Uncertainty Estimates in Computer Simulations

We use computer simulations in statistical mechanics to obtain values for quantities that can not be readily computed using direct analytical or numerical methods. We assume there is a unique "exact" result and a simulation yields an estimate for this result in the form of a value and associated "error bar". Assuming the simulation has been performed correctly, the desired exact result should lie within the range: value +/- error. These error bar estimates in computer simulations are extremely important and must always be reported as part of the results. The standard approach for error estimation is very straightforward, following the procedure we would use in experimental physics.

Definitions of Statistical Measures:

Assume we make a set of *M independent* measurements $\{A_1, A_2, ..., A_M\}$ of the quantity A. The average or mean value of A is given by

$$\langle A \rangle = \frac{1}{M} \sum_{i=1}^{M} A_i \tag{1}$$

and the variance in this set of measurements is defined as

$$\sigma_A^2 = \frac{1}{M-1} \sum_{i=1}^{M} \left(A_i - \langle A \rangle \right)^2 . \tag{2}$$

The square root of the variance, known as the standard deviation, provides our error estimate. Thus, our "result" for this set of measurements would be reported as $\langle A \rangle \pm \sigma_A$.

Estimating Error Using Block Averages:

A sometimes difficult and always important question that arises in the above analysis is what exactly constitutes an "independent" measurement? If we are using a simple growth algorithm to generate a set of self-avoiding walks, the answer is clear. Each walk is completely independent of all others in the set. However, if we are exploring the configurational space of a self-avoiding walk using a dynamic Monte Carlo method, such as the pivot algorithm, each sequential chain conformation is highly correlated with the previous conformation. Thus we need to estimate the "correlation time" of this sequence which gives the approximate number of Monte Carlo moves required to generate a statistically independent configuration. One problem with computer simulations is that locally independent samples generated from correlated sequences are generally *not* "globally independent" (i.e., they tend to be localized in a small neighborhood of configuration space). Thus for dynamic simulations, it is common to run a long simulation and to break up the results into "blocks" of data. Assuming the simulation has sufficiently explored phase space,

then the average values for each block should provide a set of *globally independent* measurements.

As an example, consider the Monte Carlo simulation of an N-bead chain using a pivot algorithm. We might assume that two conformations will be uncorrelated if they are separated by N accepted pivot moves. Thus we can make statistically independent measurements every N/f pivot attempts where f is the average acceptance fraction of these attempts. We clearly need prior knowledge of f to know how often to take data. We typically estimate this acceptance fraction during the "equilibration" part of the simulation (or for hard core systems we often use the generally accepted result that $f \approx 0.5$). To continue with our example, assume we make M measurements in each data block and that we collect B blocks of data (a popular choice is $B=10$). Thus we have B sets of M measurements (so the total simulation length would be BMN/f pivot attempts, not including equilibration). Typically we do not actually store each set of M individual measurements, rather we accumulate these measurements as the sum needed for Eq. (1). For our data analysis, we determine average values for each block of data, $\{\langle A\rangle_1, \langle A\rangle_2, \ldots, \langle A\rangle_B\}$, where each average in this set is determined using Eq. (1). We now simply analyze this set of data as done above:

$$\langle A\rangle = \frac{1}{B}\sum_{i=1}^{B}\langle A\rangle_i \tag{3}$$

and

$$\sigma_A^2 = \frac{1}{B-1}\sum_{i=1}^{B}\left(\langle A\rangle_i - \langle A\rangle\right)^2 . \tag{4}$$

As above, our "result" for this simulation would be reported as $\langle A\rangle \pm \sigma_A$. In this block averaging approach, we are treating one long simulation as B independent shorter simulations (as sketched below). Another way to achieve this same result is to actually run B independent simulations. Computer clusters are making this second approach more popular. The only drawback is that a separate equilibration must be carried out for each independent simulation.