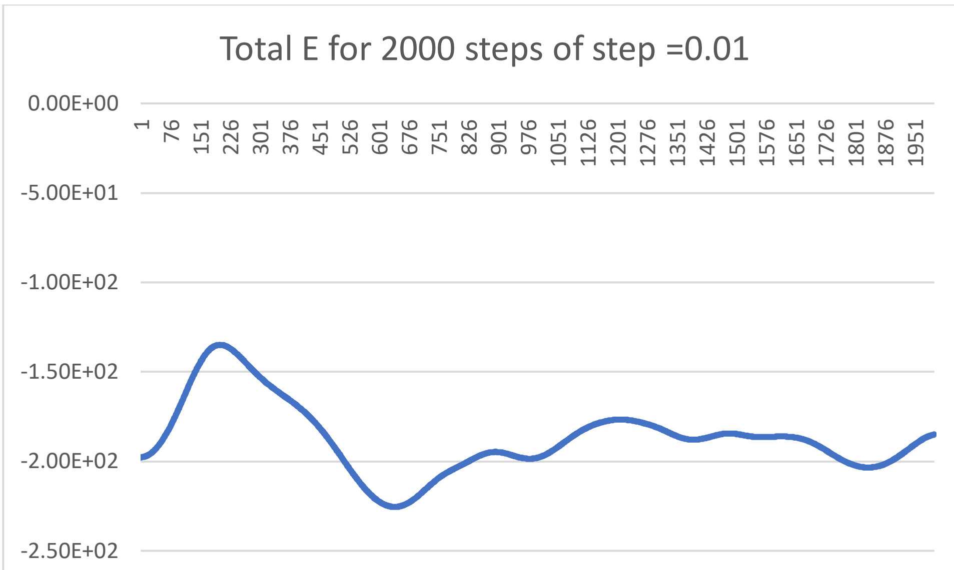
Albert Wiryawan
Avw2@illinois.edu
673431511
PHYS 466: Atomic scale simulation

Homework #2

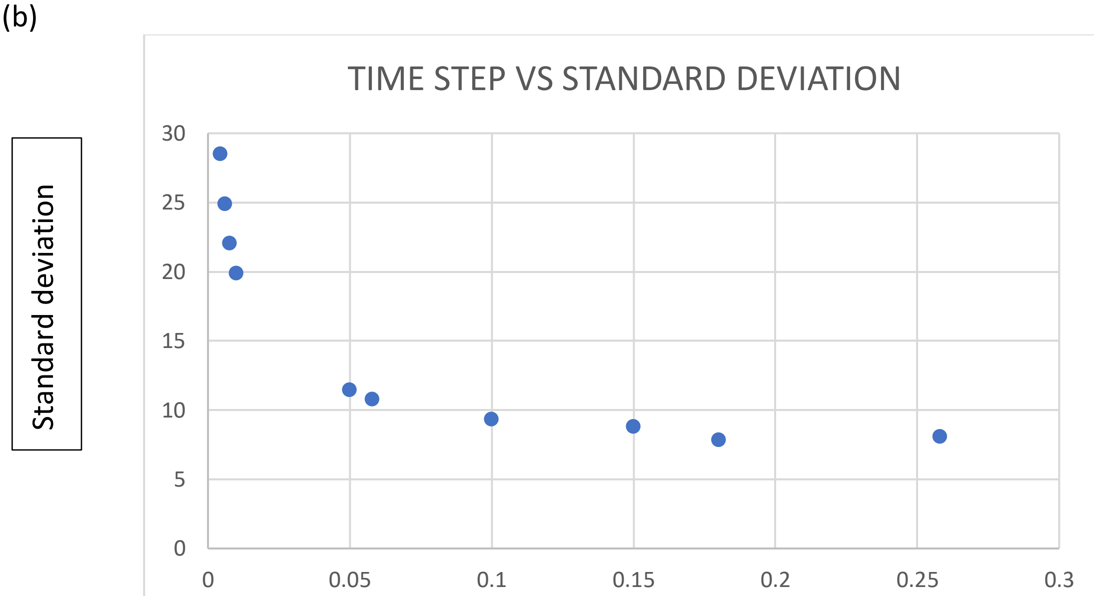
teijrhgogrojeiojgr

Problem #1

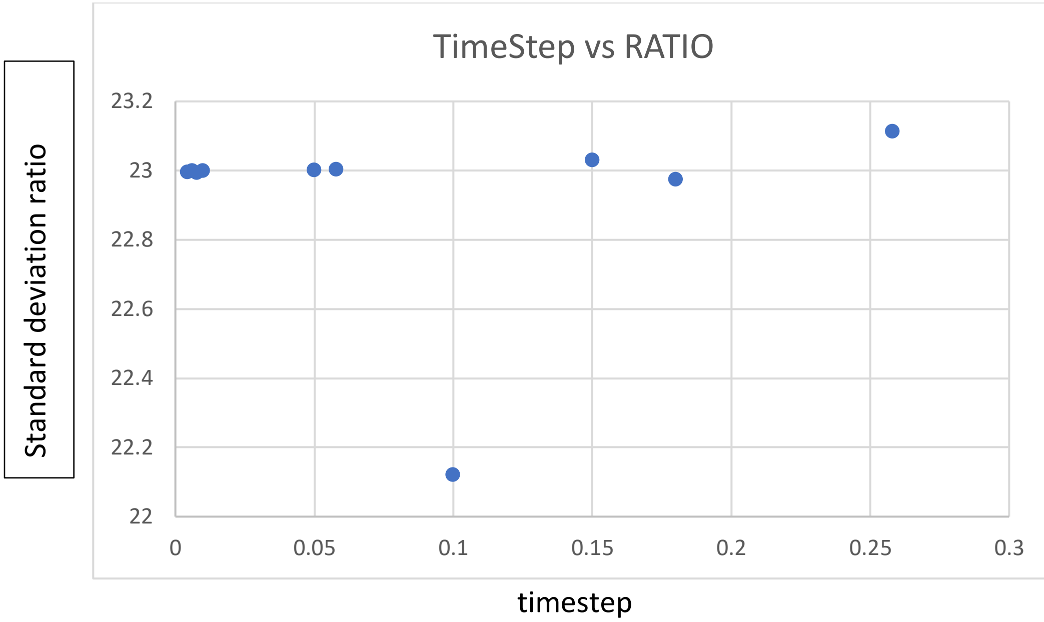
(a)



(b)



(c) timestep



(d)

If you pick a very large time step the program has an error in the potentially energy function that is caused by a division of zero

Problem #2

(a)
r(t+h) = r(t) + v(t) h + 0.5a(t) h^2
r(t-h) = r(t) +-v(t)ht + 0.5a(t) h^2

When r(t+h) and r(t-h) are added together, the total comes out to: 2r(t) -r(t-h) +a(t)h^2.
This is equal to the equation below.

r(t+h) = 2r(t) -r(t-h) +a(t)h^2

This equivalence proves time reversal invariance.

(b)

Since the float precision is precise to the 7^{th} decimal point. The h^2 term in the verlet equation which is said to have a time step h = 10^4. The decimals beyond that are essentially truncated and will not affect the estimation.

(c)

The equation for (9) is given by $r(t+h) = 2r(t) - r(t-h) + a(t)h^2$. This equation can be converted to the form of: $v\left(t - \frac{h}{2}\right) + \frac{a(t)h}{2}$. Taking this equation and applying the derivative law, the equation turns into $v(t) = \frac{r(t+h)-r(t-h)}{2h}$. Equation 10 on the other hand is $r(t+h) = r(t) = r(t) + v(t)h + \frac{a(t)h^2}{2}$ can be rearranged into $v\left(t + \frac{h}{2}\right) = v(t) + \frac{a(t)h}{2}$. Thus, this shows that (90 is equivalent to velocity Verlet.

(d)

If you pick a very time step there is a division by zero error.

Problem #3

(a)

Take the derivative of $\mathrm{u_{LJ}} = 2\epsilon\left[\mathrm{A}_{12}\left(\frac{\sigma}{r_n}\right)^{12} - \mathrm{A}_6\left(\frac{\sigma}{r_n}\right)^{6}\right]$ with respects to lattice parameter since $r_n = \frac{a}{\sqrt{2}}$and set this equal to zero.

This derivative turns out to be $\mathrm{u_{LJ}}' = 2\epsilon[-12\mathrm{A}_{12}\left(\frac{\sigma}{r_n}\right)^{13} + 6\mathrm{A}_6\left(\frac{\sigma}{r_n}\right)^{7}]$

This allows us to solve for the two parameters, thus, the $\sigma = 0.1137\ \dot{A}^{-1}$and $\epsilon = 2004.84 \text{ eV per atom/}$

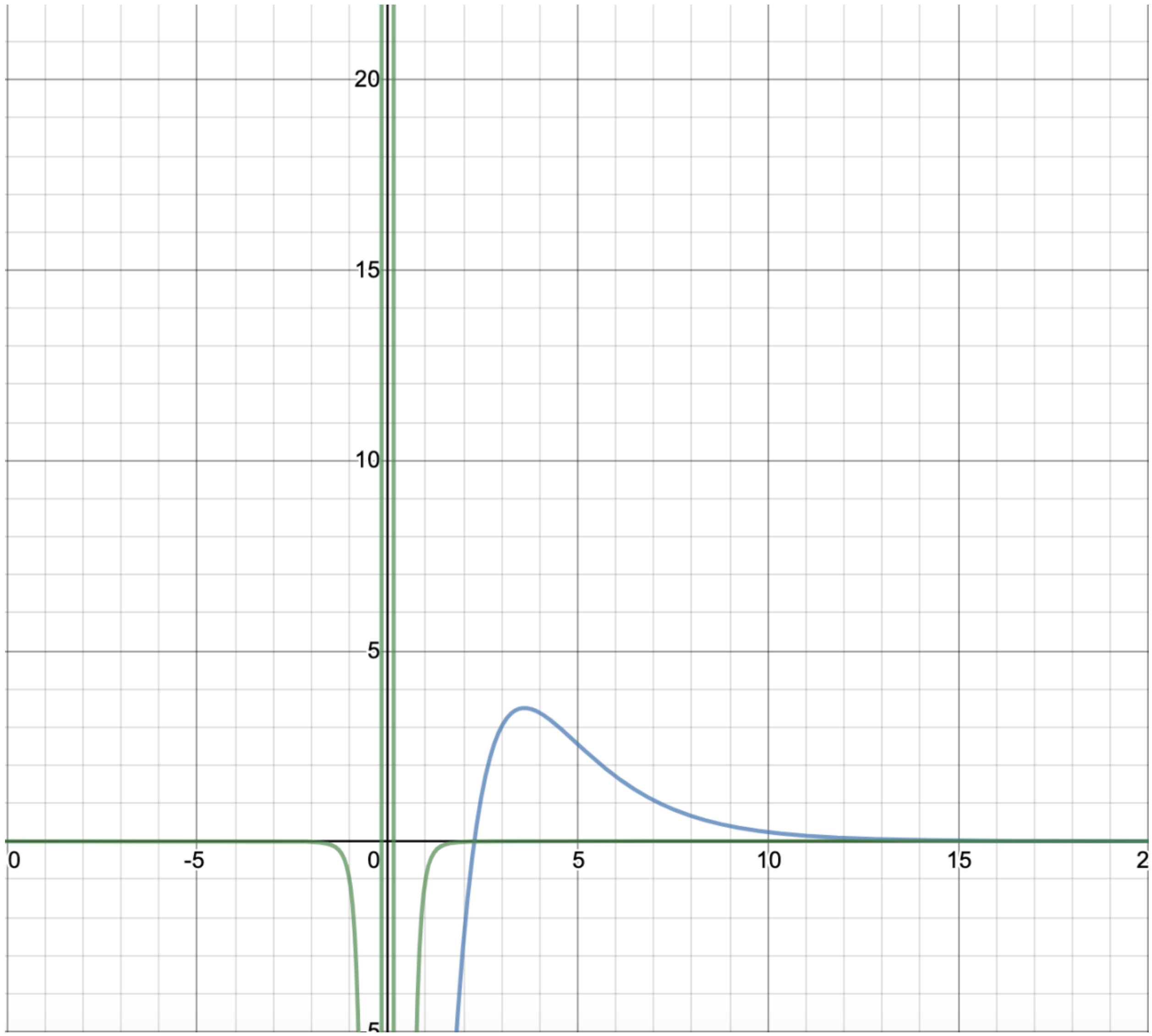
(b)

The morse potential model is given by the equation $\mathrm{u_M} = \mathrm{D_e}(e^{-2\alpha(r_n - r_e)} - 2e^{-\alpha(r_n - r_e)})$. r_e can then be found by taking the derivative of this equation with respect to the lattice parameter (a), since r_n is equal to $\frac{a}{\sqrt{2}}$. This results to $\mathrm{u_M}' = \mathrm{D_e}(-2\alpha e^{-2\alpha(r_n - r_e)} - 2\alpha e^{-\alpha(r_n - r_e)})$. Thus, $r_e = r_n = \frac{a}{\sqrt{2}} = 2.546\ \dot{A}$ as found when plugging r_e back to the original equation. From here, D_e is found to be $-u = 3.5\ eV$. Using the bulk modulus, B in the form of $B = v\frac{\partial}{\partial v}\frac{\partial u}{\partial v} = v\frac{\partial}{\left(\frac{\partial v}{\partial r}\right)^2}\frac{\partial^2 u}{\partial r^2} = \frac{r^3}{\sqrt{2}}\frac{\partial}{\frac{9r^4}{2}}\frac{\partial^2 u}{\partial r^2} = \frac{\sqrt{2}}{9r}D_e(4\alpha^2 e^{-2\alpha(r_n - r_e)} + 2\alpha^2 e^{-\alpha(r_n - r_e)})$, the constant B=134GPA can be used to find α which is $0.7437\ \dot{A}$.

(c)

In the Lennard-Jones model, the bulk's modulus equation is the same except for u. Thus, $B = v\frac{\partial}{\partial v}\frac{\partial u}{\partial v} = v\frac{\partial}{\left(\frac{\partial v}{\partial r}\right)^2}\frac{\partial^2 u}{\partial r^2} = \frac{r^3}{\sqrt{2}}\frac{\partial}{\frac{9r^4}{2}}\frac{\partial^2 u}{\partial r^2} = \frac{2\sqrt{2}\epsilon}{9r}[-156\mathrm{A}_{12}\left(\frac{\sigma}{r_n}\right)^{14} + 42\mathrm{A}_6\left(\frac{\sigma}{r_n}\right)^{8}]$. Using the parameters found from part a the Bulk's modulus was determined to be 148.52 GPa.

(d)



The green plot is given by

$$u_M = D_e\left(e^{-2\alpha(r_n - r_e)} - 2e^{-\alpha(r_n - r_e)}\right),$$

While the blue plot is given by

$$u_{LJ} = 2\epsilon\left[A_{12}\left(\frac{\sigma}{r_n}\right)^{12} - A_6\left(\frac{\sigma}{r_n}\right)^{6}\right]$$