The Social Distancing of Molecules

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In the March of 2020, the UK Government introduced several practices to combat the viral infections caused by the COVID-19. One approach is termed the Social Distancing. This refers to several behaviors which reduce virus transmission chains, including limiting social contacts, practising respiratory hygiene and, more recently, wear face coverings. An essential part of reducing the risk of transmission of COVID-19 was that people must maintain a 2-metre gap between each other. This practice is now commonly understood and referred to as social distancing. The advised distance results from an assessment of the relative risk of transmission of virus between people and is not an absolute measure of safety.

This idea can also be approached in molecular interactions. In A-level Chemistry, I have come across with the concept of intermolecular forces. Van der Waal's forces that can be described as: London dispersion forces, dipole-dipole forces and hydrogen bonding. I have also learned to compare the strengths of these forces.

Putting this concept in a nutshell, we would come out with the general formula of:

$$\text{Potential Energy(total)}=\text{Potential Energy(repulsion)}+\text{Potential Energy(attraction)}$$

But how can these interactions be compared numerically? Perhaps, creating a mathematical model is a good way to visualize it !

But before we dive into the maths, it's better to elaborate it so that we have a clear idea:

Imagine two rubber balls of equal mass and volume are separated at a very large distance, so large that their interacting potential can be considered zero. The balls are then brought closer to a certain distance, where their interacting potential is at global minimum. Ultimately, the balls are brought to the stage of touching each other. If the balls are brought even more closer, they began to repel each other since they are invading each other's space. Thus, the force of repulsion is substantially greater than the force of attraction. A schematic diagram for the description is shown below in Figure A.

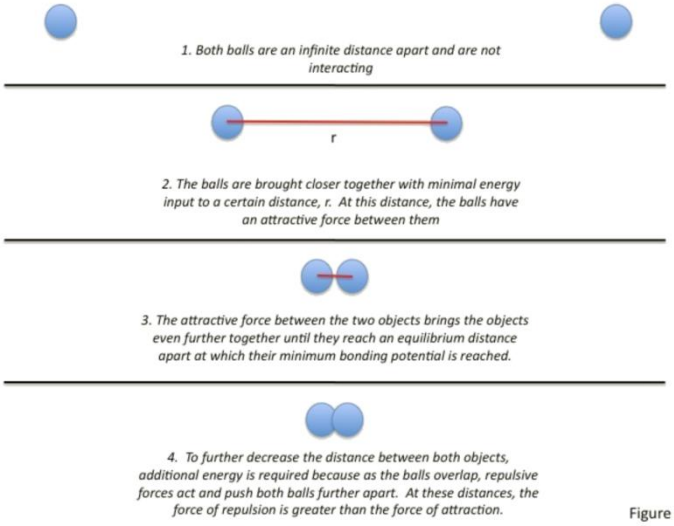

Figure A

These balls can be considered as non-bonding atoms in the microscopic world. In this case, an inert gas such as Argon(Ar) is an ideal choice. And the potential energy between the atoms are described as the Lennard-Jones Potential.

Named after Sir Lennard-Jones, who pioneered in molecular dynamics(moldy) and computational modelling, this function models mild attractive and repulsive forces for electronically neutral atoms.

An expression for the Lennard-Jones Potential function is shown below:

$$V_{\mathrm{LJ}}(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

,where r is the distance between two interacting particles (illustrated in Fig.A), ε is the well-depth potential, and σ is the distance at which the particle-particle potential energy V is zero. A graph of the Lennard-Jones potential function is shown below.

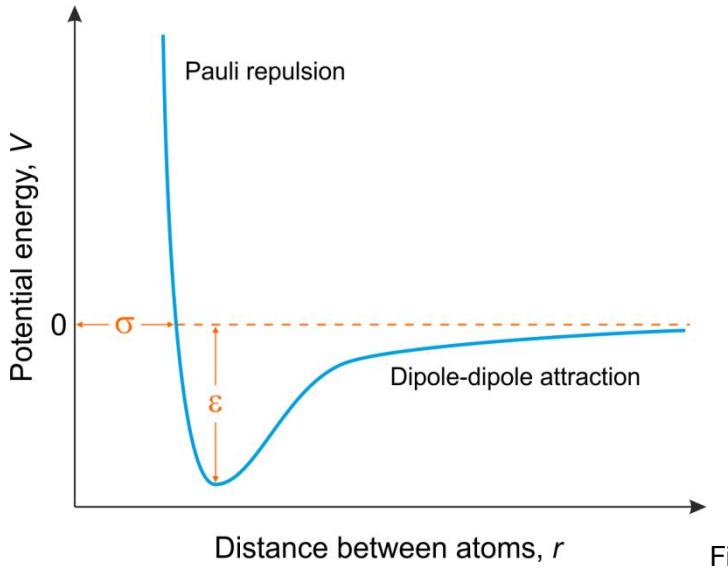

Figure B

To find the equilibrium distance of atoms, where the resultant forces are zero, this is located at the global minimum point.

Since that:

$$\mathrm{F} = \frac{\mathrm{dV}}{\mathrm{dr}}$$

, therefore we could find the stationery point by taking the first derivative of the function.

We need to rearrange this function to a new notation.

The AB form:

The Lennard-Jones potential function can also be written as:

$$\mathrm{V_{LJ}}(r) = \frac{A}{\mathrm{r}^{12}} - \frac{B}{\mathrm{r}^{6}}$$

, where $A = 4\varepsilon\sigma^{12}$ and $B = 4\varepsilon\sigma^{6}$. Conversely, $\sigma = \sqrt[6]{\frac{\mathrm{A}}{\mathrm{B}}}$, and $\varepsilon = \frac{\mathrm{B}^2}{4\mathrm{A}}$. It's interesting to note that this is the original form that Sir Lennard Jones proposed in his study in 1924.

Therefore, the derivative of this function arrives to be:

$$\frac{dV}{dr} = -12Ar^{-13} + 6Br^{-7}$$

Putting the derivative to be zero gives:

$$12\mathrm{Ar}^{-13} = 6\mathrm{Br}^{-7}$$

$$2(\frac{\mathrm{A}}{\mathrm{B}}) = \mathrm{r}^{6}$$

$$r^{6} = 2\sigma^{6}$$

$$\mathrm{r} = (\sqrt[6]{2})\,\sigma$$

For $(\mathrm{r} > 0, \sigma > 0)$

Since we mentioned σ to be the size of the particle--the distance between the centres when the atoms are just touching each other--therefore, the potential energy between the atoms can be considered as a constant.

Substituting $\mathrm{r} = (\sqrt[6]{2})\,\sigma$ into the function gives V to be:

$$\mathrm{V} = \frac{4\varepsilon\sigma^{12}}{4\sigma^{12}} - \frac{4\varepsilon\sigma^{6}}{2\sigma^{6}}$$

$$V = \varepsilon - 2\varepsilon = -\varepsilon$$

, which is consistent with Figure B.

The Lennard-Jones potential is probably the most studied model in computational chemistry as well as in computational physics. It describes the simple features between atoms and molecules: Two particles have negligible interaction at faraway distance, moderate attraction at close distance, and repel each other at very close distance, as described in Figure A. It is a paired potential which ideally limits the number of atoms to be 2.

The Practical Details of Molecular Separation:

In a closed physical system, molecules are bumping into each other with kinetic energy and I consider them nothing more than a bunch of hasty teenage hooligans. So I need a way to order the molecules to achieve the desired “tranquil” state. To do this, I need to select a generous population of molecules randomly, since a limited population might occur in biased sampling. Then, I need to optimize the population through computer simulations to find the minimum possible energy under a series of parameters.

The first step introduces the Monte Carlo method, which is another word for randomness. I believe the word originated from the city Monte-Carlo in Monaco, for it’s abundant number of casinos that represent randomness and luck. The key concept relies on random sampling to solve problems which might be deterministic in principle. In essence, the Monte Carlo method can roughly solve any problem that can be explained using probability. The law of large numbers allow us to achieve the expected value($E(x)$) of a variable through random sampling.

The Monte Carlo method can be used almost everyday in life. I recall from childhood memory about the glass marbles that I used to play with my friends. The person who shoots the marble with his hand and knocks other marbles out of bound wins the opponent’s marble. I was an avid collector and had 200 marbles at my prime.

For now, I can also use marbles to estimate constants such as π. Suppose I have a marble dropping device moving around in random paths above a rectangular table with two bowls on it. One bowl has a square cross-section with side lengths a and the other has a circular cross-section with radius a. The description is shown in Figure C.

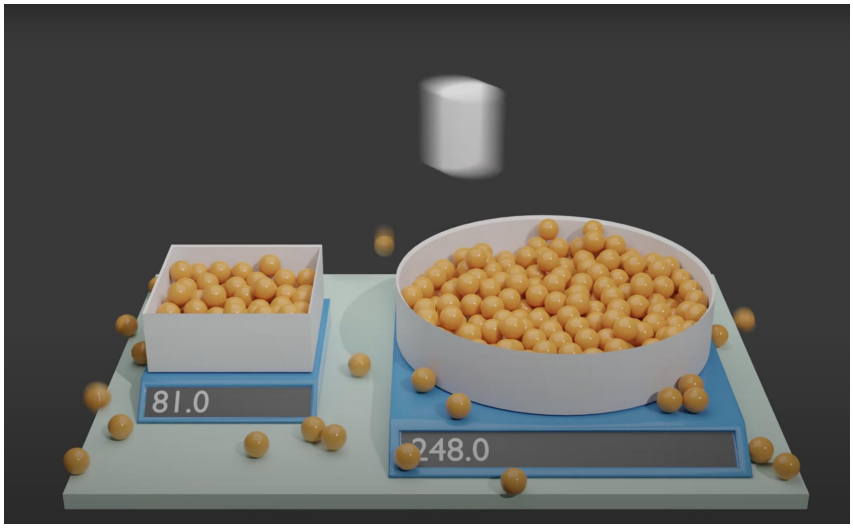

Figure C

We could establish an equation by equating the ratios of areas with the ratios of marbles, such that:

$$\frac{N_{circle}}{N_{square}} = \frac{A_{circle}}{A_{square}}$$

, where N represents the number of marbles and A represents the area of cross-section. Further simplifying this equation gives the representation:

$$\frac{N_{circle}}{N_{square}} = \frac{\pi a^2}{a^2} = \pi$$

$$(N \to \infty, \frac{N_{circle}}{N_{square}} \to \pi)$$

$$\%Uncertainty \propto \frac{1}{\sqrt{N}}$$

Conversely, we could also estimate the areas of the cross-sections using the equation. The beauty of Monte-Carlo method lies in the iterated simulations with a grand population sample. This method, of course, applies to our kinetic model of inert gases.

Our second approach aims to reach the state of minimum energy of molecules. Global optimization for the function $V_{LJ}(r)$ uses the annealing algorithm, simulated annealing. The first step is to choose a random molecule and evaluate it's potential energy, then it chooses another molecule. If the second molecule has a lower potential energy than the previous one, the algorithm accepts it probabilistically. Since the algorithm accepts the molecule with lower energy every time. Therefore, through repeated iterations we are able to obtain the molecule with the minimum energy.

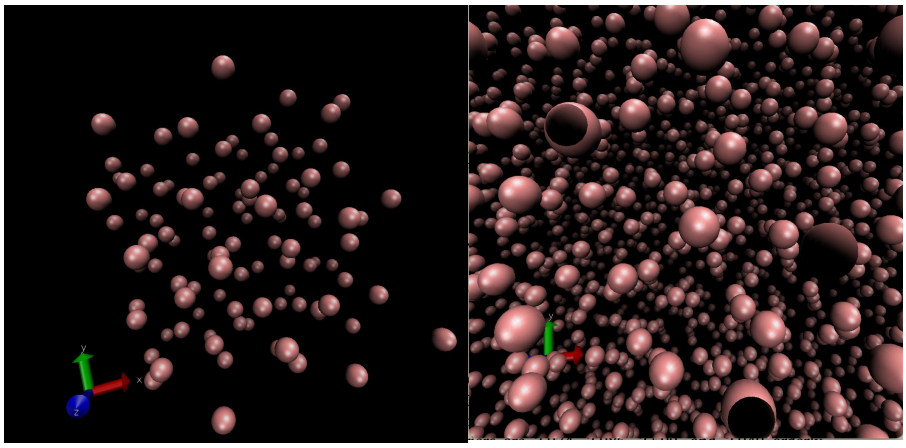

Figure D, Figure E

The application of annealing algorithm are also ubiquitous in life, especially in the logistics industry. Suppose you are a Deliveroo rider at your local town Oxford and you have 30 orders to 30 different colleges in the noon, are you going to prioritize St. Edmund Hall or Jesus? What is the shortest route? The art all lies within the annealing algorithm!

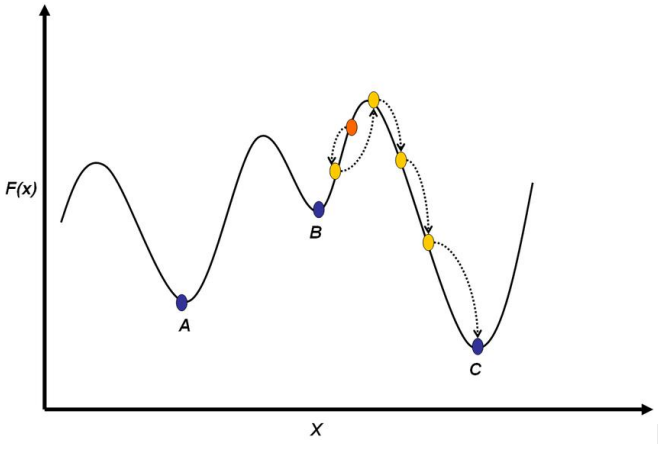

Figure F

However, a large sampling isn't always advantageous. Every computational simulation is associated with a variance that limits precision. To make a simulation statistically efficient and obtain greater precision, various reduction technique is often used. Through strategic sampling in a biased way, we can arrive at accurate results. A vivid example is frequent questions asked to potential hijackers or terrorists in Israel.(Just Pure Maths No political implications)

Conclusions:

For this essay, I have introduced molecules with interacting potential and the Lennard-Jones potential function, then using mathematical knowledge to derive the minimum potential energy of the function. Then looking into the practical details of molecular separation, introducing the Monte-Carlo method and the annealing algorithm and how are they used in everyday life. Finally, I introduced variance reduction as supplementary content. I hope the overall content is intriguing, enjoyable and related to modern computational maths. Maths is the fundamental tool for all science subjects and harnessing this art allows me to explore a broadened and integrated fields of science.

Source of Inspiration:

1. https://tomrocksmaths.com/2022/07/09/teddy-rocks-maths-essay-competition-2022-student-winner-1/
2. https://www.gov.uk/government/publications/full-guidance-on-staying-at-home-and-away-from-others
3. UK Chemistry Olympiad, UK Round 1 2021 Question 4, Royal Society of Chemistry
4. Figure C: https://www.youtube.com/watch?v=7ESK5SaP-bc
5. Figure D, Figure E: Visualizing Molecular Dynamics(VMD), University of illnois.