Event Driven Collisions

The following algorithm simulates the evolution of a system of billiard balls on a table (or, equivalently, atoms confined to a planar box). It is assumed that the collisions between the billiard balls ~~and any ball and~~ the table are elastic. In principle, given any initial position and velocity configuration, we can use Newton's Laws to evolve the system with time, using either the Euler or other higher order methods. However, given that the interactions between the balls and with the walls are contact interactions, there is an equivalent, simpler algorithm. The idea is that the force between any pair of balls is zero unless they are directly in contact, in which case it is along the line joining the centres of the two balls. Similaly, when a ball collides with a wall, the force acting on it is normal to the wall. Since these collisions are elastic, they are *specular*. That is, the relative velocity vector of any pair of balls is just 'reflected' by such a collision. The velocity vector of ball colliding with a wall is similarly reflected. First, let us consider the collision of a ball with one of the walls. Let the initial velocity of the ball be $\vec{v}$ and the velocity after collision be $\vec{v}'$

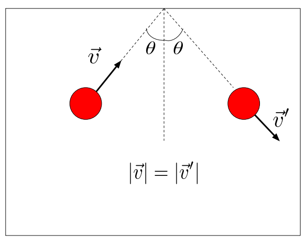

Figure 1: Specular collision of ball with wall

Then, the component of velocity tangential to the wall remains unchanged, whereas the component normal to the wall is reversed.

Next, let us consider a collision between two balls, i and j. Let the initial velocities be $\vec{v}_i$ and $\vec{v}_j$. Let the relative separation of the centres of the balls be $\vec{r}$ and their relative velocity be $\vec{v} = \vec{v}_j - \vec{v}_i$. First, we need to find a criterion for collision between these balls. Let us go to the rest frame of the i^{th} ball. Then, the j^{th} ball appears to move with velocity $\vec{v}$. Let us observe the motion of the centre of the j^{th} ball, moving with velocity $\vec{v}$. Since the combined radius of the two balls is $2R$, we imagine a sphere (actally, a circular disk) of radius $2R$ about the i^{th} ball. The balls will collide, if the centre of the j^{th} ball crosses this sphere

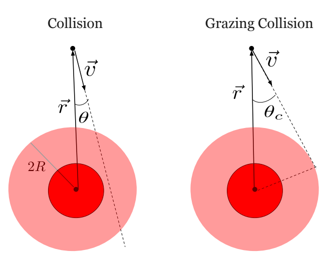

Figure 2: Condition for collision: $\theta < \theta_c$

Referring to figure 2, a collision will take place if $\theta < \theta_c$, which is equivalent to $\sin\theta < \sin\theta_c$. It is clear that $\sin\theta_c = 2R/r$, where $r = |\vec{r}|$. Simple algebra gives

$$\sin\theta = \sqrt{1 - \frac{(\vec{v}\cdot\vec{r})^2}{v^2 r^2}} \tag{1}$$

where $v = |\vec{v}|$. The condition for collision is $\sin\theta < \sin\theta_c$

$$\sqrt{1 - \frac{(\vec{v}\cdot\vec{r})^2}{v^2 r^2}} < \frac{2R}{r} \tag{2}$$

which can be written as

$$a > 0, \quad a = (\vec{v}\cdot\vec{r})^2 - v^2(r^2 - 4R^2) \tag{3}$$

This condition needs to be supplemented with the condition $\vec{r}\cdot\vec{v} < 0$ (balls moving toward each other, not away). Given these conditions are satisfied, let us compute the time it will take the balls to collide. Given the initial positions and velocities of the balls, let the collision take place after time Δt. In this time, the displacement of the centre of ball j will be $\vec{v}\Delta t$. This displacement will take the centre to a point on the surface of the disk of radius $2R$

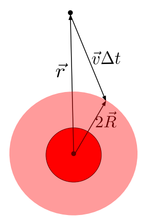

Figure 3: Collision time

If the displacement vector from the centre of ball i to this point on the disk is wriiten as $2\vec{R}$, then

$$2\vec{R} = \vec{r} + \vec{v}\Delta t \tag{4}$$

Squaring, we get a quadratic equation in Δt

$$v^2\Delta t^2 + 2(\vec{v}\cdot\vec{r})\Delta t + r^2 - 4R^2 = 0 \tag{5}$$

The appropriate root of this equation is

$$\Delta t = -\left(\frac{\vec{v}\cdot\vec{r} + \sqrt{a}}{v^2}\right) \tag{6}$$

Assuming the pair (i, j) collides, let us compute the new velocities after the collision. The velocity of the centre of mass of the pair is

$$\vec{V}_c = \frac{\vec{v}_1 + \vec{v}_2}{2} \tag{7}$$

Then, the velocity of each particle can be expressed in terms of the centre of mass velocity and their relative velocity

$$\begin{aligned} \vec{v}_i &= \vec{V} - \frac{\vec{v}}{2} \\ \vec{v}_j &= \vec{V} + \frac{\vec{v}}{2} \end{aligned} \tag{8}$$

Since $\vec{V}_c$ does not change during collision, therefore the change in velocity of the particles due to collision is given by

$$\begin{aligned} \Delta\vec{v}_i &= -\frac{\Delta\vec{v}}{2} \\ \Delta\vec{v}_j &= +\frac{\Delta\vec{v}}{2} \end{aligned} \tag{9}$$

Since the force between the particles is along the line of their relative separation (given by vector $\vec{r}$) and since it conserves momentum, the relative velocity vector is just 'reflected' about vector $\vec{r}$

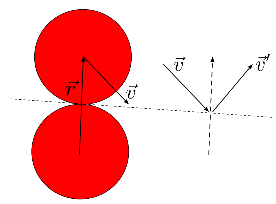

Figure 4: Change in relative velocity during collision

It is easy to check that the change in relative velocity will be

$$\Delta\vec{v} = -2(\vec{v}\cdot\hat{r})\hat{r} \tag{10}$$

where $\hat{r}$ is a unit vector along $\vec{r}$. Then, it follows from eqns.(9) that

$$\begin{aligned} \vec{v}_i' &= \vec{v}_i + (\vec{v}\cdot\hat{r})\hat{r} \\ \vec{v}_j' &= \vec{v}_j - (\vec{v}\cdot\hat{r})\hat{r} \end{aligned} \tag{11}$$

The 'Event Driven' collision algorithm proceeds as follows

- Given the initial configuration (position and velocity of every atom), the time it takes every atom to collide against the nearest wall is computed.
- For every pair of atom, collision time is calculated.
- The minimum of all these times gives the next event.
- The atoms are moved freely till this next event.
- If the next event is a wall-collision event, the identity of the atom undergoing this collision is determined, and its velocity changed.
- On the other hand, if the next event is a pair-collision event, the identities of the pair are determined and their velocities changed according to (11).
- This now forms the new configuration, and we start all over again (till a certain number of events, which we can choose).