Adiabatic compression

Derek W. Harrison

October 2, 2020

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:

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

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 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:

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

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:

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

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:

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

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

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

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

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:

$$\mathbf{J} = J_n\mathbf{n} + J_t\mathbf{t} \tag{10}$$

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:

$$\mathbf{n} = \frac{\mathbf{r}_a - \mathbf{r}_b}{|\mathbf{r}_a - \mathbf{r}_b|} \tag{11}$$

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

The normal component of the impulse vector is:

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

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:

$$B_2 = \frac{1}{m_a} + \frac{1}{m_b} \tag{14}$$

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

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

Where ω_a is the rotational velocity vector of particle a and ω_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:

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

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

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

Where μ is the coefficient of friction, β_0 the coefficient of tangential restitution and B_1 is given by:

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

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

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

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

$$J_t = -\mu J_n \tag{20}$$

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:

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

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:

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

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:

$$U = \frac{3}{2}NkT \tag{23}$$

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

$$dw = pdV \tag{24}$$

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

$$dw = \frac{NkTdV}{V} \tag{25}$$

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

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

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

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

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:

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

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