runs under Linux and provides a web interface to selected back-end NEMO modeling and analysis tools, and several integration methods which can optionally use an MD-GRAPE2 supercomputer card in the server to accelerate calculation of particle-particle forces. The testbed provides a framework for using and experimenting with the main components of N-body simulations: data models and transformations, numerical integration of the equations of motion, analysis and visualization products, and acceleration techniques (in this case, special purpose hardware). The testbed can be used by students with no knowledge of programming or Unix, freeing such students and their instructor to spend more time on scientific experimentation. The advanced student can extend the testbed software and/or more quickly transition to the use of more advanced Unix-based toolsets such as NEMO, Starlab and model builders such as GalactICS. Cosmology students at Pomona College used the testbed to study collisions of galaxies with different speeds, masses, densities, collision angles, angular momentum, etc., attempting to simulate, for example, the Tadpole Galaxy and the Antenna Galaxies. The testbed framework is available as open-source to assist other researchers and educators. Recommendations are made for testbed enhancements.

1. Introduction and Motivations

NBodyLab¹ is a web-based N-body simulation testbed for undergraduate astronomy students. It was developed for the Astronomical Computing Initiative at Pomona College and used initially to support the curriculum for a course in

¹<http://www.nbodylab.com>

cosmology. Students can use the testbed to simulate stellar dynamics: dynamics of single galaxies (relaxation, scattering and collapse); interacting galaxies (collisions and mergers); and to explore interesting structures like tidal tails.

At Pomona, a liberal arts college, students work primarily with Microsoft products and some students, even physics seniors, are unfamiliar with Unix and/or programming. NBodyLab runs server-side, under Linux, and supports a CGI-based web interface for ease of use by students with little background in computing. Its open-source framework was designed to enable students with programming ability to learn scientific computing and refine the software components. NEMO programs provide commonly used data models and analysis functions. NEMO is a widely used, advanced stellar dynamics toolbox that runs under Unix. Students with astrophysics knowledge can add additional data models and analysis programs from NEMO, or write their own, and they are encouraged to master NEMO natively under Unix. A menu of data sets is also offered, including, for example, disk-halo-bulge models of Andromeda and the Milky Way, produced by the package GalactICS (Kuijken & Dubinski 1995). To accelerate the particle-particle force calculations, a desktop supercomputer card, the MD-GRAPE2, may optionally be used.

2. Input Data Parameter Selection

Using a web interface, the user can select the number of galaxies to be modeled, and for each, the model type, number of particles for a model, scale factor and type, rotation about axes, shift, and addition of velocity addition and spin. Models include, from NEMO, Plummer, baredisk, exponential disk, homogeneous sphere, polytrope and spiral. Scale factor choices include scaling mass and velocities, positions, or positions and velocities while retaining the virial ratio.

3. Model Generation and Data Selection

If a model is selected, the appropriate NEMO program is called. Prebuilt datasets, not generated from NEMO programs, include combined and separate disk, bulge and halo components of Milky Way and Andromeda models, produced by the galactICS model builder.

The model and/or datasets are transformed, if requested, and stacked into one data file in preparation for the numerical integration.

4. N-body Evolution and MD-GRAPE2

The user inputs integration options for the type of integrator, number of iterations, output increment, $\Delta-t$, and the softening factor.

The force exerted on each of the N particles by all of the other $N-1$ particles is computed for each time step, from Newton's law of gravitation. By Newton's second law of motion, the force calculation has yielded the acceleration for each particle. Two first-order differential equations involving acceleration and velocity must be solved, using numerical integration, to estimate new positions and

velocities of each particle for the next time step. Integration options include NEMO's `hackcode1`, 2nd order leapfrog, 2nd, 4th and 6th order symplectic, 4th order Runge-Kutta, and others. Except for `hackcode1`, all may run optionally with the MD-GRAPE2.

The MD-GRAPE2 is designed specifically to accelerate force calculations between a list of particles. The MD-GRAPE2 (molecular dynamics-gravity pipeline) card runs at 64 GFlops, peak, has a PCI interface, and can provide the computational power of, roughly, a 24 node Beowulf cluster for direct summation of forces. The MD-GRAPE board has memory for five hundred thousand particle positions. The card is manufactured in Japan, costs less than \$20,000, and can also be used for forces used in molecular dynamics simulations.

5. Analyses, Displays and Viewers

The user specifies the plot observation plane, plot axes range, and whether the following should be produced: animated GIF, image and velocity maps, radial profiles, slit spectrogram simulation, and debugging information. These analyses products and displays are presented on the resulting web pages and are produced by corresponding NEMO programs.

An ASCII dataset is produced by the initial and final states. A binary-only Windows OpenGL viewer supplied by the MD-GRAPE2 vendor allows the user to visualize, rotate and scale the results in three-space.

6. Examples of Student Exercises

Examples of student exercises include:

- *Single galaxy* – How does a Plummer model evolve with time? What are the central mass distributions and velocity dispersions? Experiment with an exponential disk: what does its rotation curve look like? Comment on the effects of the addition of angular momentum.
- *Dynamics of two galaxies* – Make two Plummer spheres interact by colliding and merging. How does the new equilibrium configuration compare in shape and size to the original? Try glancing blows where the spheres are sent at various impact parameters and constant velocity. Try to create a polar ring galaxy by dropping a compact dense galaxy normal to a disk galaxy in a path perpendicular to the disk.

7. Future Plans

Due to limitations in time and budget, many desirable features were not implemented, including a scheduler to handle concurrent requests for the MD-GRAPE2, better error handling, more data modeling capabilities, a simple open-source OpenGL visualizer, instructions and translations for using `partiview` (Teuben et al. 2001), a popular viewer, more efficient and accurate integration methods, and a library of student experiments. Pomona College has recently upgraded its telescopes (14 inch and one meter) and future research projects could relate observational data to simulations.

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References

- Kuijken, K. & Dubinski, J., 1995, *MNRAS*, 277, 1341
Narumi, T. et al. 1999, *Molecular Simulation*, 21, 401
Stein, L., 1998, *Guide to Programming with CGI.pm* (New York: Wiley)
Teuben, P. J. 1994, in *ASP Conf. Ser.*, Vol. 77, *Astronomical Data Analysis Software and Systems IV*, ed. R. A. Shaw, H. E. Payne, & J. J. E. Hayes (San Francisco: ASP), 398
Teuben, P. J. et al. 2001, in *ASP Conf. Ser.*, Vol. 238, *Astronomical Data Analysis Software and Systems X*, ed. F. R. Harnden, Jr., F. A. Primini, & H. E. Payne (San Francisco: ASP), 499