

Notes on Project 3

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I. MULTIPLE COMPONENT LENNARD JONES FLUID

Suppose a binary mixture of components 1 and 2 are in the same box.

A. Long Range Correction

$$\begin{aligned} U_{lrc} = & \frac{N_1\rho_1}{2} \int_{r_c}^{\infty} u_{11}(r)4\pi r^2 dr \\ & + \frac{N_2\rho_2}{2} \int_{r_c}^{\infty} u_{22}(r)4\pi r^2 dr \\ & + \frac{1}{2} \left(N_1\rho_2 \int_{r_c}^{\infty} u_{12}(r)4\pi r^2 dr + N_2\rho_1 \int_{r_c}^{\infty} u_{12}(r)4\pi r^2 dr \right) \end{aligned} \tag{1}$$

B. Creation/Destruction

1. creation of a new particle: pick molecule type first, then generate a random position in the control volume.
2. destruction of an existing particle: pick molecule type first, then pick a random particle of that type in the control volume.