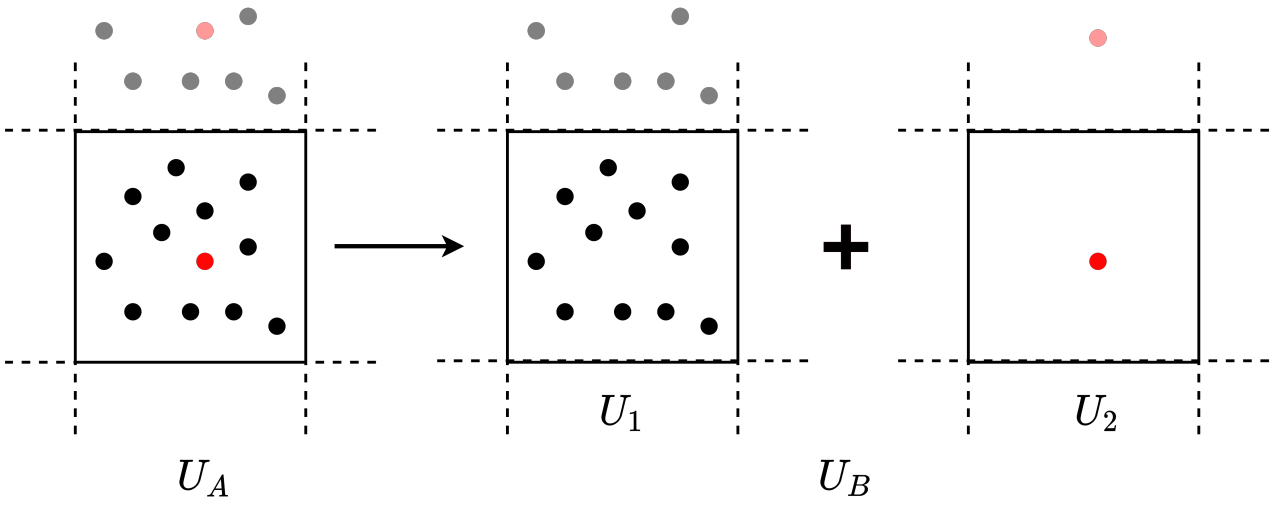
Alchemical Simulation Protocol for Deepmd-kit

Here we want to build a protocol for alchemical simulation with Deepmd-kit. Also, this protocol can be used for other neural network potential model.



The basic protocol model is showed as above.

We want to construct the alchemical process between U_A and U_B based on Deepmd-kit. First, the alchemical system potential energy can be written as

$$U := \lambda \cdot U_A + (1-\lambda) \cdot U_B = \lambda \cdot U_A + (1-\lambda)(U_1(\{j\}) + U_2(\{i\})) \tag{1}$$

U_1 is the function of atoms $\{j\}$'s coordinates while U_2 is the function of atoms $\{i\}$'s coordinates only. The force on each particle can easily derived from U.

$$F_i = \lambda \cdot F_A + (1-\lambda) \cdot F_2 \tag{2}$$
$$F_j = \lambda \cdot F_A + (1-\lambda) \cdot F_1 \tag{3}$$

With this simple protocol, we need three trained graphs actually in real cases. These three graphs are used for the calculation of U_A, U_1, U_2 separately.

Back to the hydration free energy calculation of water based on this protocol. We need three graphs in principle. However, due to the homogenous system of water bulk, one graph might be enough for hydration free energy calculation.