24-623 2010 HW#4

Assigned: February 22, 2010.
Due: March 24, 2010 at the beginning of class. Please use the Blackboard discussion board to ask questions of the instructor or the other students.

1. (10 points) To perform MD in the NVT ensemble using the Nose-Hoover thermostat, the following equations of motion are used:

$$\begin{aligned} \dot{\mathbf{r}}_i &= \frac{\mathbf{p}_i}{m_i} \\ \dot{\mathbf{p}}_i &= \mathbf{F}_i - \eta \mathbf{p}_i \\ \dot{\eta} &= \frac{1}{\tau_T^2}\left(\frac{T}{T_{set}} - 1\right). \end{aligned}$$

Prove that the implementation for the velocity Verlet algorithm is:

$$\begin{aligned} &1.\, \mathbf{p}_i(t + \Delta t/2) = \mathbf{p}_i(t) + [\mathbf{F}_i(t) - \eta(t)\mathbf{p}_i(t)]\Delta t/2 \\ &2.\, \mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \frac{\mathbf{p}_i(t + \Delta t/2)\Delta t}{m_i} \\ &3.\, \eta(t + \Delta t) = \eta(t) + \frac{\Delta t}{\tau_T^2}\left[\frac{T(t)}{T_{set}} - 1\right] \\ &4.\, \mathbf{p}_i(t + \Delta t) = \frac{\mathbf{p}_i(t + \Delta t/2) + \mathbf{F}_i(t + \Delta t)\Delta t/2}{1 + \eta(t + \Delta t)\Delta t/2}. \end{aligned}$$

2. (10 points) Read the paper: E. S. Landry, S. Mikkilineni, M. Paharia, and A. J. H. McGaughey, "Droplet Evaporation: A Molecular Dynamics Investigation." *Journal of Applied Physics* **102** (2007) 124301, available at http://ntpl.me.cmu.edu/pubs/landry_jap07_droplet.pdf.

Pretend that you are reviewing this paper for *Journal of Applied Physics*. Prepare a 1-2 page review where you describe: (a) the objective(s), (b) the important conclusions, (c) concerns you have with the MD simulations and/or data analysis. Based on your review, comment on whether or not the paper is suitable for publication and what changes you want the authors to make in a revised version.

3. (10 points) If we define $f(x, y) = 1$ for $x^2 + y^2 \leq 1$ and $f(x, y) = 0$ for $x^2 + y^2 > 1$, then

$$\int_{-1}^{1}\int_{-1}^{1} f(x, y)dxdy = \pi.$$

Write a C++ code to compute π by evaluating this double integral using Monte Carlo sampling. Use N = 10, 100, 1000, and 10,000 samples. In each case, run your code 5 times and report the average value of π and the estimated uncertainty. Based on your results, predict how many samples you would need to compute π to 20 significant figures.

4. (20 points) In this problem, you will use Monte Carlo simulations to study the properties of the single oscillators from HW#2, which had potential energies (i) $U = x^2/2$ and (ii) $U = x^4 - 2x^2 + 1$.

(a) Determine $\langle U \rangle$, $\langle x \rangle$, and $\langle x^2 \rangle$ for $\beta = 0.1$, 1, 5, and 10 for oscillator (i) by directly evaluating the appropriate integrals (either analytically or numerically). Write a C++ code that uses Metropolis Monte Carlo to compute $\langle U \rangle$, $\langle x \rangle$, and $\langle x^2 \rangle$ for $\beta = 0.1$, 1, 5, and 10 for (i) and compare to the direct predictions. Describe how you debugged your code and how you chose the parameters you used to collect your data (e.g., maximum step size, number of trial moves).

(b) Repeat part (a) for oscillator (ii). Compare your results to the behavior you observed in HW#2.

BONUS WORK:

(10 points) The Metropolis acceptance/rejection criterion is not unique. There are other acceptance/rejection criteria that can be used to perform Monte Carlo calculations in the NVT ensemble. Repeat 4.(a) by computing the acceptance probability for all moves as

$$acc(old \rightarrow new) = \frac{\exp(-\beta \delta E/2)}{\exp(-\beta \delta E/2) + \exp(\beta \delta E/2)},$$

where $\delta E = U(new) - U(old)$. Simulations performed with this criterion are referred to as Kawasaki Monte Carlo. In addition to implementing Kawasaki Monte Carlo in your C++ code, show analytically that this criterion satisfies detailed balance.