PHY 607 Project 2 Proposal

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Project Description

Consider a 2D system containing a large number of identical non-interacting non-relativistic (subject to change) particles confined by thermal walls with temperature T. The particles move freely governed by the equation of motion

$$m\ddot{r}_i = 0, \tag{1}$$

where i denotes the i's particle. In general, we might have non-trivial potentials on the right-hand side of the above equation, but for simplicity we set it to 0 for now. When a particle hits the wall, it has probability p that it will have an elastic collision, leading to

$$v_\perp \to -v_\perp, \quad v_\parallel \to v_\parallel \tag{2}$$

i.e., changing the sign for the perpendicular component and leaving the parallel component unchanged. The particle also has the probability $1-p$ to have a thermal reflection where the wall acts as a thermal bath at temperature T. The particle picks up a new velocity sampled from a Maxwell-Boltzmann distribution of thermal velocities at that temperature

$$f(v_x, v_y) = \frac{m|\mathbf{v}|}{k_B T} \exp\left(-\frac{m|\mathbf{v}|^2}{2k_B T}\right), \tag{3}$$

where $|\mathbf{v}| = \sqrt{v_x^2 + v_y^2}$ is the velocity norm, m is the mass of the particle, k_B is the Boltzmann constant. This stochastic resampling is the Monte Carlo step, randomizing the velocity vector according to physical probability distributions.

All particles start with arbitrary positions and velocities, and evolve according to the equation of motion (1). For each time step, the position is determined by

$$r_i(t + \Delta t) = r_i(t) + \mathbf{v}_i(t)\Delta t. \tag{4}$$

After a long enough time, the velocity distribution is driven to equilibrium and obeys the Maxwell-Boltzmann distribution

$$P(v)\,\mathrm{d}v = \frac{mv}{k_B T} \exp\left(-\frac{mv^2}{2k_B T}\right) \mathrm{d}v\,. \tag{5}$$

Here, v represents the magnitude of the velocity and $P(v)$ denotes the probability of the velocity between v and $v + \mathrm{d}v$.

One may check the pressure of this model from wall collisions. Note that pressure is defined by momentum transfer per unit time per unit area. In fact, if collisions occur i times, then the pressure is given by

$$p = \frac{1}{A\Delta t} \sum_i 2m|v_{\perp,i}|. \tag{6}$$

At equilibrium of the simulation, the pressure of the system is expected to satisfy the ideal gas law

$$pA = Nk_BT. \tag{7}$$

Another physical quantity that can be checked in the simulation is the mean kinetic energy. For the thermal system, the mean kinetic energy per particle is theoretically given by

$$\frac{1}{2}m\langle v^2\rangle = k_BT. \tag{8}$$

An extension of the model is to add a potential $V(r)$ to the system, so that the equation of motion becomes

$$m\ddot{r}_i = -\nabla V(r_i). \tag{9}$$

The process can be simulated via the ODE methods used in the last project, such as the Euler's methods and the Runge-Kutta method. For nontrivial potentials, if we repeat the simulation, the expected distribution should also obey the Maxwell-Boltzmann distribution with the modified weight

$$f(\mathbf{r},\mathbf{v}) \propto \exp\left[-\frac{1}{k_BT}\left(\frac{1}{2}m|\mathbf{v}|^2 + V(\mathbf{r})\right)\right], \tag{10}$$

where the normalization factor depends on the exact form of the potential.

Specifically, for a harmonic trap

$$V = \frac{1}{2}k\left(x^2+y^2\right), \tag{11}$$

we expect the equipartition

$$\left\langle\frac{1}{2}mv_x^2\right\rangle = \left\langle\frac{1}{2}mv_y^2\right\rangle = \left\langle\frac{1}{2}kx^2\right\rangle = \left\langle\frac{1}{2}ky^2\right\rangle = \frac{1}{2}k_BT. \tag{12}$$

Moreover, x and y each have a Gaussian distribution with variance $\sigma_x^2 = \sigma_y^2 = k_BT/k$, which can seen from the above Maxwell-Boltzmann distribution.

Pseudocode

1. Main methods
   (a) Initialize a run of the simulation, given an initial probability distribution for speeds, number of particles, particle type, and thermal bath temperature
   (b) Evolve 1 time step
      i. For each particle, get interactions with other particles and evolve velocity & position
      ii. For each particle, check for interactions with walls and update velocity according to rule, update position to make sure particles don't get out of bounds
   (c) Run simulation for N time steps
      i. For each time step, record the speed distribution, the total perpendicular components of the velocities involved in wall collisions
2. Parent class: particle

(a) Utility methods: Get/set velocity, get/set position, get speed

(b) Method to get interaction rule with walls: See equation (3)

3. Subclass 1: Central force particles

   (a) Inherits utility & wall-interaction methods from Particle class

      i. Returns v_new

   (b) Method to get interaction rule with other particles: 1/r potential, i.e. Coulomb force between positively charged particles

      i. Parameters: One other particle's position, velocity

      ii. Returns v_new

4. Subclass 2: Particles without central force

   (a) Inherits utility & wall-interaction methods from Particle class

      i. Returns v_{new}

   (b) Particle-particle interactions: If particles are within a small distance of each other, do an elastic collision. Otherwise, particles do not interact

      i. Parameters: One other particle's position, velocity

      ii. Returns v_{new}

5. Plots

   (a) Initial and final speed distributions for a given simulation

   (b) Mean kinetic energy per particle over time

   (c) Pressure, as computed via proposal eqn. 6, over time

Work Division

Code:

- Main methods (Carter)
  - Simulation initialization
  - Single-timestep evolution
  - Run simulation
- Particle parent class (Fangyi)
- Central force particle subclass (Fangyi)
- Non-central force particle subclass (Fangyi)
- Plots (Fangyi)
- Benchmarks (Carter)

Report:

- Introduction/background (Fangyi)
- Results (Carter)
- Validation (Fangyi)
- Error analysis (Carter)
- Code benchmarks (Carter)
- Discussion & conclusion (Fangyi)