# Adiabatic compression

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# Introduction

3D simulation of adiabatic compression of a system of 60 spherical particles, each with a mass of 1.0 kg and with radii of 0.02 m. Initial velocity components of the particles are uniformly distributed random values between -9.0 m/s and 9.0 m/s. The size of the system is initially 8 x 8 x 8 m and compressed to 5.2 x 5.2 x 5.2 m. Compression occurs between 5 and 12 s (simulation time) at a rate of 0.2 m/s.

# Model equations

## Collisions

In order to update the positions of the particles the collision time between particles and between particles and boundaries needs to be determined. Collision times $t_{ab}$ between particles are computed by:

$$t_{ab} = \frac{-\mathbf{r}_{ab} \cdot \mathbf{v}_{ab} - \sqrt{(\mathbf{r}_{ab} \cdot \mathbf{v}_{ab})^2 - \mathbf{v}_{ab} \cdot \mathbf{v}_{ab}(\mathbf{r}_{ab} \cdot \mathbf{r}_{ab} - (R_a + R_b)^2)}}{\mathbf{v}_{ab} \cdot \mathbf{v}_{ab}} \tag{1}$$

Where $R_a$ is the radius of particle $a$, $R_b$ is the radius of particle $b$, $\mathbf{r}_{ab}$ is the relative position $\mathbf{r}_a - \mathbf{r}_b$ with $\mathbf{r}_a$ the position of particle $a$ and $\mathbf{r}_b$ the position of particle $b$ and $\mathbf{v}_{ab}$ is the relative velocity $\mathbf{v}_a - \mathbf{v}_b$ with $\mathbf{v}_a$ the velocity of particle $a$ and $\mathbf{v}_b$ the velocity of particle $b$:

$$\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b \tag{2}$$

$$\mathbf{v}_{ab} = \mathbf{v}_a - \mathbf{v}_b \tag{3}$$

Collision times $t_c$ between particles and boundaries are computed by:

$$t_c = \frac{\mathbf{t} \cdot (\mathbf{L} - \mathbf{r}_i)}{\mathbf{t} \cdot \mathbf{v}_i} \tag{4}$$

Where $\mathbf{t}$ is the unit vector normal to the boundaries (and directed inward), $\mathbf{L}$ is the vector $(L, L, L)$ with $L$ the location of the boundary minus the radius of the particle colliding with the boundary (which in this work is taken to be $\pm(3 - R_i)$) with $R_i$ the radius of particle $i$, $\mathbf{r}_i$ is the position vector of particle $i$ and $\mathbf{v}_i$ is the velocity vector of particle $i$.

The collision times between all particles and between all particles and boundaries are computed. Then, the minimum collision time is taken and used to update the particle positions. Should the minimum collision time be between two particles the velocities of the colliding particles are updated as follows:

$$m_a(\mathbf{v}_{a,n+1} - \mathbf{v}_{a,n}) = \mathbf{J} \tag{5}$$

$$m_b(\mathbf{v}_{b,n+1} - \mathbf{v}_{b,n}) = -\mathbf{J} \tag{6}$$

Where $\mathbf{J}$ is the impulse vector, $m_a$ is the mass of particle $a$, $m_b$ is the mass of particle $b$, $\mathbf{v}_{a,n}$ the velocity of particle $a$ at timestep $n$ and $\mathbf{v}_{b,n}$ the velocity of particle $b$ at timestep $n$. The impulse vector is calculated as follows:

$$\mathbf{J} = J_n\mathbf{n} + J_t\mathbf{t} \tag{7}$$

Where $J_n$ is the normal component of the impulse vector, $J_t$ is the tangential component of the impulse vector, $\mathbf{n}$ is the unit vector normal to the contact point and $\mathbf{t}$ is the unit vector tangent to the contact point. The unit vector normal to the contact point and the unit vector tangent to the contact point are given by:

$$\mathbf{n} = \frac{\mathbf{r}_a - \mathbf{r}_b}{|\mathbf{r}_a - \mathbf{r}_b|} \tag{8}$$

$$\mathbf{t} = \frac{\mathbf{v}_{ab,c} - \mathbf{n}(\mathbf{v}_{ab,c} \cdot \mathbf{n})}{|\mathbf{v}_{ab,c} - \mathbf{n}(\mathbf{v}_{ab,c} \cdot \mathbf{n})|} \tag{9}$$

The normal component of the impulse vector is:

$$J_n = -(1+e)\frac{\mathbf{v}_{ab,c} \cdot \mathbf{n}}{B_2} \tag{10}$$

Where $e$ is the coefficient of normal restitution, $\mathbf{v}_{ab,c}$ is the relative velocity between particle $a$ and $b$ at the contact point. The quantity $B_2$ depends on the masses of the particles and is given by:

$$B_2 = \frac{1}{m_a} + \frac{1}{m_b} \tag{11}$$

The relative velocity between particle $a$ and $b$ at the contact point $\mathbf{v}_{ab,c}$ is computed as:

$$\mathbf{v}_{ab,c} = \mathbf{v}_a - \mathbf{v}_b - (R_a\omega_a + R_b\omega_b) \times \mathbf{n} \tag{12}$$

Where $\omega_a$ is the rotational velocity vector of particle $a$ and $\omega_b$ the rotational velocity of particle $b$. The tangential component of the impulse vector depends on the relative velocity between the particles at the contact point and the masses of the particles. If the relative velocity is large enough collisions will be of the sliding type:

$$\mu < \frac{(1+\beta_0)\mathbf{v}_{ab,c} \cdot \mathbf{t}}{J_n B_1} \tag{13}$$

If the relative velocity is low collisions will be of the sticking type:

$$\mu \geq \frac{(1+\beta_0)\mathbf{v}_{ab,c} \cdot \mathbf{t}}{J_n B_1} \tag{14}$$

Where $\mu$ is the coefficient of friction, $\beta_0$ the coefficient of tangential restitution and $B_1$ is given by:

$$B_1 = \frac{7}{2}(\frac{1}{m_a} + \frac{1}{m_b}) \tag{15}$$

When collisions are of the sticking type the tangential impulse is given by:

$$J_t = -(1+\beta_0)\frac{\mathbf{v}_{ab,c}\cdot\mathbf{t}}{B_1} \tag{16}$$

When collisions are of the sliding type the tangential impulse is given by:

$$J_t = -\mu J_n \tag{17}$$

Should the minimum collision time be between a particle and the boundary the velocities are simply reflected. For collisions with the upper or lower boundaries the reflection is defined by $f : \mathbb{R}^3 \to \mathbb{R}^3$:

$$f((v_x, v_y, v_z)) = (v_x, -v_y, v_z) \tag{18}$$

For collisions with the left or right boundaries the reflection is defined by $g : \mathbb{R}^3 \to \mathbb{R}^3$:

$$g((v_x, v_y, v_z)) = (-v_x, v_y, v_z) \tag{19}$$

For collisions with the bottom and top boundaries the reflection is $h : \mathbb{R}^3 \to \mathbb{R}^3$:

$$h((v_x, v_y, v_z)) = (v_x, v_y, -v_z) \tag{20}$$

## Compression

Compression increases the momentum of the particles colliding with the moving boundaries. Consequently, the average kinetic energy of the system increases. The total kinetic energy of the particles $U$ in the system is:

$$U = \frac{3}{2}NkT \tag{21}$$

Work $w$ is required to compress the system. The work required $dw$ to compress the system an amount $dV$ is:

$$dw = pdV \tag{22}$$

Where $p$ is the pressure of the system and $V$ the volume. Application of the ideal gas law to (22) gives:

$$dw = \frac{NkTdV}{V} \tag{23}$$

Where $N$ is the number of particles, $k$ the Boltzmann constant and $T$ the temperature. An energy balance over the system $dU = dw$ gives:

$$d(\frac{3}{2}NkT) = \frac{NkTdV}{V} \tag{24}$$

From the equation above the following relation between volume and temperature can be obtained:

$$\frac{T_2}{T_1} = (\frac{V_1}{V_2})^{2/3} \tag{25}$$

Where $T_1$ and $T_2$ are the temperatures before and after compression, respectively. Likewise, $V_1$ and $V_2$ are the volumes before and after compression. The above result can be compared with the actual temperature increase observed in the system. For the simulated system the kinetic energy of the system is proportional with the system temperature. Therefore, the temperature ratio can be estimated via:

$$\frac{T_2}{T_1} = \frac{E_{k2}}{E_{k1}} = \frac{\Sigma(v_{2,i})^2}{\Sigma(v_{1,i})^2} \tag{26}$$

Where $E_{k2}$ is the average kinetic energy of the system after compression, $E_{k1}$ is the average kinetic energy of the system before compression, $v_{2,i}$ is the speed of particle $i$ after compression and $v_{1,i}$ the speed of particle $i$ before compression.

# Results

In one particular simulation the temperature ratio $T_2/T_1$ obtained from (26) is 2.37 (2.3703). From the thermodynamic relation (25) the ratio obtained is 2.37 (2.3681) . The relative difference between simulation and theoretical prediction is within 1 %. Numerous simulations show that the results obtained from simulation agree well with the theoretical predictions (based on kinetic theory).