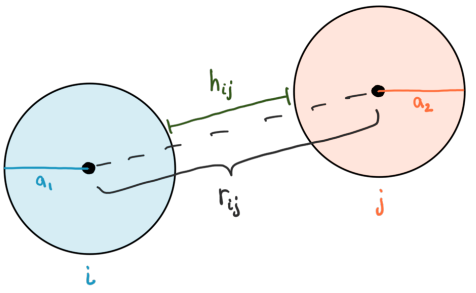
Morse Potential

One option for modeling particle pair interactions

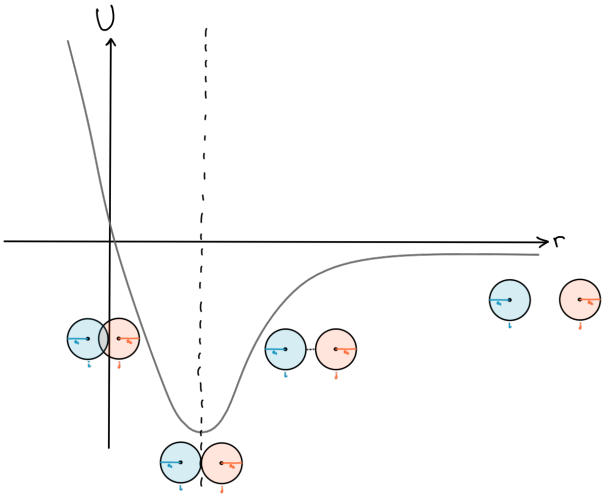
particle i & particle j separated by a center-center distance r_{ij}

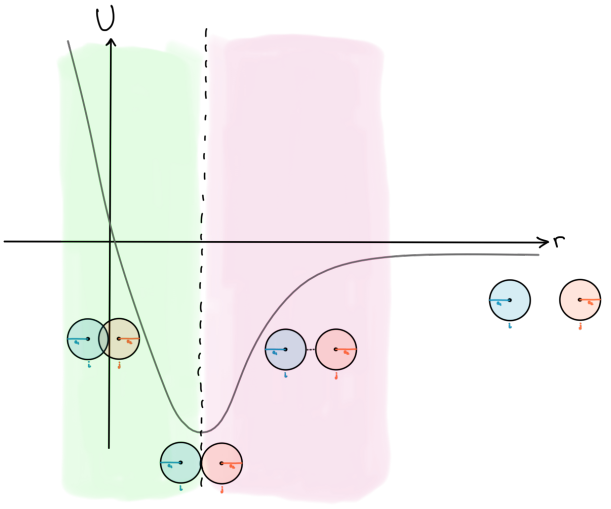
(AKA surface-surface distance $h_{ij} = r_{ij} - (a_i + a_j)$)



Morse Potential is a formula for a potential energy well that two particles "fall" into when they form a bond.

It includes ATTRACTION and REPULSION.



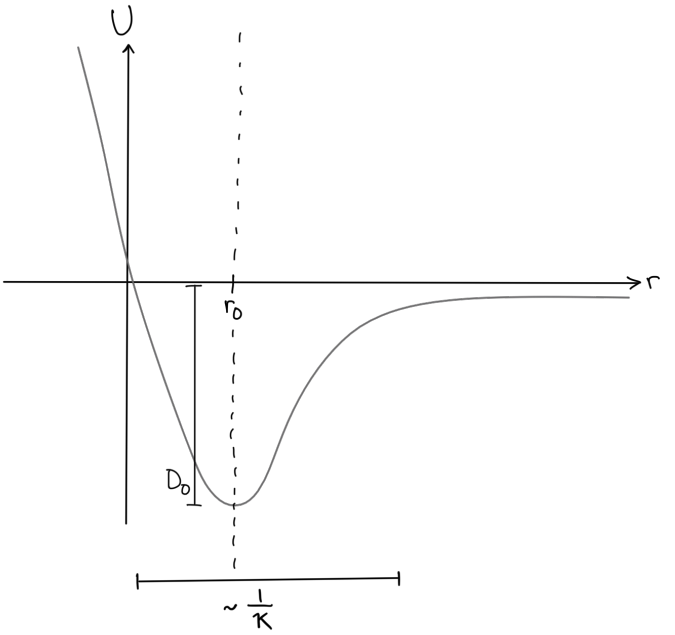


MORSE POTENTIAL ENERGY : $U(r) = D_0 \left(e^{-2\kappa(r - r_0)} - 2e^{-\kappa(r - r_0)} \right)$

The depth of the energy well is scaled by the strength of the interparticle bond (AKA the energy required to break the bond, called the "bond-dissociation energy") D_0, which we typically call attraction strength.

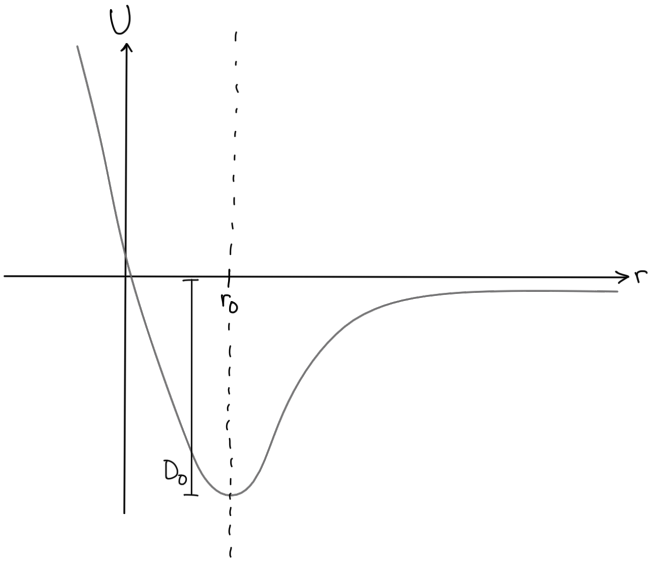
The width of the energy well is scaled by the parameter κ (also called α), which has units $[\text{length}]^{-1}$ (i.e. $\frac{1}{\kappa}$ has units of length)
A SMALLER value for κ creates a WIDER well.

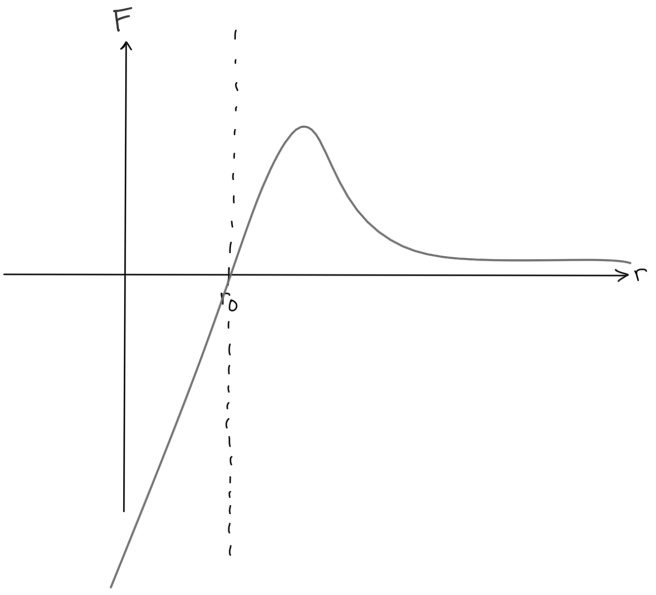
The position r_0 is the center of the well. ($r_0 = 0$ results in NO repulsive component)



The Morse force between two particles is the derivative of the Morse Potential

$$\text{MORSE FORCE: } F = \frac{dU}{dr} = -2\kappa D_0 \left(e^{-2\kappa(r_{ij}-r_0)} - e^{-\kappa(r_{ij}-r_0)} \right)$$

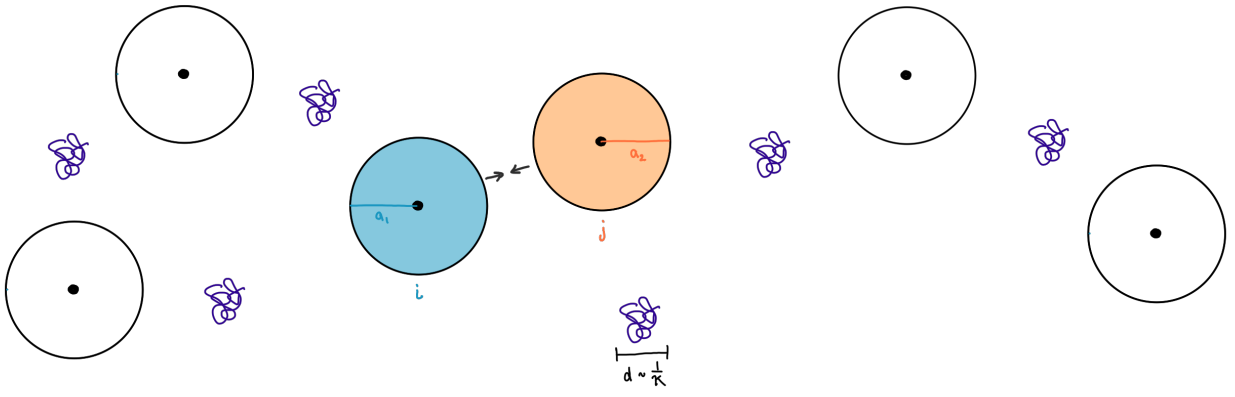




Modeling Real Systems

Our simulations typically model colloidal systems where interparticle attraction in induced by POLYMER DEPLETION, i.e. the particles themselves are not attractive or repulsive, instead the interparticle attraction is caused by changes in local concentration of a polymer.

In this case, we can use the kappa term (κ) to match (or predict) the behavior in a system with a specific size polymer depletant (polymer diameter $d \sim \frac{1}{\kappa}$).



To correctly model the behavior of these colloidal systems with the Morse Potential we use $r_0 = 0$ (i.e. no Morse repulsion) and then resolve particle contact/overlap with a separate contact force that makes the colloids hard particles.