Demonstrating Basic Simulation Efficacy

I made my own code, which while it allows us to do some more stuff with it, I still probably should demonstrate that it’s not too shitty. There are some simple tests that we can run to demonstrate that this software works accurately.

First we’re running some simulations of pure gases and testing if the results agree with experimental data as well as our equations of state. A unit cell of gas should behave exactly the same as our reservoir under the same conditions. The only difference is that we’re looking at it.

Do the Isotherms make sense?

Pressure of system vs pressure of reservoir

Chemical Potential of system vs chemical potential of reservoir

3 Temperatures

10 or 20 Pressures

3 Replicates

Same box size as X and Y in carbon experiment

Run time?

Block size 100

Gas Mixtures w/ experimental data

As above but with 0.2, 0.4, 0.6, 0.8 yCO

Pure Gas Demonstrations:

1. Isotherms in direct comparison (with error bars?)
2. Pressure Drift (y = x plot)
3. Chemical Potential Drift (y=x plot)

Mixture Demonstrations:

1. Isotherms in direct comparison for each mole fraction (with all 3 temps shown)
2. Isotherms in direct comparison for each temperature (with each mole fraction shown)
3. Pressure Drift per mole fraction
4. Chemical Potential Drift
5. Mole Fraction Drift