Assignment: Multi-particle dynamics between two parallel walls

Consider a number of N particles randomly distributed between two walls having different temperatures (T_1 and T_2). The domain between the walls is divided within cells such that there are at least 50 particles in each cell. Each particle is represented by its location r_i and its velocity v_i. The particle evolution is integrated in time steps of duration delta_t and consists of two distinct phases: moving and collision of particles. In the moving procedure, the particles are moved as if they did not interact and their position are updated to r_i+v_i*delta_t.
When a particle strikes a wall with temperature T_w, all three compenents of the velocity are reset as follows:

$$v_x = \sqrt{\frac{kT_w}{m}}\, r_G,$$

$$v_y = \sqrt{\frac{kT_w}{m}}\, r'_G + u_w,$$

$$v_z = \sqrt{-\frac{2kT_w}{m}\ln r},$$

where r is a uniformly distributed random number in (0,1) and r_G, r_G' are Gaussian-distributed random numbers with zero mean and unit variance. In our case u_w corresponding to the wall velocity is zero.
After all the particles have been moved, a given pair is randomly selected for collisions. Only those particles that are near each other are allowed to interact. To implement this condition we sort the particles into spatial cells and allow only particles in the same cell to collide. In each cell, a set of representative collisions is processes at each time step. All pairs of particles in a cell considered to be candidate collision partners, regardless their positions within the cell. Because only the magnitude of the relative velocity between particles is used in determining their collision probability, even particle that move away from each other may collide. This condition allows particles to collide by simply being located in the same cell.

The collision probability for a pair i and j is proportional to their relative speed and the following rejection-acceptance scheme is used to select collision pairs in each cell:

(1) A pair of potential collision partners, i and j, is chosen at random from the particles within the cell.
(2) The pair is accepted as collision partners if

$$\frac{|\mathbf{v}_i - \mathbf{v}_j|}{v_{r,max}} > r, \qquad (8)$$

where $v_{r,max}$ is the maximum relative speed in the cell and r is a uniform deviate in (0, 1).
(3) If the pair is accepted, the collision is processed and the velocities of the particles are reset as discussed below.
(4) After the collision is processed or if the pair is rejected, the routine moves again to step (1) until the required number of candidate pairs M_{coll} in the cell has been processed. The value of M_{coll} is discussed in the following.

The method is also exact if we overestimate the value of v_r,max, although it is less efficient in the sense that more candidates are rejected. It is computationally cheaper to make an intelligent guess that overestimates vr_max rather than recomputed it at each time step.

After the collision pair is chosen, their postcollision velocities $\mathbf{v}_i'$ and $\mathbf{v}_j'$, need to be evaluated. Conservation of linear momentum tells us that the centre-of mass (cm) velocity remains unchanged by the collision.

$$\mathbf{v}_i' = \mathbf{v}_{cm}' + \tfrac{1}{2}\mathbf{v}_r'$$

$$\mathbf{v}_j' = \mathbf{v}_{cm}' - \tfrac{1}{2}\mathbf{v}_r' .$$

$$\mathbf{v}_{cm} = \tfrac{1}{2}(\mathbf{v}_i + \mathbf{v}_j) = \tfrac{1}{2}(\mathbf{v}_i' + \mathbf{v}_j') = \mathbf{v}_{cm}' .$$

$$v_r = |\mathbf{v}_i - \mathbf{v}_j| = |\mathbf{v}_i' - \mathbf{v}_j'| = v_r' .$$

$$\mathbf{v}_r' = v_r\,[(\sin\theta\cos\phi)\hat{\mathbf{x}} + (\sin\theta\sin\phi)\hat{\mathbf{y}} + \cos\theta\,\hat{\mathbf{z}}].$$

where

$$q = 2r - 1,$$

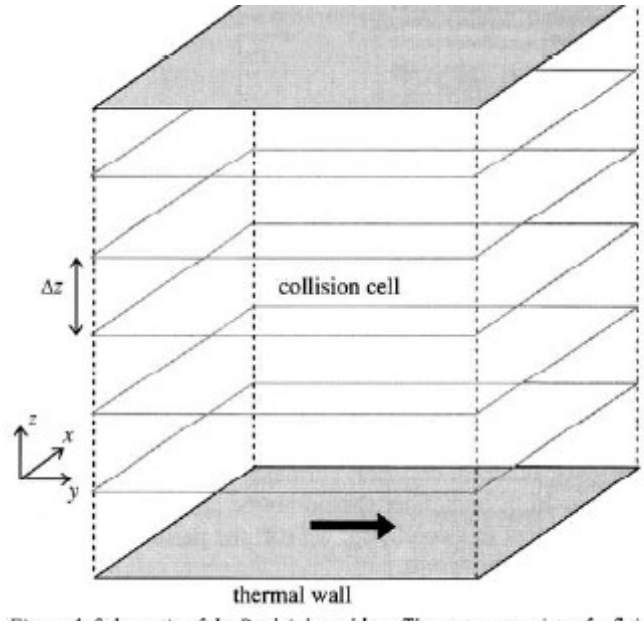
$$\cos\theta = q,$$

$$\sin\theta = \sqrt{1 - q^2}.$$

The total number of collisions that should take place in a cell during a time step is given by:

$$M_{coll} = \frac{N_c^2 \pi \sigma^2 \langle v_r \rangle N_e \Delta t}{2V_c},$$

where V_c=volume of the cell, N_c=number of particles per cell, and <V_r> is the average relative velocity in the cell.



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Constants:
      pi = 3.141592654
      boltz = 1.3806e-23     ! Boltzmann's constant (J/K)
      mass = 6.63e-26        ! Mass of argon atom (kg)
      diam = 3.66e-10        ! Effective diameter of argon atom (m)
      T = 273                ! Temperature (K)
      density = 2.685e25     ! Number density of argon at STP (m^-3)
      L = 1e-6               ! System size is one micron
      T1=300K
      T2=450K
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a) Implement the collisions per cell in case of a 1D grid (see figure) and compute the density and velocity profiles in the system.
b) Calculate the time step for a certain grid (The most probable initial velocity is given by `mpv = sqrt(2*boltz*T/mass) )`
c) Study the performance of the collision algorithm in case v_r=<v_r> and in case v_r=v_r_max.
d) Analyze the performance of the routine to sort particles within cells and indicate how could be optimised.
e) Consider now that the particle in a cell can interact with particles in nearby cells, modify the collision procedure to include these interactions.
f) Consider now instead of a 1D grid, a two dimensional grid and the collisions of particles taking place per cell. Compare the density profiles in the system with the 1D situation.
g) As there are no direct conflicts between collisions in cells, modify the algorithms to support parallelism.