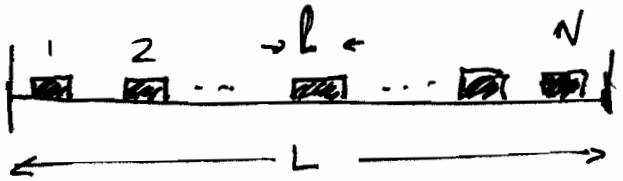
A simple application

Calculate the equation of state for a system of N hard rods, each of length ℓ, in a line of length L.



Virtual NPT simulation, volume creation/annihilation

$$P_{acc} = \min\left(1, \exp(-\beta\Delta\mathcal{U} - \beta P \Delta V)\right)$$

$\Delta\mathcal{U} = 0$ since no interactions

At equilibrium, $P_{acc}^{+} = P_{acc}^{-}$ for any small ΔL

$$P_{acc}^{+} = \exp(-\beta P \Delta L) \simeq 1 - \beta P \Delta L$$

$\beta P \Delta L \ll 1$

$P_{acc}^{-} = ?$ same as for ideal gases, except now the effective density in free space is higher due to the volume exclusion of the rods

$$P_{acc}^{-} = \left(1 - \frac{\Delta L}{L - \ell N}\right)^{N} \simeq 1 - \frac{\rho \Delta L}{1 - \rho \ell}, \text{ where } \rho = \frac{N}{L}$$

Setting $P_{acc}^{+} = P_{acc}^{-} \Rightarrow$

$$1 - \beta P \Delta L = 1 - \frac{\rho \Delta L}{1 - \rho l} \Rightarrow \boxed{\beta P = \frac{\rho}{1 - \rho l}}$$

This is exact in 1-D and is similar to the first (repulsive) term of the van der waals equation-of state.