

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:

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

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 are computed by:

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

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.

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:

$$U = \frac{3}{2}NkT \quad (5)$$

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

$$dw = pdV \quad (6)$$

Where p is the pressure of the system and V the volume. Application of the ideal gas law to (6) gives:

$$dw = \frac{NkTdV}{V} \quad (7)$$

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

$$d(\frac{3}{2}NkT) = \frac{NkTdV}{V} \quad (8)$$

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

$$\frac{T_2}{T_1} = (\frac{V_1}{V_2})^{2/3} \quad (9)$$

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:

$$\frac{T_2}{T_1} = \frac{E_{k2}}{E_{k1}} = \frac{\Sigma(v_{2,i})^2}{\Sigma(v_{1,i})^2} \quad (10)$$

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 (10) is 2.37 (2.3703). From the thermodynamic relation (9) 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).