Simple Math for Interacting Gases

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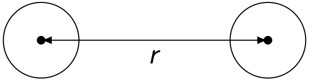
Lennard-Jones Potential

$$U(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$



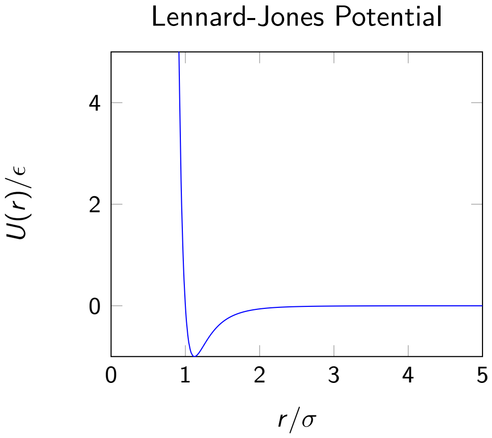
Lennard-Jones Potential

$$U(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

- ϵ represents the energy of the interaction.
- σ represents the lengths scale of the interaction.
- Outdated for detailed work, but useful for something like this.
- Bad infinity at short distances.

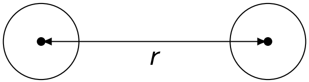
Lennard-Jones Potential

$$U(r) = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$



Morse Potential

$$U(r) = D_e\left(1 - e^{-a(r-r_e)}\right)^2$$



- Often used in advanced undergraduate chemistry to describe vibrations of diatomic molecules.
- Can also be used in this context.
- Also an older model, but good for illustrative work.

Morse Potential

$$U(r) = D_e \left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)} \right)$$

- Can be rewritten in this form (note that there is an offset that has been omitted).
- Morse potential stays finite.

Morse Potential

$$U(r) = D_e \left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)} \right)$$
$$r_e = 2^{\frac{1}{6}}\sigma$$
$$D_e = \epsilon$$
$$a = \frac{6}{2^{\frac{1}{6}}\sigma}$$

- Parameters can be set in terms of Lennard-Jones potential parameters.
- For this to work, we need to add the restriction that the minima must be the same.

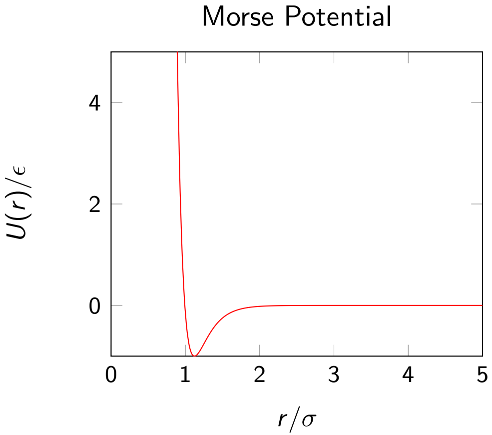
Morse Potential

$$U(r) = D_e \left(e^{-2a(r-r_e)} - 2e^{-a(r-r_e)} \right)$$

$$r_e = 2^{\frac{1}{6}}\sigma$$

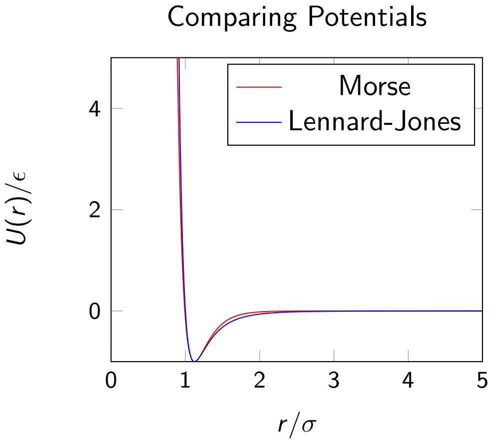
$$D_e = \epsilon$$

$$a = \frac{6}{2^{\frac{1}{6}}\sigma}$$



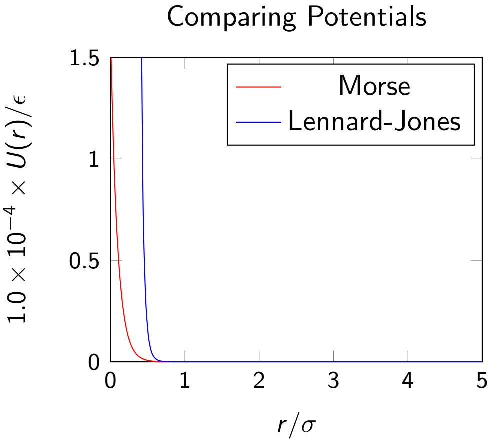
Direct Comparison

- The two potentials look quite similar at this scale.



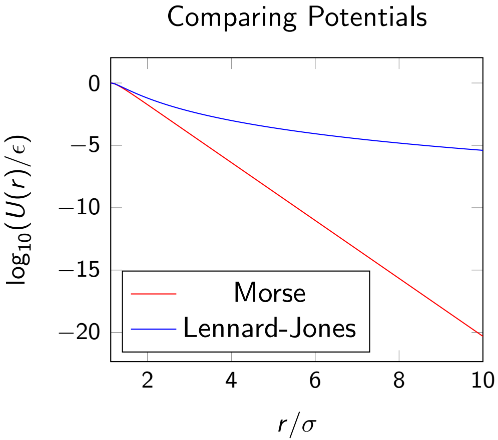
Direct Comparison

- When we look at the small r values, the difference becomes aparent.
- At small separation, the Morse potential stays finite.
- The Lennard-Jones potential goes asymptotically to infinity.
- Makes turning potentials off and on unstable for Lennard-Jones.



Direct Comparison

- Looking at long range, the Morse potential goes to zero faster than the Lennard-Jones potential.
- Makes it easier to ignore long-distance interactions with Morse.

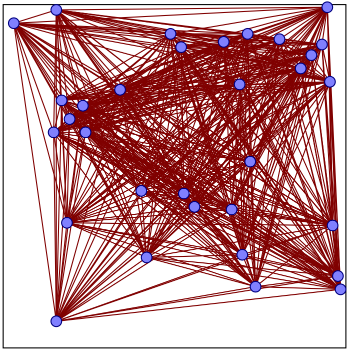


Acceleration Is a Bottleneck

- We need to compare every particle to every other particle.
- This means we need to do

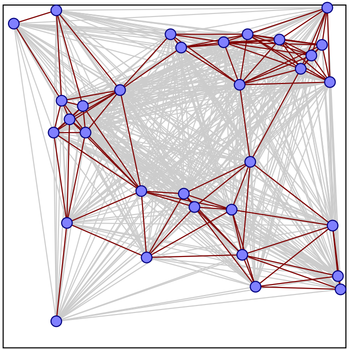
$$N_{comp} = \frac{1}{2} N_{part} \left(N_{part} - 1 \right)$$

  comparisons.
- Going from 512 particles to 4096 increases the time for updating the accelerations by a factor of about 64.



Acceleration Is a Bottleneck

- Improved this a bit by abandoning some calculations particles were farther than some threshold.
- Still need enough calculation to check the threshold.
- Any further strategy will require excluding some of the early calculations that can't be in the threshold.



Acceleration Is a Bottleneck

- One approach is to divide the box into sectors.
- Sectors should be small enough that particles can only interact with others in the same sector or neighboring sectors.
- This might also make concurency easier to do safely.