Graph Algorithm for the Simulation of the Interaction between Particles

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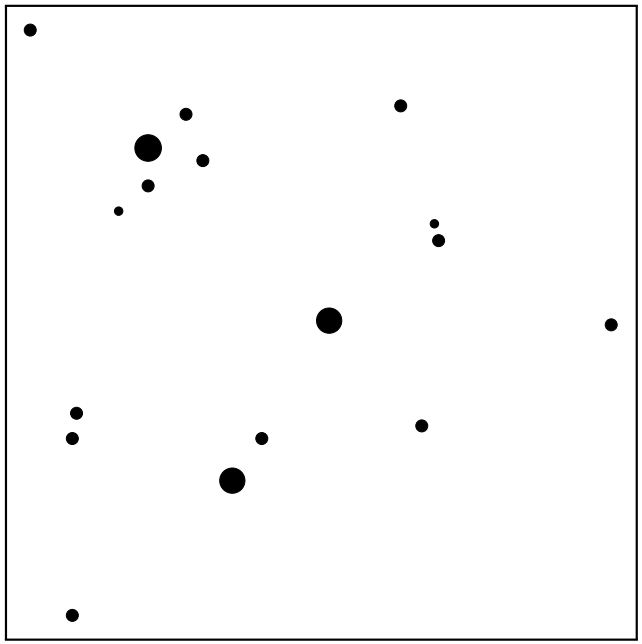
Dynamical system of interacting particles

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

Newton's second law of motion:

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



Hamiltonian equation

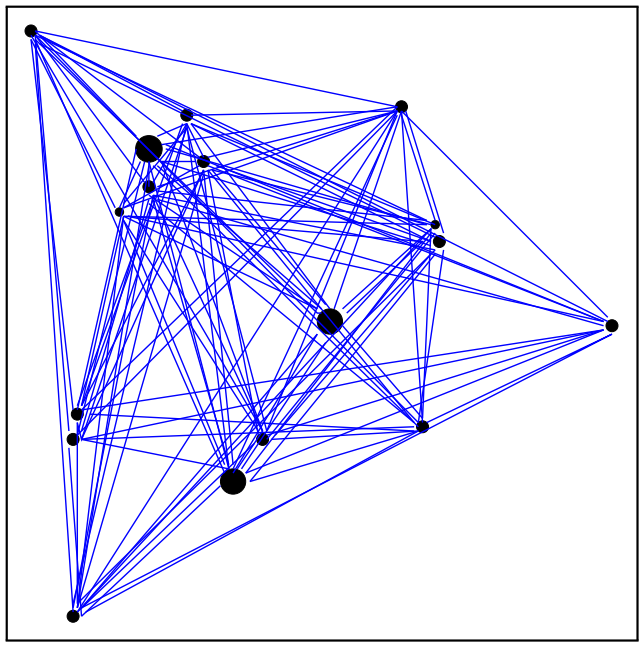
$$H(\chi,\pi) = \sum_i \frac{||\pi_i||^2}{2m_i} - \sum_{i<k} G\frac{m_i m_k}{|\chi_i - \chi_k|}$$

Equation of motion

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

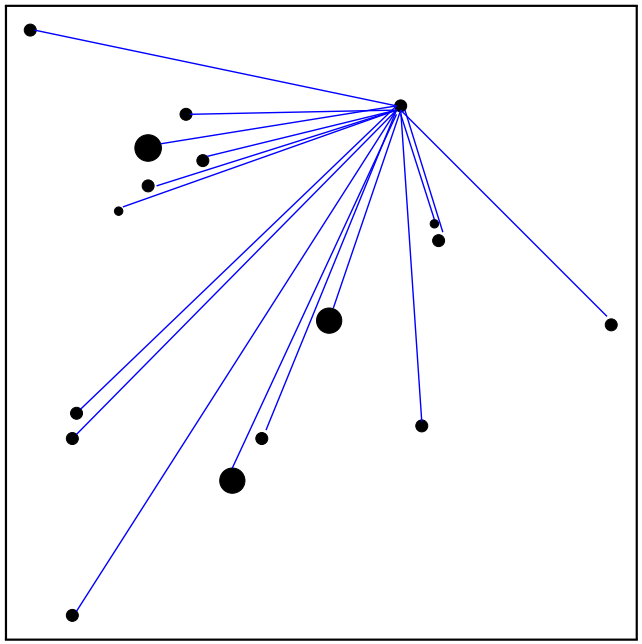
Problems of direct integration

- time computation
- stability
- scale problems



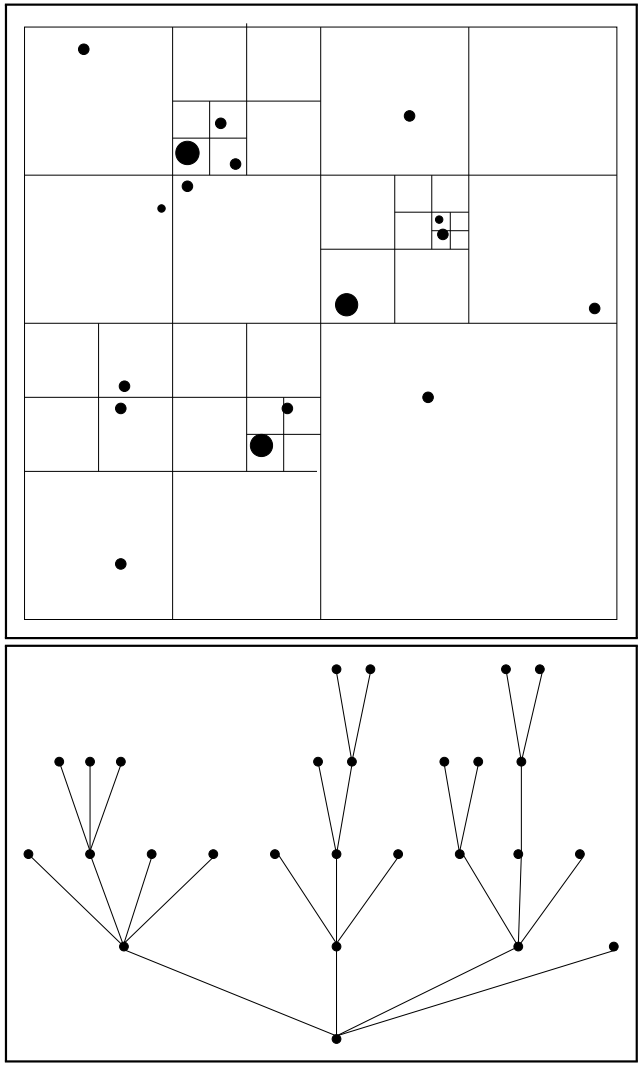
N-body simulation

- 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]



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 $R << H_A$
    - H_A : The sum of Keplerian Hamiltonians
    - R : the residual mutual perturbations

The Nbodies Softwares

Sverre Aarseth's Institute of Astronomy Homepage http://www.ast.cam.ac.uk/~sverre/

Sverre Aarseth

All-Round N-Body Guy, Mountaineer and Wild-Life Enthusiast

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N-Body

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.

Code Group	Filename	Filesize (Kb)	Notes
	CODES	2	General textual description of the codes.
nbody1	README	1	The version nbody1.tar.Z is in full REAL*8.
	nbody1.tar.Z	26	The file nbody1_real4.tar.Z is the old version with mixed REAL*4/*8 precision which is kept for historical reasons.
	nbody1_real4.tar.Z	26	The recent file nbody1h.tar.gz is the Hermite block-step formulation for workstations and (micro-)GRAPE, developed with Jun Makino in 1991.
	nbody1h.tar.gz	140	
nbody2	nbody2.tar.Z	213	Directory nbody2 contains the code NBODY2 and an article describing it. 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 NBODY2H is the Hermite block-step version of NBODY2.
	nbody2h.tar.Z	185	
nbody3	nbody3.tar.Z	204	One force polynomial with full regularization.
nbody4	README	1	The public GRAPE-6 or micro-Grape code NBODY4
	nbody4.tar.gz	360	and the equivalent brute force code for workstations or laptops called BRUT4.
	brut4.tar.gz	340	The current versions were updated 12 March 2006.
	intro_nbody4.pdf	1	Introduction to running simulations.
nbody5	README	1	The code NBODY5 has been heavily used but
	nbody5.tar.Z	289	is no longer updated. NBODY6 is recommended instead.
nbody6	README	1	README contains some past history of NBODY6.
	nbody6.tar.gz	980	Further practical info can be found in directory Docs.
	old6.tar.gz	640	nbody6.tar.gz holds the new standard code NBODY6.
	man6.pdf	200	The previous 2006 version has been renamed as old6.tar.gz.
	old6.ps	306	The postscript file man6.pdf is the new manual.
	intro_nbody6.pdf	1	The 2006 manual has been renamed as ps file old6.ps.
	README2	1	Rainer Spurzem's corresponding parallel code, nbody6++, can be obtained here.
	guide.pdf	30	Introduction to running simulations.
	gpu.tar.gz	65	README2 contains input file for using GPU with nbody6. guide.pdf is guide for SSE and GPU with nbody6. Tar file for the GPU directory and library.

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Outlines

- Tree model of the hierarchical partition
  $\Rightarrow$ extract more information than Barns and Hut
- change of coordinates and symplectic integration
  $\Rightarrow$ extension of Beust method
- Algorithm and Software

Graph model

Complete graph $\mathcal{G}$ of interactions

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

Partition of $\mathcal{G}$ of parameter ϵ . 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 ϵ

Complexity of the hierarchical partition algorithm: $O(N \log N)$

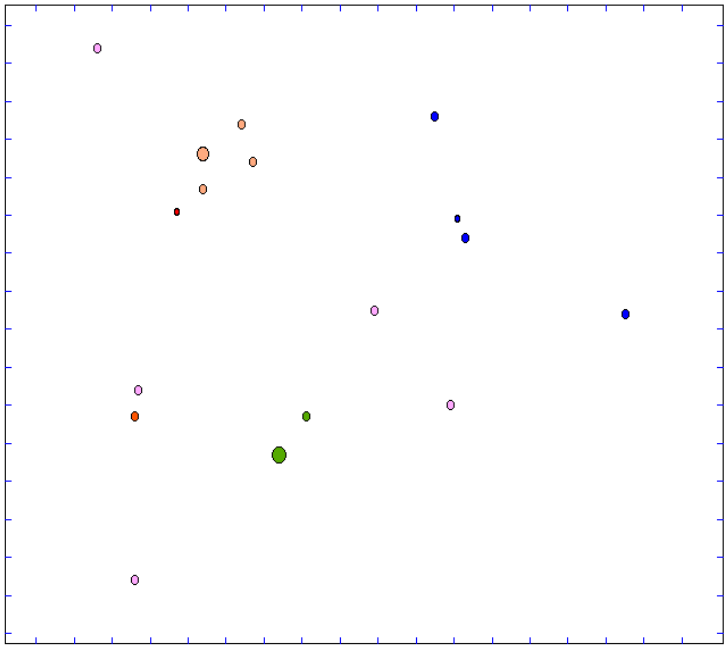
The adjacency matrix of $\mathcal{G}$: $A = \begin{cases} a_{ij} = & \frac{m_i m_j}{\|\chi_i - \chi_j\|} \text{ if } i \neq j \\ & -\sum_{j, j \neq i} a_{ij} \text{ else} \end{cases}$

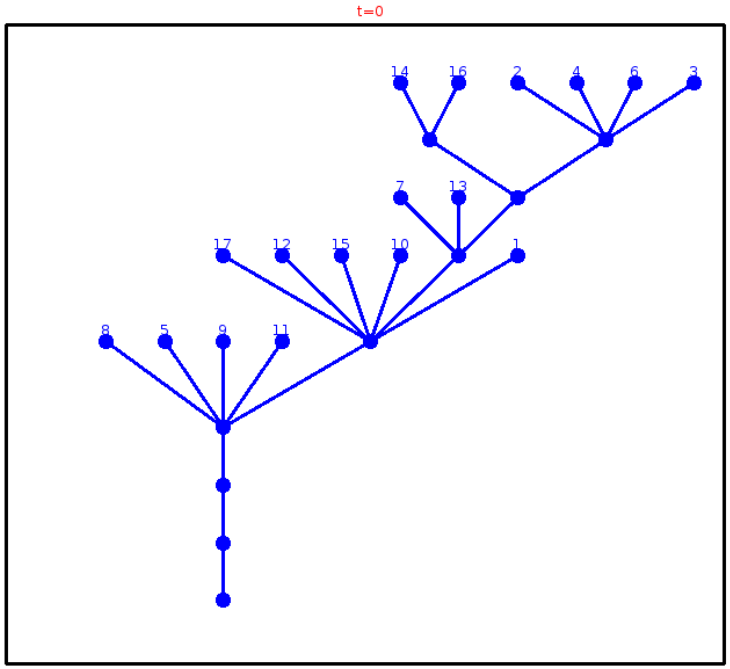
The partition is obtained by :

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

A is equivalent to $D_A = \begin{pmatrix} \boxed{B_1(\epsilon)} & & \\ \leq \epsilon & \ddots & \leq \epsilon \\ & & \boxed{B_k(\epsilon)} \end{pmatrix}$

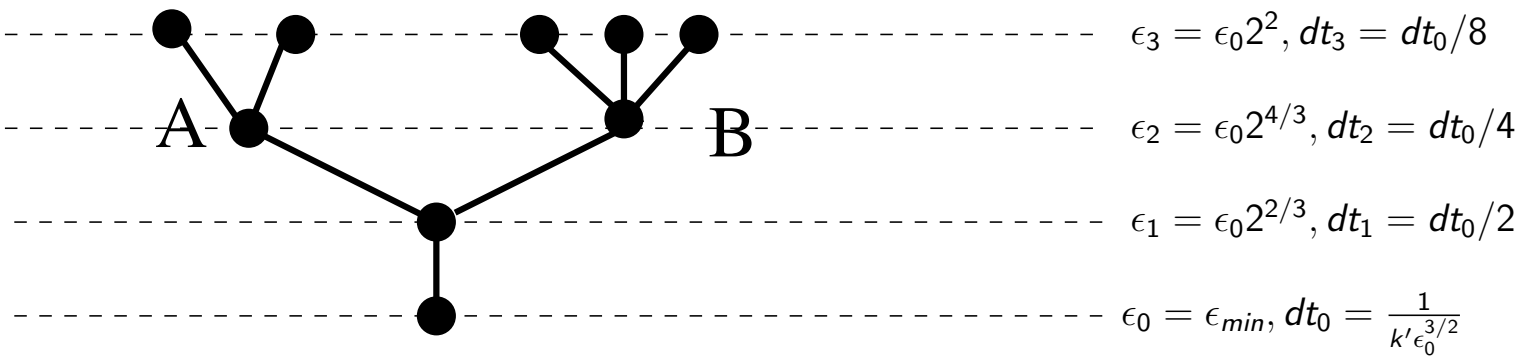
Partition tree





- The set of interactions $particle_A \leftrightarrow particle_B$ are approximated by an interaction $center\_mass\_A \leftrightarrow center\_mass\_B$
- The time step of integration depends on the level in the tree.

ϵ is multiplied by $2^{2/3}$ at each step $\Longrightarrow$ the time step of integration is divided by 2



ϵ lower bound

Theorem

- Let λ_2 be the second eigenvalue of the Laplacian matrix
$$L = \begin{cases} l_{ij} = & -w_{ij} \text{ if } i \neq j \\ & -\sum_{j,j\neq i} l_{ij} \text{ else} \end{cases}$$
- let n the size of the matrix L.

Then for all

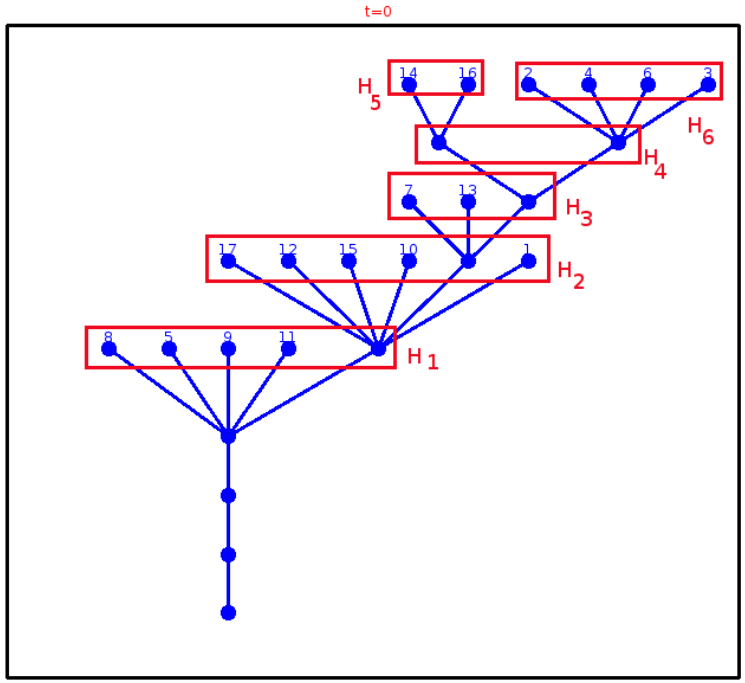
$$\epsilon < \frac{\lambda_2}{n}$$

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

$$x = A\chi \quad and \quad p = C\pi$$

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

$$H(\chi, \pi) = \pi^T \Delta \pi + f(\chi), \tag{1}$$

in the new coordinates, H has a similar expression

$$H(x, p) = p^T D p + F(x). \tag{2}$$

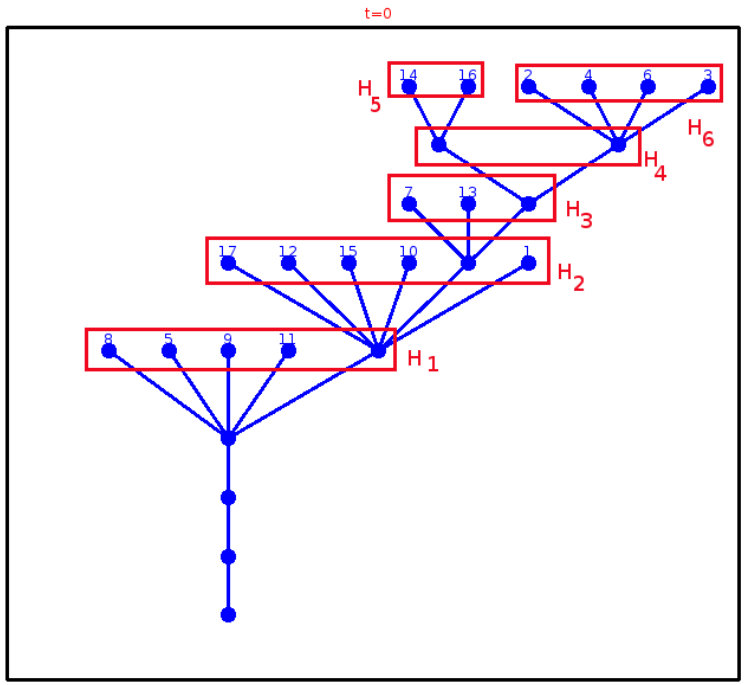
Theorem

- *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 $H(x,p) = \sum H_i(x,p) + R(x)$

$$H(x,p) = \sum H_i(x,p) + R(x)$$

- The H_i are integrated separatly in the (x,p) coordinates.
  - If H_i contains 2 particles $\rightarrow$ Kepler method
  - else Runge Kutta is used with a time step determined by the tree.
- R is integrated.



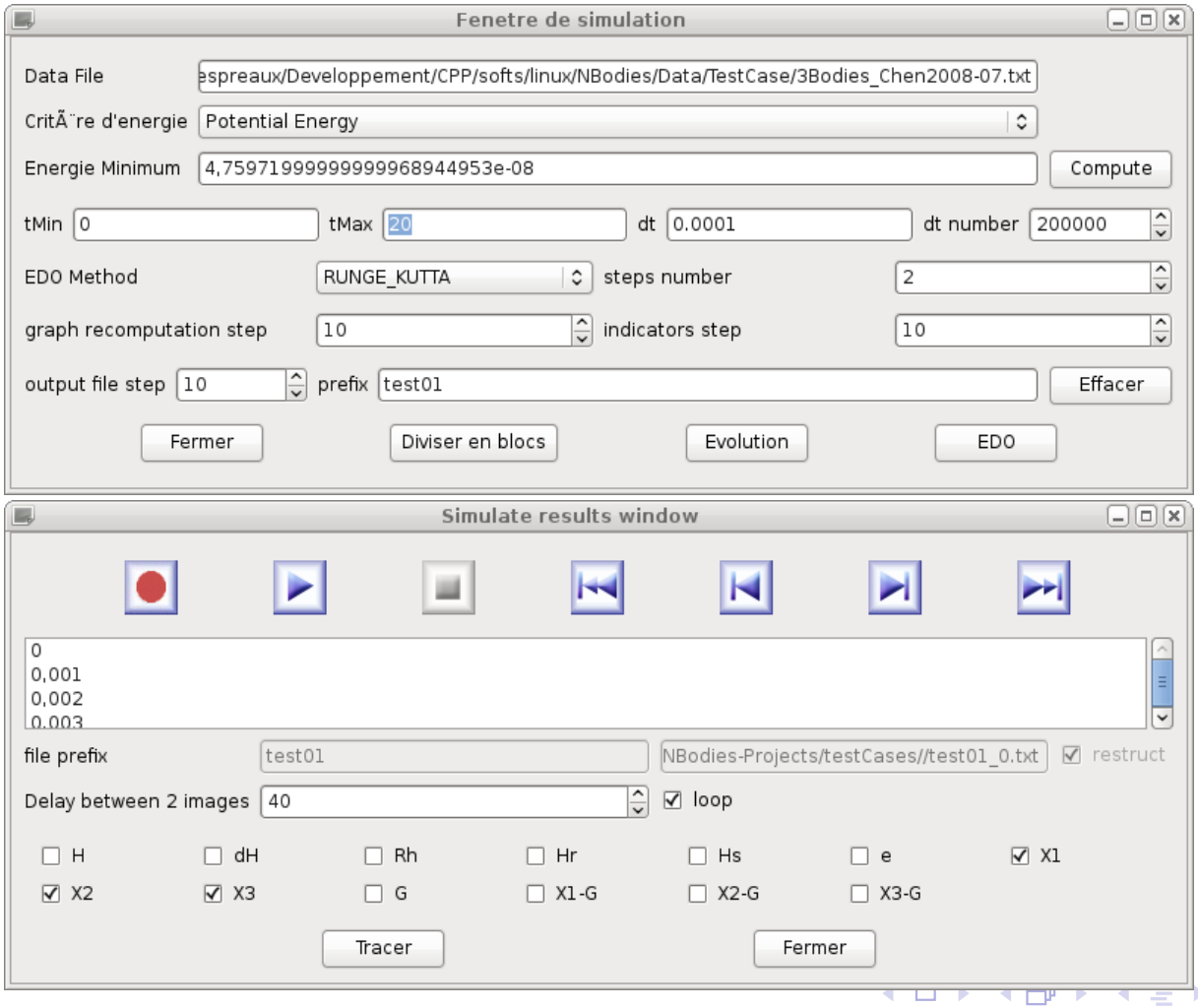
Symplectic integration part of $H(x,p) = \sum H_i(x,p) + R(x)$ in $[t, t+\tau]$

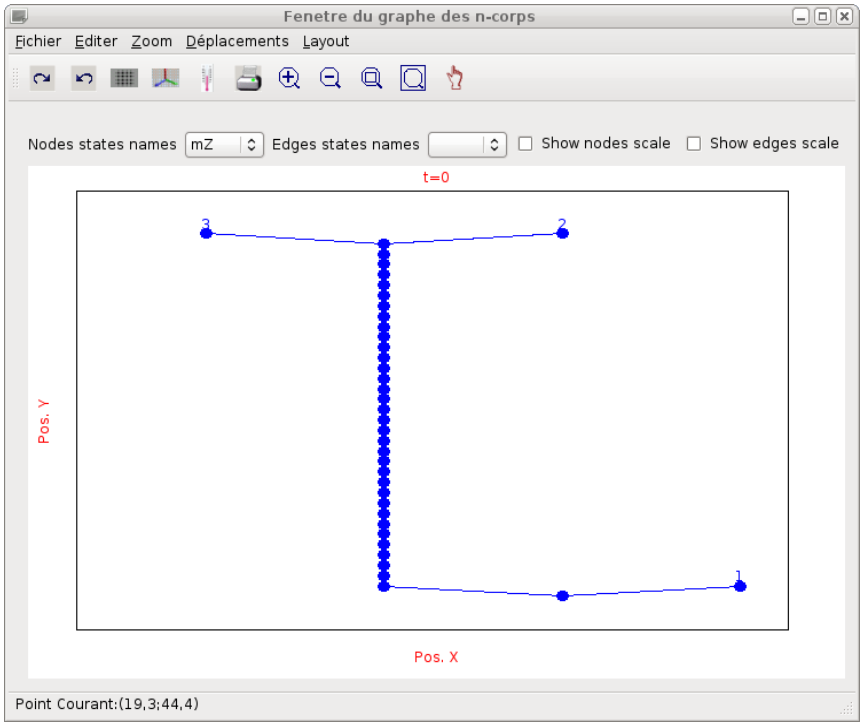
1. Integration of $\sum H_i(x,p)$ at a time step $\tau/2$. We obtain $(\tilde{x}(t+\tau/2), \tilde{p}(t+\tau/2)) = (x(t), p(t)) + \int_t^{\tau/2} (\frac{\partial \sum H_i}{\partial p}, -\frac{\partial \sum H_i}{\partial x})$
2. Integration of R at a time step τ. We obtain $(x', p') = (\tilde{x}(t+\tau/2), \tilde{p}(t+\tau/2)) + \tau \frac{\partial R}{\partial x}(\tilde{x}(t+\tau/2))$
3. Integration of $\sum H_i$ at a time step $\tau/2$. Finally, $(\tilde{x}(t+\tau), \tilde{p}(t+\tau)) = (x', p') + \int_{t+\tau/2}^{t+\tau} (\frac{\partial \sum H_i}{\partial p}, -\frac{\partial \sum H_i}{\partial x})$.

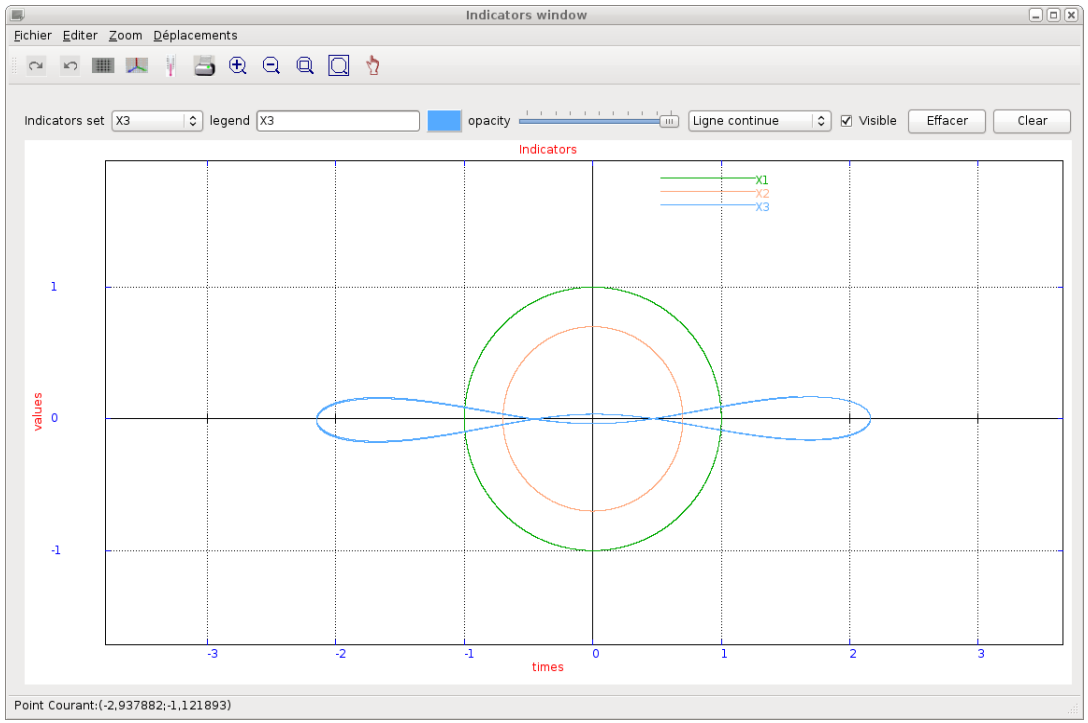
$(\tilde{x}(t+\tau), \tilde{p}(t+\tau))$ is the approximation of $(x(t+\tau), p(t+\tau))$.

Algorithm

1. $t = t_{min}$
2. While $(t < tMax)$ 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 $(n < nTreeSteps)$ and $(t < tMax)$ 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 $\tau = \frac{1}{k\epsilon^{3/2}}$.
     - $n = n + 1$
     - $t = t + \tau$
   - Perform the reverse coordinate transformation:
     $(x, p) \rightarrow (\chi = C^T x, \pi = A^T p)$


Fenetre de simulation
Data File
espreaux/Developpement/CPP/softs/linux/NBodies/Data/TestCase/3Bodies_Chen2008-07.txt
CritÃ¨re d'energie
Potential Energy
Energie Minimum
4,75971999999999968944953e-08
Compute
tMin
0
tMax
20
dt
0.0001
dt number
200000
EDO Method
RUNGE_KUTTA
steps number
2
graph recomputation step
10
indicators step
10
output file step
10
prefix
test01
Effacer
Fermer
Diviser en blocs
Evolution
EDO
Simulate results window
0
0,001
0,002
0,003
file prefix
test01
NBodies-Projects/testCases//test01_0.txt
restruct
Delay between 2 images
40
loop
H
dH
Rh
Hr
Hs
e
X1
X2
X3
G
X1-G
X2-G
X3-G
Tracer
Fermer


Fenetre du graphe des n-corps
Fichier Editer Zoom Déplacements Layout
Nodes states names mZ Edges states names Show nodes scale Show edges scale
t=0
3
2
1
Pos. Y
Pos. X
Point Courant:(19,3;44,4)


Indicators window
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Indicators set X3 legend X3 opacity Ligne continue Visible Effacer Clear
Indicators
X1
X2
X3
values
times
Point Courant:(-2,937882;-1,121893)

Conclusion

Software 

- Dynamical partition tree
  - $\Rightarrow$ Flocking simulation
  - $\Rightarrow$ Wireless sensor networks
- New augmented coordinates system generalized the base of Jacobi.