

Other topics in Metropolis Monte Carlo.

### 1. systems with continuous potential energy surfaces

First consider a simple 1D potential such as that shown in 1D\_potential.mcd

In this case, attempted moves will be given by

$$x_{\text{new}} = x_{\text{old}} + \text{maxstep} * [\text{rnd}(1) * 0.5]$$

In general, one wants about 50% of the attempted moves to be accepted. Based on test runs, a value of maxstep is chosen to assure this. Note that maxstep will vary with T.

This could be a potential such as that between a collection of Ar atoms.

### 2. Simulated annealing.

Here one starts at high T, and gradually lowers the temperature in an attempt to locate the global minimum.

This approach has been used to "solve" the travelling salesman problem. There are many web pages discussing TSP and with java applets you can run. See, e.g., <http://www.heatonresearch.com/articles/64/page1.html> and <http://www.ph.biu.ac.il/~rapaport/java-apps/travel.html>.

In this algorithm we use the "Boltzmann" factors  $\exp(-\Delta L/T)$ , where L is the length of the path and T plays the role of "temperature"

One chooses an initial path, and then randomly attempts various modifications of the path, using a Metropolis acceptance criterion.

