# Statistical Analysis for Monte Carlo Simulations

# Markov Chains

- A Markov Chain is a random walk in state space
  - $S_1 \rightarrow S_2 \rightarrow S_3 \ldots$
- The transition probability that takes us from one state to the next is a stochastic matrix:

$$P(s \rightarrow s') \geq 0 \; and \; \sum_i P_i = 1$$

- The probability of states at a given iteration

$$f_{n+1}(s') = \sum_s f_n(s) P(s \rightarrow s')$$

- The stationary states of this are eigenstates of P
- If the random walk is ergodic, there will be a unique equilibrium state

# The Monte Carlo methods we will learn about are largely Markov Chains

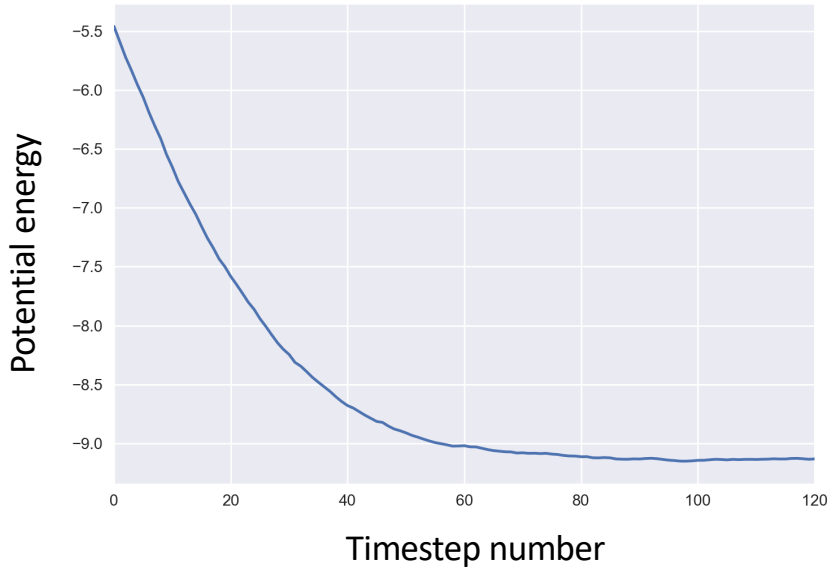
- Need to be able to understand the statistical data from them
- A classic example of a Markov Chain is Brownian Motion
  - Imagine scattering some larger particles in a fluid
  - The initial positions are random
  - The positions of the particles evolve by collisions with the rest of the fluid
  - After some equilibration, the position of the particles satisfies the diffusion equation

# Example Code

- In the Day 1 directory of the git repository (https://github.com/lkwagner/StochasticSchool.git)
- The code RandomWalk.py simulates a random walk of N particles in a quartic potential
- Parameters such as the time step of the propagation, the number of walkers and the total number of time steps can be changed in the top of the file

# Example Code continued

- Run the application with 128 walkers and a timestep of 0.01 to generate a time series like the following:
- This is can be divided into phases, equilibration and equilibrium



# Exercise #1

- Create an algorithm to divide the time series into equilibration and equilibrated phases
  - Hint: start from the end of the calculation

# Calculating properties

- Now that equilibrium phase is identified, want to calculate statistics
  - Sample Mean: $\bar{a} = \sum_i \frac{a_i}{N}$
  - How well is this mean known?
    - If all samples from the Markov chain were uncorrelated:
      - standard deviation of the samples: $\sigma = \sqrt{\frac{1}{N-1}\sum_i (a_i - \bar{a})^2}$
      - standard error of the mean: $err(\bar{a}) = \sigma/\sqrt{N}$

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  - Unfortunately, the data is NOT uncorrelated
  - Knowing where the walkers were at step n gives a good idea of where they will be at step n+1
  - Need to know the time it takes to “forget” this history (autocorrelation time)

# Two commonly used methods of handling this

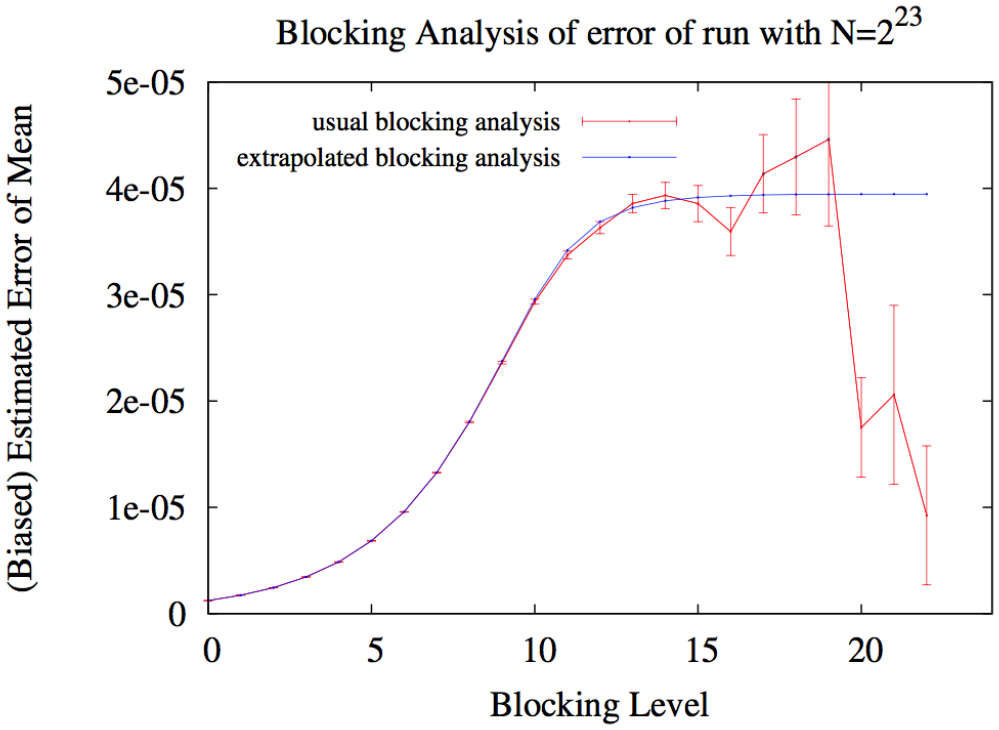
- Blocking
- Direct use of autocorrelation function

# Blocking method

- Group data into successively larger blocks and compute the error using this blocked data
  - For correlated data this will increase until roughly block size equals the autocorrelation time
  - Specifically, calculate $\frac{1}{N_b(N_b-1)}\sum_{i=1}^{N_b}(m_i-\bar{a})^2$
    - Where the number of samples in each block is growing (doubling is convenient) and $m_i$ is the average of the data in each block
    - Can also estimate the error in the error estimates as: error estimate / $\sqrt{2(N_b-1)}$

# Blocking method example (courtesy C. Umrigar)

**Blocking Analysis for error of mean of autocorrelated variables**



# Direct calculation of autocorrelation function

- Calculate the autocorrelation function: f(k) = $\frac{\sum_{i=1}^{N-k}(a_i-\bar{a})(a_{i+k}-\bar{a})}{\sum_{i=1}^{N}(a_i-\bar{a})^2}$
  - Measure of how correlated data is with data k units of time away
- Define autocorrelation time: $\kappa = 1 + 2\sum_{i=1}^{N} f(k) \approx 1 + 2\sum_{i=1}^{f(k)>0} f(k)$
- Now the number of samples used in determining the error is reduced by a factor of $\kappa$
- $err(\bar{a}) = \sigma/\sqrt{N/\kappa}$

# Exercise #2

- Implement either the blocking method or the autocorrelation method to determine the average and error in that average for data from the equilibrated part of a Markov chain

# Exercise #3

- Combine the algorithms from exercises 1 and 2 and analyze the data from RandomWalk.py
  - Perform an initial calculation with 128 walkers, 2000 steps and a timestep of 0.005
  - Using the same number of walkers, how many steps would be necessary to get the same error bar with a timestep of 0.0025?
  - If you double the number of walkers, how many steps are necessary to get the same error bar?

# Digression on ergodicity

- In everything previous we have assumed ergodicity
  - Basically that given enough propagation time, a walker can come arbitrarily close to any point in space
  - Must always be aware of the possibility that this could be violated

# Exercise #4

- Alter RandomWalk.py so that walkers are initially distributed from -4 to 4 (rather than 2-3, see line ~45)
- For various values of the timestep is it possible to enter into a nonergodic calculation?
  - Look at timeseries of energies
  - Use histogram of final positions (example code at end of file)

# A set of advice from a D. Ceperely lecture…

- "Shouldn't the energy settle down to a constant"
  - NO. It fluctuates forever. It is the overall mean which converges.
- "The cumulative energy has converged".
  - BEWARE. Even pathological cases have smooth cumulative energy curves.
- "Data set A differs from B by 2 error bars. Therefore it must be different".
  - This is normal in 1 out of 10 cases. If things agree too well, something is wrong!
- "My procedure is too complicated to compute errors"
  - NO! NEVER! Run your whole code 10 times and compute the mean and variance from the different runs. If a quantity is important, you MUST estimate its errors.