1 Metropolis Acceptance Criterion

1. (TA comment: η stands for the Gaussian random number needed to move from x to x', while η' stands for that needed for the reverse move)

$$T(x \to x') = p(\eta) = p(x' - x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x'-x)^2/2\sigma^2}$$

$$T(x' \to x) = p(\eta') = p(x - x') = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-x')^2/2\sigma^2}$$

2. Since $(x - x')^2 = (x' - x)^2 \Longrightarrow T(x \to x') = T(x' \to x) \Longrightarrow \frac{T(x \to x')}{T(x' \to x)} = 1$

3.

$$A(x \to x') = min\{1, e^{\beta(V(x')-V(x))}\}$$

2 Monitoring Acceptance and Setting Up Runs

1. For $\sigma = 0.04$ the acceptance ratio came to be 0.5661, which is in the acceptable range.

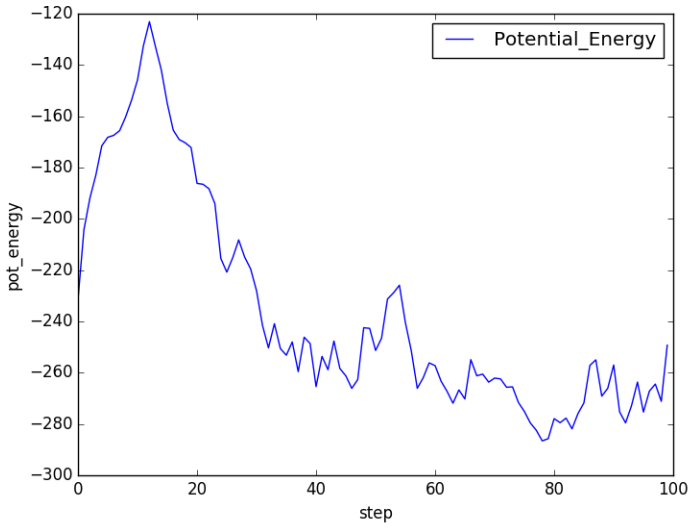

Figure 1: $\sigma = 0.04$ potential energy trace for 100MC steps

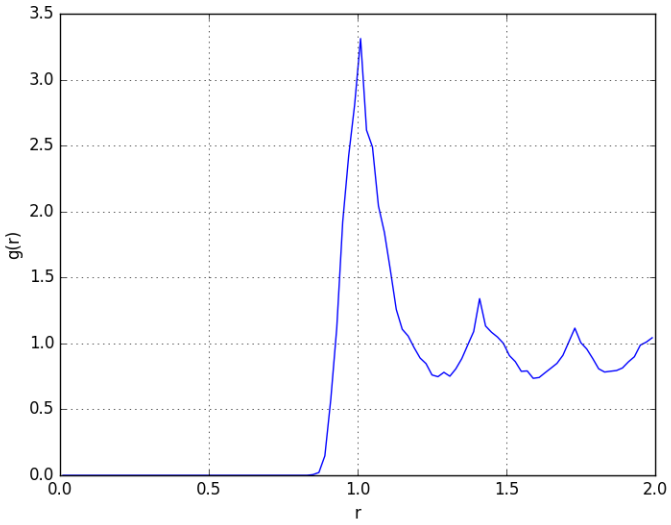

Figure 2: $\sigma = 0.04$ RDF for 100MC steps

2. For $\sigma = 2.5 * 10^{-5}$ the acceptance ratio came to be 1.0.

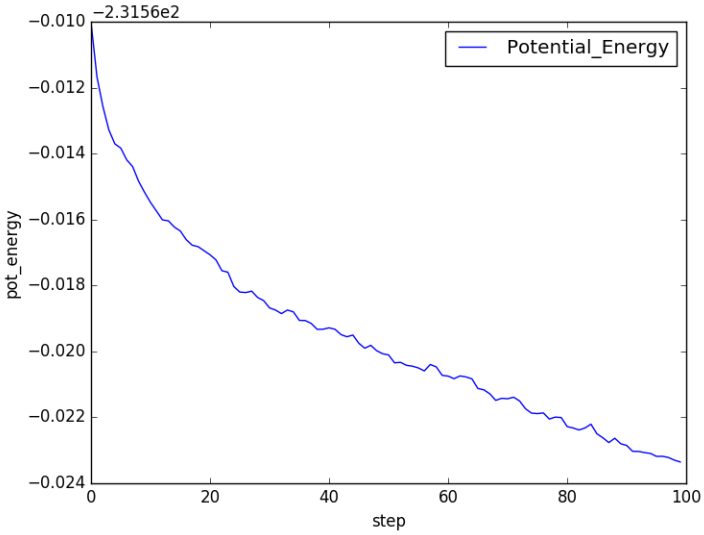

Figure 3: $\sigma = 2.5 * 10^{-5}$ potential energy trace for 100MC steps

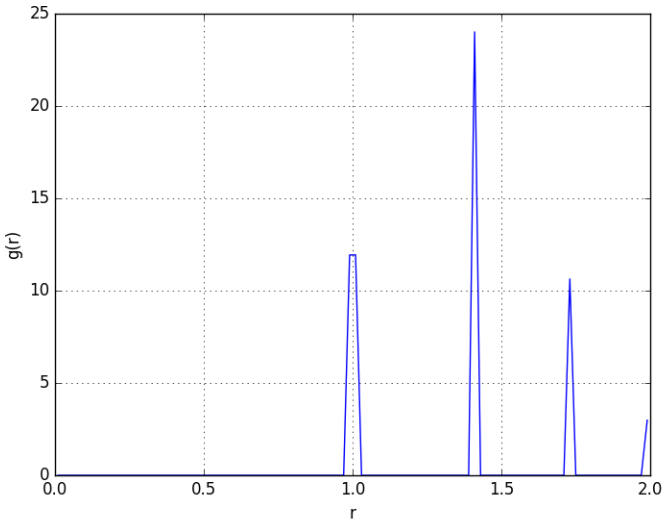

Figure 4: $\sigma = 2.5 * 10^{-5}$ RDF for 100MC steps

3. For $\sigma = 1.0$ the acceptance ratio came to be 0.00016.

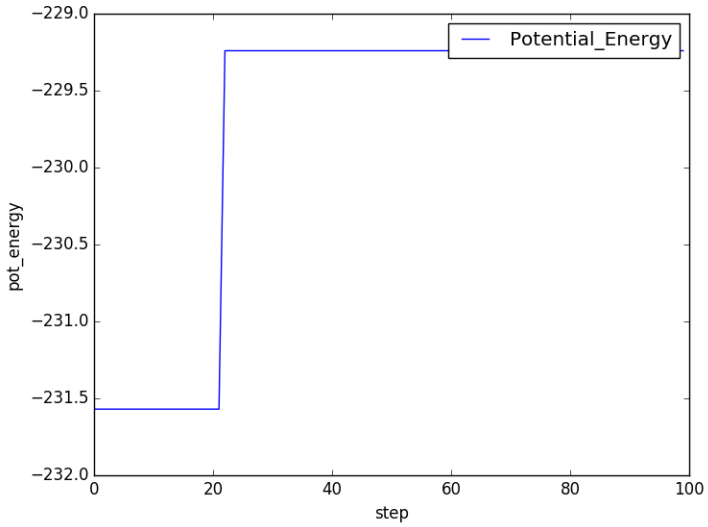

Figure 5: $\sigma = 1.0$ potential energy trace for 100MC steps

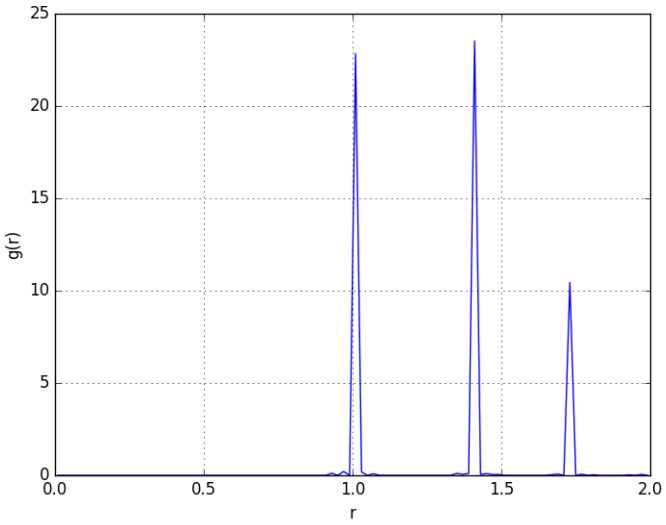

Figure 6: $\sigma = 1.0$ RDF for 100MC steps

4. When the sampling frequency is very high, the sigma we are using is very small, therefore for 100 steps the potential energy did not change by less than 1%. The RDF shows that the particles almost stayed in defined positions where the RDF shows clear peaks. in addition to the small step, this may be also due to the fact that different steps may not have a huge difference in thier acceptance probability, making on the directions for all the particles almost equiprobable during different steps. Since η is sampled from a random distribution, this will let the particles on average have a zero distance travelled. When the sampling frequency is very low, the particles will almost stay stationary, changing there potential energy in jumps with very small probability. Also the fact that fig 4 and 6 have the same peak positions, tells us that the low sampling frequency also led to having the particles almost stay in their initial configuration and not sample thes sample space efficiently.

5. $P.E = -278.7732 \pm 2.6605$. The number of steps is 2000. The first 100 steps were disregarded in the averaging process. (TA comment: you do not need to show the peak at k=0 for S(k))

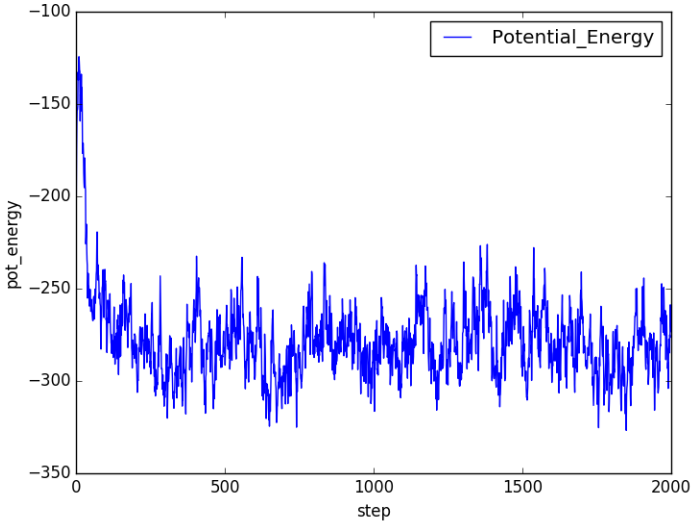

Figure 7: T=2.0 potential energy trace for 2000MC steps

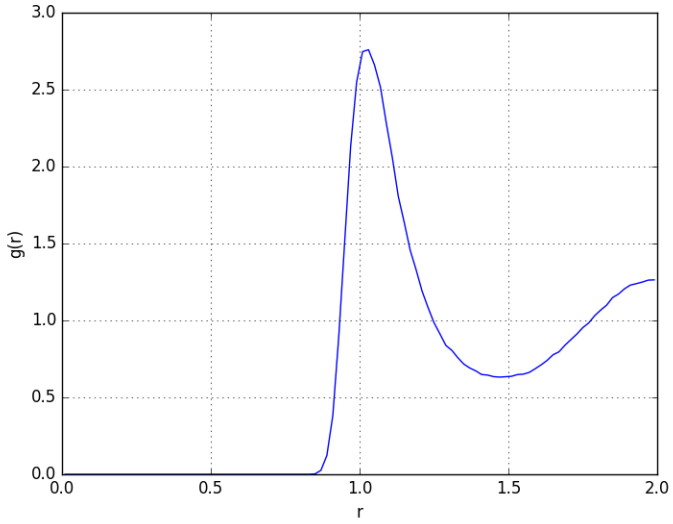

Figure 8: T=2.0 RDF for 2000MC steps

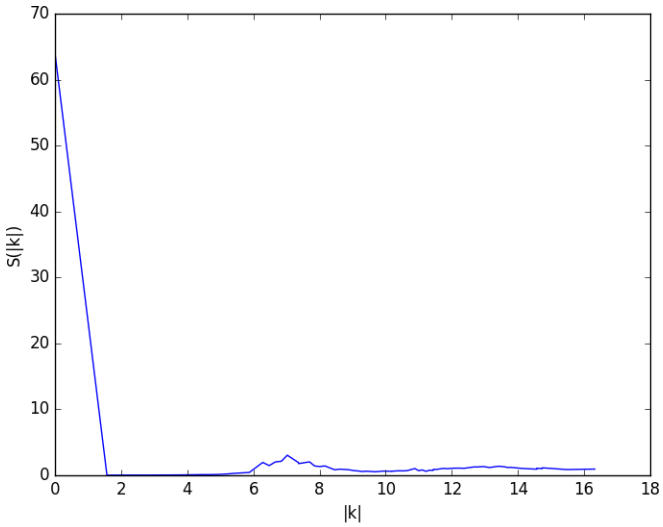

Figure 9: T=2.0 S(k) for 2000MC steps

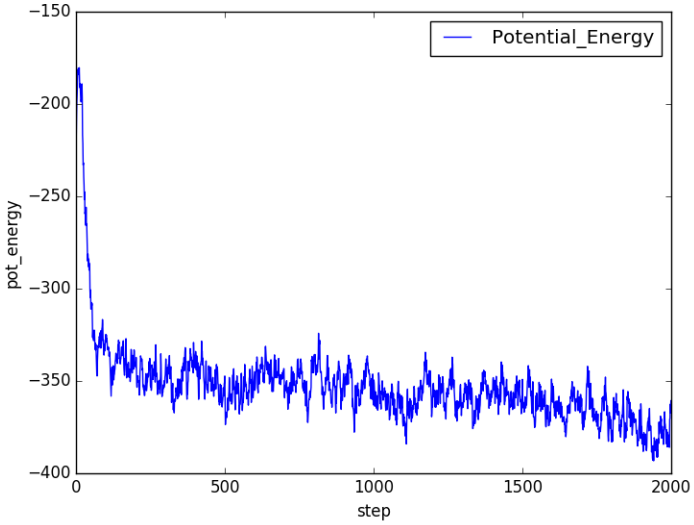

Figure 10: T=1.0 potential energy trace for 2000MC steps

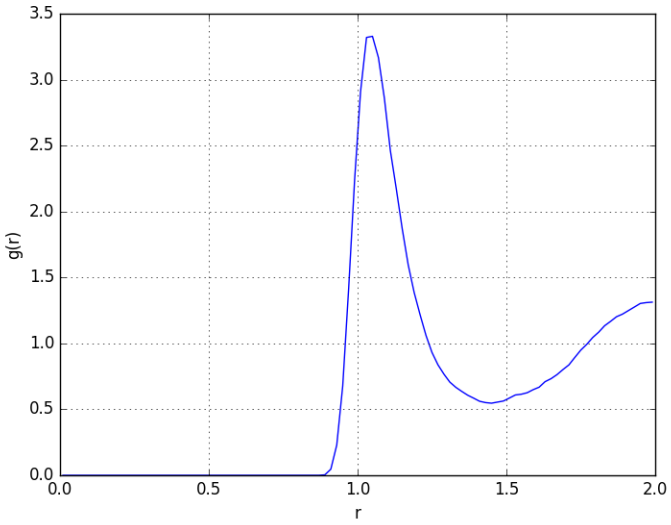

Figure 11: T=1.0 RDF for 2000MC steps

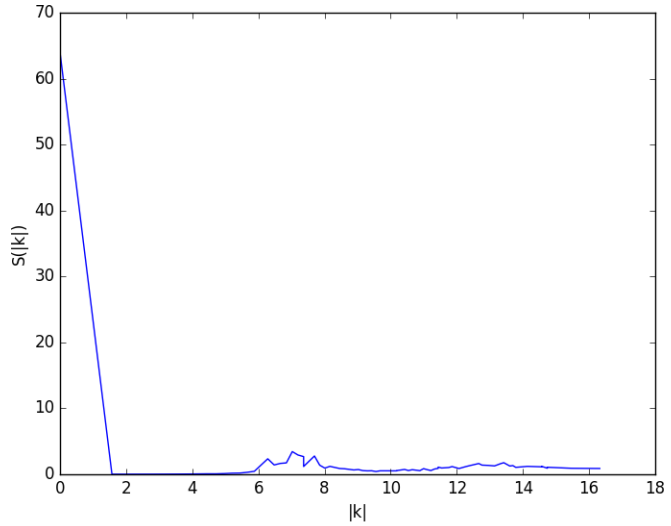

Figure 12: T=1.0 S(k) for 2000MC steps

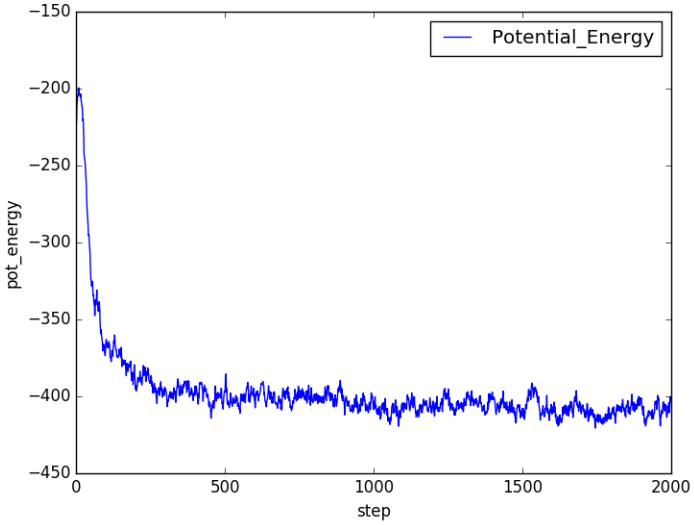

Figure 13: T=0.5 potential energy trace for 2000MC steps

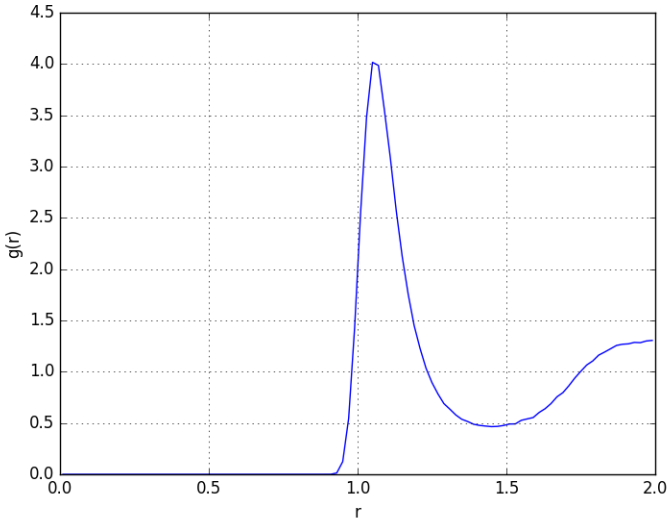

Figure 14: T=0.5 RDF for 2000MC steps

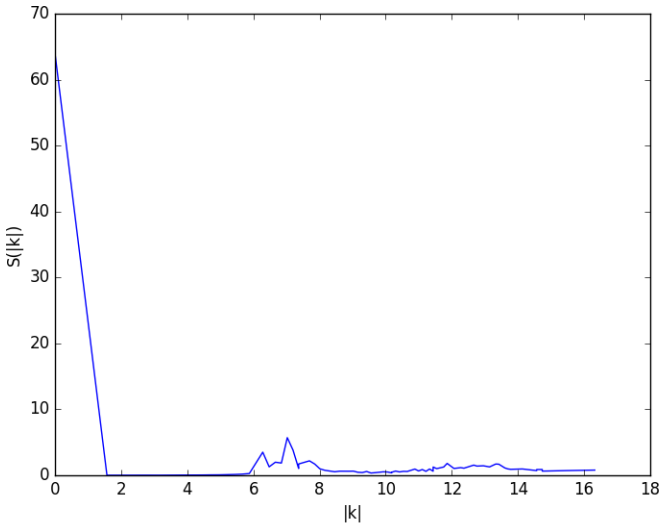

Figure 15: T=0.5 S(k) for 2000MC steps

6.

7. Very similar behaviour was observed for the MD simulations were the peaks in the spatial correlation functions decay as the temperature increase. Nevertheless here we were able to capture the structure without computing any forces and just from energy considerations.

3 Detailed Balance and acceptance criterion

From the definition of the acceptance criterion we can deduce that if $A(x \to x') < 1$ and $\frac{\pi(x')T(x' \to x)}{\pi(x)T(x \to x')} < 1$ then $A(x' \to x) = 1$. So in this case $\pi(x)T(x \to x')A(x \to x') = \pi(x')T(x' \to x) = \pi(x')T(x' \to x)A(x' \to x)$.
If $A(x \to x') = 1$ and $\frac{\pi(x')T(x' \to x)}{\pi(x)T(x \to x')} > 1$ then $A(x' \to x) = \frac{\pi(x)T(x \to x')}{\pi(x')T(x' \to x)}$. So in this case $\pi(x)T(x \to x')A(x \to x') = \pi(x \to x')T(x \to x') = \pi(x')T(x' \to x)A(x' \to x)$.

4 Force-Bias MC

1.

$$T(x \to x') = p(\eta) = p(x' - x - x_{adjustcenter}) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x'-x-x_{adjustcenter})^2/2\sigma^2}$$

and

$$T(x \to x') = p(\eta) = p(x - x' - x'_{adjustcenter}) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-x'-x'_{adjustcenter})^2/2\sigma^2}$$

$$A(x \to x') = min\{1, e^{\beta(V(x')-V(x))} \frac{e^{-(x-x'-x'_{adjustcenter})^2/2\sigma^2}}{e^{-(x'-x-x_{adjustcenter})^2/2\sigma^2}}\}$$

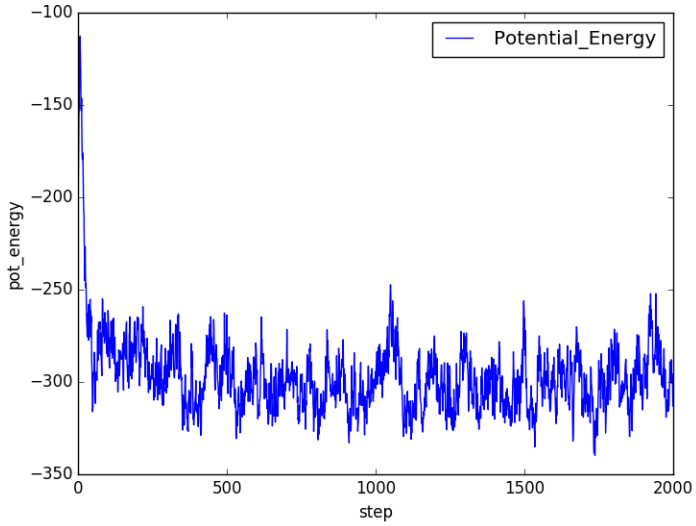

Figure 16: Force-Bias Method Potential Energy Trace

2. $P.E = -301 \pm 1.4793$.The standard error for this simulation is 1.4793, which is less than the standard error reported for the more naive way which was 2.66. The runtime for the force-biased simulation was about 32 mins, where for the more naive way it was about 23 mins. If we compare the errors to the mean value of the potential energy, not much improvement was observed. Therefore we may say that the more naive way is more efficient.
Simulation parameters: $\sigma = 0.04$ and $\delta t = 0.06$

5 Your Own Move

Instead of choosing sigma(roughly the length scale of the random fluctions) randomly, the random movement step η will be computed using $\eta = V\delta t$, where V is sampled from the maxwell-boltzmann distribution. in this way we will have the same runtime as the implemented random guasian method, but the movement will more realistic based on the temperature of the system. $T(x \to x') = p(\eta) = p(x' - x) = p(V)$ where $V = \frac{(r'-r)}{\delta t}$, therefore

$$T(x \to x') = (\frac{m}{2\pi KT})^{3/2} e^{-mV^2/KT}$$

Similarly $T(x' \to x) = p(\eta) = p(x - x') = p(V')$ where $V' = \frac{(r-r')}{\delta t}$, therefore

$$T(x \to x') = (\frac{m}{2\pi KT})^{3/2} e^{-mV'^2/KT} = T(x \to x')$$

since $V^2 = V'^2$ Therefore

$$A(x \to x') = min\{1, e^{\beta(V(x')-V(x))}\}$$