Homework 5: Molecular and Langevin Dynamics, NPT, and grand canonical ensembles

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1. (Computational) Follow the instructions in the Introduction to Molecular Dynamics and Langevin Dynamics notebook in the MolecularDynamics assignment on RCNYU or under molecular-dynamics/ at:
https://github.com/hockyg/chem-ga-2600/
Submit the MD via RCNYU or email, but you don’t have to turn in anything for the Langevin dynamics part.

2. Ideal gas law at constant pressure. Derive the equivalent of the ideal gas law in the (N,P,T) ensemble. See Tuckerman Chapter 5.5.

3. Volume fluctuations at constant pressure. Derive the relationship between the isothermal compressibility \( \kappa = -\frac{1}{V}(\frac{\partial V}{\partial p})_{N,T} \) and the variance in the volume \( \text{Var}(V) = \langle V^2 \rangle - \langle V \rangle^2 \).

You should be able to do this starting by plugging \( V = -k_B T \left(\frac{\partial \ln \Delta}{\partial p}\right)_{N,T} \) in to the definition of \( \kappa \).

4. Sackur-Tetrode equation for the grand canonical ensemble. Write the entropy of an ideal gas in the (\( \mu, V, T \)) ensemble. See Tuckerman Chapter 6.5.