

Exact Timestep for a Pairwise Coulomb Collision

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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

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

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 ,

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

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

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

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

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

$$u' = \frac{du}{d\theta} = \frac{du}{dr} \frac{dr}{dt} \frac{dt}{d\theta} = \frac{-1}{r^2} \dot{r} \frac{1}{\dot{\theta}}.$$

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

$$\begin{aligned} (A \cos \theta_0)^2 + (-A \sin \theta_0)^2 &= A^2 = \left(\frac{1}{|\mathbf{x}_1|} - C \right)^2 + \left(\frac{-\mathbf{x}_1 \cdot \mathbf{v}_1}{|\mathbf{x}_1| h} \right)^2 \\ \Rightarrow A &= \frac{1}{|\mathbf{x}_1|} \sqrt{(1 - |\mathbf{x}_1| C)^2 + \left(\frac{\mathbf{x}_1 \cdot \mathbf{v}_1}{h} \right)^2}. \end{aligned}$$

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, $\dot{\theta} = \frac{d\theta}{dt} = hu^2$. The equation to solve is

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

Kepler's eccentric anomaly E is defined via

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

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

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

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

$$\begin{aligned} \sin\{h\} E &= \pm \sqrt{\{-\}(1 - \cos\{h\}^2 E)} = \pm \sqrt{\{-\} \left(1 - \frac{(e + \cos \theta)^2}{(1 + e \cos \theta)^2} \right)} \\ &= \pm \sqrt{\{-\} \left(\frac{1 + 2e \cos \theta + e^2 \cos^2 \theta - e^2 - 2e \cos \theta - \cos^2 \theta}{(1 + e \cos \theta)^2} \right)} \\ &= \pm \frac{\sqrt{\{-\}(1 - e^2 - \cos^2 \theta + e^2 \cos^2 \theta)}}{1 + e \cos \theta} = \pm \frac{\sqrt{|1 - e^2|(1 - \cos^2 \theta)}}{1 + e \cos \theta} = \frac{\sqrt{|1 - e^2|} \sin \theta}{|1 + e \cos \theta|}. \end{aligned}$$

Substituting this back in,

$$\begin{aligned} \frac{dE}{dt} &= \frac{\sin \theta}{\sin\{h\} E} |1 - e^2| h \frac{(A \cos \theta + C)^2}{(1 + e \cos \theta)^2} = \frac{|1 + e \cos \theta|}{\sqrt{|1 - e^2|}} |1 - e^2| h \frac{(A \cos \theta + C)^2}{(1 + e \cos \theta)^2} \\ &= \sqrt{|1 - e^2|} h \frac{(A \cos \theta + C)^2}{|1 + e \cos \theta|} = \sqrt{|1 - e^2|} h C^2 \frac{(1 + \frac{A}{C} \cos \theta)^2}{|1 + e \cos \theta|}. \end{aligned}$$

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

$$\frac{dE}{dt} = \sqrt{|1 - e^2|} h C^2 |1 + e \cos \theta|.$$

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 $\frac{dE}{dt}$ back in terms of E , note that

$$\begin{aligned} \cos\{h\} E - \frac{1}{e} &= \frac{e - \frac{1}{e}}{1 + e \cos \theta} \\ \Rightarrow 1 + e \cos \theta &= \frac{e - \frac{1}{e}}{\cos\{h\} E - \frac{1}{e}} = \frac{e^2 - 1}{e \cos\{h\} E - 1}. \end{aligned}$$

Therefore

$$\frac{dE}{dt} = \sqrt{|1 - e^2|} h C^2 \frac{|1 - e^2|}{|1 - e \cos\{h\} E|} = \frac{|1 - e^2|^{3/2} h C^2}{|1 - e \cos\{h\} E|}.$$

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

$$q = \frac{dE}{dt} - e \cos\{h\} E \frac{dE}{dt} = (1 - e \cos\{h\} E) \frac{dE}{dt}$$

and substituting the $\frac{dE}{dt}$ found above gives

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

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

- 1 for elliptic orbits ($0 \leq e < 1$),
- -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

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

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

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

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

$$\frac{dr}{dt} = \frac{dr}{du} \frac{du}{d\theta} \frac{d\theta}{dt} = \frac{-1}{u^2} (-A \sin \theta) hu^2 = Ah \sin \theta.$$