MAKING SIMULATIONS SIMPLER

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1. Improved data analysis

1.1. **Radial distribution function.** The result obtained by Borgis et al. [1, 2] can be obtained in two lines. We start with the identity:

$$g(r) = \int_0^r dr' \, \frac{\partial g(r')}{\partial r'} \,, \tag{1}$$

which is correct for particles that have a strong repulsive interaction at short distances, such that $g(r = 0)$=0. Next, we note that the potential of mean force is defined as $U_{MF}(r) \equiv -k_B T \ln g(r)$. Therefore

$$\begin{aligned} g(r) &= \int_0^r dr' \, \frac{e^{-\beta U_{MF}(r')}}{\partial r'} \\ &= -\beta \int_0^r dr \; e^{-\beta U_{MF}(r')} \frac{\partial U_{MF}(r')}{\partial r'} = \beta \int_0^r dr' \; g(r) F_r(r) \end{aligned} \tag{2}$$

where F_r is the radial component of the potential of mean force. Eqn. 2 is equivalent to

$$g(r) = \frac{\beta}{4\pi\rho} \left\langle \sum_{j \neq i}^{N} \mathbf{F}_j \cdot \frac{\mathbf{r}_{ij}}{r_{ij}^3} \theta(r - r_{ij}) \right\rangle \,, \tag{3}$$

which is the Borgis et al. expression.

References

[1] D. Borgis et al. Mol Phys 111, 3486 (2013)
[2] D. de las Heras & M. Schmidt, Phys Rev Lett 120, 218001 (2018)
[3] D. Frenkel and B. Smit, *Understanding Molecular Simulation: From Algorithms to Applications*, Academic Press, second edition, 2002.

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