Ideal Gas Applet

UMB CS 410 SE project outline

Constantin “Ted” Malliaris

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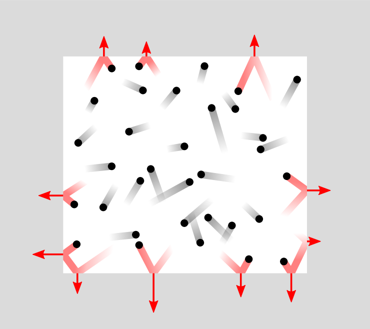
 [1]

[1] all graphics from Wikipedia unless otherwise noted

Ideal Gas Law refresher

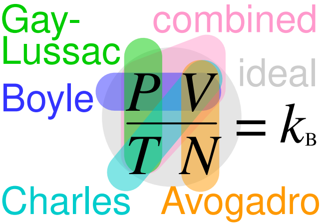
- you might recall (from high school chem or later):

$$pV = nRT, \quad \text{where}$$

  - p is the gas pressure (others use upper case P)
  - V is the volume occupied by gas
  - n is number of gas particles (e.g., in moles)
  - R is the ideal gas constant
  - T is <u>absolute</u> temperature of the gas
- units:
  - T must be in Kelvin!
  - units of p, V, and n are flexible, but...
  - units of R must "match"; common values include:

$$R = 8.314\frac{\text{J}}{\text{mol}\cdot\text{K}} \qquad R = 0.08206\frac{\text{L}\cdot\text{atm}}{\text{mol}\cdot\text{K}}$$

  - $R = N_A k_B \longrightarrow$ alternative form of ideal gas law: $pV = Nk_BT$



What's Ideal?

- helpful to "observe" a sample of gas and note:
  - mostly empty space ($\rho_{\text{gas}} \sim \frac{1}{1000}\rho_{\text{liquid}}$)
  - nature of n, V straightforward
  - nature of T: average kinetic "thermal" energy of particles
  - nature of p?

    → randomly moving fluid particles exert pressure through collisions
- what's "ideal" about the ideal gas law?
  - "ideal" in that (i) each particle takes up zero volume

    (ii) no inter-particle interactions

    → no attraction/repulsion, so no inter-particle collisions

    → collisions with wall are "allowed"...

    → will never "condense" into a liquid
- the ideal gas law (IGL) is an *equation of state*

  → more accurate equation of state from van der Waals:

$$p = \frac{RT}{V/n - b} - \frac{a}{(V/n)^2}$$

Implementation, Computation

- on paper, IGL is straightforward: knowns, unknowns, plug in, etc...
  → but this applet must *simulate* the dynamics of the IG particles
- preliminary considerations
  - for now, keep $N = nN_A$ fixed and small, e.g., $N = 10$ particles
  - real gases live in 3 spatial dimensions, but can we implement in 2D?
  - let's stick to monatomic gas "point" particles
- system state
  - how about a length 10 array of `Particle` objects?
  - what should each `Particle` object contain?
    → probably at least `float`'s x, y, v_x, v_y
  - these $10 \times 4 = 40$ `float`'s give a "snapshot" of the system
- system update equations/algorithm
  → how do we use state at t to generate state at $t + \Delta t$?
  - away from walls, $\sum \mathbf{F} = m\mathbf{a} = \mathbf{0}$ tells us:

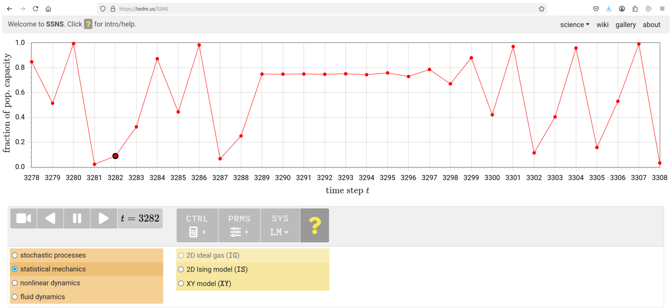
$$\begin{aligned} v_{x,\text{new}} &= v_x \\ v_{y,\text{new}} &= v_y \\ x_{\text{new}} &= x + v_x \Delta t \\ y_{\text{new}} &= y + v_y \Delta t \end{aligned}$$

  - (assumed elastic) collision at (locally flat) section of wall $\perp \hat{x}$:

$$\begin{aligned} v_{x,\text{new}} &= -v_x \\ v_{y,\text{new}} &= v_y \\ x_{\text{new}} &= \ldots \quad \text{(left as exercise)} \\ y_{\text{new}} &= y + v_y \Delta t \end{aligned}$$

Integration into existing js code

- integrate into existing SSNS web app
  - SSNS is an existing set of interactive STEM applets with common UI
  - Javascript codebase at `https://github.com/malliaris/SSNS`
  - live version on my personal site at `https://tedm.us/SSNS`
  - **SSNS** = **S**imple **S**tochastic and **N**onlinear **S**imulator



- existing codebase provides both support and constraints
  - e.g., good `js` pseudorandom number capabilities already in place → I will help team use them to generate proper initial gas states
  - e.g., existing class hierarchy for handling visualization via HTML `canvas` and external plotting library `https://www.flotcharts.org/` → must extend `PlotType` class, but very flexibile beyond that...

References

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8. https://en.wikipedia.org/wiki/Van_der_Waals_equation
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11. Atkins et al., *Atkins' Physical Chemistry*, 12th Ed., Oxford University Press, 2023.

    → accessible undergraduate text; see chapter 1 ("Focus 1")
12. Kittel & Kroemer, *Thermal Physics*, 2nd Ed., W. H. Freeman, 1980.

    → undergraduate text for physics majors; see chapters 3, 6