Graph Algorithm for the Simulation of the Interaction between Particles

Stéphane Despréaux, Roland Hildebrand, Aude Maignan

September 24 2012
The Classical $N$-body problem

Dynamical system of interacting particles

- Mass $m_i$
- Position $\chi_i(t)$
- Momentum $\pi_i(t) = m_i\dot{\chi}_i(t)$

Newton’s second law of motion:

$$m_i\ddot{\chi}_i = G \sum_{k \neq i} \frac{m_i m_k (\chi_k - \chi_i)}{|\chi_k - \chi_i|^3}$$
The Classical $N$-body problem

Hamiltonian equation

$$H(\chi, \pi) = \sum_i \frac{||\pi_i||^2}{2m_i} - \sum_{i<k} G \frac{m_i m_k}{|\chi_i - \chi_k|}$$

Equation of motion

$$\begin{cases} \frac{d\chi}{dt} = \frac{\partial H}{\partial \pi} \\ \frac{d\pi}{dt} = -\frac{\partial H}{\partial \chi} \end{cases}$$

Problems of direct integration

- time computation
- stability
- scale problems
The Classical $N$-body problem

$N$-body simulation

- Evaluating the forces on individual particles
- Integrating the orbits of particles
Evaluating the forces on individual particles: Tree methods

- Barns and Hut [1986, 1989]
- Fast multipole method [Carrier, Greengard, 1988]
The Classical $N$-body problem

Integrating the orbit of particles

- Kepler laws for $n = 2$
- Runge-Kutta with adaptive time step
- Symplectic integration [Hierarchical Jacobi Symplectic, Beust 2003]
Integrating the orbit of particles

- Kepler laws for \( n = 2 \)
- Runge-Kutta with adaptive time step
- Symplectic integration [Hierarchical Jacobi Symplectic, Beust 2003]
  - the stellar system is static and modelled with a binary hierarchical tree.
  - \( H = H_A + R \) with \( R \ll H_A \)
    - \( H_A \): The sum of Keplerian Hamiltonians
    - \( R \): the residual mutual perturbations
Introduction

My research into numerical simulations of many-body (N-body) gravitational interactions spans over 40 years, and is reported in several publications and my book. I have developed a set of FORTRAN codes which describe the dynamics very closely, and these are regarded by many as the de facto standard. I have explained below how you can download these codes for execution on your local computer system.

Downloads

For those of you with an FTP tool, you can access my public N-Body directory at ftp://ftp.ast.cam.ac.uk/pub/sverre/. Your browser (such as Microsoft's Internet Explorer) should present you with an FTP viewer window when you click on this link. If so, you should be able to copy whole code group directories at a time. Otherwise please use the links below to identify and download the specific files that you need.

At any time if you’d like further information, please do contact me.

<table>
<thead>
<tr>
<th>Code Group</th>
<th>Filename</th>
<th>Filesize (Kb)</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>CODES</td>
<td>README</td>
<td>2</td>
<td>General textual description of the codes.</td>
</tr>
<tr>
<td>nbody1</td>
<td>README</td>
<td>1</td>
<td>The version nbody1.tar.Z is in full REAL*8.</td>
</tr>
<tr>
<td></td>
<td>nbody1.tar.Z</td>
<td>26</td>
<td>The file nbody1.tar.Z is the old version with mixed REAL*4/*8 precision which is kept for historical reasons.</td>
</tr>
<tr>
<td></td>
<td>nbody1h.tar.gz</td>
<td>140</td>
<td>The recent file nbody1h.tar.gz is the Hermite block-step formulation for workstations and micro-GRAPE, developed with Jun Makino in 1991.</td>
</tr>
<tr>
<td>nbody1h</td>
<td>README</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>nbody1_real4.tar.Z</td>
<td>26</td>
<td></td>
</tr>
<tr>
<td></td>
<td>nbody1h.tar.gz</td>
<td>90</td>
<td></td>
</tr>
<tr>
<td>nbody2</td>
<td>README</td>
<td>1</td>
<td>The whole file is called nbody2.tar.Z. Inside is the code, the article chap9.tex and also chap9.ps. The article may be produced in TeX using the enclosed macro svnyp.sty (or see New Ast. 6, 277). The code NODY2H is the Hermite block-step version of NODY2H.</td>
</tr>
<tr>
<td></td>
<td>nbody2.tar.Z</td>
<td>213</td>
<td>Directory nbody2 contains the code NODY2H and an article describing it.</td>
</tr>
<tr>
<td></td>
<td>nbody2h.tar.gz</td>
<td>185</td>
<td></td>
</tr>
<tr>
<td>nbody3</td>
<td>README</td>
<td>1</td>
<td>The code NODY3 has been heavily used but is no longer updated. NODY3 is recommended instead.</td>
</tr>
<tr>
<td></td>
<td>nbody3.tar.Z</td>
<td>204</td>
<td>One force polynomial with full organization.</td>
</tr>
<tr>
<td>nbody4</td>
<td>README</td>
<td>1</td>
<td>The public GRAPE-6 or micro-GRAPE code NODY4 and the equivalent brute force code for workstations or laptops called BRUT4.</td>
</tr>
<tr>
<td></td>
<td>nbody4.tar.gz</td>
<td>360</td>
<td>The current versions were updated 12 March 2006. The article may be produced in TeX using the enclosed macro svnyp.sty (or see New Ast. 6, 277). The code NODY6H is the Hermite block-step version of NODY6H.</td>
</tr>
<tr>
<td></td>
<td>intro_nbody4.pdf</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>guide.pdf</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td>nbody5</td>
<td>README</td>
<td>1</td>
<td>The code NODY5 has been heavily used but is no longer updated. NODY5 is recommended instead.</td>
</tr>
<tr>
<td></td>
<td>nbody5.tar.Z</td>
<td>299</td>
<td></td>
</tr>
<tr>
<td>nbody6</td>
<td>README</td>
<td>1</td>
<td>The code NODY6 has been heavily used but is no longer updated. NODY6 is recommended instead.</td>
</tr>
<tr>
<td></td>
<td>nbody6.tar.Z</td>
<td>980</td>
<td></td>
</tr>
<tr>
<td></td>
<td>old6.tar.gz</td>
<td>640</td>
<td>The previous 2006 version has been renamed as old6.tar.gz.</td>
</tr>
<tr>
<td></td>
<td>man6.pdf</td>
<td>260</td>
<td>The 2006 manual has been released as ps-file add6.ps.</td>
</tr>
<tr>
<td></td>
<td>old6.ps</td>
<td>305</td>
<td>The full manual is available as ps file add6.ps.</td>
</tr>
<tr>
<td></td>
<td>intro_nbody6.pdf</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>guide.pdf</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>nbody6.tar.gz</td>
<td>980</td>
<td></td>
</tr>
<tr>
<td></td>
<td>old6.tar.gz</td>
<td>640</td>
<td></td>
</tr>
<tr>
<td></td>
<td>man6.pdf</td>
<td>260</td>
<td></td>
</tr>
<tr>
<td></td>
<td>old6.ps</td>
<td>305</td>
<td></td>
</tr>
<tr>
<td></td>
<td>intro_nbody6.pdf</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td></td>
<td>guide.pdf</td>
<td>30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>nbody6.tar.gz</td>
<td>980</td>
<td></td>
</tr>
</tbody>
</table>
Outlines

- Tree model of the hierarchical partition
  ⇒ extract more information than Barns and Hut
- change of coordinates and symplectic integration
  ⇒ extension of Beust method

- Algorithm and Software

GASIP
Graph model

Complete graph $G$ of interactions

- Node $i$ : Particle
- Weighted edge $(i, j) : w_{ij} = G \frac{m_im_j}{|\chi_i - \chi_j|}$

Partition of $G$ of parameter $\epsilon$ . If $A$ and $B$ are 2 parts of the partition :

- $i \in A$ and $j \in B \implies w_{ij} \leq \epsilon$
- $i \in A$ and $j \in A \implies$ there exists a path from $i$ to $j$ such that every edge weight are greater than $\epsilon$

Complexity of the hierarchical partition algorithm: $O(N \log N)$
The adjacency matrix of $G$: $A = \begin{cases} 
a_{ij} = \frac{m_im_j}{||x_i-x_j||} & \text{if } i \neq j \\
-\sum_{j,j \neq i} a_{ij} & \text{else}
\end{cases}$

The partition is obtained by:

- Comparing at most one time the coefficients of $A$ with the value of $\epsilon$
- Executing rows and columns permutations.

$A$ is equivalent to $D_A = \begin{pmatrix} 
B_1(\epsilon) \\
& \leq \epsilon \\
& \quad \cdot \\
& \quad \cdot \\
& \quad \cdot \\
& \leq \epsilon \\
B_k(\epsilon)
\end{pmatrix}$
Partition tree
- The set of interactions \( \text{particle}_A \leftrightarrow \text{particle}_B \) are approximated by an interaction \( \text{center}_A \text{mass}_A \leftrightarrow \text{center}_B \text{mass}_B \)

- The time step of integration depends on the level in the tree.

\[ \epsilon \text{ is multiplied by } 2^{2/3} \text{ at each step } \]

\[ \text{the time step of integration is divided by } 2 \]

\[ \epsilon_3 = \epsilon_0 2^2, dt_3 = \frac{dt_0}{8} \]

\[ \epsilon_2 = \epsilon_0 2^{4/3}, dt_2 = \frac{dt_0}{4} \]

\[ \epsilon_1 = \epsilon_0 2^{2/3}, dt_1 = \frac{dt_0}{2} \]

\[ \epsilon_0 = \epsilon_{\text{min}}, dt_0 = \frac{1}{k' \epsilon_0^{3/2}} \]
Theorem

- Let $\lambda_2$ be the second eigenvalue of the Laplacian matrix $L$

$$L = \begin{cases} 
  l_{ij} = -w_{ij} & \text{if } i \neq j \\
  -\sum_{j, j \neq i} l_{ij} & \text{else}
\end{cases}$$

- let $n$ the size of the matrix $L$.

Then for all

$$\epsilon < \frac{\lambda_2}{n}$$

the partition is reduced to the trivial partition.
Symplectic integration

\[ H = H_A + R \]

- \( H_A = H_1 + H_2 + H_3 + H_4 + H_5 + H_6 \) contains the main interactions
- \( R \) contains all the residual interactions

Coordinates change is performed in order to incorporate the tree structure explicitly.
Extended Basis

Coordinate change $(\chi_i, \pi_i)_{i \in \{1..n\}} \rightarrow (x_i, p_i)_{i \in \{1..N\}}$ with

- $n$: number of particles
- $N$: number of nodes

Coordinate change Formulas

$$x = A \chi \quad \text{and} \quad p = C \pi$$

with $A \in \mathcal{M}_{3N \times 3n}$ and $C \in \mathcal{M}_{3N \times 3n}$ depend on

- the masses
- the structure of the tree.

Extended coordinates is a generalization of the base of Jacobi
The original Hamiltonian

\[ H(\chi, \pi) = \pi^T \Delta \pi + f(\chi), \quad (1) \]

in the new coordinates, \( H \) has a similar expression

\[ H(x, p) = p^T Dp + F(x). \quad (2) \]

**Theorem**

- Let \( (\chi(t), \pi(t)) \) be a trajectory of system (1). Then \( (x(t), p(t)) = (A\chi(t), C\pi(t)) \) is a trajectory of system (2).

- Let \( (x(t), p(t)) \) be a trajectory of system (2). Then \( (\chi(t), \pi(t)) = (C^T x(t), A^T p(t)) \) is a trajectory of system (1).
Integration of $H(x, p) = \sum H_i(x, p) + R(x)$

- The $H_i$ are integrated separately in the $(x, p)$ coordinates.
  - If $H_i$ contains 2 particles → Kepler method
  - else Runge Kutta is used with a time step determined by the tree.
- $R$ is integrated.
Symplectic integration part of
\[ H(x, p) = \sum H_i(x, p) + R(x) \text{ in } [t, t + \tau] \]

1. Integration of \( \sum H_i(x, p) \) at a time step \( \tau/2 \). We obtain
   \[
   (\tilde{x}(t + \tau/2), \tilde{p}(t + \tau/2)) \equiv (x(t), p(t)) + \int_{t}^{t + \tau/2} \left( \frac{\partial \sum H_i}{\partial p}, - \frac{\partial \sum H_i}{\partial x} \right)
   \]

2. Integration of \( R \) at a time step \( \tau \). We obtain
   \[
   (x', p') = (\tilde{x}(t + \tau/2), \tilde{p}(t + \tau/2)) + \tau \frac{\partial R}{\partial x}(\tilde{x}(t + \tau/2))
   \]

3. Integration of \( \sum H_i \) at a time step \( \tau/2 \). Finally,
   \[
   (\tilde{x}(t + \tau), \tilde{p}(t + \tau)) \equiv (x', p') + \int_{t + \tau/2}^{t + \tau} \left( \frac{\partial \sum H_i}{\partial p}, - \frac{\partial \sum H_i}{\partial x} \right).
   \]

\((\tilde{x}(t + \tau), \tilde{p}(t + \tau))\) is the approximation of \((x(t + \tau), p(t + \tau))\).
Algorithm

1. \( t = t_{\text{min}} \)
2. While \((t < t_{\text{Max}})\) do
   - Compute the tree
   - Perform the coordinate transformation \((\chi, \pi) \rightarrow (x, p)\)
   - Construct the individual parts of the Hamiltonian in the new coordinate system:
     \[
     H(x, p) = \sum H_i(x, p) + R(x)
     \]
   - \( n = 0 \)
   - While \((n < n_{\text{TreeSteps}})\) and \((t < t_{\text{Max}})\) do
     - Integrate \((\dot{x}, \dot{p}) = (\frac{\partial H}{\partial p}, -\frac{\partial H}{\partial x})\) with the combined integration method and a bottom time step of \(\tau = \frac{1}{k^{3/2}}\).
     - \( n = n + 1 \)
     - \( t = t + \tau \)
   - Perform the reverse coordinate transformation:
     \((x, p) \rightarrow (\chi = C^T x, \pi = A^T p)\)
Conclusion

Software

- Dynamical partition tree
  - ⇒ Flocking simulation
  - ⇒ Wireless sensor networks

- New augmented coordinates system generalized the base of Jacobi.