Simulations based Inference

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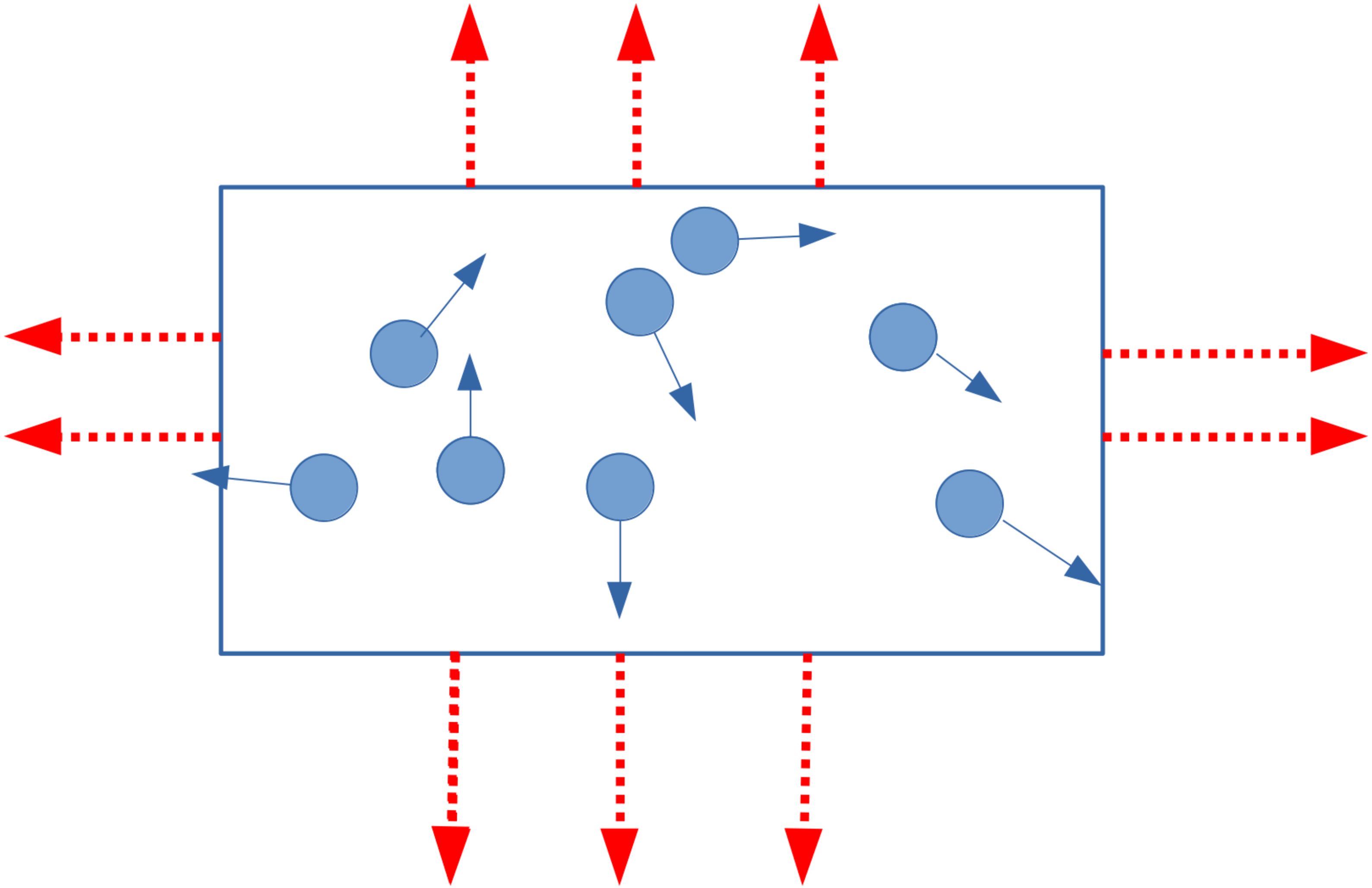
Simulation based Inference

- In this week's lab, we simulate particles moving and colliding with a 2 dimensional bounding box.
- Now, we will use this simulation to do some actual science.

Ideal Gas

- Imagine a $5m \times 5m$ 2-dimensional box filled with some kind of gas.
- We assume the gas is ideal.
    - No interaction/collision between gas molecules.
    - Gas molecules moves randomly.
- The walls of the box will feel **the pressure of the gas** since molecules collide with the walls.

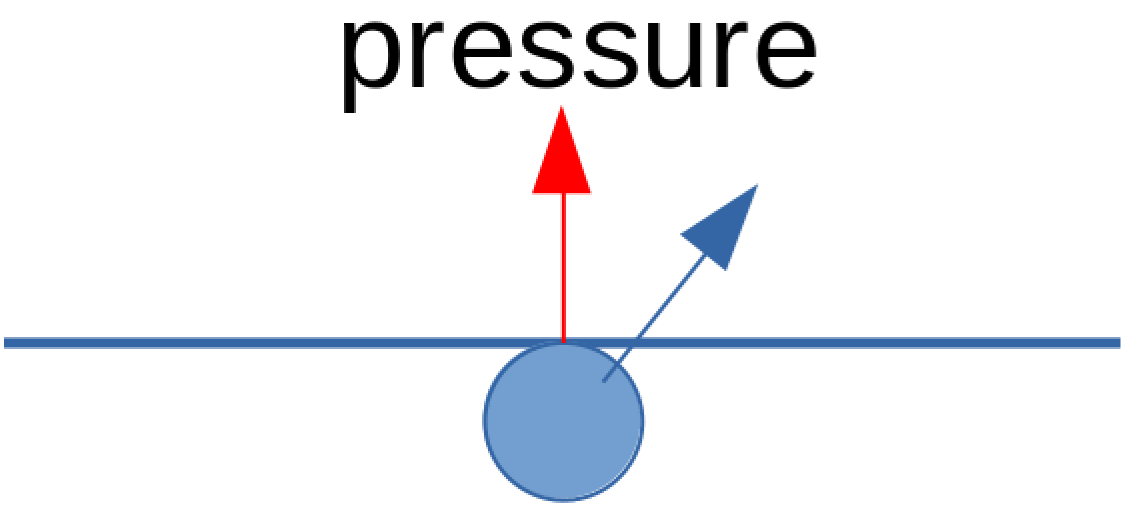
Ideal Gas



The Pressure

- The pressure to the wall is the average force applied perpendicular to the surface per unit area.
- Can we calculate the pressure of the wall using our simulation?
  - Suppose each "point" we plot using the lab code is an ideal gas molecule and the time interval between two `update` functions is exactly 1s.
  - Pressure created by a single wall-colliding molecule is **the velocity that is perpendicular to the wall**.
    - assuming each molecule has unit weight.
  - Adding up all pressures created by wall-colliding molecules, divide by the surface area, you get the average pressure.

The Pressure of a Single Wall-colliding Particle



- Hint: Pressure does not have directions, so you only need to take **the magnitude** of the perpendicular velocity.

Simulation based Inference

- Imagine the code we wrote during the lab is a simulation of ideal gas, where each "point" is an air molecule.
- Modify your lab code (for the 2nd task), so that it simulates the ideal gas for 500 iterations (seconds) and **compute the average pressure received by the box**.
- Run such simulations 100 times with randomly generated `x` and `v`.
- Plot the histogram of the average pressure computed from 100 simulations.
    - Hint: `?hist`

Simulation based Inference

- What is the relationship between the average pressure and number of molecules in the box?
- What is the relationship between the average pressure and velocities of molecules?
  - Hint: You can scale the velocities of molecules by `v<-matrix(runif(n * 2, -.5, .5), nrow = n)*C`, where `C` is a scaling factor.
- Is your finding consistent with Kinetic Theory?
  - $PV = RNm\bar{v^2}$, where R is a constant, P is the average pressure, N is the number of molecules, V is the volume of the gas and $\bar{v^2}$ is the average of squared molecules velocities.