Gaussian Pairwise Interations

Previously we were using a Lennard Jones pair-wise interaction to minimize our particle distributions. This pair-wise potential needs to be defined locally, if this interaction extends to long distances it will change the global distribution of the particles. Previously we used the Lennard-Jones Potential, however, in high-dimensions this will no longer be local, but become long-ranged.

A better approach will be to use a gaussian potential for minimizing the pairwise interactions. Consider a quasi-Gaussian pairwise interaction ($\mathbf{U}_{ij}$)

$$\begin{aligned} \mathbf{U}_{ij}(\mathbf{x}_i, \mathbf{x}_j) &:= -\exp\left\{\frac{(|\mathbf{x}_{ij}| - \sigma_i)^2}{(\gamma\ \sigma_i)^2}\right\} \\ |\mathbf{x}_{ij}| &= \sum (\mathbf{x}_i - \mathbf{x}_j)^2 \end{aligned} \tag{1}$$

Where γ is a constant defining the width of the Gaussian (can be paramaterized, try γ=0.1 for testing purposes).

σ represents the distance between nearest neighbors for our regularly distributed $\mathbf{P}$ grid-points.

$$\sigma_i = \sigma(\mathbf{x}_i) := c \cdot [N \cdot P(\mathbf{x}_i)]^{-1/d} \tag{2}$$

The constant c should be on the order of 1, ensuring particles do not form clusters (c is too small) or expand to the surface (c is too large).

Distribution of Interest

The distribution of interest ($\mathbf{P}$) is defined in terms of the Morse Potential

$$\begin{aligned} \mathbf{P}(\mathbf{x}) &:= \frac{E_{cut} - \mathbf{V}(\mathbf{x})}{\int d\mathbf{x}\ E_{cut} - \mathbf{V}(\mathbf{x})} \\ \mathbf{V}(\mathbf{x}) &:= D \sum_i \left(e^{-w_i \mathbf{x}_i} - 1\right)^2 \end{aligned} \tag{3}$$

Where we define a maximum energy contour (E_{cut})

$$\begin{cases} \mathbf{P}(\mathbf{x}) = 0 & \mathbf{V}(\mathbf{x}) > E_{cut} \\ \mathbf{P}(\mathbf{x}) > 0 & \mathbf{V}(\mathbf{x}) < E_{cut} \end{cases}$$

σ represents the distance between nearest neighbors for our regularly distributed $\mathbf{P}$ grid-points.

$$\sigma_i = \sigma(\mathbf{x}_i) := c \cdot \left[N \cdot P\left(\mathbf{x}_i\right)\right]^{-1/d} \tag{4}$$