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

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Due: November 24, 2020

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 $\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_{N,T}$ and the variance in the volume $\mathrm{Var}(V) = \langle V^2 \rangle - \langle V \rangle^2$.

   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.