Intro to Monte Carlo Methods

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Basic Aspects of MC Applications

- Stochastic – i.e., some element of randomness.
- Contrast with standard integration algorithms.
- When is MC useful?

Problem from Friday Class

- Compute an integral of p(q)f(q)dq where p(q) is a probability distribution.
- You could do it by sampling {q1,q2,q3,...} from the distribution p(q), and then just averaging

  <f> ~ {f(q1)+f(q2)+...+f(q3)}/N

  and that as N gets large this average will approach the value of the desired integral.

Basic MC Application – 2d integration

- Calculate value of Pi
- http://www.eveandersson.com/pi/monte-carlo-demo.tcl

Comparisons of accuracy

- MC – accuracy ~ $N^{-0.5}$
- Other methods – accuracy ~ $N^{-1/d}$

Problem with Random States

- Ex: calculation for area of hyper-sphere for calculation of Pi. Chance of ‘hit’->0.

- Importance Sampling – concentrates sampling in regions of higher probability

Idea of Phase Space

- Represents the entire set of states that can be occupied by the ‘system’.
- Ex: all values for which p(x) is not 0.
- What if phase space represents a very small portion of the randomly generated possibilities?: ex. Bonded molecule.

Ergodicity

- MC often used to simulate time-dependent processes, although there is no ‘time’ in MC simulations.
- Ergodic Theorem: Phase space average is identical to the time average.

Metropolis Method

- If the attempted move lowers the energy, it is automatically accepted.
- If the attempted move increases the energy, it is accepted with probability $p(x)=\exp(\Delta E/kT)$
- Only need RELATIVE probabilities

Metropolis Method (cont.)

- The attempted configuration represents a deviation from a previous configuration.
- Important: If a move is rejected the ‘old’ state is counted again.
- Does this make sense?

MC vs. MD

- Equilibrium vs. Dynamics

Orientation of Polymers using MC

- MD cannot typically probe large (ms) time scales
- MC can find equilibrium sets of configurations – typically shorter correlations because of the possibility of unphysical moves.

Example – evolution of torsions using MC

- Statistical sampling of the phase space