Our model system has two local minima, one at approximately 1.9 atomic units and another at approximately 2.4 atomic units.

1. Set the r\_init to 1.8 atomic units (i.e. somewhat near the minimum of the energy landscape for the system) and run the simulation a few times.
   1. Does the final value for the position of H always, usually, sometimes or rarely converge to the “equilibrium” value?
      1. **Looks like the final value for the position of H sometimes changes when running the simulation.**
   2. Does the final value for the position of H ever converge to the other, non-global local minimum in the energy landscape?
      1. **The final value for the position of H does converge to the other non-global local minimum in the energy landscape.**
   3. How well, in general, does the final value for the potential energy match the minimum of the energy landscape?
      1. **In general, the final value for the potential energy matches to the minimum of the energy landscape.**
2. Set the r\_init to 2.4 atomic units (i.e. very near the other, non-global local minimum in the energy landscape) and run the simulation a few times.
   1. Does the final value for the position of H always, usually, sometimes or rarely converge to the “equilibrium” value?
      1. **The final value of H usually converges to the equilibrium value.**
   2. Does the final value for the position of H ever converge to the other, non-global local minimum in the energy landscape (i.e. does the position of H ever end up more or less where it started, even after “exploring” positions with lower energy?)?
      1. **The position of H does end up converging.**
   3. How well, in general, does the final value for the potential energy match the minimum of the energy landscape?
      1. **It matches well the final value for the potential energy to the minimum of the energy landscape.**
3. Note that the value of g used in this week’s exercise is higher than the value of g used in the previous computational exercise (which itself was on the high side for Langevin dynamics).
   1. What effect, if any, does lowering the value of g have? In particular, when you start with r\_init being 2.4 atomic units, do you often see the position of H explore values near the global energy minimum in the landscape and then return to the local minimum occurring when the position of H is near 2.4 atomic units?
      1. **When lowering the value of gamma, the position of H is a slight change. The H values near the global energy minimum in the landscape and then return to the local minimum the position was near 2.4 units.**
   2. What does lowering the value of g mean, conceptually speaking? Do your observations of what happens when you lower the value of g make sense in terms of what g means as a “drag” parameter?
      1. **When looking at gamma when lowering the value it seems like it does act in the terms of what gamma means a drag parameter and it is lowering the drag force in the system.**
4. Convert the initial temperature and hot temperature to kelvin (using the conversion factor ): what would actually happen if you heated an aqueous solution of HF to the hottest temperature used in our simulation?
   * 1. **When changing the temperature and converted it to kelvin the value of the position H changed and decreased. This could mean that we would not be able to see the molecule because it would be to hot.**
5. Change the value of g back to 0.02 and change the initial temperature and hot temperature to 0 (essentially using the drag term in the Langevin equation to minimize energy). How do your answers to the questions in parts 1 & 2 above change? In particular, if you start with r\_init = 2.4 atomic units, does the position of H ever converge to the global minimum? You may also want to try using a hotter temperatures than you did with your first
   * 1. **When setting the gamma to 0.02 and changing all the temperatures to 0, the answers to question 1 and 2 do change. Looks like the position of H barley converges to the global minimum.**