Kinetic Theory using Simulations

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Simulation based Inference

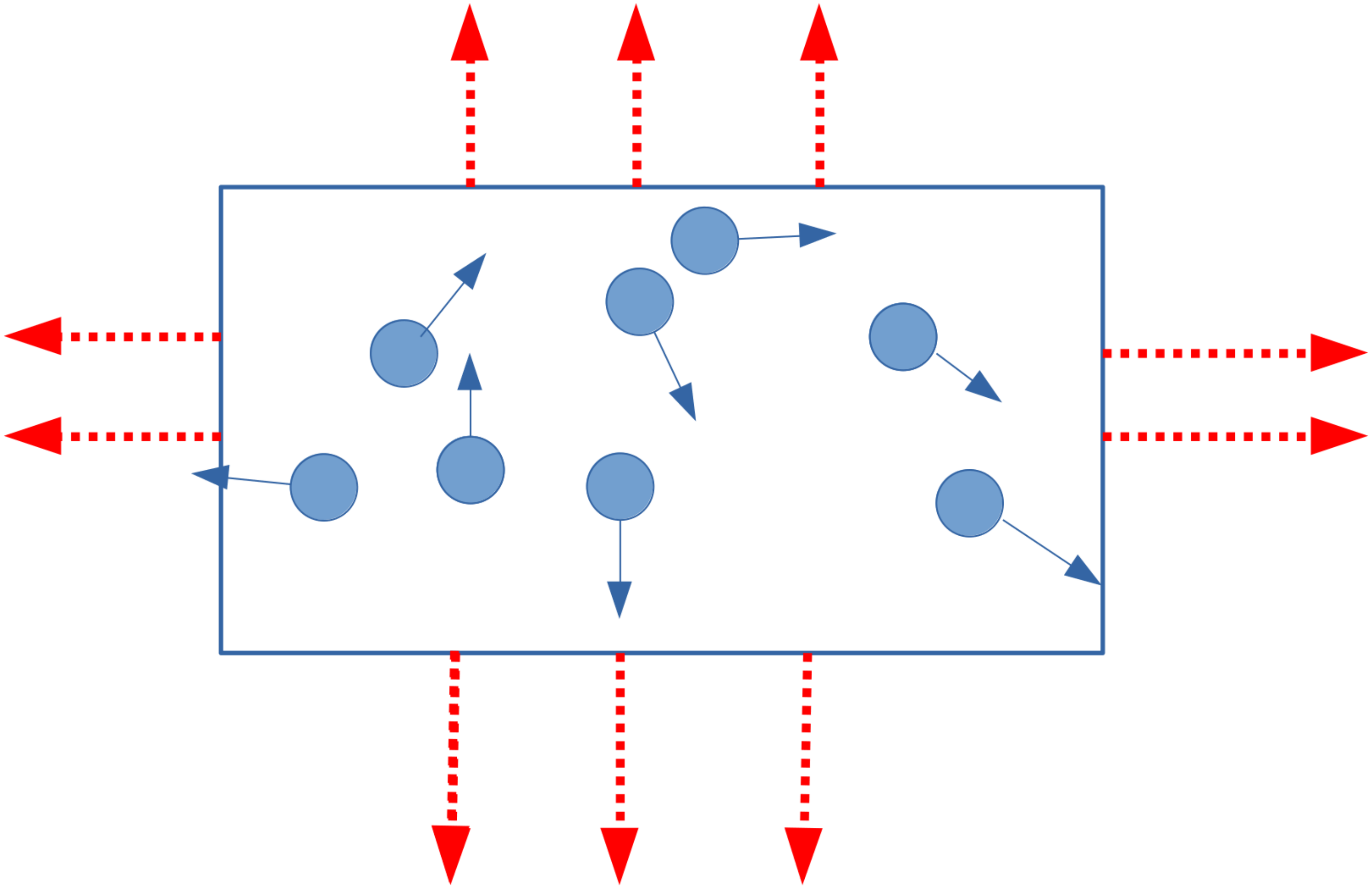
- In this week's lab, we simulate particles moving and colliding with a 2 dimensional bounding box.
- Now, we will use this simulation to do some actual science, with a technique called **simulation based inference**.

Ideal Gas

The Pressure of a Single Wall-colliding Particle

Hint:
`abs(v[(x[, 1] > 5 | x[, 1] < -5), 1])` gives you the absolute values of

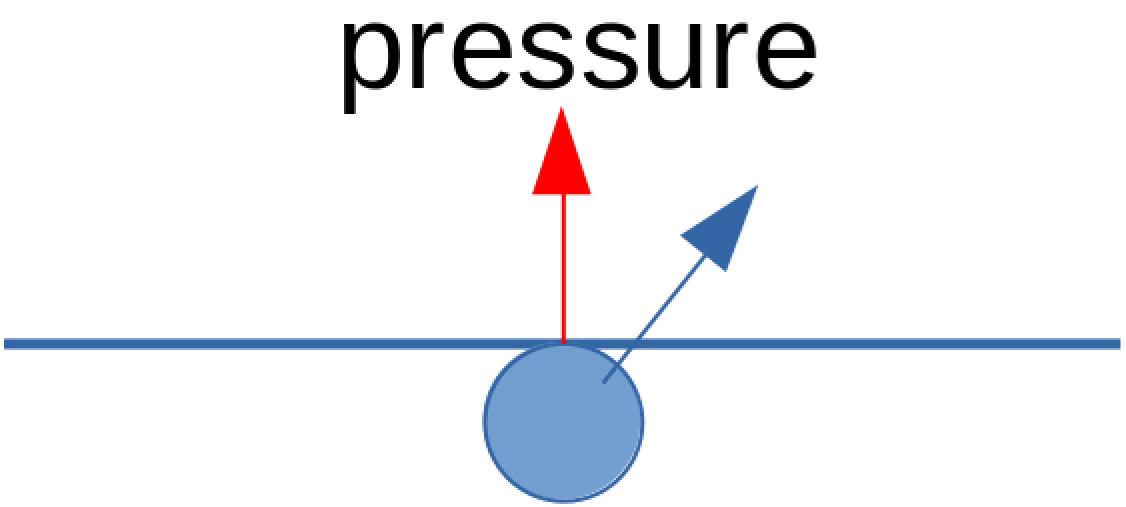
Ideal Gas



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 of our particles 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**.
  - 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



Simulation based Inference

- Modify your lab code (2nd task), so that it simulates the ideal gas for 500s and compute the average pressure.
- 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 pressure and number of molecules in the box?
- What is the relationship between the 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?
    - $PV = CNm\bar{v}^2$, where C is a constant.