**Ab Initio MD of vibrational motion of HF**

Computational Lab recovered by Dr. Foley under recovered Computational Lab 3….

1. **How are the dynamics different when the *ab* *initio* forces are used? Try to identify at least two quantitative ways in which you can distinguish the harmonic motion from the motion deriving from the *ab* *initio* forces.**

* When using ab initio forces, you can observe the system at a fixed time. The harmonic motion will start and finish were it started whereas the ab initio potential will be great in the begining and then decrease. We can use newton’s equation to distinguish harmonic motion.

1. **Can you estimate the frequency from the *ab* *initio* trajectories? How does this frequency compare with the Harmonic approximation and with the experimental value?**

* Yes,

frequency = 1/(2\*np.pi) \* np.sqrt(Force\_constant/mu)

I would assume they would all be the same since the u (reduced mass) & k (force constant) will remain the same.