

Metropolis Monte Carlo Simulation: Q & A

Aiichiro Nakano

Collaboratory for Advanced Computing & Simulations

Department of Computer Science

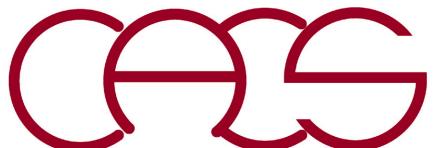
Department of Physics & Astronomy

Department of Chemical Engineering & Materials Science

Department of Quantitative & Computational Biology

University of Southern California

Email: anakano@usc.edu



Q: What Is α_{mn} in Ising MC?

States: $m, n \in \left\{ s^N = \begin{pmatrix} s_1 \\ s_2 \\ \vdots \\ s_N \end{pmatrix} \middle| s_i = \uparrow, \downarrow; i = 1, \dots, N \right\}$

$$\pi_{m,n} = \overbrace{\min\left(\frac{\rho_m}{\rho_n}, 1\right)}^{\text{accept/reject}} \overbrace{\tilde{\alpha}_{m,n}}^{\text{attempt}}$$

Attempt matrix: $\alpha_{m,n} = \begin{cases} 1/N & \text{Hamming_distance}(m, n) = 1 \\ 0 & \text{else} \end{cases}$

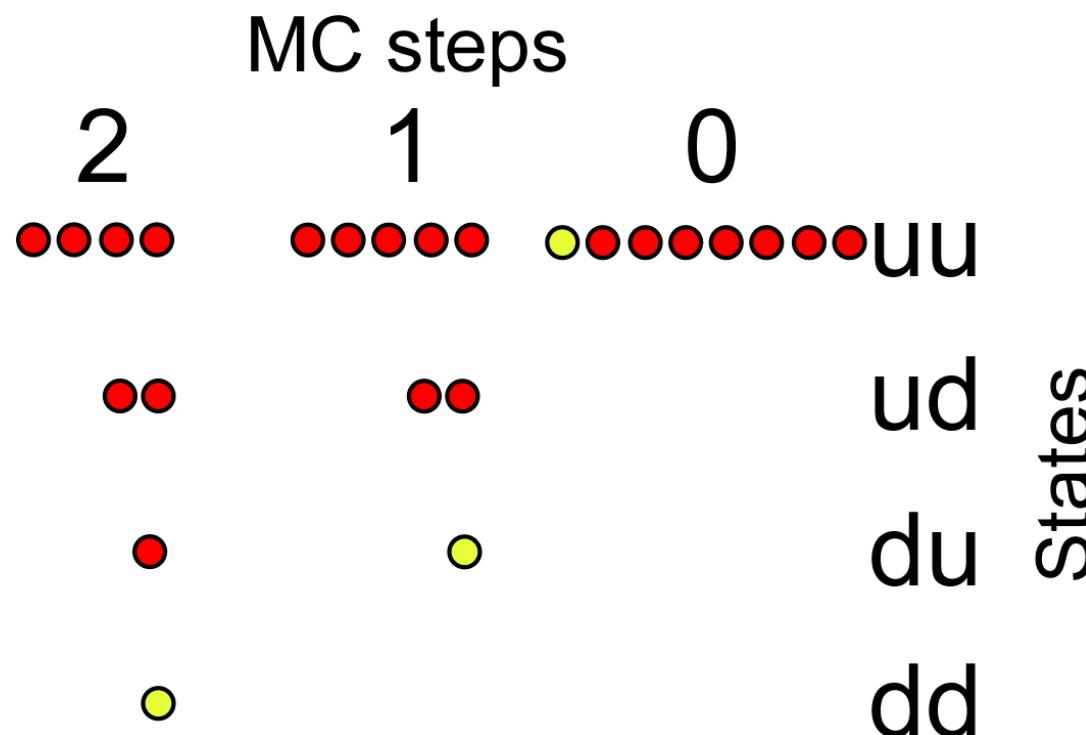
Example: $N = 3$ ($2^N = 8$ states)

$$\begin{pmatrix} \uparrow \uparrow \uparrow \\ \uparrow \uparrow \downarrow \\ \uparrow \downarrow \uparrow \\ \uparrow \downarrow \downarrow \\ \downarrow \uparrow \uparrow \\ \downarrow \uparrow \downarrow \\ \downarrow \downarrow \uparrow \\ \downarrow \downarrow \downarrow \end{pmatrix} = \begin{pmatrix} 1/3 & 1/3 & 1/3 & & & \\ 1/3 & & 1/3 & 1/3 & & \\ 1/3 & & 1/3 & & 1/3 & \\ & 1/3 & 1/3 & & & 1/3 \\ 1/3 & & & 1/3 & 1/3 & \\ & 1/3 & & 1/3 & & 1/3 \\ & & 1/3 & 1/3 & & \\ & & & 1/3 & 1/3 & 1/3 \end{pmatrix} \begin{pmatrix} \uparrow \uparrow \uparrow \\ \uparrow \uparrow \downarrow \\ \uparrow \downarrow \uparrow \\ \uparrow \downarrow \downarrow \\ \downarrow \uparrow \uparrow \\ \downarrow \uparrow \downarrow \\ \downarrow \downarrow \uparrow \\ \downarrow \downarrow \downarrow \end{pmatrix}$$

Q: Where Is Matrix-Vector Multiplication?

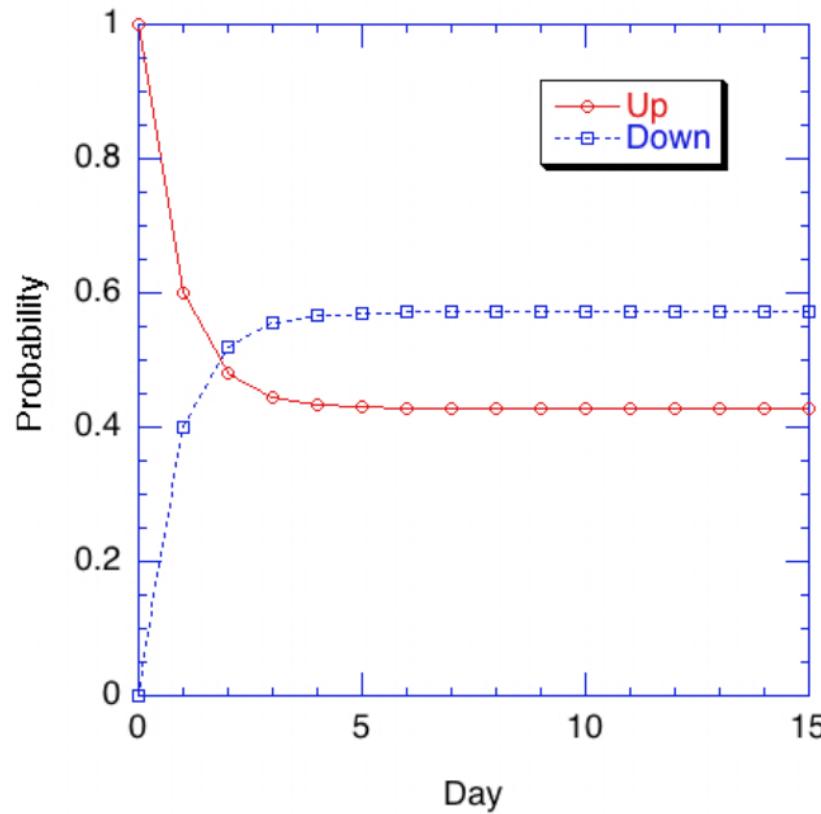
A: The probability density vector is replaced by an ensemble of individual MC sequences in Markov-chain MC; the ensemble average is then replaced by time average.

$$\rho^{(t+1)} = \Pi \rho^{(t)}$$



Example: Two-Level System

$$\Pi = \begin{pmatrix} \uparrow & \downarrow \\ \uparrow & \begin{pmatrix} a & 1-b \\ 1-a & b \end{pmatrix} \\ \downarrow & \end{pmatrix} = \begin{pmatrix} 0.6 & 0.3 \\ 0.4 & 0.7 \end{pmatrix} \quad (a = 0.6, b = 0.7)$$



$$\begin{pmatrix} p_{\uparrow}^{(t)} \\ p_{\downarrow}^{(t)} \end{pmatrix} = \begin{pmatrix} 0.6 & 0.3 \\ 0.4 & 0.7 \end{pmatrix}^t \begin{pmatrix} 1 \\ 0 \end{pmatrix} \xrightarrow[t \rightarrow \infty]{} \begin{pmatrix} 0.4286 \\ 0.5714 \end{pmatrix} \begin{matrix} 3/7 \\ 4/7 \end{matrix}$$

A Metropolis Monte Carlo

Your only knowledge = equilibrium probability distribution

$$\rho = \begin{pmatrix} 3/7 \\ 4/7 \end{pmatrix}$$

A choice of attempt matrix

$$\alpha_{\uparrow\downarrow} = \alpha_{\downarrow\uparrow} = 1$$

Detailed-balanced transition-probability matrix

$$\begin{aligned}\Pi &= \begin{pmatrix} \pi_{\uparrow\uparrow} & \pi_{\uparrow\downarrow} \\ \pi_{\downarrow\uparrow} & \pi_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} 1 - \alpha_{\downarrow\uparrow} & \alpha_{\uparrow\downarrow}(\rho_{\uparrow}/\rho_{\downarrow}) \\ \alpha_{\downarrow\uparrow} & 1 - \alpha_{\uparrow\downarrow}(\rho_{\uparrow}/\rho_{\downarrow}) \end{pmatrix} \\ &= \begin{pmatrix} 1 - 1 & 1 \cdot 3/4 \\ 1 & 1 - 1 \cdot 3/4 \end{pmatrix} = \begin{pmatrix} 0 & 3/4 \\ 1 & 1/4 \end{pmatrix}\end{aligned}$$

Q: How to represent the probability distribution?

A: An ensemble of many samples

Ensemble-Average MC

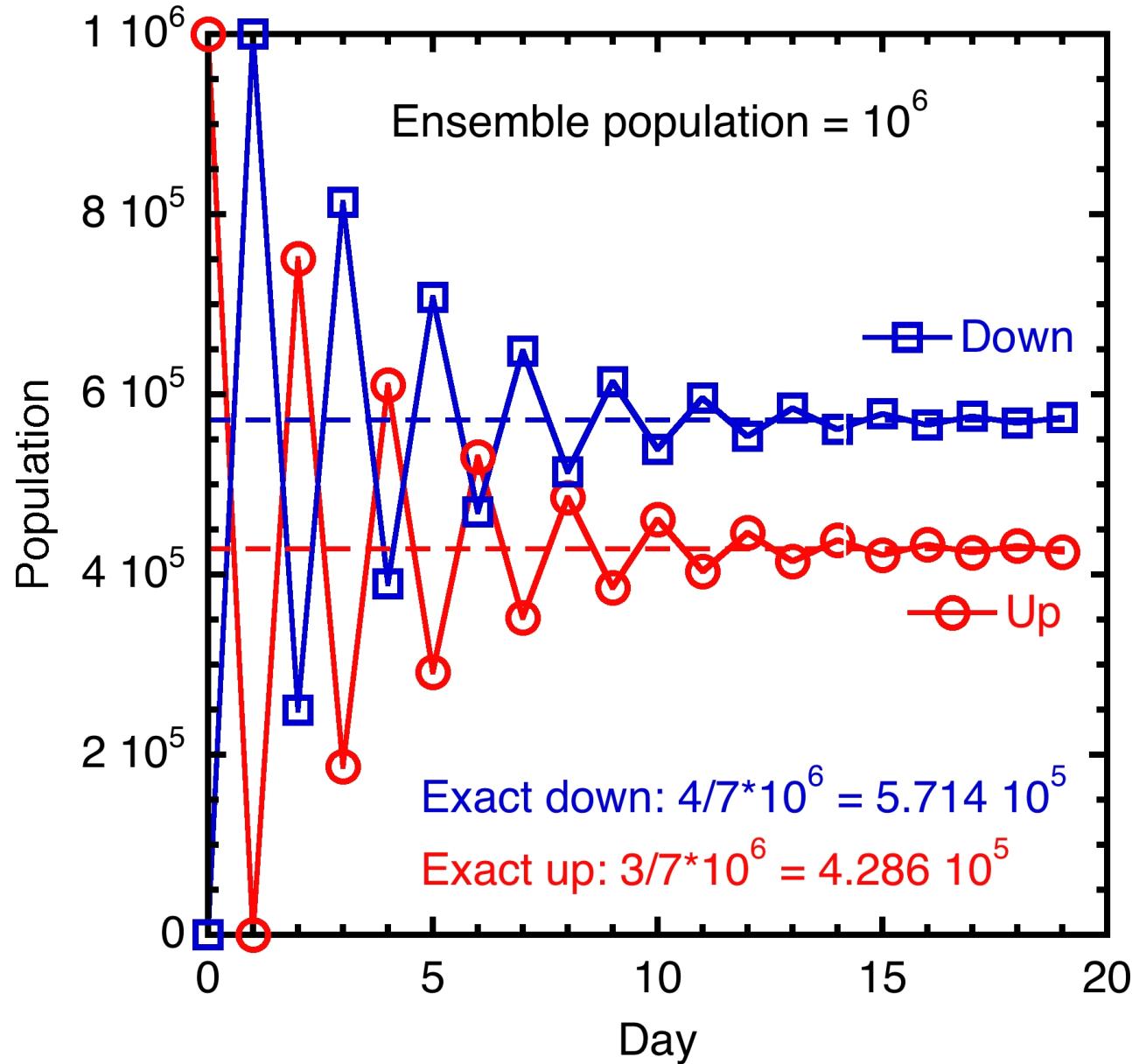
```
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#define NTRY 20 /* # of MC trials */
#define NENS 1000000 /* ensemble size */
#define TRNS 3.0/4.0 /* up-to-down conditional probability */

int main() {
    int s; /* spin state: 0 = up; 1 = down */
    int hist[NTRY][2]; /* histgram */
    int try,walker;

    srand((unsigned)time((long *)0));
    for (try=0; try<NTRY; try++) for (s=0; s<2; s++) hist[try][s] = 0;

    for (walker=0; walker<NENS; walker++) {
        s = 0; /* up on day 0 */
        ++(hist[0][s]);
        for (try=1; try<NTRY; try++) {
            if (s == 0) s = 1; /* unconditional down move */
            else if (rand()/(double)RAND_MAX < TRNS) s = 0; /* conditional up move */
            ++(hist[try][s]); /* accumulate the average */
        }
    }
    for (try=0; try<NTRY; try++) printf("%d %d %d\n",try,hist[try][0],hist[try][1]);
    return 0;
}
```

Ensemble-Average MC Result



Time-Average MC

```
#include <stdio.h>
#include <stdlib.h>
#include <time.h>
#define NTRY 1000 /* ensemble size */
#define TRNS 3.0/4.0 /* up-to-down conditional probability */

int main() {
    int s; /* spin state: 0 = up; 1 = down */
    int hist[NTRY][2]; /* histogram */
    int try,i;

    srand((unsigned)time((long *)0));
    for (try=0; try<NTRY; try++) for (s=0; s<2; s++) hist[try][s] = 0;

    s = 0; /* up on day 0 */
    ++(hist[0][s]);
    for (try=1; try<NTRY; try++) {
        if (s == 0) s = 1; /* unconditional down move */
        else if (rand()/(double)RAND_MAX < TRNS) s = 0; /* conditional up move */
        for (i=0; i<2; i++) hist[try][i] = hist[try-1][i];
        ++(hist[try][s]); /* accumulate the average */
    }

    for (try=0; try<NTRY; try++)
        printf("%d %d %d\n",try,hist[try][0],hist[try][1]);

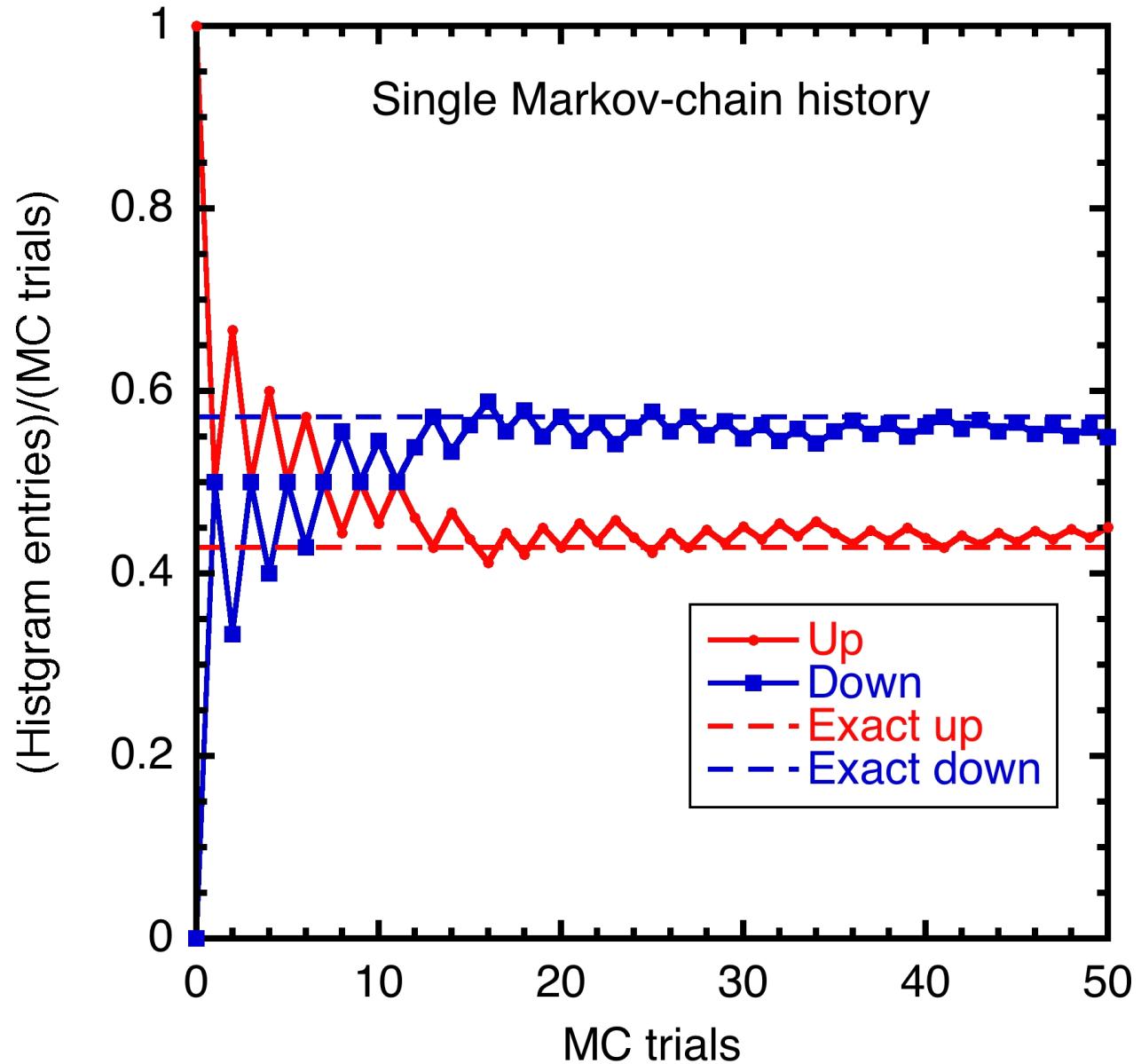
    return 0;
}
```

Ergodic hypothesis

Time-Average MC Result

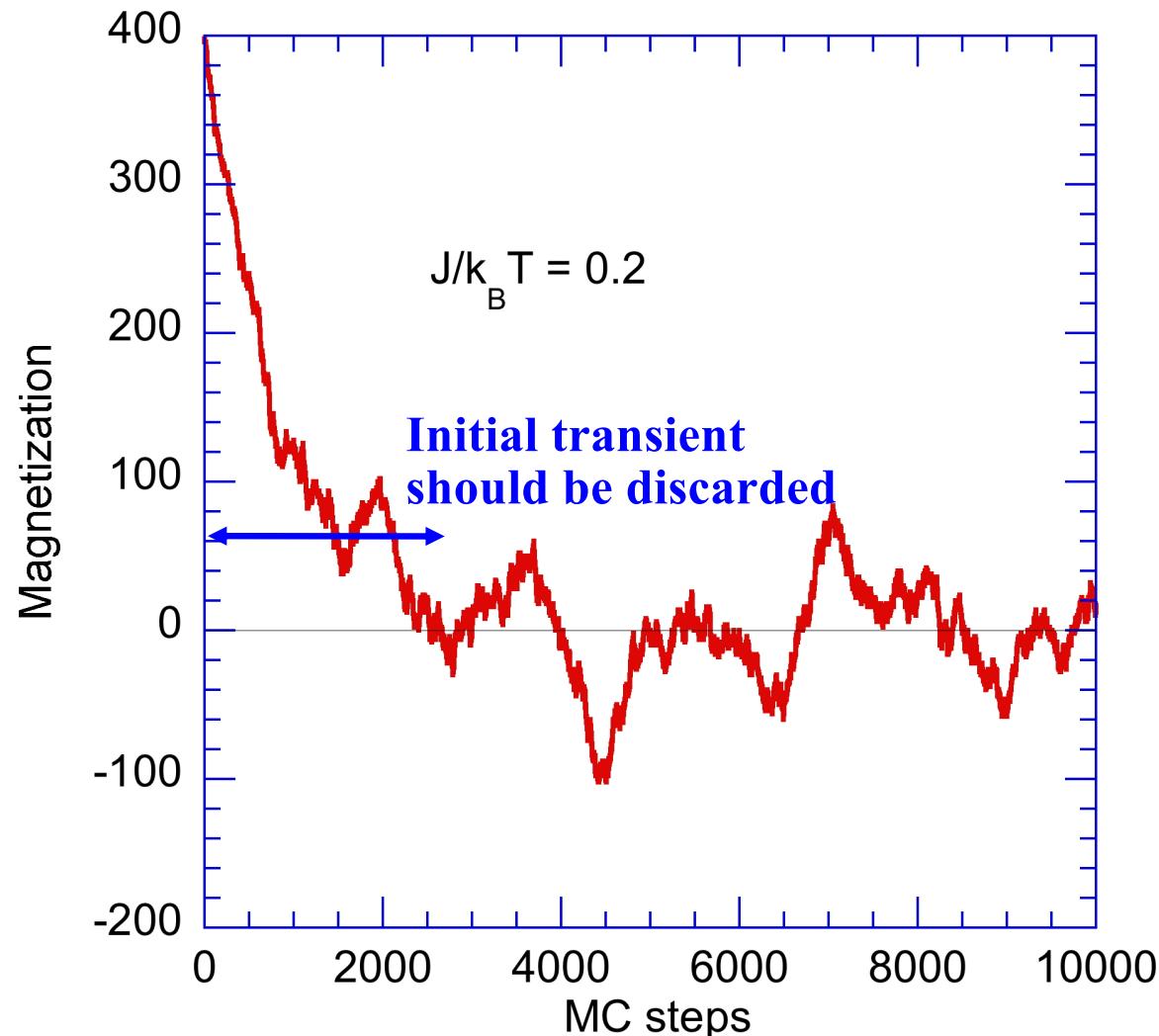
Try	Up	Down
0	1	0
1	1	1
2	2	1
3	2	2
4	3	2
5	3	3
6	4	3
7	4	4
8	4	5
9	5	5
10	5	6
11	6	6
12	6	7
13	6	8
14	7	8
15	7	9
16	7	10
17	8	10
18	8	11
19	9	11
20	9	12

Cumulative
histogram



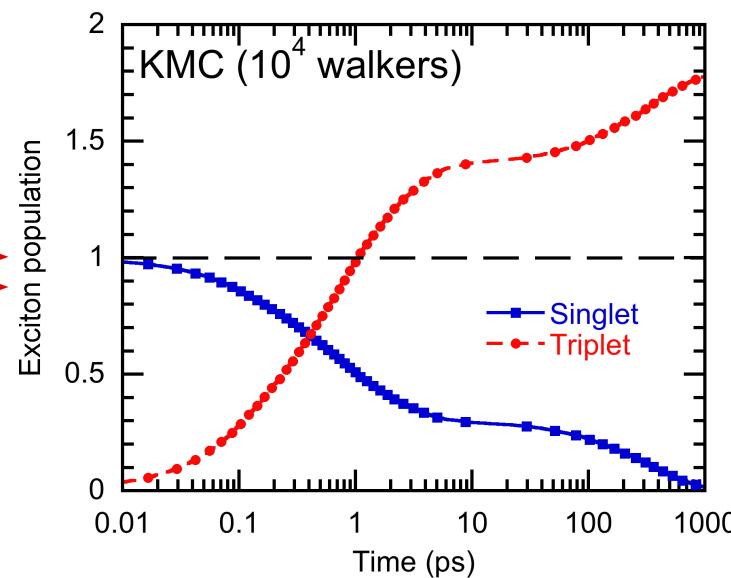
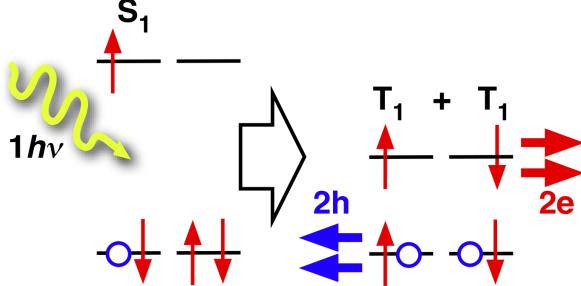
Q: Need Equilibration Steps?

A: Yes, statistics should be taken after the memory of the initial configuration is lost

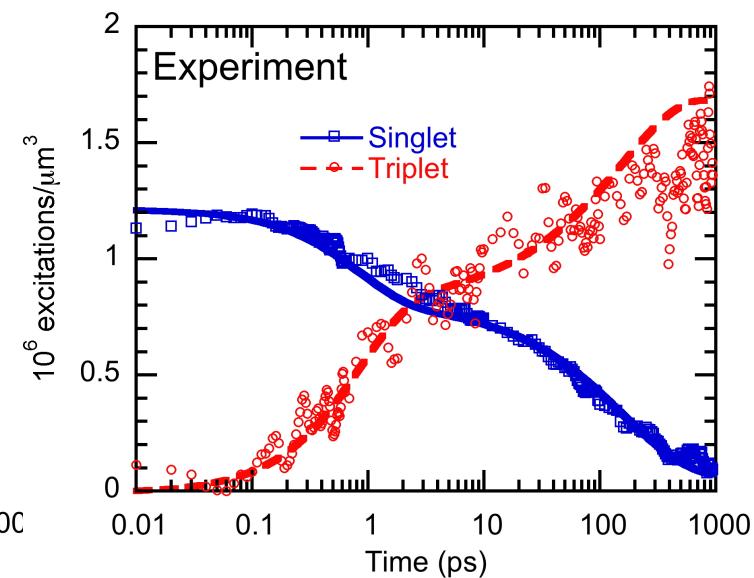


Metropolis MC vs. Kinetic MC

- **Metropolis MC:** Given probability density ρ_α ($\alpha = 1, \dots, N_{\text{states}}$) calculate statistical average of a physical quantity as $\langle A \rangle = \sum_\alpha \rho_\alpha A_\alpha$ where the transition-probability matrix $\pi_{\alpha\beta}$ is an artifact for importance sampling
- **Kinetic MC:** Given transition-rate matrix $\pi_{\alpha\beta}$ (calculated, e.g., based on the transition state theory) & initial distribution $\rho_\alpha(t=0)$, obtain the time variation of $\rho_\alpha(t)$ by solving the master equation represented by an ensemble of state samples, $d\rho_\alpha/dt = -\sum_\beta \pi_{\beta\alpha} \rho_\alpha + \sum_\beta \pi_{\alpha\beta} \rho_\beta$



W. Mou et al.
APL 102, 173301 ('13)



S. T. Roberts et al.
JACS 134, 6388 ('12)

Coordinate Transformation?

- **Box-Muller algorithm:** For a harmonic oscillator, $u(x) = Kx^2/2$, Boltzmann probability density (which is Gaussian $p(x) \propto \exp(-u(x)/k_B T) = \exp(-Kx^2/2k_B T)$) can be generated by coordinate transformation
- **Boltzmann generator:** Machine learning of coordinate transformation such that the probability density is Gaussian in the transformed coordinate system, $z(x)$, for complex, multidimensional $u(x)$

F. Noe et al.
Science 365, 1001 ('19)

