DRP

Take N particles $X_i \in \mathbb{R}^3$ $i = 1, \ldots, N$. The energy function is given by

$$E(X_1, \ldots, X_N) \stackrel{\text{def}}{=} \frac{1}{2N} \sum_{i \neq j} K_{\alpha,\lambda}(|X_i - X_j|)$$

where the interaction kernel is

$$K_{\alpha,\lambda}(r) \stackrel{\text{def}}{=} \frac{1}{\alpha} r^{\alpha} + \frac{1}{\lambda} r^{-\lambda}, \quad \alpha \in (0, \infty), \quad \lambda \in (0, 3).$$

- Idea: for a big number of particles N, use Backward mode Automatic Differentiation to compute the gradient of the energy function. Then use gradient descent to find the local minimizers of the energy function.
- Implementation details: we need an implementation of the energy function compatible with Zygote.jl (the library for automatic differentiation in Julia). The energy function should be able to take any number of particles N and any pair of parameters α and λ.

Note: Given two particles $X_1 = (x_1, y_1, z_1)$ and $X_2 = (x_2, y_2, z_2)$ in $\mathbb{R}^3$. The distance between them $|X_1 - X_2|$ is given by

$$|X_1 - X_2| = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}.$$