# Adiabatic compression

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# Introduction

3D adiabatic compression is simulated using a system of 60 spherical particles in a cubic domain. The average increase in temperature observed in simulation is compared with the increase in temperature predicted by kinetic theory.

# Method

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.

## Collisions

Collisions occur between particles and particles and boundaries. To update the position of the particles collision times need to be computed. These are computed based on relative positions and velocities of particles and boundaries. Particle velocities are updated following the methods in [1] when collision occurs between particles and reflected when collision occurs with a wall. A more detailed discussion of collisions is given in the Appendix.

## Compression

Compression increases the momentum of the particles colliding with the moving boundaries. Consequently, the average kinetic energy of the system increases. From kinetic theory a relation between temperature and volume can be obtained for adiabatic compression:

$$\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{2/3} \tag{1}$$

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. A more detailed discussion on compression based on kinetic theory is provided in the Appendix.

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:

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

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 (2). These results are then compared with those obtained from the thermodynamic relation (1). 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 |

# References

[1] Foerster, S.F., Louge, M.Y., Chang, H. and Allia, K. (1994). Measurements of the collision properties of small spheres. *Phys. Fluids*, 6, 1108.

# Appendix

## 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:

$$t_{ab} = \frac{-\mathbf{r}_{ab} \cdot \mathbf{v}_{ab} - \sqrt{(\mathbf{r}_{ab} \cdot \mathbf{v}_{ab})^2 - \mathbf{v}_{ab}^2(\mathbf{r}_{ab}^2 - (R_a + R_b)^2)}}{\mathbf{v}_{ab}^2} \tag{3}$$

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

Collision times $t_c$ between particles and boundaries depend on the relative distance $\Delta s$ and velocity $\Delta v$ between particles and boundaries.

$$t_c = \frac{\Delta s}{\Delta v} \tag{4}$$

Collisions between particles are modeled using the methods of [1]:

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

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

$$I_a(\omega_{a,n+1} - \omega_{a,n}) = -(R_a\mathbf{n}) \times \mathbf{J} \tag{7}$$

$$I_b(\omega_{b,n+1} - \omega_{b,n}) = (R_b\mathbf{n}) \times (-\mathbf{J}) \tag{8}$$

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:

$$\mathbf{J} = J_n\mathbf{n} + J_t\mathbf{t} \tag{9}$$

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:

$$\mathbf{n} = \frac{\mathbf{r}_a - \mathbf{r}_b}{|\mathbf{r}_a - \mathbf{r}_b|} \tag{10}$$

$$\mathbf{t} = \frac{\mathbf{v}_{ab,c} - \mathbf{n}(\mathbf{v}_{ab,c} \cdot \mathbf{n})}{|\mathbf{v}_{ab,c} - \mathbf{n}(\mathbf{v}_{ab,c} \cdot \mathbf{n})|} \tag{11}$$

The normal component of the impulse vector is:

$$J_n = -(1+e)\frac{\mathbf{v}_{ab,c} \cdot \mathbf{n}}{B_2} \tag{12}$$

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:

$$B_2 = \frac{1}{m_a} + \frac{1}{m_b} \tag{13}$$

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

$$\mathbf{v}_{ab,c} = \mathbf{v}_a - \mathbf{v}_b - (R_a\omega_a + R_b\omega_b) \times \mathbf{n} \tag{14}$$

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:

$$\mu < \frac{(1+\beta_0)\mathbf{v}_{ab,c} \cdot \mathbf{t}}{J_n B_1} \tag{15}$$

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

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

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

$$B_1 = \frac{7}{2}(\frac{1}{m_a} + \frac{1}{m_b}) \tag{17}$$

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

$$J_t = -(1+\beta_0)\frac{\mathbf{v}_{ab,c} \cdot \mathbf{t}}{B_1} \tag{18}$$

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

$$J_t = -\mu J_n \tag{19}$$

For collisions with walls the velocities are reflected, taking into account the velocity of the walls $v_w$ during compression:

$$v_i^{p+1} = 2v_w - v_i^p \tag{20}$$

Where $v_i^p$ is the component of the velocity of particle $i$ at timestep $p$.

## Compression

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:

$$dw = \frac{NkT}{V} dV \tag{23}$$

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

$$d\left(\frac{3}{2}NkT\right) = \frac{NkT}{V} dV \tag{24}$$

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

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