Adiabatic compression

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Introduction

Simulations are performed of adiabatic compression of a system of particles in a cubic domain. Particles collide with one another and with the boundaries. Compression increases the temperature of the system and the average increase in temperature observed in simulation is compared with the increase in temperature predicted by kinetic theory.

Method

Adiabatic compression is simulated by computing the motion and collisions of 60 spherical particles in a cubic domain, taking into account conservation of energy and momentum. 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.

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:

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

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 by computing the change in the speeds of the particles:

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

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 based on relative positions and velocities:

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

Collision times t_c between particles and boundaries depend on the relative distance Δs and velocity Δv between particles and boundaries:

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

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

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

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

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

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

The impulse vector is composed of a tangential and normal component:

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

The unit normal and tangential vectors are:

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

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

The normal component of the impulse vector is:

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

The factor B_2 depends on the masses of the particles:

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

The relative velocities at the contact point depend on the relative and rotational velocities of the particles at collision time:

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

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:

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

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

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

The factor B_1 depends on the masses of the particles:

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

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

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

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 during compression:

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

Compression

The total kinetic energy U of the particles in the system is:

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

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

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

Application of the ideal gas law to (22) gives:

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

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:

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

Nomenclature

B_1	Factor depending of the masses of colliding particles (kg^{-1})
B_2	Factor depending of the masses of colliding particles (kg^{-1})
e	Coefficient of normal restitution $(-)$
E_{ki}	Kinetic energy of the system in state i (J)
I_x	Moment of inertia of particle x $(kg \cdot m^2)$
J_i	Component of flux vector $(kg \cdot m \cdot s^{-1}$
$\mathbf{J}$	Impulse vector $(kg \cdot m \cdot s^{-1}$
k	Boltzmann constant $(J \cdot K^{-1})$
m_x	Mass of particle x (kg)
N	Number of particles $(-)$
$\mathbf{n}$	Unit normal vector $(-)$
p	Pressure of the system $(N \cdot m^{-2})$
R_x	Radius of particle x (m)
$\mathbf{r}_x$	Position of particle x (m)
$\mathbf{r}_{xy}$	Relative position between particle x and y (m)
s	Distance to boundary (m)
t_c	Collision time between particles and boundaries (s)
t_{xy}	Collision time between particle x and y (s)
T	Temperature of the system (K)
T_i	Temperature of the system in state i (K)
$\mathbf{t}$	Unit vector tangent to the contact point $(-)$
U	Total kinetic energy of the system (J)
V	Volume of the system (m^3)
v_w	Wall velocity $(m \cdot s^{-1})$
v_i^p	Velocity component of particle i at timestep p $(m \cdot s^{-1})$
V_i	Volume of the system in state i (m^3)
$v_{i,k}$	Speed of particle k in state i $(m \cdot s^{-1})$
$\mathbf{v}_x$	Velocity of particle x $(m \cdot s^{-1})$
$\mathbf{v}_{xy}$	Relative velocity between particles x and y $(m \cdot s^{-1})$
$\mathbf{v}_{x,n}$	the velocity of particle x at timestep n (m^2)
$\mathbf{v}_{xy,c}$	Relative velocity between particle x and y at the contact point $(m \cdot s^{-1})$
w	Work required to compress the system (J)

Greek

β	the coefficient of tangential restitution $(-)$
μ	is the coefficient of friction $(-)$
$\omega_{x,n}$	Rotational velocity vector of particle x at timestep n (s^{-1})

Subscripts

1	Compression state, factor label (−)
2	Compression state, factor label (−)
c	Collision, contact (−)
i	Particle index (−)
k	Kinetic energy, particle index (−)
n	Timestep (−)
w	Wall (−)
x	Particle index (−)
y	Particle index (−)

Superscripts

p	Timestep (−)