# Scientific Computing, Homework 4

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## Monte Carlo Metropolis Algorithm in Argon Molecular Dynamics

For this homework, we are asked to replace the Verlet algorithm in the molecular dynamics code with a Metropolis update. The basic Scheme of the algorithm is as follows:

1. Initialize the starting positions and velocities of all N=864 particles in the region of interest. The positions are set by placing each particle at small, random deviations from a uniform grid. The velocities are set by giving each particle a random $v_x$, $v_y$, $v_z$ between -.45 and +.45.
2. For each timestep, choose a random particle, and displace it by a small, random amount in phase space - a random walk in both position and velocity.
3. Calculate the change in potential energy $\Delta PE$ in the system corresponding to this change.
4. If $\Delta PE < 0$, accept the changes made, and go back to step 2.
5. If $\Delta PE \geq 0$, select a random number R, between 0 and 1, and:
   (a) If $e^{\frac{-\Delta PE}{kT}} < R$, accept the changes that were made, and go back to step 2.
   (b) If $e^{\frac{-\Delta PE}{kT}} \geq R$, reject the changes, and keep the original phase space coordinates, and go back to step 2.

In this algorithm, each iteration is independent of the previous one, meaning there does not have to be stored memomry. However, since we want to find Temperature, Potential Energy and $\frac{p}{T}$, we will need to calculate and store these values at each iteration. Following Verlet's paper, the temperature is given by

$$T = 16 \sum_i \frac{v_i^2}{N}$$

Where $v_i$ are the particles velocities. The Potential Energy is calculated by the Lenerd Jones Potential, and the quantity $p/T$ is calculated via:

$$\frac{p}{T} = 1 - \frac{\rho}{6T} * (virial)$$

To calculate the error, we calculate the integrated correlation time, $\tau_{int}$, first by computing the self-correlation of a variable A:

$$C_A(t) = \langle (A_i - \langle A \rangle)(A_{i+t} - \langle A \rangle) \rangle$$

Then we can define a parameter:

$$\Gamma(t) = \frac{C_A(t)}{C_A(0)}$$

Finally, we find that

$$\tau_{int} = \int_0^\infty \Gamma(t)dt$$

We can find the estimate for the error by multiplying the naiive estimate of the error in the mean by $\sqrt{2\tau_{int}}$. The results for T = 1.069 and $\rho = 0.75$, are below.

| Variable | Value after 1200 iterations | Value from Verlet paper |
|---|---|---|
| Temperature | 1.087 ± 0.004 | 1.069 ± 0.004 |
| Potential E | -4360.0 ± 80.0 | -5190 ± 20 |
| p/T | 0.98 ± 0.3 | 0.90 ± 0.01 |