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:

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

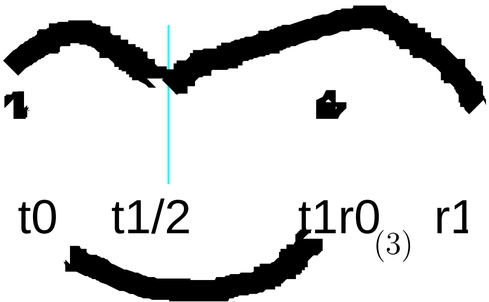
In the "Leap Frog" we start with an initial time step $h/2$:

h = t1 - t0

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

Then taking turns:

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



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):

$$\begin{aligned} \mathbf{x}_p(t) &= \frac{1}{6}(t-t_0)^3\dot{\mathbf{a}}_0 + \frac{1}{2}(t-t_0)^2\mathbf{a}_0 + (t-t_0)\mathbf{v}_0 + \mathbf{x}_0 \\ \mathbf{v}_p(t) &= \frac{1}{2}(t-t_0)^2\dot{\mathbf{a}}_0 + (t-t_0)\mathbf{a}_0 + \mathbf{v}_0 \end{aligned} \tag{4}$$

We get then the corrector step for the i particle (index i dropped here):

$$
\begin{aligned}
\mathbf{x}_c(t) &= \mathbf{x}_p(t) + \frac{1}{24}(t-t_0)^4\mathbf{a}^{(2)} + \frac{1}{120}(t-t_0)^5\mathbf{a}^{(3)} \\
\mathbf{v}_c(t) &= \mathbf{v}_p(t) + \frac{1}{6}(t-t_0)^3\mathbf{a}^{(2)} + \frac{1}{24}(t-t_0)^4\mathbf{a}^{(3)} \ . \qquad (5)
\end{aligned}
$$

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). This method is **not** time symmetric. It means that our numerical solution does not belong to a Hamiltonian function; the best we can say is following Quinlan & Tremain (1995) that it jumps from one Hamiltonian to another one, never leaving the "possible" space of solutions.

Makino (1997) has proposed to drop the highest order term in $\mathbf{x}$, and shown that then the method is still 4th order and time-symmetric:

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

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. In that way we avoid the spurious trick to use low-order predicted coordinates.

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

3 Regularisation as canonical transformation

We used in classical KS (Kustaanheimo & Stiefel) regularisation:

$$g(\mathbf{r},\mathbf{p},t)ds = \mathbf{r}ds = dt \qquad (7)$$

r = u**2

and the Poincaré-Transformation of the Hamiltonian

$$\Gamma = g(H-E) \qquad (8)$$

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

$$
\begin{aligned}
\mathbf{p}' &= -\frac{\partial\Gamma}{\partial\mathbf{q}} \\
\mathbf{q}' &= \frac{\partial\Gamma}{\partial\mathbf{p}} \\
t' &= \frac{\partial\Gamma}{\partial p_0} = g \qquad (9)
\end{aligned}
$$

r!

r'

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

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

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 **u** and **p**.

4 Algorithmic Regularisation

This new idea of Mikkola (2000) and also Preto & Tremaine (1999) we start again with the isolated two-body Hamiltonian:

$$H = H_1(\mathbf{p}) + H_2(\mathbf{r}) = T(\mathbf{p}) + U(\mathbf{r}) \tag{12}$$

Now a new regularising time transformation is used:

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

and the Poincaré transformed Hamiltonian is

$$\Gamma = |U|^{-1}\Big(T(\mathbf{p}) + U(\mathbf{r}) - E\Big) \tag{14}$$

It is not separable, so it looks bad, but

$$\Lambda = \log(1+\Gamma) = \log\Big(T(\mathbf{p}) - E\Big) - \log\Big|U(\mathbf{r})\Big| \tag{15}$$

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 C

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

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