

# 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.

## 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:

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

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  $b$ :

$$\mathbf{r}_{ab} = \mathbf{r}_a - \mathbf{r}_b \quad (2)$$

$$\mathbf{v}_{ab} = \mathbf{v}_a - \mathbf{v}_b \quad (3)$$

Collision times  $t_c$  between particles and boundaries depend on the relative distance and velocity between particles and boundaries. For collisions between particles and the west boundary the collision time is computed as follows:

$$t_c = \frac{x_{c,i} - L_W - R_i}{v_{w,W} - v_{x,i}} \quad (4)$$

Where  $x_{c,i}$  the  $x$  coordinate of particle  $i$ ,  $L_W$  the location of the west boundary,  $R_i$  the radius of particle  $i$ ,  $v_{w,W}$  is the velocity of the west boundary and  $v_{x,i}$  the  $x$  component of the velocity of particle  $i$ . For collisions between particles and the east boundary the collision time is:

$$t_c = \frac{x_{c,i} - L_E + R_i}{v_{w,E} - v_{x,i}} \quad (5)$$

Where  $L_E$  is the location of the east boundary and  $v_{w,E}$  the velocity of the east boundary. The collision times between the particles and the remaining boundaries are computed in a similar manner.

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:

$$m_a(\mathbf{v}_{a,n+1} - \mathbf{v}_{a,n}) = \mathbf{J} \quad (6)$$

$$m_b(\mathbf{v}_{b,n+1} - \mathbf{v}_{b,n}) = -\mathbf{J} \quad (7)$$

$$I_a(\omega_{a,n+1} - \omega_{a,n}) = -(R_a \mathbf{n}) \times \mathbf{J} \quad (8)$$

$$I_b(\omega_{b,n+1} - \omega_{b,n}) = (R_b \mathbf{n}) \times (-\mathbf{J}) \quad (9)$$

Where  $\mathbf{J}$  is the impulse vector,  $\omega_{a,n}$  is the rotational velocity vector of particle  $a$  at timestep  $n$ ,  $\omega_{b,n}$  the rotational velocity vector of particle  $b$  at timestep  $n$ ,  $I_a$  is the moment of inertia of particle  $a$ ,  $I_b$  is the moment of inertia of particle  $b$ ,  $m_a$  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:

$$\mathbf{J} = J_n \mathbf{n} + J_t \mathbf{t} \quad (10)$$

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:

$$\mathbf{n} = \frac{\mathbf{r}_a - \mathbf{r}_b}{|\mathbf{r}_a - \mathbf{r}_b|} \quad (11)$$

$$\mathbf{t} = \frac{\mathbf{v}_{ab,c} - \mathbf{n}(\mathbf{v}_{ab,c} \cdot \mathbf{n})}{|\mathbf{v}_{ab,c} - \mathbf{n}(\mathbf{v}_{ab,c} \cdot \mathbf{n})|} \quad (12)$$

The normal component of the impulse vector is:

$$J_n = -(1 + e) \frac{\mathbf{v}_{ab,c} \cdot \mathbf{n}}{B_2} \quad (13)$$

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:

$$B_2 = \frac{1}{m_a} + \frac{1}{m_b} \quad (14)$$

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

$$\mathbf{v}_{ab,c} = \mathbf{v}_a - \mathbf{v}_b - (R_a \omega_a + R_b \omega_b) \times \mathbf{n} \quad (15)$$

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:

$$\mu < \frac{(1 + \beta_0)\mathbf{v}_{ab,c} \cdot \mathbf{t}}{J_n B_1} \quad (16)$$

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

$$\mu \geq \frac{(1 + \beta_0)\mathbf{v}_{ab,c} \cdot \mathbf{t}}{J_n B_1} \quad (17)$$

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

$$B_1 = \frac{7}{2} \left( \frac{1}{m_a} + \frac{1}{m_b} \right) \quad (18)$$

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

$$J_t = -(1 + \beta_0) \frac{\mathbf{v}_{ab,c} \cdot \mathbf{t}}{B_1} \quad (19)$$

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

$$J_t = -\mu J_n \quad (20)$$

Should the minimum collision time be between a particle and the boundary the velocities are reflected, taking into account the velocity of the walls during compression. For collisions between particles and the east boundary the velocity is updated as:

$$v_{x,i,p+1} = 2v_{w,E} - v_{x,i,p} \quad (21)$$

Where  $v_{x,i,p}$  is the  $x$  component of the velocity of particle  $i$  at timestep  $p$ . For collisions between particles and the west boundary the velocity is updated as follows:

$$v_{x,i,p+1} = 2v_{w,W} - v_{x,i,p} \quad (22)$$

For collisions with the remaining boundaries the velocities are updated in a similar manner.

## 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:

$$U = \frac{3}{2} N k T \quad (23)$$

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

$$dw = p dV \quad (24)$$

Where  $p$  is the pressure of the system and  $V$  the volume. Application of the ideal gas law to (24) gives:

$$dw = \frac{NkTdV}{V} \quad (25)$$

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

$$d(\frac{3}{2}NkT) = \frac{NkTdV}{V} \quad (26)$$

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

$$\frac{T_2}{T_1} = (\frac{V_1}{V_2})^{2/3} \quad (27)$$

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:

$$\frac{T_2}{T_1} = \frac{E_{k2}}{E_{k1}} = \frac{\Sigma(v_{2,i})^2}{\Sigma(v_{1,i})^2} \quad (28)$$

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

The temperature ratio  $T_2/T_1$  is computed for several compression ratios  $V_1/V_2$  using equation (28). These results are then compared with those obtained from the thermodynamic relation (27). The comparison is shown in table 1. The relative differences between simulations and corresponding theoretical predictions are within 1 %.

Table 1: Temperature ratio determined from thermodynamic relations and from simulation.

$V_1/V_2$	$T_2/T_1$ analytical	$T_2/T_1$ simulation
1.17	1.11	1.11
1.37	1.23	1.23
1.63	1.38	1.38
1.95	1.56	1.57
2.37	1.78	1.78
2.92	2.04	2.04
3.64	2.37	2.38