Time Symmetry

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1 “Leap Frog”

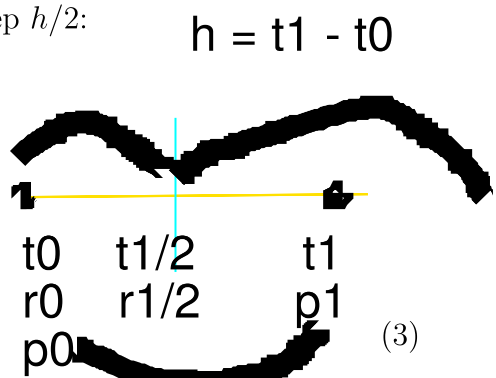
Hamiltonian, relative two-body motion without perturbers

$$H = \frac{\mathbf{p}^2}{2\mu} - \frac{GMm}{|\mathbf{r}|} \tag{1}$$

with canonical conjugate variables $\mathbf{p} = \mu\mathbf{v}$, and $\mathbf{r}$; H is separable:

$$H = H_1(\mathbf{p}) + H_2(\mathbf{r}) = \frac{\mathbf{p}^2}{2\mu} + U(\mathbf{r}) \tag{2}$$

In the “Leap Frog” we start with an initial time step $h/2$:



$$r_{1/2} = r_0 + \frac{1}{2}hp_0$$

Then taking turns:

$$\begin{aligned} p_1 &= p_0 - h\frac{dU}{dr}\Big|_{r=r_{1/2}} \\ r_{3/2} &= r_{1/2} + hp_1 \end{aligned} \tag{3}$$

This solution is time symmetric (for more than two particles: only if all particles have the same time step). It means that the numerical solution is the solution of an approximate Hamiltonian $H = H_0 + hH_1 + \ldots$.

symplectic

2 Hermite

Remember from our previous lectures, we first do the predictor step (for all particles in regular step, and for all neighbours in irregular step):

[illegible] (4)

We get then the corrector step for the i particle (in[redacted] here):

$$\begin{aligned} \mathbf{x}_c(t) &= \mathbf{x}_p(t) + \frac{1}{24}(t-t_0)^4\mathbf{a}^{(2)} + \frac{1}{20}(t-t_0)^5\mathbf{a}^{(3)} \\ \mathbf{v}_c(t) &= \mathbf{v}_p(t) + \frac{1}{6}(t-t_0)^3\mathbf{a}^{(2)} + \frac{1}{24}(t-t_0)^4\mathbf{a}^{(3)} \,. \end{aligned} \tag{5}$$

Remember, that $\mathbf{a}^{(2)}$ and $\mathbf{a}^{(3)}$ have been obtained from the special Hermite step (Taylor series for accelerations), while $\mathbf{a}$ and $\dot{\mathbf{a}}$ have been computed directly from Newton's law and its time derivative (sums over all other particles).

he best we can say is following that it jumps from one Hamiltonian to another one, never leaving the "possible" space of solutions.

and shown that then the method is still 4th order and time-symmetric:

$$\begin{aligned} \mathbf{v}_c(t) &= \mathbf{v}_0(t) + \frac{1}{2}(t-t_0)\Big(\mathbf{a}_1 + \mathbf{a}_0\Big) - \frac{1}{12}(t-t_0)^2\Big(\dot{\mathbf{a}}_1 - \dot{\mathbf{a}}_0\Big) \\ \mathbf{x}_c(t) &= \mathbf{x}_0(t) + \frac{1}{2}(t-t_0)\Big(\mathbf{v}_c + \mathbf{v}_0\Big) - \frac{1}{12}(t-t_0)^2\Big(\mathbf{a}_1 - \mathbf{a}_0\Big) \,. \end{aligned} \tag{6}$$

You can use the Hermite interpolation formulae (previous lecture manuscript) and show the equivalence. This method can be also used to iterate to higher precision, by using $\mathbf{x}_c$ and $\mathbf{v}_c$ in a second step to re-compute $\mathbf{a}_1$ and $\dot{\mathbf{a}}_1$, until convergence is reached.

Eq. (5) and Eq. (6) are equivalent, use Hermite step

3 Regularisation as canonical transformation

r = u**2 (7)

and the Poincaré-Transformation of the Hamiltonian

(8)

leads to the following canonical equations (the last equation originates from taking $p_0 = E$ as canonically conjugate to the time t):

r!

r'

with the derivative $'$ with respect to s. For the isolated two-body problem we get the new Poincaré-Hamiltonian

$$\Gamma = u^2\Big(\frac{\mathbf{p}^2}{8u^2} - \frac{GM}{u^2} - E\Big) \tag{10}$$

so for $E < 0$:

$$\Gamma = \frac{1}{8}\mathbf{p}^2 + |E|\mathbf{u}^2 = GM \tag{11}$$

Note that in case of 3D particle coordinate space we have to use the 4D quaternion space for the vectors $\mathbf{u}$ and $\mathbf{p}$.

4 Algorithmic Regularisation

we start again with the isolated two-body Hamiltonian:

$$\tag{12}$$

Now a new regularising time transformation is used:

$$|U|^{-1}ds = dt\ . \tag{13}$$

and the Poincaré transformed Hamiltonian is

$$\tag{14}$$

It is not separable, so it looks bad, but

$$\Lambda = \log(1+\Gamma) = \tag{15}$$

is separable!! And one can show that now new canonical equations are valid:

logarithmic Hamiltonian

$$\begin{aligned}
\mathbf{p}' = -\frac{\partial \Lambda}{\partial \mathbf{r}} &= -\frac{1}{1+\Gamma}\cdot\frac{\partial \Gamma}{\partial \mathbf{r}} \\
\mathbf{r}' = \frac{\partial \Lambda}{\partial \mathbf{p}} &= \frac{1}{1+\Gamma}\cdot\frac{\partial \Gamma}{\partial \mathbf{p}} \\
t' = \frac{\partial \Lambda}{\partial p_0} &= \frac{1}{1+\Gamma}\cdot\frac{\partial \Gamma}{\partial p_0}
\end{aligned} \tag{16}$$

p' = dp/ds ~ (p1-p0)/ds

AR regularization (2 bodies)
AR Chain (>2 bodies)
NBODY7 (Banerjee, Sambaran)

$$\begin{aligned}
\mathbf{p}' &= -\frac{1}{|U|}\frac{\partial U}{\partial \mathbf{r}} \\
\mathbf{r}' &= \frac{1}{T-E}\cdot\frac{\mathbf{p}}{m} \\
t' &= \frac{1}{T-E}
\end{aligned} \tag{17}$$

These equations can be used to make a new "Leap Frog" - the time-transformed leap frog. Algorithmic regularization is based on this.

5 New Developments - very short

GPU

Rantala, Naab, Springel, et al. 2021: frost: a momentum-conserving CUDA implementation of a hierarchical fourth-order forward symplectic integrator

Rantala et al. 2020: MSTAR - a fast parallelized algorithmically regularized integrator with minimum spanning tree coordinates

Chin & Chen 2005: Symplectic Integrators

Planetary Systems: Mercury, new variants of Hernandez

Wang, Iwasawa, Nitadori, Makino 2020: PETAR: a high-performance N-body code for modelling massive collisional stellar systems