Exact Timestep for a Pairwise Coulomb Collision

Stephen Brooks

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1 Introduction

Standard numerical integrators work well for many-body Coulomb repulsion problems when the timestep is much shorter than the timescale of relative position changes. However, for 'hard' collisions in which two particles have a near miss and exchange a lot of momentum within one timestep, they understandably struggle. This note proposes using the exact solution of Keplerian two-body orbits (usually hyperbolic) to calculate the momentum exchange with other particles: either a selection of the 'closest' ones or all of them.

2 Pairwise Collision in Central Frame

Take the masses of two particles to be $m_{1,2}$ and their charges to be $q_{1,2}$. Adopt the frame where the total momentum $\mathbf{p} = m_1\mathbf{v}_1 + m_2\mathbf{v}_2 = \mathbf{0}$ and also the centre of mass $m_1\mathbf{x}_1 + m_2\mathbf{x}_2 = \mathbf{0}$ is at the origin. From this, it is always true that $\mathbf{x}_2 = -\frac{m_1}{m_2}\mathbf{x}_1$ and $\mathbf{x}_1 - \mathbf{x}_2 = \frac{m_1+m_2}{m_2}\mathbf{x}_1$. Similar relations hold for $\mathbf{v}_1$, meaning the problem is restricted to a two dimensional subspace spanned by $\mathbf{x}_1$ and $\mathbf{v}_1$. The radial Coulomb force on the first particle is

$$\mathbf{F}_1(|\mathbf{x}_1|) = \frac{q_1q_2}{4\pi\epsilon_0}\frac{\mathbf{x}_1 - \mathbf{x}_2}{|\mathbf{x}_1 - \mathbf{x}_2|^3} = \frac{q_1q_2}{4\pi\epsilon_0}\frac{\frac{m_1+m_2}{m_2}\mathbf{x}_1}{(\frac{m_1+m_2}{m_2})^3|\mathbf{x}_1|^3} = \frac{q_1q_2}{4\pi\epsilon_0}\left(\frac{m_2}{m_1+m_2}\right)^2\frac{\mathbf{x}_1}{|\mathbf{x}_1|^3}.$$

Defining $r = |\mathbf{x}_1|$, this is a central force of magnitude

$$F_1(r) = \frac{q_1q_2}{4\pi\epsilon_0}\left(\frac{m_2}{m_1+m_2}\right)^2\frac{1}{r^2}.$$

3 Binet Equation

The trajectory shape can be conveniently found from the Binet equation. Defining $u = 1/r$ and using polar coordinates, it states, for a central force F,

$$F = -mh^2u^2\left(\frac{\mathrm{d}^2u}{\mathrm{d}\theta^2} + u\right),$$

where $h = r^2\dot{\theta}$ is a conserved angular-momentum-like quantity. For this problem, $F = ku^2$ where $k = \frac{q_1q_2}{4\pi\epsilon_0}(\frac{m_2}{m_1+m_2})^2$. Thus,

$$ku^2 = -m_1h^2u^2\left(\frac{\mathrm{d}^2u}{\mathrm{d}\theta^2} + u\right) \qquad \Rightarrow \qquad \frac{\mathrm{d}^2u}{\mathrm{d}\theta^2} + u = -\frac{k}{m_1h^2}$$

$$\Rightarrow \qquad u(\theta) = A\cos\theta + B\sin\theta - \frac{k}{m_1 h^2}$$

for some constants A, B. The origin for θ is free to choose at this point, so it simplifies the calculation to choose it such that $B = 0$ and $A \geq 0$. The solution is now

$$u(\theta) = A\cos\theta + C$$

where $C = -\frac{k}{m_1 h^2}$ is a constant that is negative for repelling particles with $q_1 q_2 > 0$ and positive for attracting particles with $q_1 q_2 < 0$.

4 Initial Conditions

Call the value of θ corresponding to the initial condition θ_0, so that

$$u(\theta_0) = \frac{1}{|\mathbf{x}_1|} = A\cos\theta_0 + C,$$

where in this section $\mathbf{x}_1$ and $\mathbf{v}_1$ are evaluated at the initial condition.

The first derivative satisfies

$$u' = \frac{\mathrm{d}u}{\mathrm{d}\theta} = \frac{\mathrm{d}u}{\mathrm{d}r}\frac{\mathrm{d}r}{\mathrm{d}t}\frac{\mathrm{d}t}{\mathrm{d}\theta} = \frac{-1}{r^2}\dot{r}\frac{1}{\dot{\theta}}.$$

Initially we have $\dot{r} = \mathbf{v}_1 \cdot \mathbf{x}_1 / |\mathbf{x}_1|$ and $\dot{\theta} = |\mathbf{x}_1 \times \mathbf{v}_1| / |\mathbf{x}_1|^2$, so

$$u'(\theta_0) = \frac{-1}{|\mathbf{x}_1|^2}\frac{\mathbf{v}_1 \cdot \mathbf{x}_1}{|\mathbf{x}_1|}\frac{|\mathbf{x}_1|^2}{|\mathbf{x}_1 \times \mathbf{v}_1|} = \frac{-\mathbf{x}_1 \cdot \mathbf{v}_1}{|\mathbf{x}_1||\mathbf{x}_1 \times \mathbf{v}_1|}.$$

These initial conditions also determine

$$h = r^2\dot{\theta} = |\mathbf{x}_1|^2\frac{|\mathbf{x}_1 \times \mathbf{v}_1|}{|\mathbf{x}_1|^2} = |\mathbf{x}_1 \times \mathbf{v}_1|,$$

which is a conserved quantity proportional to angular momentum. Using the solution for $u(\theta)$ gives

$$u'(\theta_0) = \frac{-\mathbf{x}_1 \cdot \mathbf{v}_1}{|\mathbf{x}_1|h} = -A\sin\theta_0.$$

Taking the sum of squares gives

$$(A\cos\theta_0)^2 + (-A\sin\theta_0)^2 = A^2 = \left(\frac{1}{|\mathbf{x}_1|} - C\right)^2 + \left(\frac{-\mathbf{x}_1 \cdot \mathbf{v}_1}{|\mathbf{x}_1|h}\right)^2$$

$$\Rightarrow \qquad A = \frac{1}{|\mathbf{x}_1|}\sqrt{(1 - |\mathbf{x}_1|C)^2 + \left(\frac{\mathbf{x}_1 \cdot \mathbf{v}_1}{h}\right)^2}.$$

Taking the ratio gives

$$\frac{A\sin\theta_0}{A\cos\theta_0} = \tan\theta_0 = \frac{\frac{\mathbf{x}_1 \cdot \mathbf{v}_1}{|\mathbf{x}_1|h}}{\frac{1}{|\mathbf{x}_1|} - C} = \frac{\mathbf{x}_1 \cdot \mathbf{v}_1}{(1 - |\mathbf{x}_1|C)h}.$$

But also

$$\cos\theta_0 = \frac{\frac{1}{|\mathbf{x}_1|} - C}{A} = \frac{1 - |\mathbf{x}_1|C}{|\mathbf{x}_1|A}$$

is useful.

5 Time Dependence and the Eccentric Anomaly

As $h = r^2\dot\theta$ is a constant found in the previous section, $\dot\theta = \frac{\mathrm{d}\theta}{\mathrm{d}t} = hu^2$. The equation to solve is

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = hu^2 = h(A\cos\theta + C)^2.$$

Kepler's eccentric anomaly E is defined via

$$\cos\{\mathrm{h}\}\, E = \frac{e + \cos\theta}{1 + e\cos\theta}$$

for some eccentricity e that will be found later. Terms in {brackets} are used for the hyperbolic form when $|e| > 1$. The sign of $\sin\{\mathrm{h}\}\, E$ is defined to be the same as $\sin\theta$. The variable of the differential equation can be changed to E via the chain rule:

$$\begin{aligned}
\frac{\mathrm{d}E}{\mathrm{d}t} &= \frac{\mathrm{d}E}{\mathrm{d}\cos\{\mathrm{h}\}\, E}\frac{\mathrm{d}\cos\{\mathrm{h}\}\, E}{\mathrm{d}t} \\
&= \frac{\{-\}1}{-\sin\{\mathrm{h}\}\, E}\left(\frac{1}{1+e\cos\theta}\frac{\mathrm{d}\cos\theta}{\mathrm{d}t} + (e+\cos\theta)\frac{-1}{(1+e\cos\theta)^2}e\frac{\mathrm{d}\cos\theta}{\mathrm{d}t}\right) \\
&= \frac{\{-\}1}{-\sin\{\mathrm{h}\}\, E}\left(\frac{1}{1+e\cos\theta} + \frac{-e(e+\cos\theta)}{(1+e\cos\theta)^2}\right)\frac{\mathrm{d}\cos\theta}{\mathrm{d}t} \\
&= \frac{\{-\}1}{-\sin\{\mathrm{h}\}\, E}\frac{1+e\cos\theta - e^2 - e\cos\theta}{(1+e\cos\theta)^2}(-\sin\theta)h(A\cos\theta + C)^2 \\
&= \frac{\{-\}\sin\theta}{\sin\{\mathrm{h}\}\, E}(1-e^2)h\frac{(A\cos\theta+C)^2}{(1+e\cos\theta)^2} \\
&= \frac{\sin\theta}{\sin\{\mathrm{h}\}\, E}|1-e^2|h\frac{(A\cos\theta+C)^2}{(1+e\cos\theta)^2}.
\end{aligned}$$

Next, $\sin\{\mathrm{h}\}\, E$ needs to be evaluated:

$$\sin\{\mathrm{h}\}\, E = \pm\sqrt{\{-\}(1 - \cos\{\mathrm{h}\}^2 E)} = \pm\sqrt{\{-\}\left(1 - \frac{(e+\cos\theta)^2}{(1+e\cos\theta)^2}\right)}$$

$$= \pm\sqrt{\{-\}\left(\frac{1 + 2e\cos\theta + e^2\cos^2\theta - e^2 - 2e\cos\theta - \cos^2\theta}{(1+e\cos\theta)^2}\right)}$$

$$= \pm\frac{\sqrt{\{-\}(1 - e^2 - \cos^2\theta + e^2\cos^2\theta)}}{1+e\cos\theta} = \pm\frac{\sqrt{|1-e^2|(1-\cos^2\theta)}}{1+e\cos\theta} = \frac{\sqrt{|1-e^2|}\sin\theta}{|1+e\cos\theta|}.$$

Substituting this back in,

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \frac{\sin\theta}{\sin\{\mathrm{h}\}\, E}|1-e^2|h\frac{(A\cos\theta+C)^2}{(1+e\cos\theta)^2} = \frac{|1+e\cos\theta|}{\sqrt{|1-e^2|}}|1-e^2|h\frac{(A\cos\theta+C)^2}{(1+e\cos\theta)^2}$$

$$= \sqrt{|1-e^2|}h\frac{(A\cos\theta+C)^2}{|1+e\cos\theta|} = \sqrt{|1-e^2|}hC^2\frac{(1+\frac{A}{C}\cos\theta)^2}{|1+e\cos\theta|}.$$

Setting $e = \frac{A}{C}$ gives

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sqrt{|1-e^2|}hC^2|1+e\cos\theta|.$$

Note that this e has the same sign as C, so is the usual definition of eccentricity for attracting particles, but negative for repelling particles.

To express $\frac{\mathrm{d}E}{\mathrm{d}t}$ back in terms of E, note that

$$\cos\{h\} E - \frac{1}{e} = \frac{e - \frac{1}{e}}{1 + e\cos\theta}$$

$$\Rightarrow \qquad 1 + e\cos\theta = \frac{e - \frac{1}{e}}{\cos\{h\} E - \frac{1}{e}} = \frac{e^2 - 1}{e\cos\{h\} E - 1}.$$

Therefore

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \sqrt{|1-e^2|}hC^2 \frac{|1-e^2|}{|1 - e\cos\{h\} E|} = \frac{|1-e^2|^{3/2}hC^2}{|1 - e\cos\{h\} E|}.$$

Kepler's equation suggests an implicit solution of the form

$$qt = E - e\sin\{h\} E$$

for some constant q. Differentiating both sides with respect to t gives

$$q = \frac{\mathrm{d}E}{\mathrm{d}t} - e\cos\{h\} E \frac{\mathrm{d}E}{\mathrm{d}t} = (1 - e\cos\{h\} E)\frac{\mathrm{d}E}{\mathrm{d}t}$$

and substituting the $\frac{\mathrm{d}E}{\mathrm{d}t}$ found above gives

$$q = (1 - e\cos\{h\} E)\frac{|1-e^2|^{3/2}hC^2}{|1 - e\cos\{h\} E|} = \sigma|1-e^2|^{3/2}hC^2,$$

which is indeed a constant. The sign σ of $1 - e\cos\{h\} E$ is

- 1 for elliptic orbits ($0 \le e < 1$),
- -1 for hyperbolic attractive orbits ($e > 1$, $C > 0$) and
- 1 for hyperbolic repulsive orbits ($e < -1$, $C < 0$).

6 Time Step

With A and θ_0 known, calculate $e = \frac{A}{C}$ and proceed via

$$\cos\{h\} E_0 = \frac{e + \cos\theta_0}{1 + e\cos\theta_0}, \qquad qt_0 = E_0 - e\sin\{h\} E_0$$

to find the initial time t_0 in Kepler's equation.

Suppose the position is required at $t = t_0 + \delta t$ for some time step δt. A solution of $qt = E - e\sin\{h\} E$ is needed. This does not have a closed-form solution but Newton–Raphson iterations exist (see Appendices). Then

$$\cos\theta = \frac{e - \cos\{h\} E}{e\cos\{h\} E - 1}, \qquad \sin\theta = \frac{|1 + e\cos\theta|}{\sqrt{|1-e^2|}}\sin\{h\} E$$

and

$$u(\theta) = A\cos\theta + C.$$

A convenient way of handling the frames of reference is to rotate $\mathbf{x}_1$ by angle $\theta - \theta_0$ about the $\mathbf{x}_1 \times \mathbf{v}_1$ axis and then scale by $r/r_0 = u(\theta_0)/u(\theta)$.

To find the velocity, it is easier to use the known differential equations $\dot\theta = hu^2$ and $u'(\theta) = -A\sin\theta$ to get

$$\frac{\mathrm{d}r}{\mathrm{d}t} = \frac{\mathrm{d}r}{\mathrm{d}u}\frac{\mathrm{d}u}{\mathrm{d}\theta}\frac{\mathrm{d}\theta}{\mathrm{d}t} = \frac{-1}{u^2}(-A\sin\theta)hu^2 = Ah\sin\theta.$$