"But what ... is it good for?"

--Engineer at the Advanced Computing Systems Division of IBM, 1968, commenting on the microchip.

Metropolis Monte Carlo

Theory, Simulation Analysis, Thermodynamic Properties

Bentley Strockbine

Overview

-Introduce Monte Carlo

-Monte Carlo In Dynamics

-Metropolis Monte Carlo

-The Algorithm

-The Thermodynamic Consequences of Metropolis

-Strengths and Weaknesses

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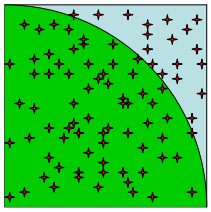
A Monte Carlo Calculation of Pi



8/10=.8
.8*4=3.2

71/90=.789
.789*4=3.15

$$\frac{\text{———}}{r^2} = \frac{\frac{1}{4}\pi r^2}{r^2} = \frac{1}{4}\pi$$

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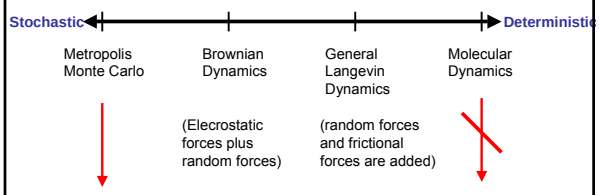
Molecular Simulation

1. Construction of a Model
   - Parameter Set (Force Field)
   - Coordinates

2. Calculation of Molecular Trajectories
   - M.D., Monte Carlo …

3. Analysis to Obtain Property Values
   - RMSD, Native Contacts, Distances
   - Convergence



Markov Chain

1. The outcome of each trial depends only on the Preceeding trial.
(in MD the states are connected in time.)

2. Each trial belongs to a finite set of possible outcomes.

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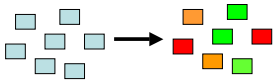
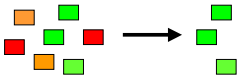
Monte carlo generates states with equal probability and assigns them weight with Boltzman factor



Metropolis generates states with a Boltzman factor probability and assigns them equal weight.



(Less new structures)

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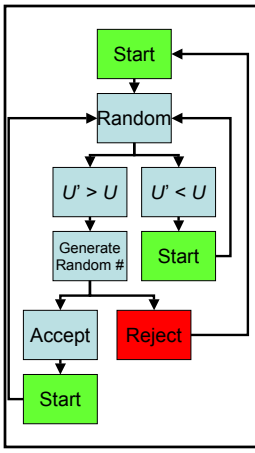

-Pick a starting state

-Create a new state (Randomly)

-Compare the potential energies of the two states

-If $U' < U$ than the second state becomes the new current state

-If $U' > U$ than accept with a probability proportional to the factor $e^{-\Delta U/kt}$, where $\Delta U = U' - U$

(k is Boltzman's Constant)

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Thermodynamics

The energy function we use is independent of the momenta of the atoms.

MD uses the momenta only for predicting the next structure.

If a simulation is run to convergence, Metropolis can predict the thermodynamic properties as well as MD (limited by your energy function)

(This works because states with high probabilities are those that contribute most to the thermodynamic properties)

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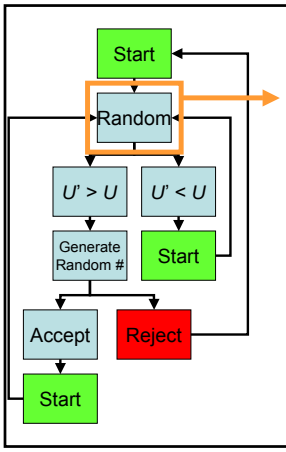
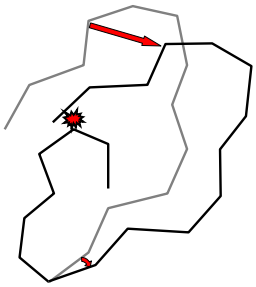


1 Change (i.e. a change in a Cartesian Coordinate)

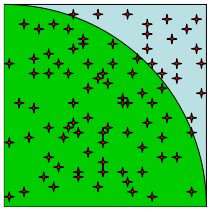
Very Slow

Changes in all degrees of Freedom

Requires small changes



Small changes can have big effects



Limited degrees of limit the results

Advantages

Random Sampling

(Barriers are less of an issue)

Large movements are easy to accommodate

(Fast sampling of conformational space)

Particularly effective for small molecules or systems with frozen internal degrees of freedom

(Freezing degrees of freedom will limit the sampling)

Take Home Message

Monte Carlo = Metropolis = Monte Carlo
(At least as far as simulations are concerned)

Random sampling of conformational space
(With a Boltzman weighting factor)

If a simulation is converged, the thermodynamic properties are as good as the energy function
(If the simulation is converged)