Each Team Must Complete the following two tasks.

Task 1. Simulate Cl₂ in the gas phase at T = 600 K and approximately 1 atm. Use an accurate EOS to predict the fluid density.

First,
- Verify that rcut, rnbr, maxeqb, maxstp, N, Δt are all legitimate values.

Second,
- Explicitly report pressure, self-diffusivity and potential energy with error bars.
- Explicitly report all parameters used in the simulation.

Third,
- Explore temperature dependence of pressure, self-diffusivity and potential energy from 400 K to 700 K at constant density.
- Explore density dependence of pressure, self-diffusivity and potential energy in gas phase at constant T of 600 K.

Fourth,
- prepare a written document summarizing your results in an organized manner.
- This report must contain all the tasks listed above summarized in graphical or tabular (or both) form.
- Compare the (i) magnitude and (ii) temperature-dependence of your pressure with the ideal gas law.
- Compare the (i) magnitude, (ii) temperature-dependence, and (iii) pressure dependence of your self-diffusivity with the prediction of Kinetic Theory.
Task 2. Simulate CCl₄ (Carbon Tetrachloride) in the liquid phase at T = 300 K and approximately 1 atm. Use the Lennard-Jones EOS to predict the fluid density.

First,
- Verify that rcut, rnbr, maxeqb, maxstp, N, Δt are all legitimate values.

Second,
- Explicitly report pressure, self-diffusivity and potential energy with error bars.
- Explicitly report all parameters used in the simulation.

Third,
- Explore temperature dependence of pressure, self-diffusivity and potential energy from 100 K to 400 K at constant density.
- Explore density dependence of pressure, self-diffusivity and potential energy in gas phase at constant T of 250 K.

Fourth,
- prepare a written document summarizing your results in an organized manner.
- This report must contain all the tasks listed above summarized in graphical or tabular (or both) form.
- Compare the (i) magnitude and (ii) temperature-dependence of your pressure with the Lennard Jones Equation of State.
- Compare the (i) magnitude, (ii) temperature-dependence, and (iii) pressure dependence of your self-diffusivity with the prediction from the corresponding states chart in Chapter 17 of BSL 2.