Markov Chain Monte Carlo

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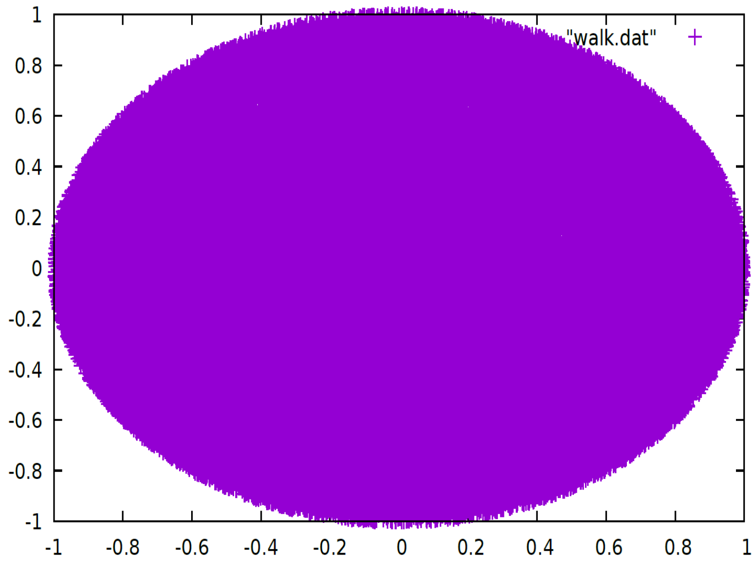
Contents

- Following "**Group action Markov chain Monte Carlo for accelerated sampling of energy landscapes with discrete symmetries and energy barriers**" by Matthew Grasinger (Apr 2022)
  - arXiv:2205.00028 **[cond-mat.stat-mech]**
- Monte Carlo background
- Example
- Simple Harmonic Oscillator (SHO)
- Double Well
- Conclusion

Monte Carlo Differences

Regular Monte Carlo (MC)

- Uniform Random Sampling
  - Good for finding area of a circle

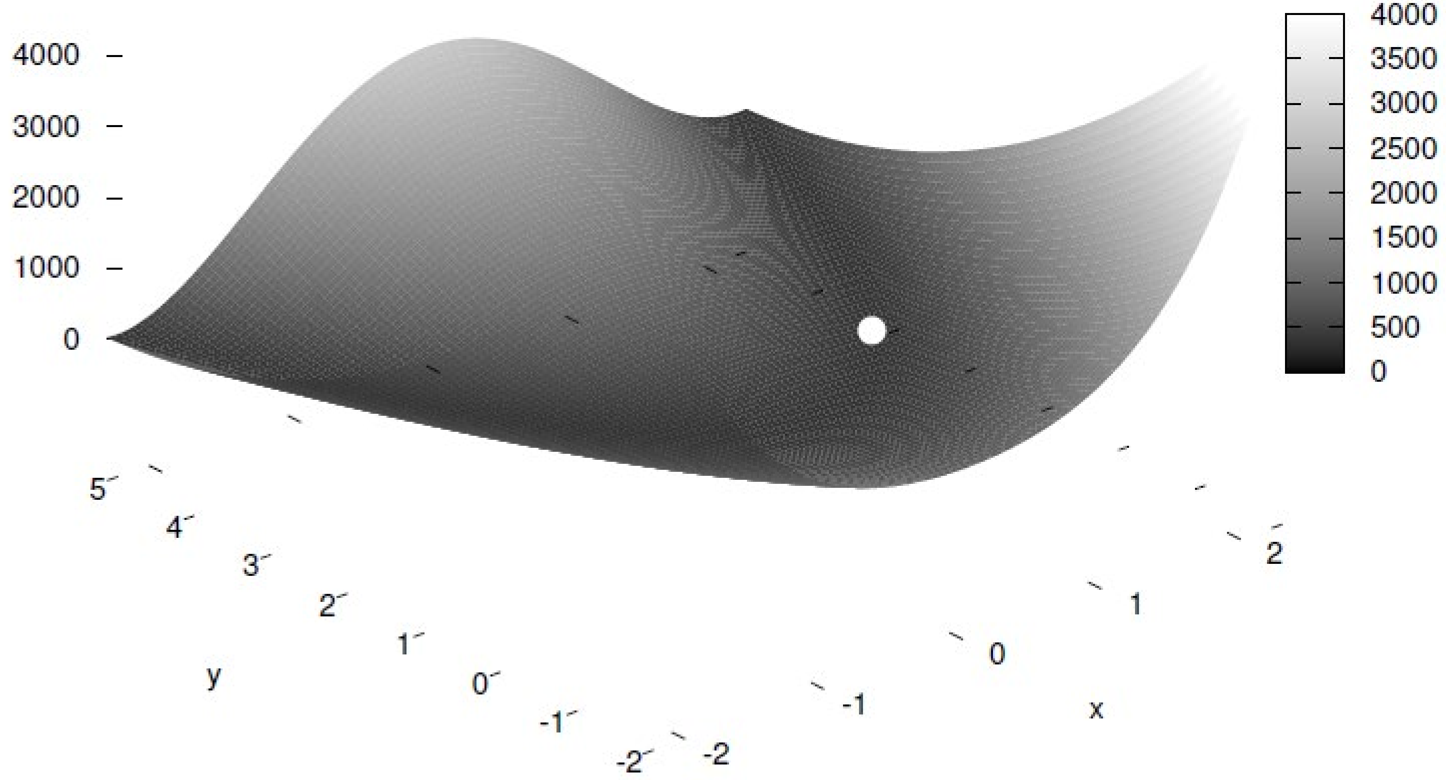


Markov Chain Monte Carlo (MCMC)

- Next data point depends on previous data point
  - Correlated data
- Works better on complicated objects or functions
  - difficult to sample directly
- Some burn in time necessary

Markov Chain Example

- Rosenbrock function
  $f(x, y) = (a - x)^2 + b(y - x^2)^2$
- Difficult function to sample via MC
- MCMC can find path to minimum



Markov Chain Example

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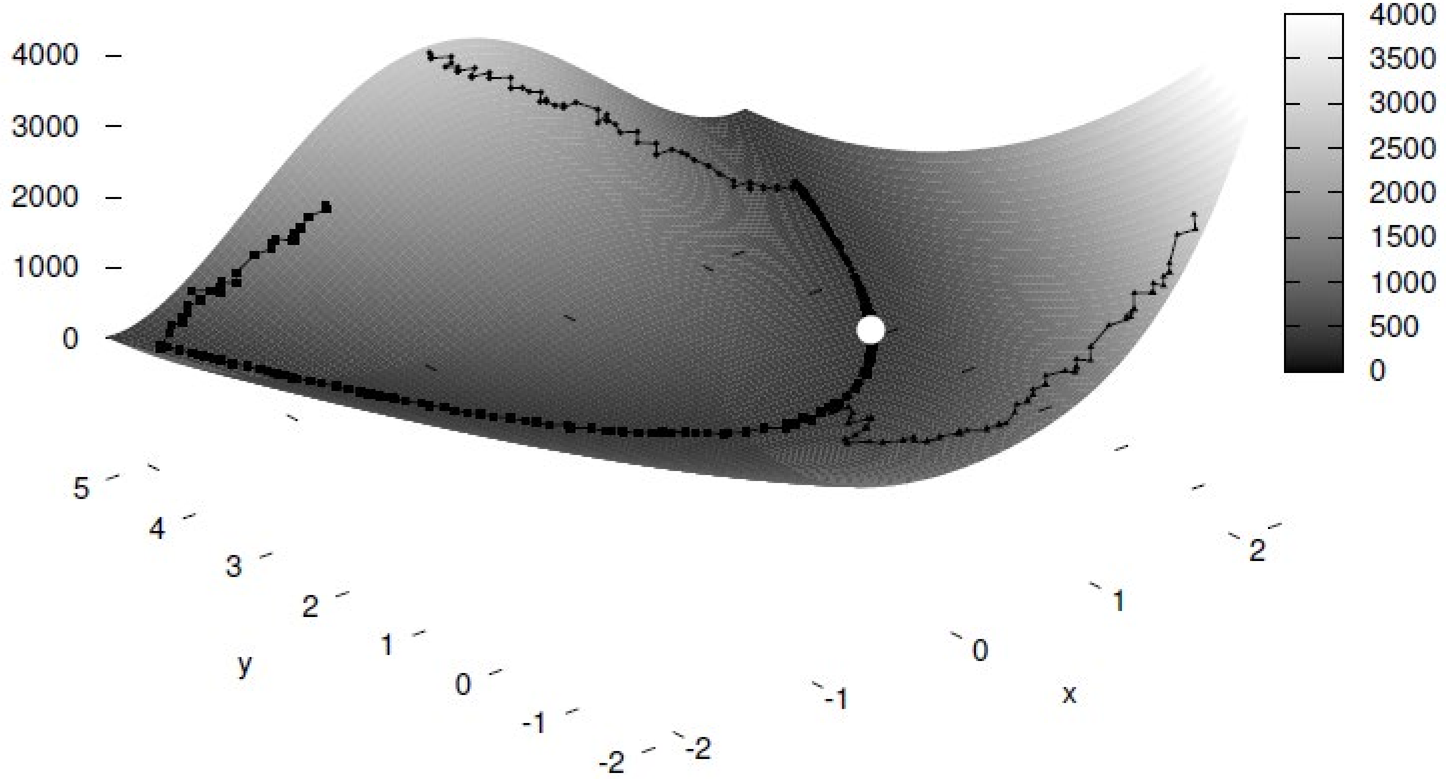


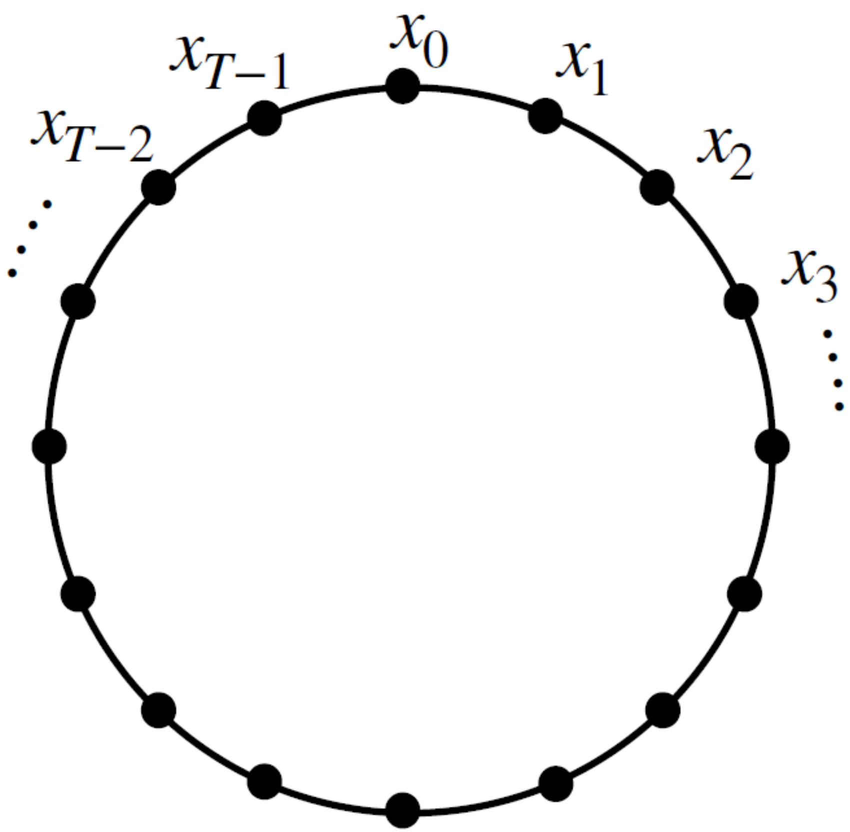
MCMC and Feynman Path Integrals

- In QM, transition amplitude
  - Probability amplitude for particle to go from x_i at t_i to x_f at t_f
  - $\langle x_f(t_f) | x_i(t_i) \rangle$
- Path Integral
  - Transition amplitude connected to classical action, S
  - $S = \int L(x, \dot{x})\, dt$
  - This can be the criteria for MCMC updates

MCMC SHO

- $S = \int d\tau \, (\frac{m\dot{x}^2}{2} + \frac{m\omega^2 x^2}{2})$
- Consider lattice
- Change in action given by

$$\delta S_L = \frac{\widehat{m}}{2} \sum_{n=0}^{N_\tau - 1} \Big\{ (\widehat{x}_{n+1} - \widehat{x}_n^{new})^2 - (\widehat{x}_{n+1} - \widehat{x}_n)^2 + \frac{\widehat{\omega}^2}{4} (\widehat{x}_{n+1} + \widehat{x}_n^{new})^2 - \frac{\widehat{\omega}^2}{4} (\widehat{x}_{n+1} + \widehat{x}_n)^2 \Big\}$$



SHO Implementation

$$\delta S_L = \frac{\widehat{m}}{2} \sum_{n=0}^{N_\tau - 1} \Big\{ \left(\widehat{x}_{n+1} - \widehat{x}_n^{new}\right)^2 - \left(\widehat{x}_{n+1} - \widehat{x}_n\right)^2 + \frac{\widehat{\omega}^2}{4}\left(\widehat{x}_{n+1} + \widehat{x}_n^{new}\right)^2 - \frac{\widehat{\omega}^2}{4}\left(\widehat{x}_{n+1} + \widehat{x}_n\right)^2 \Big\}$$

- Change in action

```
dS=(pow((site[tau+1]-new_site[tau]),2.0)
    +0.25*omega*omega*pow((site[tau+1]+new_site[tau]),2.0))
    -(pow((site[tau+1]-old_site[tau]),2.0)
    +0.25*omega*omega*pow((site[tau+1]+old_site[tau]),2.0));
dS=(m/2.0)*dS;
```

- Metropolis Update

```
u=drand48();
if(u<exp(-dS)){
    site[tau]=new_site[tau];
}
else{
    site[tau]=old_site[tau];
}
```

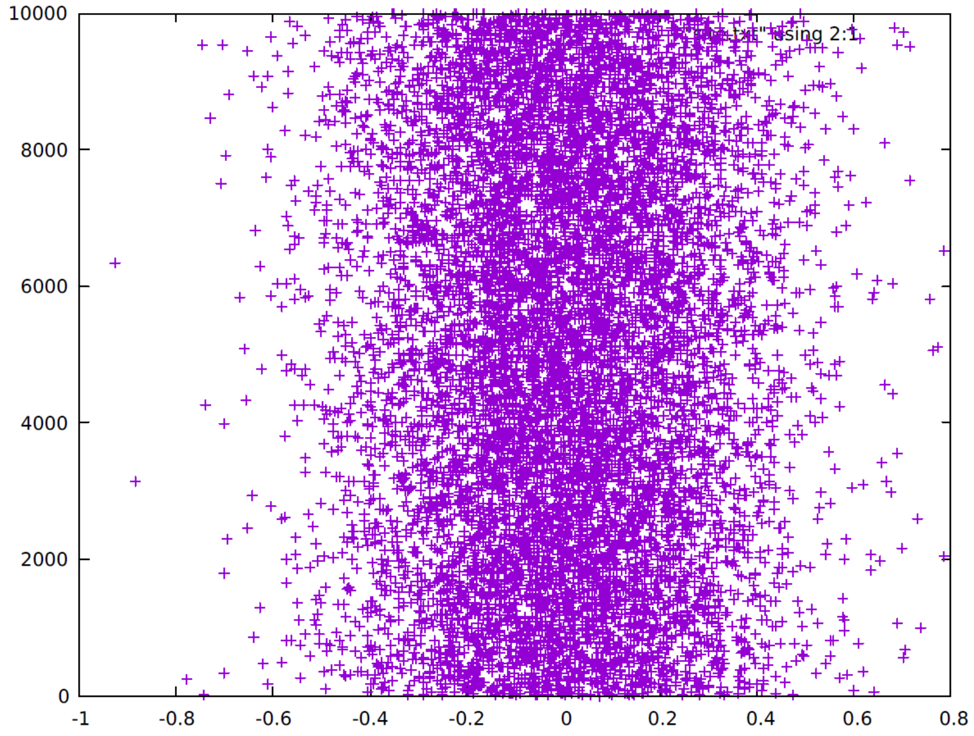
Burn in Time:

```
//begin thermalization MC sweeps
for(int i=1; i<=THERM; i++){
```

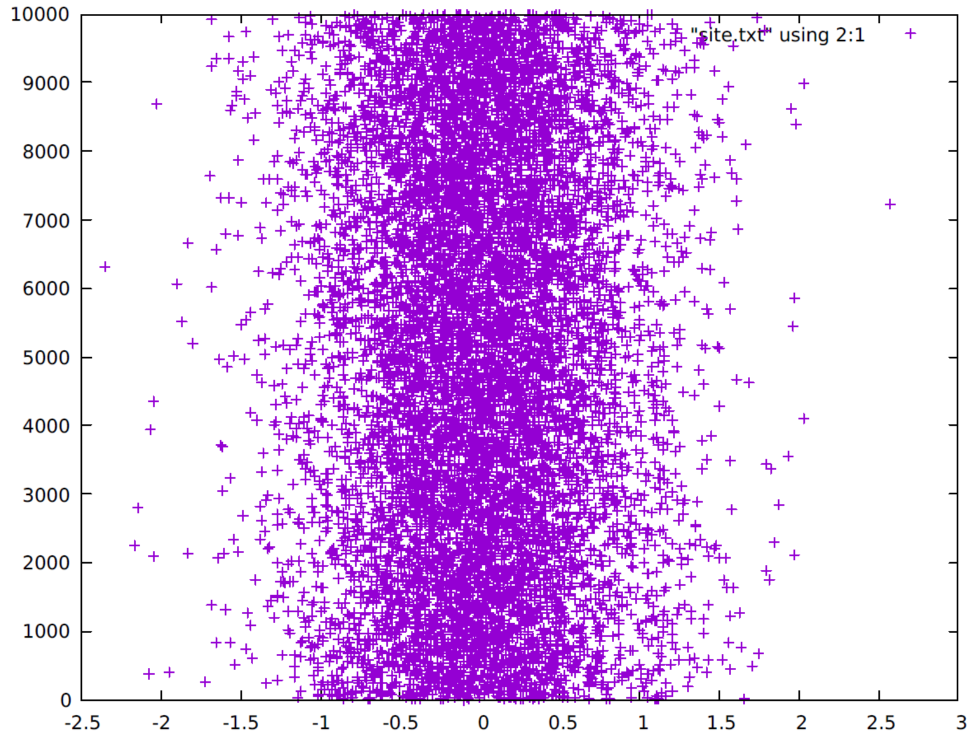
```
//amount of random shift for position at tau
shift=2.0*DELTA*(drand48()-0.5);
```

SHO Results

$\omega = 2$ and $m = 10$

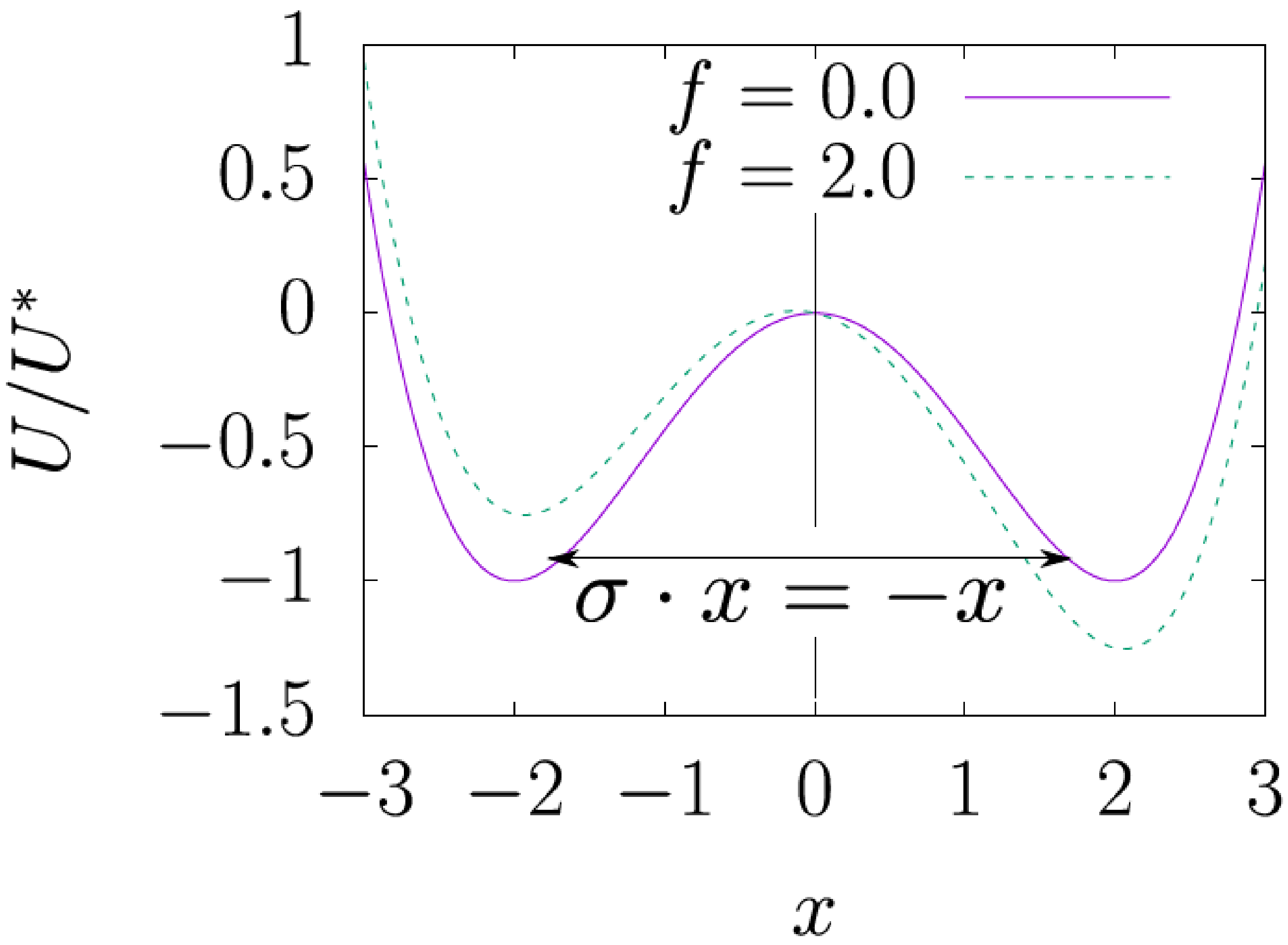


$\omega = 100$ and $m = 0.5$



Double Well

- $U = ax^4 - bx^2 - fx$
  - $a = 1$
  - $b = 8$
  - $U^* = \frac{b^2}{4a}$
- Use this as new potential in path integral



Double Well Implementation

- Change in action:

```
dS=(1/2)*(-a*(pow((site[tau+1]+new_site[tau]),4.0))
        +b*((pow((site[tau+1]+new_site[tau]),2.0)))
        +f*(site[tau+1]+new_site[tau])
        -a*(pow((site[tau+1]+old_site[tau]),4.0))
        +b*((pow((site[tau+1]+old_site[tau]),2.0)))
        +f*(site[tau+1]+old_site[tau]));
```

- Metropolis Update:

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u=drand48();
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Burn in time:

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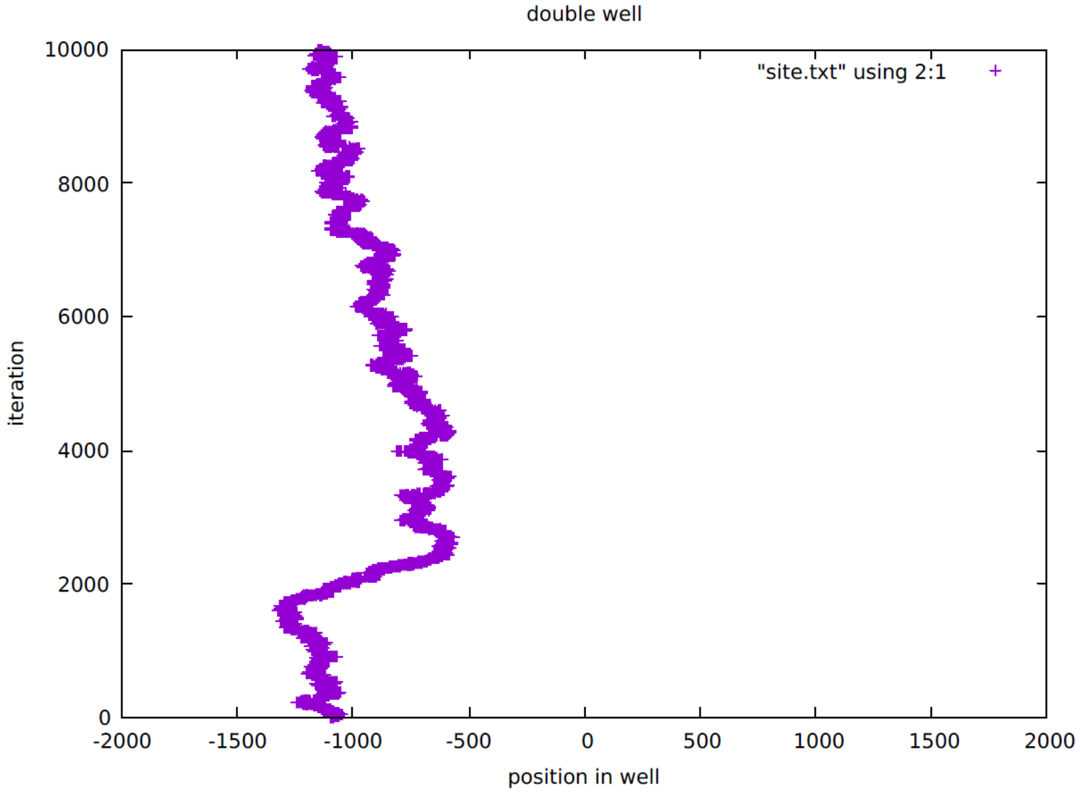
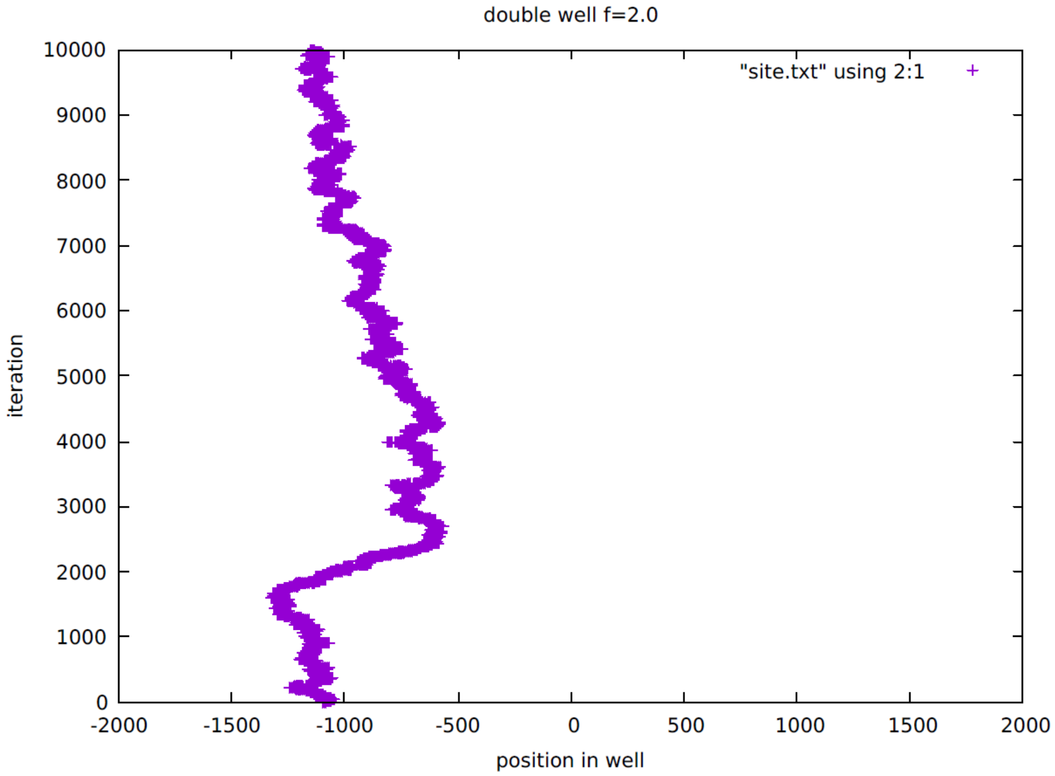
```

Double Well Results

Symmetric Well, $f = 0$

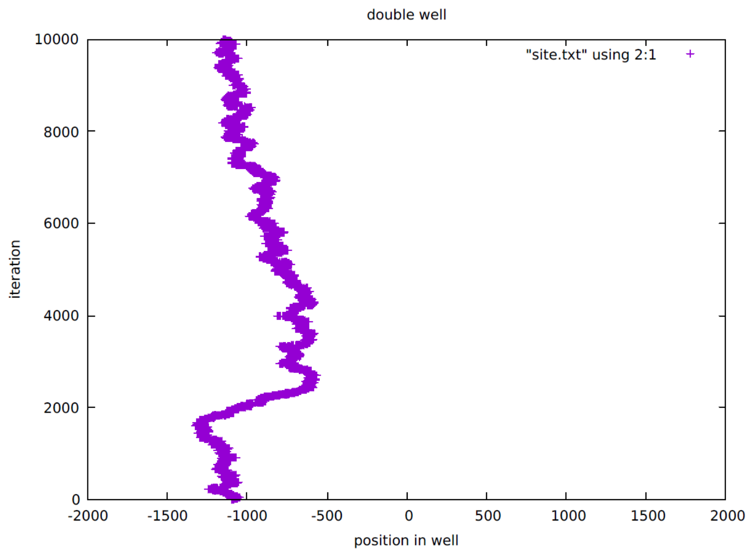


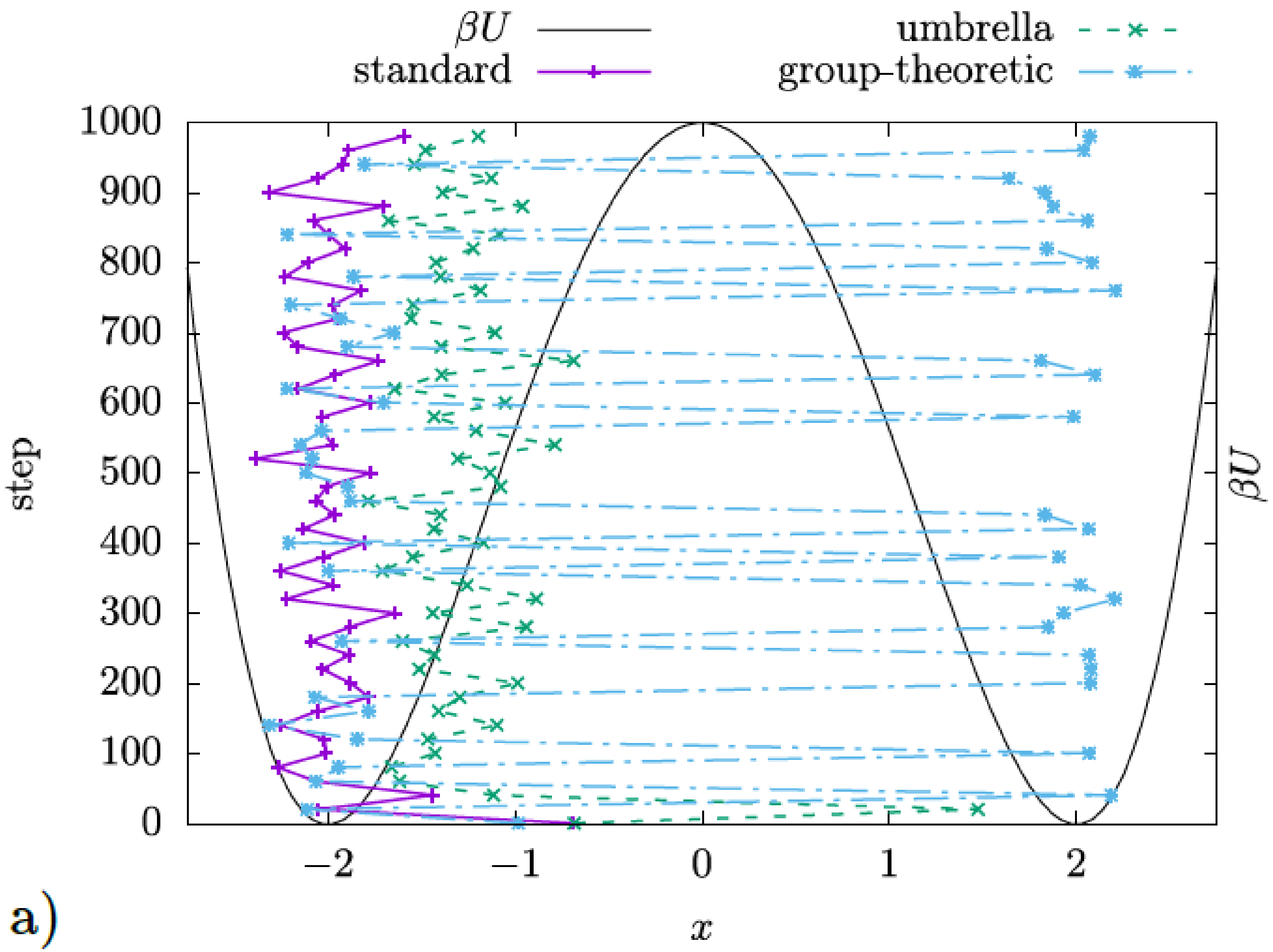
Asymmetric Well, $f = 2$



Paper Results

- Comparing results
- MCMC is not perfect
  - Different ways to optimize





Conclusion

- MCMC can describe difficult functions
  - More efficient than regular MC
- Not perfect, so lots of room for research
- Current research tool at UTK
  - At least in Condensed Matter

Thank you

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