Studying the impact of multiple, localized, gauge-fixed subvolumes with coherent conjugate momenta on the Hybrid Monte Carlo

Robert Mawhinney
Columbia University

Lattice 2026
July 28, 2026
The University of Maryland, College Park

Work done in collaboration with Rajiv Eranki of Columbia

Introduction

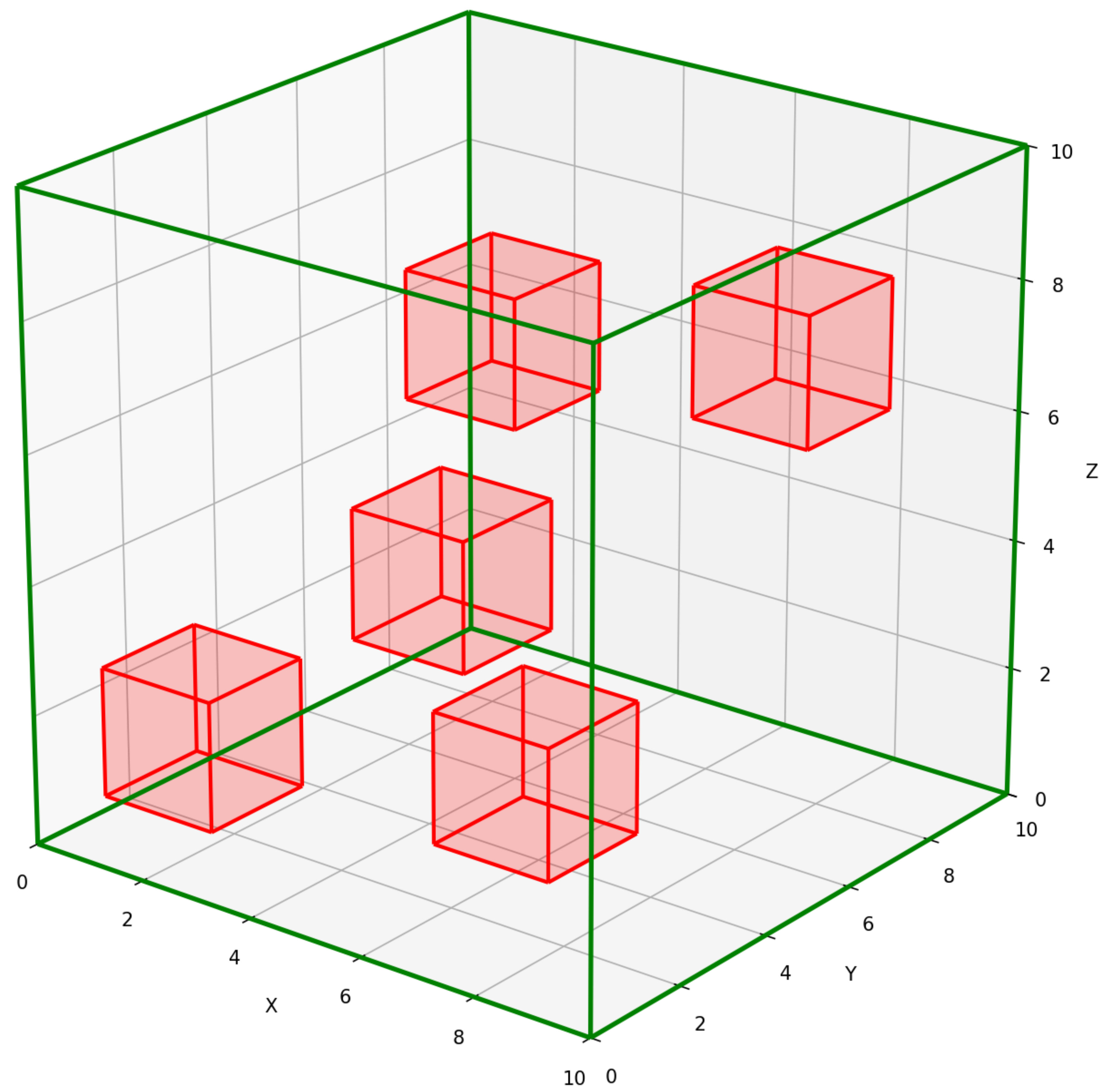
- Hybrid Monte Carlo (HMC) is the dominant evolution algorithm, but there is need for faster de-correlation of lattices and improved topological sampling.

- Many efforts to adjust which d.o.f. receive the most computer effort to improve the sampling of phase space: Riemannian Manifold Hybrid Monte Carlo (RMHMC), Field Transformation HMC, flows …

- In this talk, we present ongoing work that investigates the utility of conjugate momenta that are composed of spatial and color coherent modes.

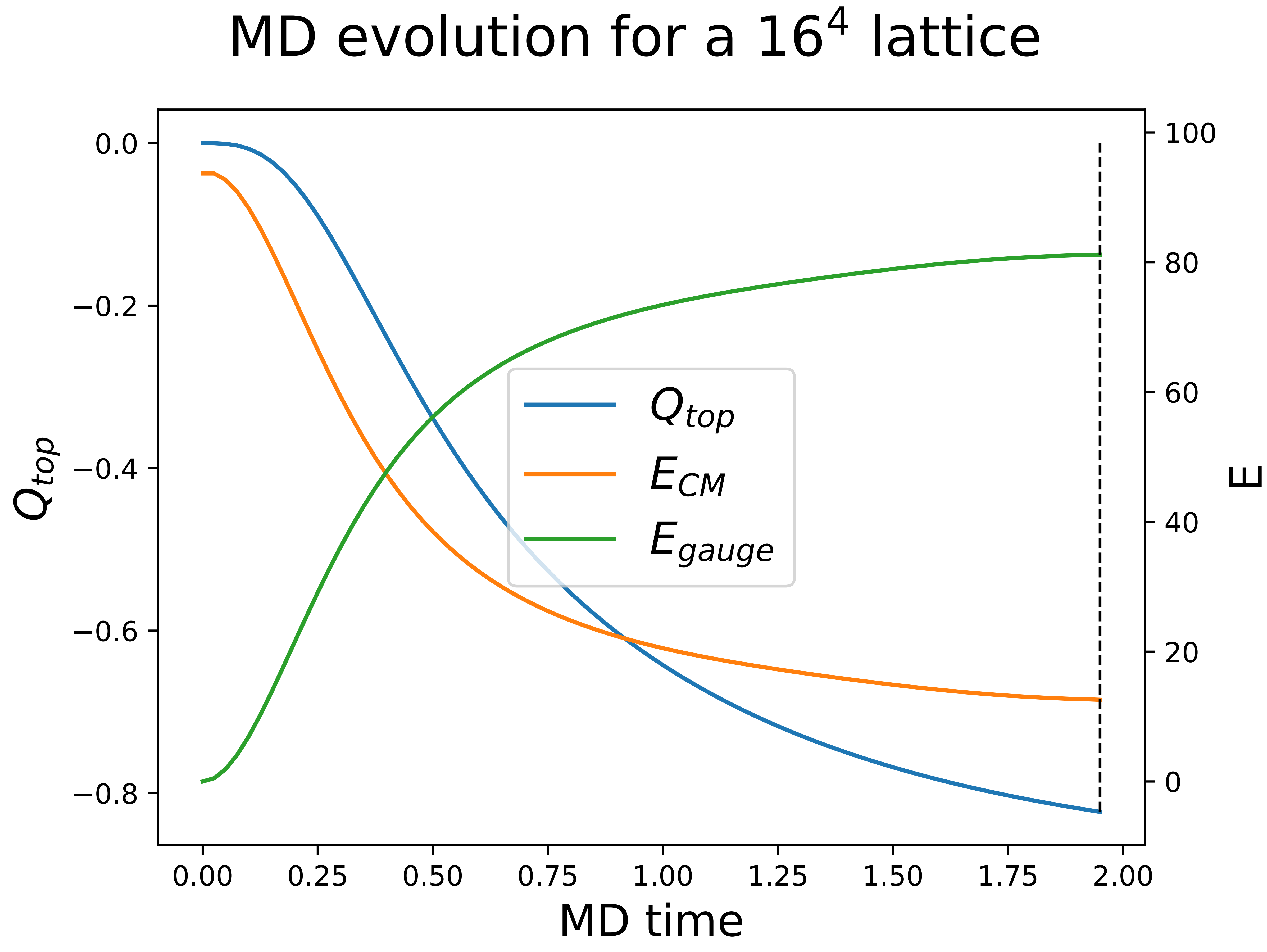
Lattice Subvolumes

- QCD vacuum should only support coherence over ~1/2 fermi, so will investigate coherent conjugate momenta in subvolumes.
- Gauge invariance of HMC requires a fixed gauge in the sub volumes for coherence.
- Maximal tree gauges can be readily evolved by the HMC by keeping conjugate momenta zero on gauge fixed links
- Choose random locations for subvolumes and can also vary features of the maximal tree gauge.



Lattice Evolution to Produce Topology

- Starting from a lactic with all links unity,choose conjugate momenta to create an approximate classical instanton after some number of MD steps.
- Can we use coherent conjugate momenta like this in the HMC?
- If we can, will this have any impact on the rate at which we sample phase space?



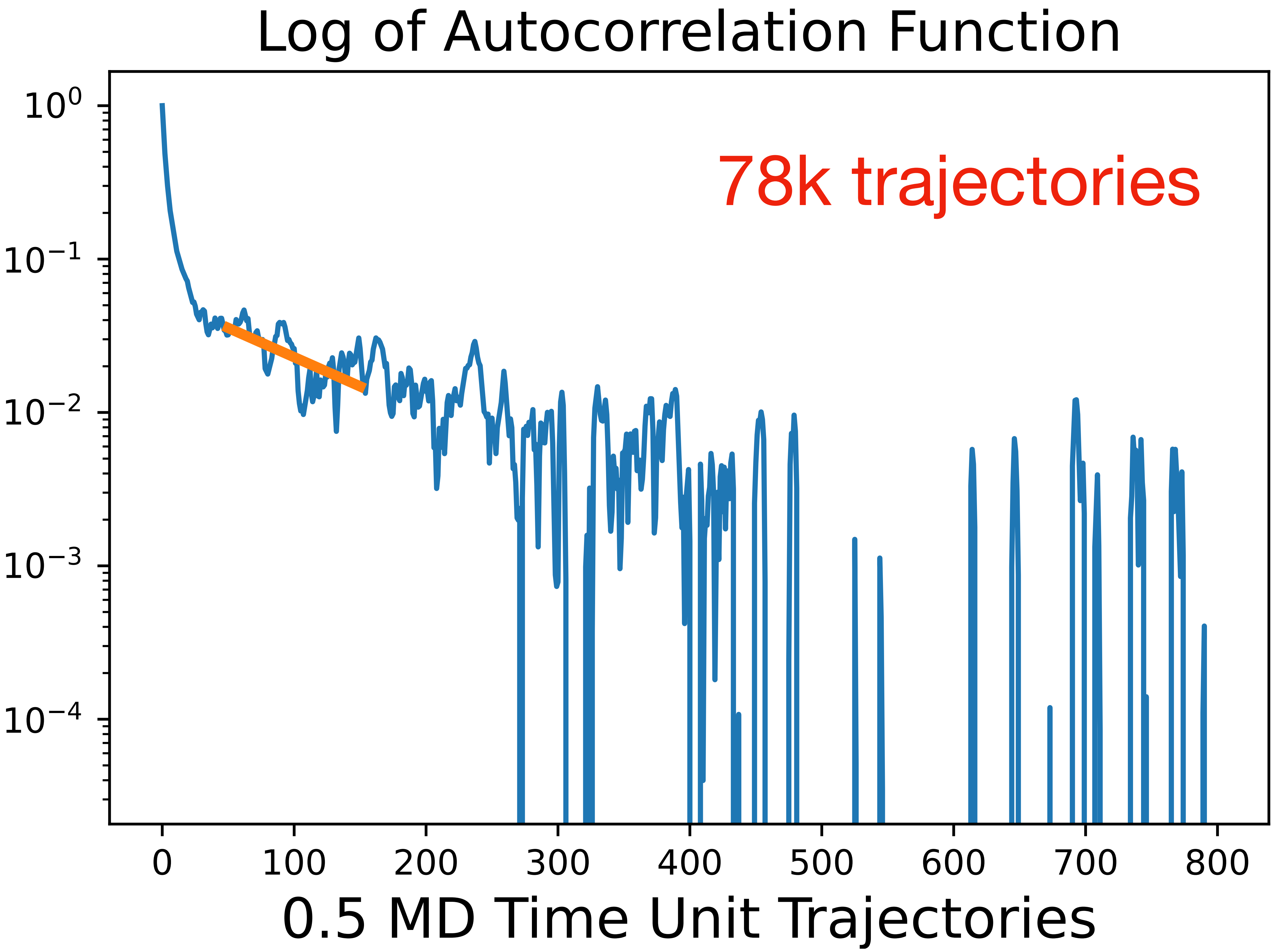
Standard Leap-Frog Molecular Dynamics in HMC

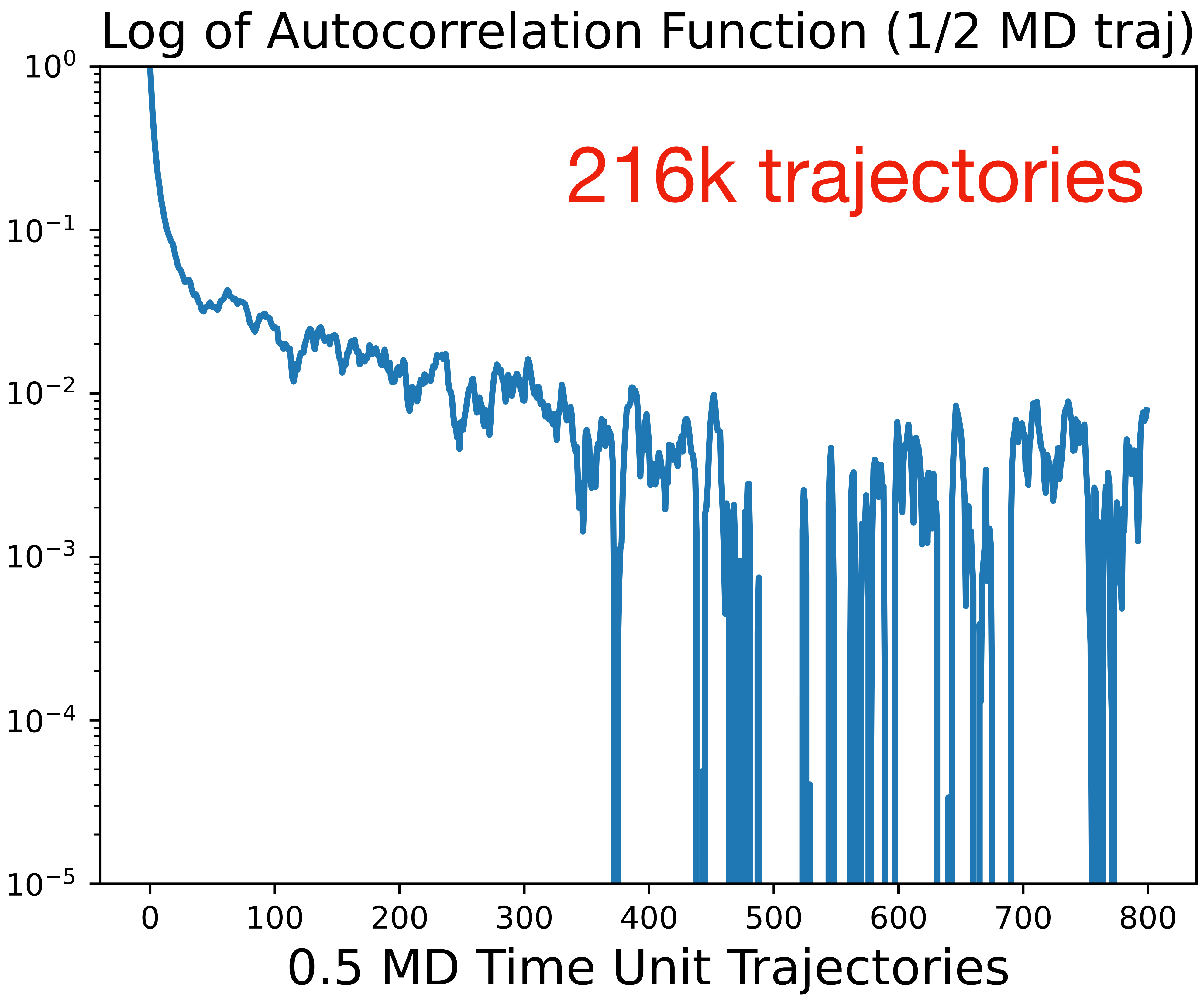
- $\dot{U}_{j,\mu} = iH_{j,\mu}\, U_{j,\mu}$ with $H_{j,\mu} = \sum_a \lambda_a h_{j,\mu.a}$ $h_{j,\mu,a}$ are the conjugate momenta for each site, link and color
- $i\dot{H}_{j,\mu} = -\frac{\beta}{3}\left[U_{j,\mu}\, V_{j,\mu}\right]_{\mathrm{TA}}$ with $V_{j,\mu}$ the sum of staples and TA = traceless and antihermitian
- Draw $h_{j,\mu,a}$ from $\int [dh_{j,\mu,a}]\ \exp\left(-\sum_{j,\mu,a} h^2_{j,\mu,a}\right)$ at beginning of a trajectory
- $H_{j,\mu}(t+\Delta t/2) - H_{j,\mu}(t-\Delta t/2) = \dot{H}_{j,\mu}(t)\cdot\Delta t + O(\Delta t^3)$
- $U_{j,\mu}(t+\Delta t) = \exp[iH(t+\Delta t/2)\cdot\Delta t]\cdot U_{j,\mu}(t) + O(\Delta t^3)$

Plaquette Autocorrelation Function

- As a code check and to establish baseline auto correlations, started with SU(3) pure gauge evolution, on 24^4 lattice, with Wilson action and $\beta = 6.0$, $1/a \sim 2$ GeV

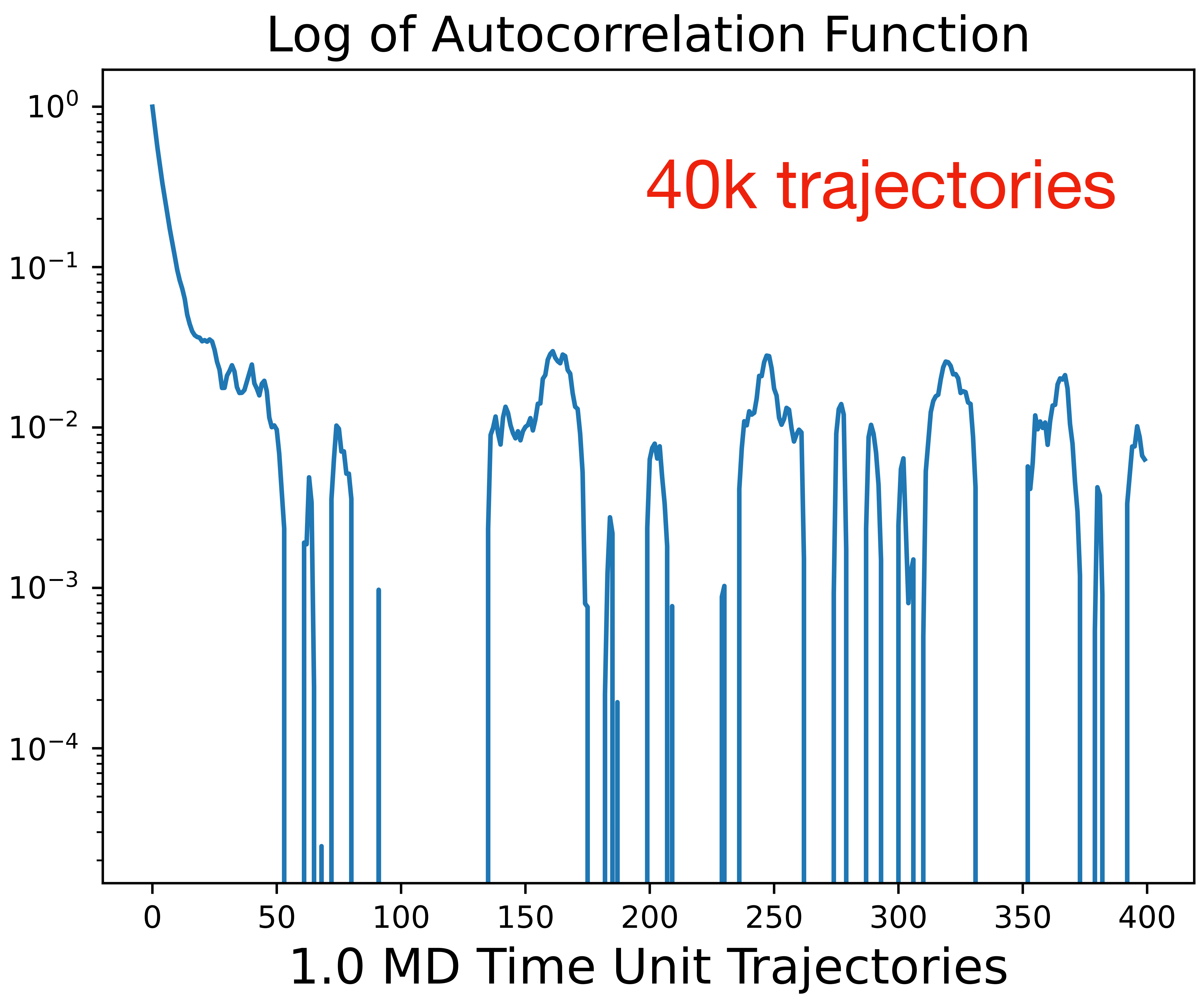
- Long exponential tail clearly visible.

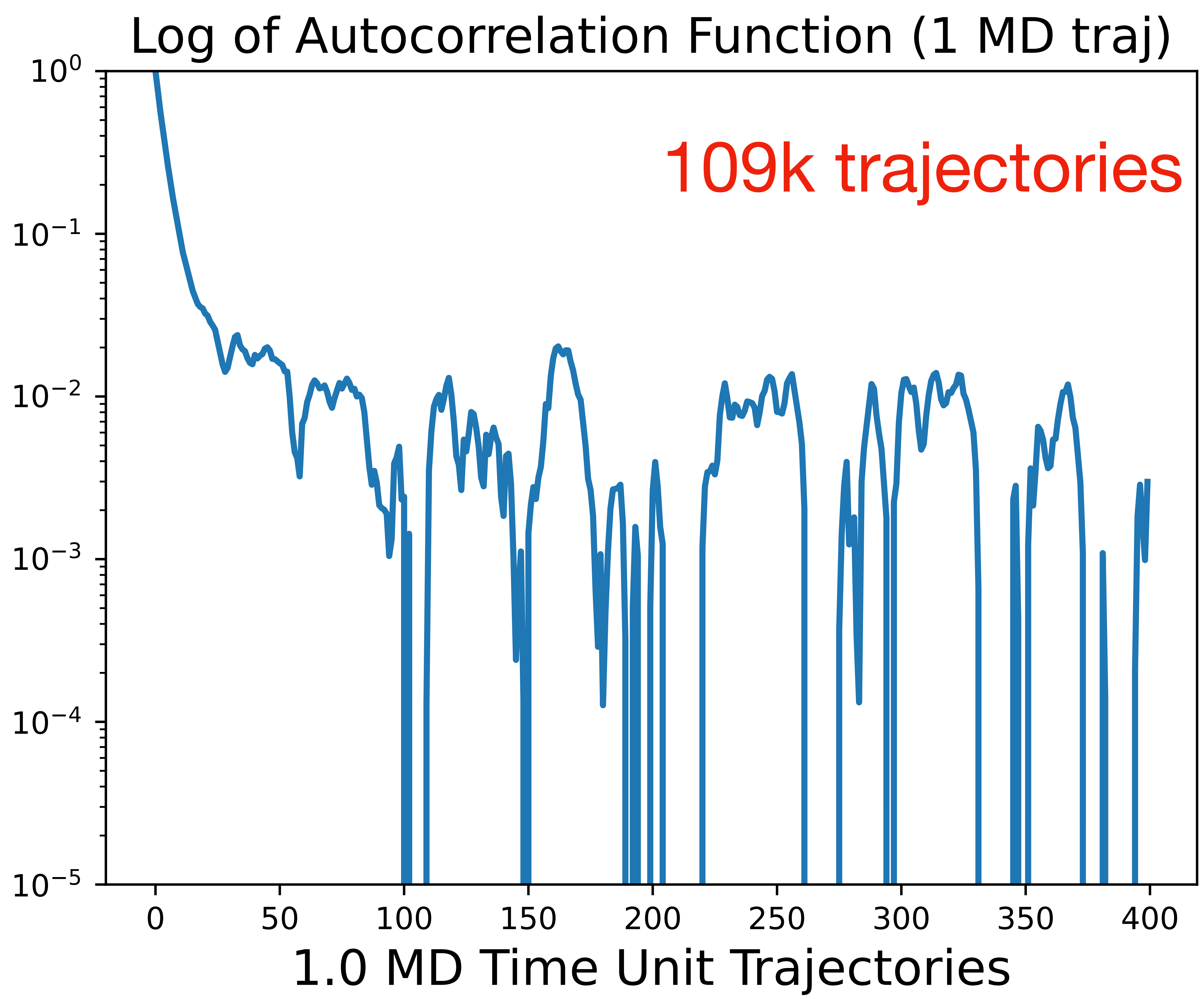




Effect of Trajectory Length

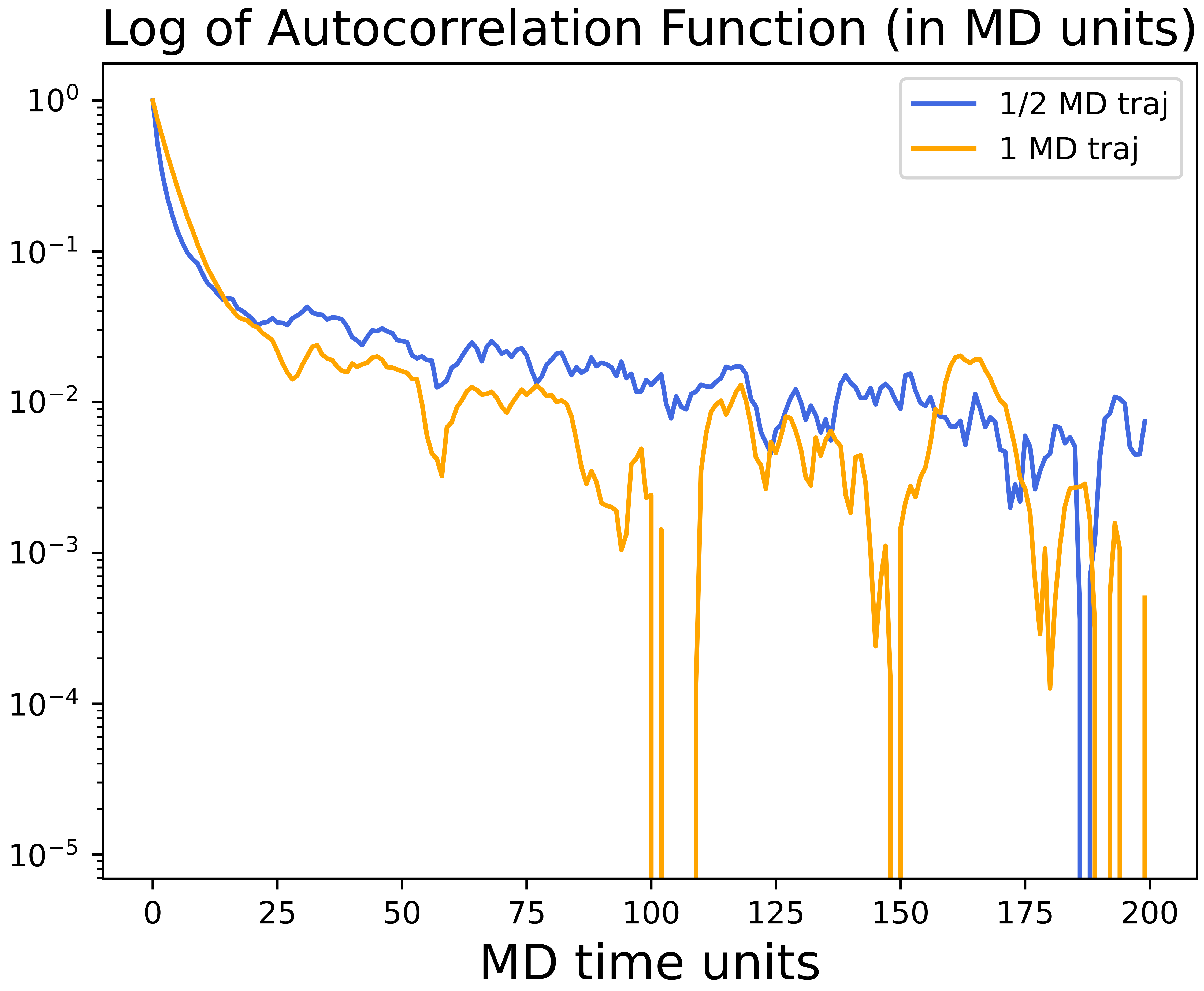
- Same system, but 1 MD time unit trajectories.

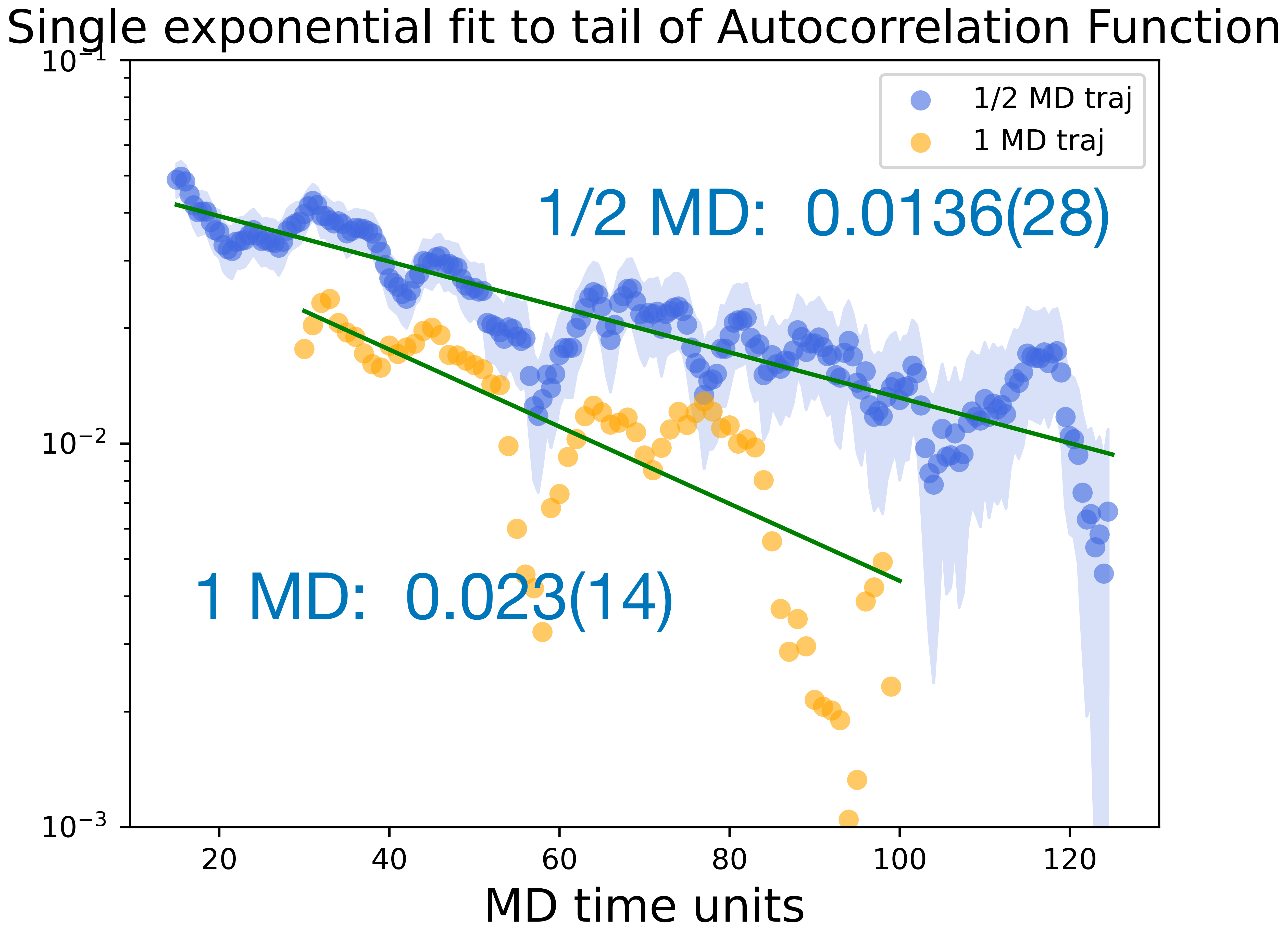




Comparing 1/2 and 1 MD autocorrelations

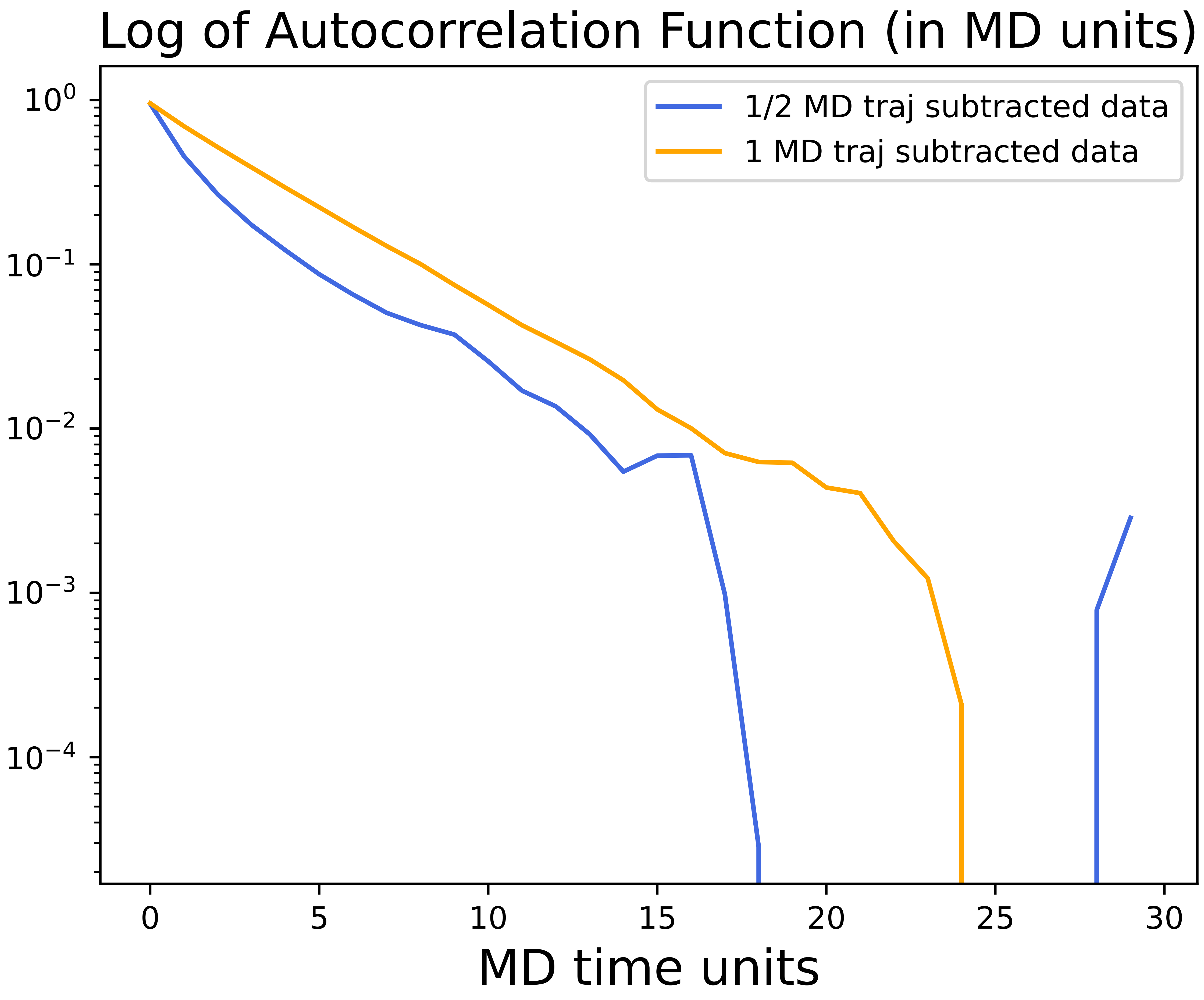
- Autocorrelation function for 1/2 MD trajectory length falls faster initially.
- Fits are uncorrelated, but done under a jackknife blocking: $a \times \exp(-bx)$

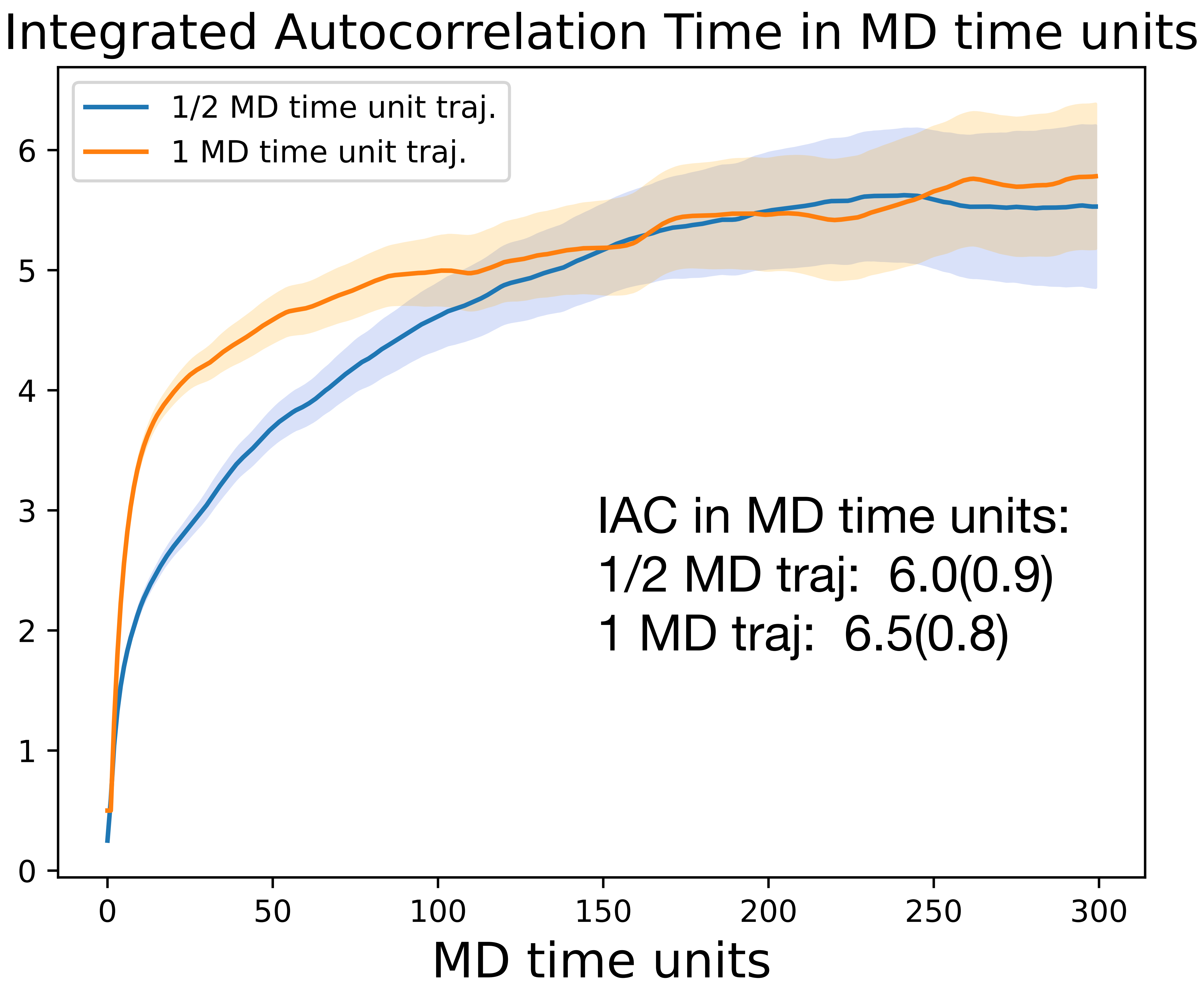




Comparing 1/2 and 1 MD IAC and errors

- The error on the plaquette is the same within its errors for ~110k MD time units, whether that comes in 1/2 or 1 MD time unit trajectories.





Comparing 1/2 and 1 MD errors

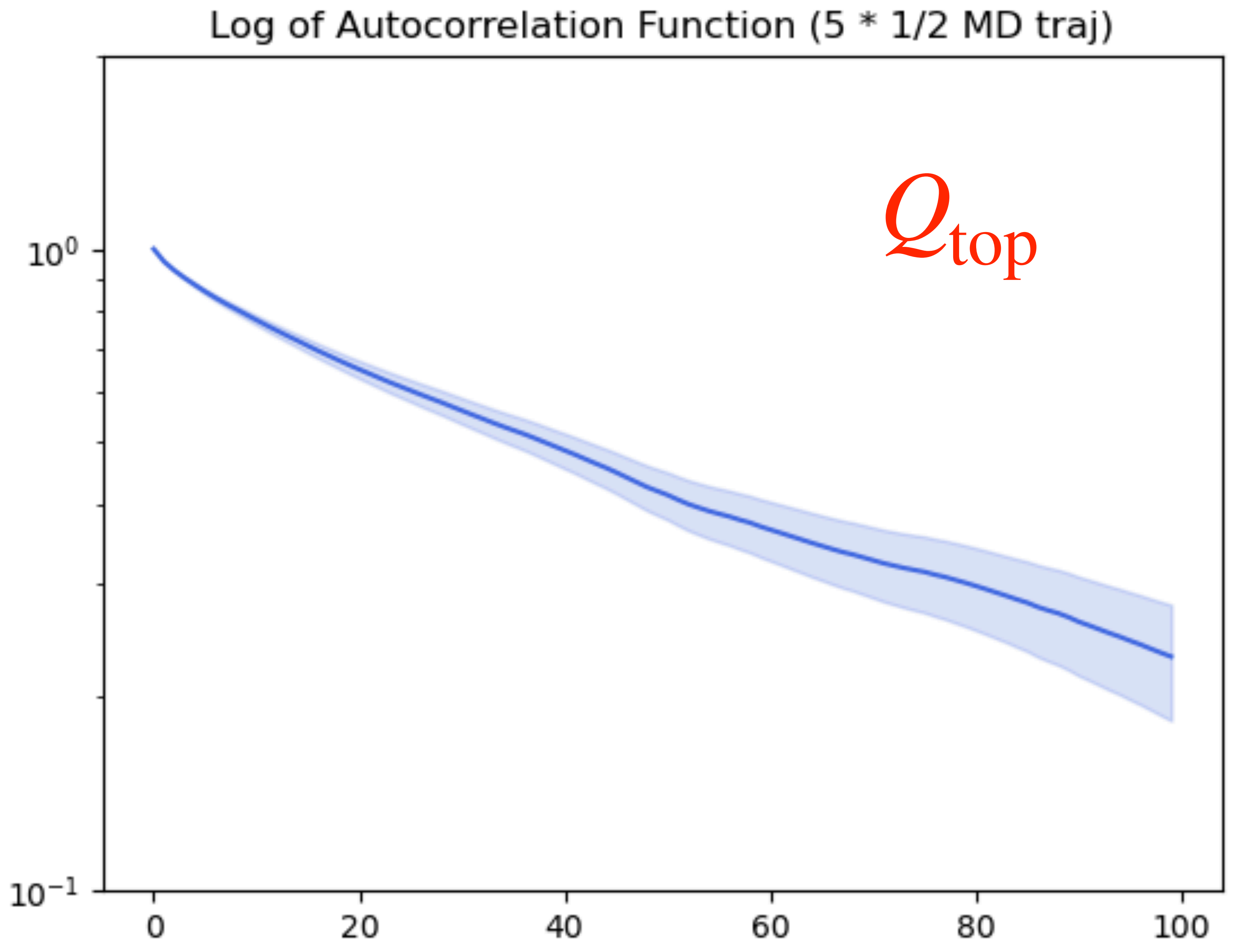
- 216k, 1/2 MD trajectories blocked in groups of 2000
  - plaquette = 0.5936859(25)
- 109k, 1 MD trajectories blocked in groups of 1000
  - plaquette = 0.5936850(26)
- Fitting exponential tail to $a \times \exp(-bx)$ gives (in MD time units)
  - 1/2 MD traj: a = 0.051(0.06), b = 0.0136(28)
  - 1 MD traj: a = 0.044(31), b = 0.023(14)

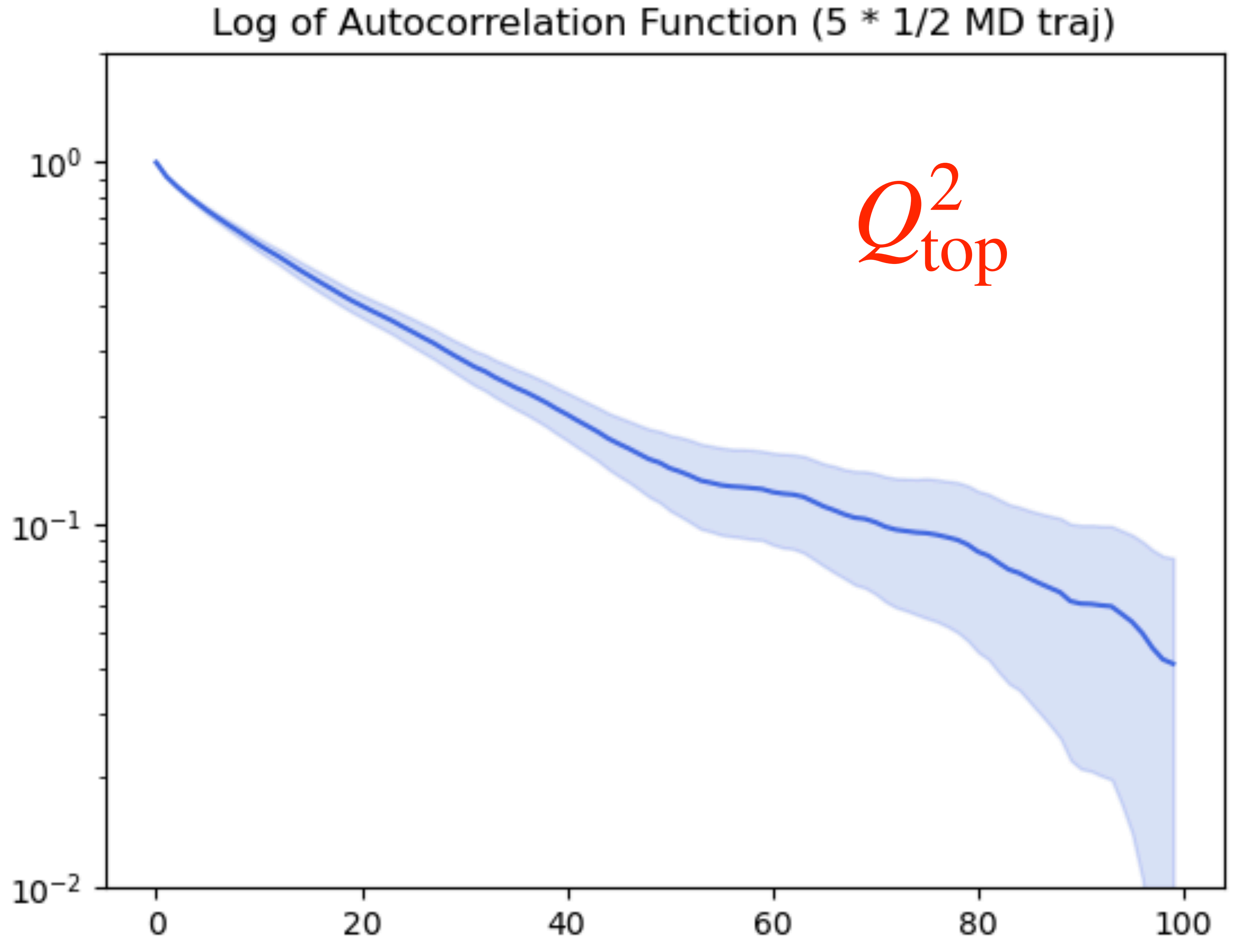
Autocorrelation Functions for $Q_{\rm top}$ and $Q_{\rm top}^2$

- Using Grid and Force Gradient integrator, have 159k trajectories of length 1/2 MD time unit (Rajiv).

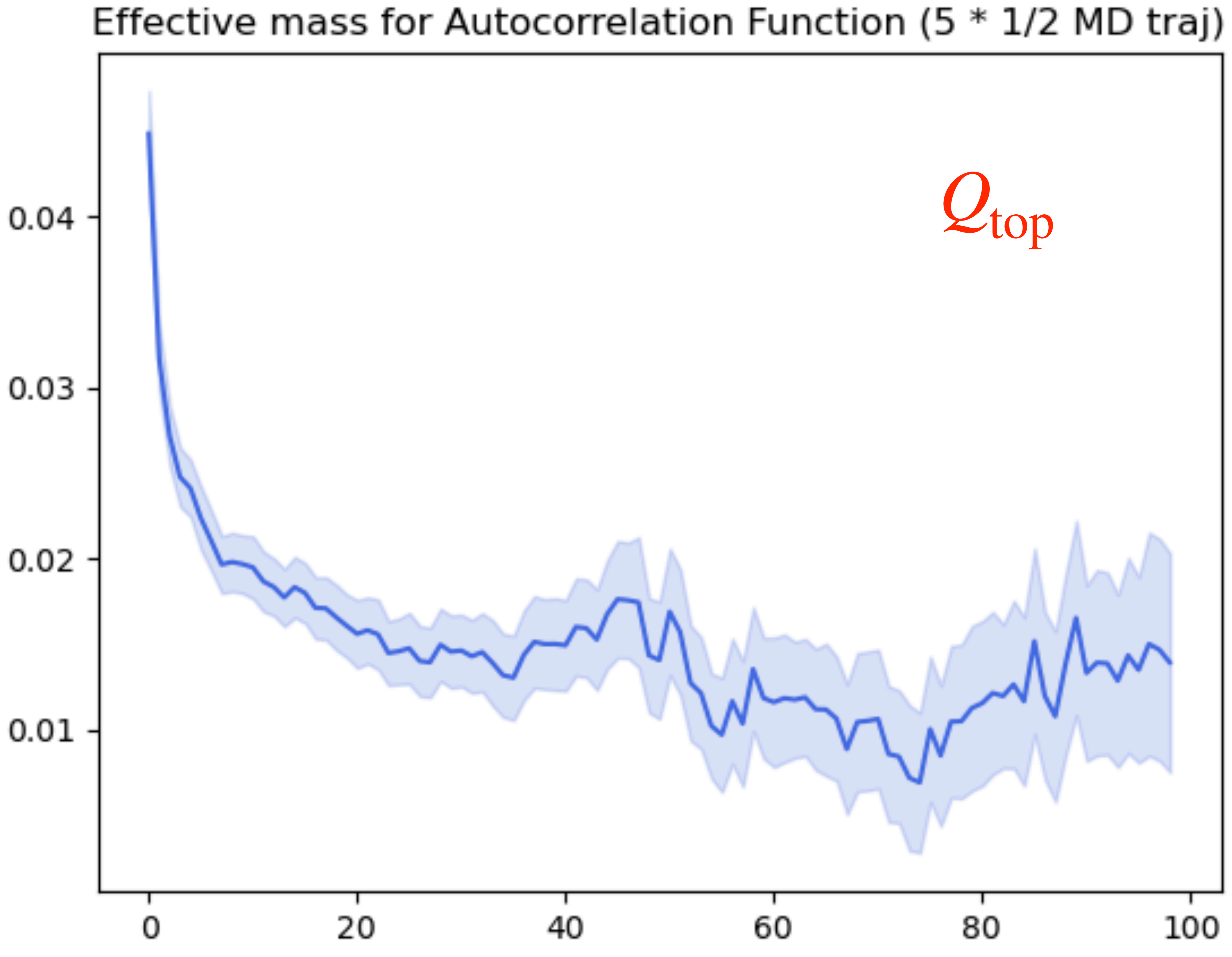
- Acceptance = 84% very close to 81% acceptance with leap-frog.

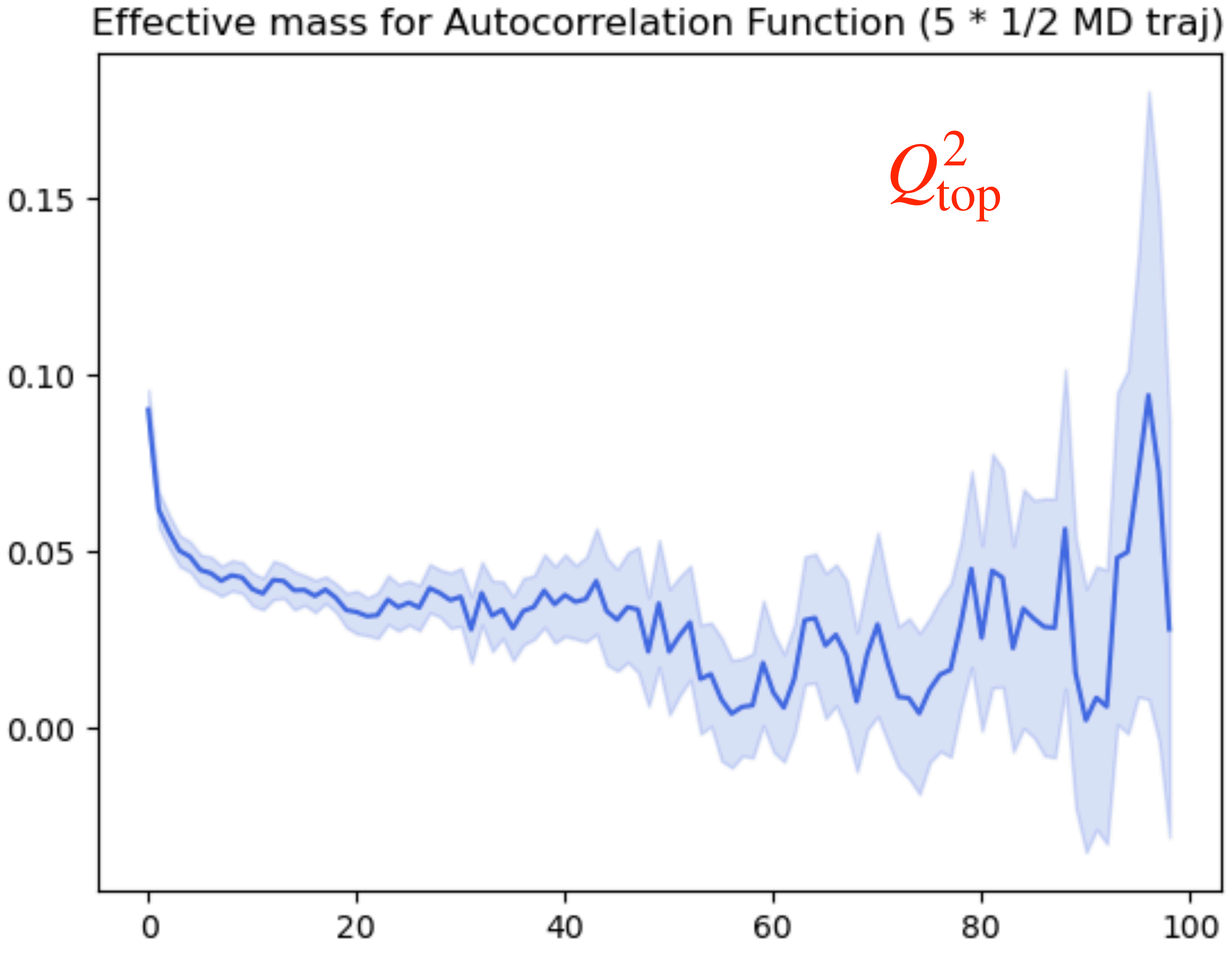
- Have autocorrelation functions for $Q_{\rm top}$ and $Q_{\rm top}^2$ at Wilson flow time.





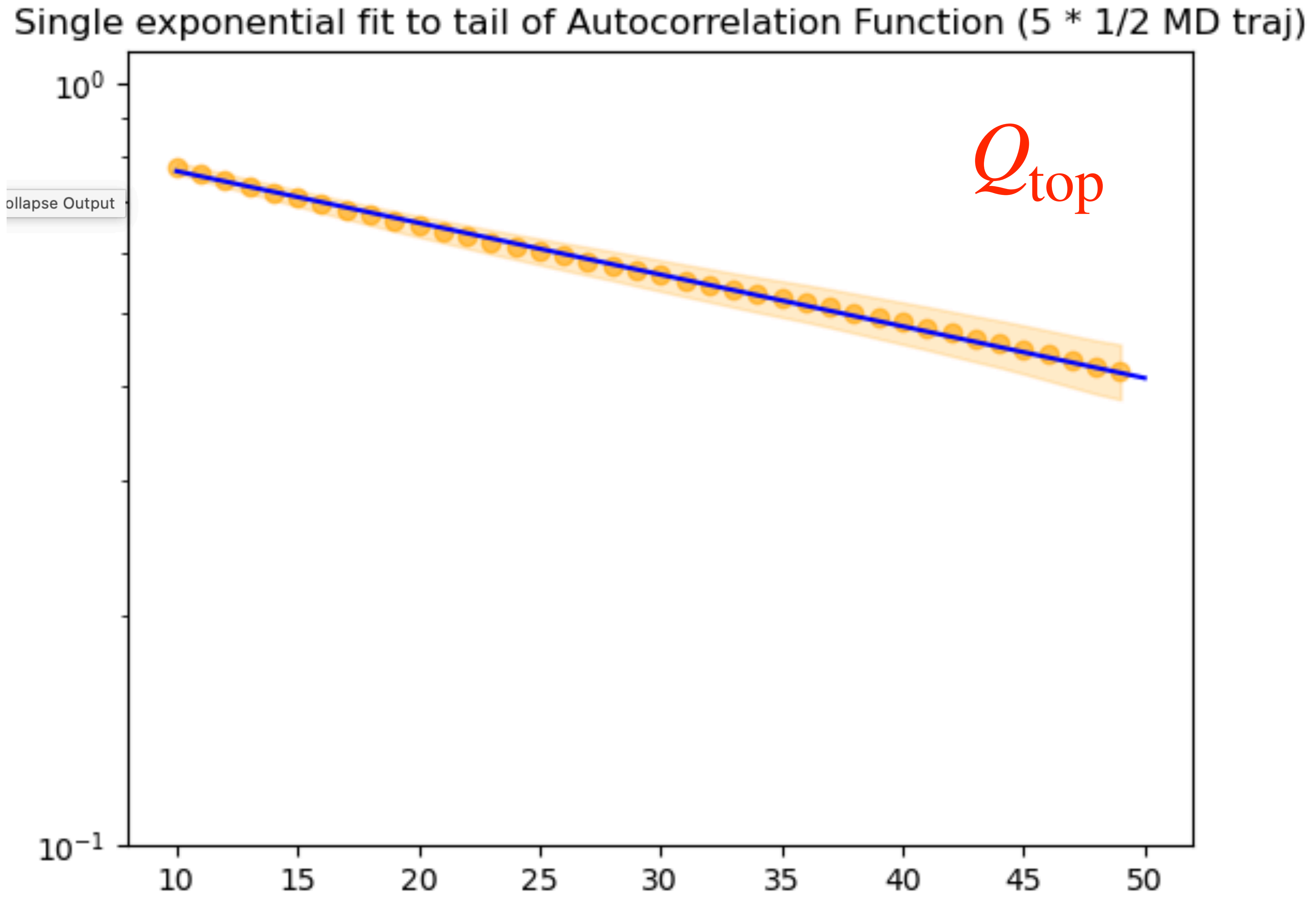
“Effective Mass” for Autocorrelation Functions for Q_{top} and Q^2_{top}



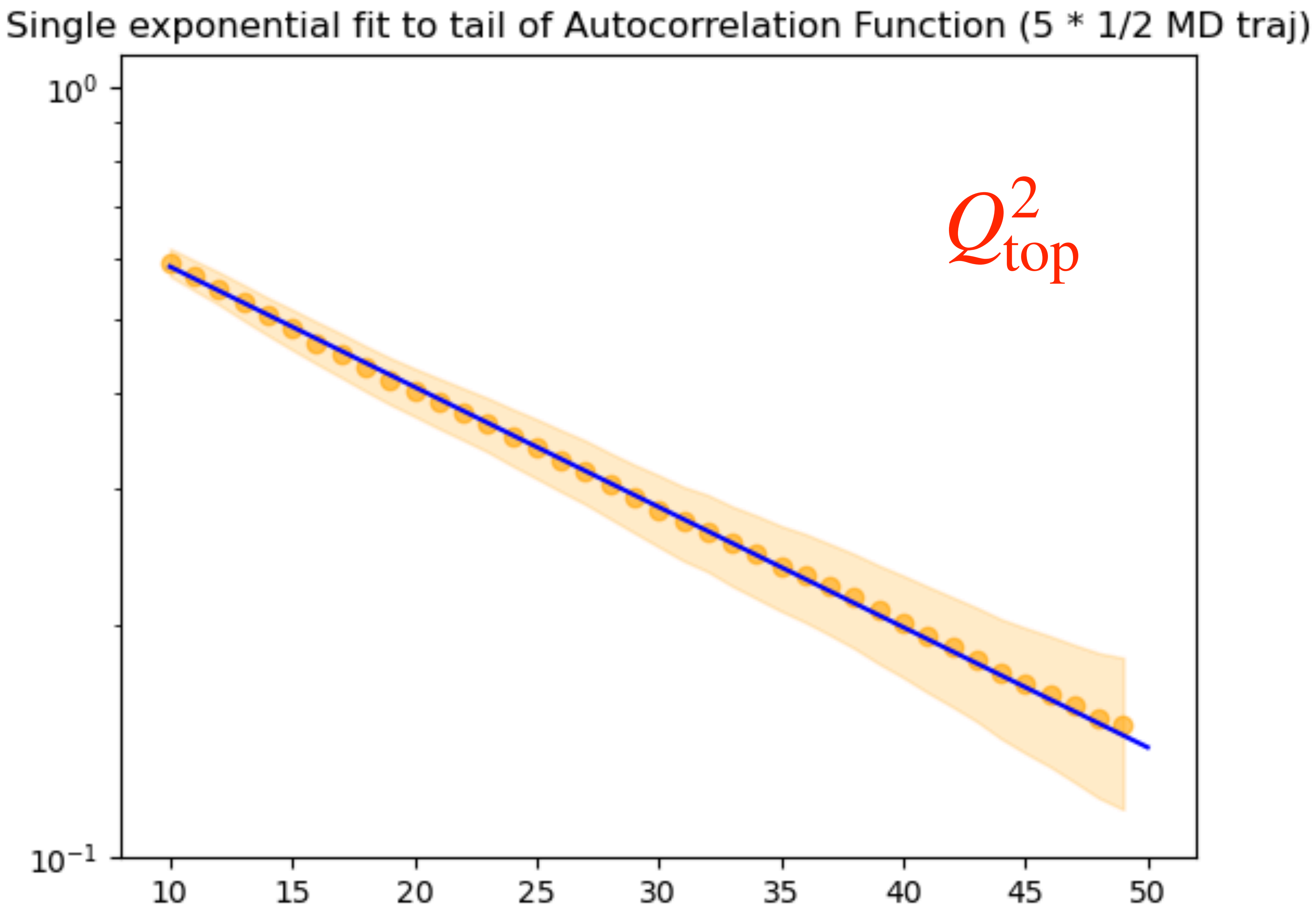


Fits toAutocorrelation Functions for $Q_{\rm top}$ and $Q^2_{\rm top}$

- Single exponential fits from 25 to 125 MD time units: $a \times \exp(-bx)$
- Decay rate in tail of plaquette AC function same, within errors as for $Q^2_{\rm top}$



b = 0.00624(68), IAC = 127(7) (MD time units)



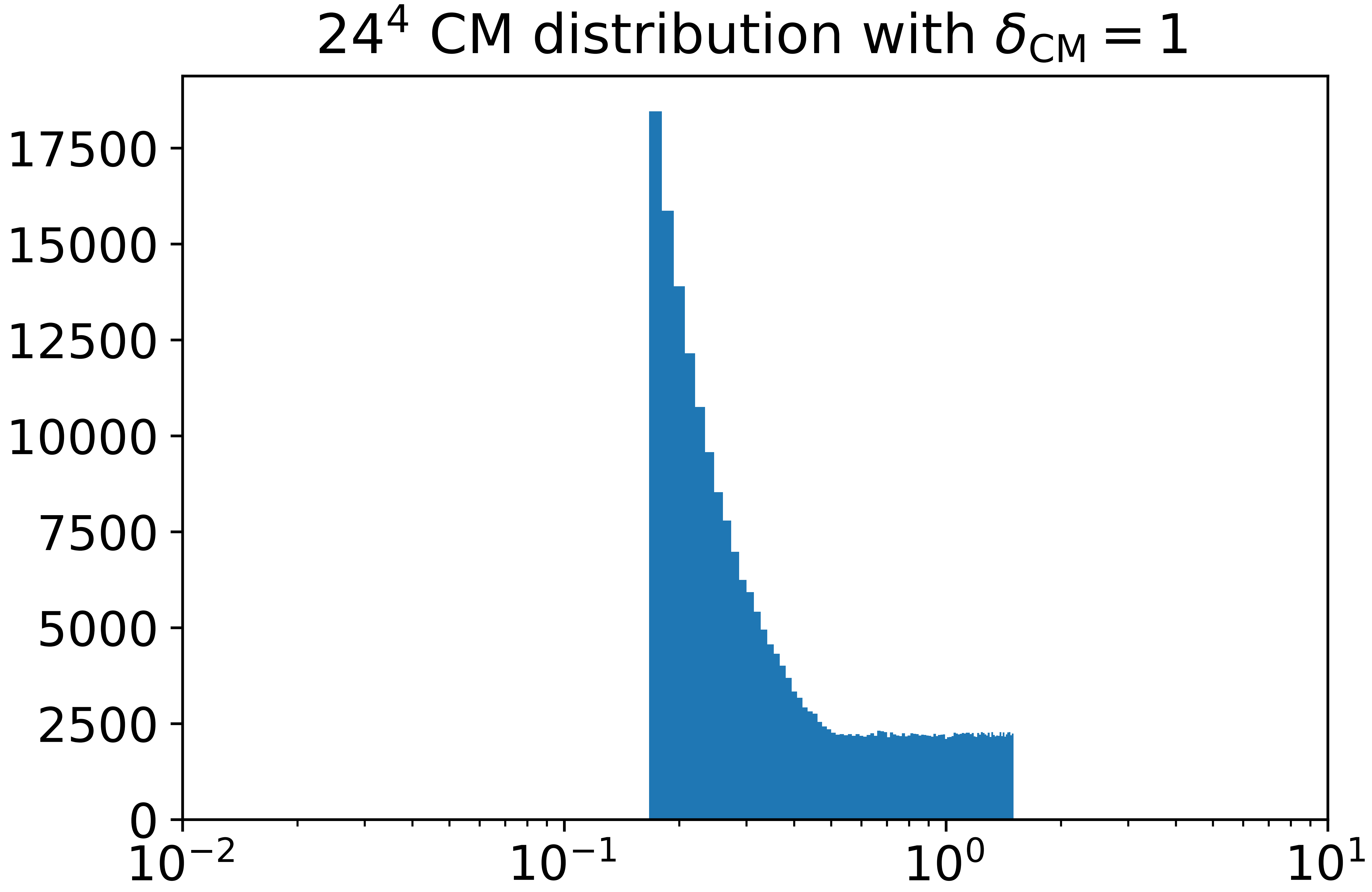
b = 0.0144(17), IAC = 51(5) (MD time units)
b = 0.0136(28) from plaquette

Variable Width Conjugate Momenta

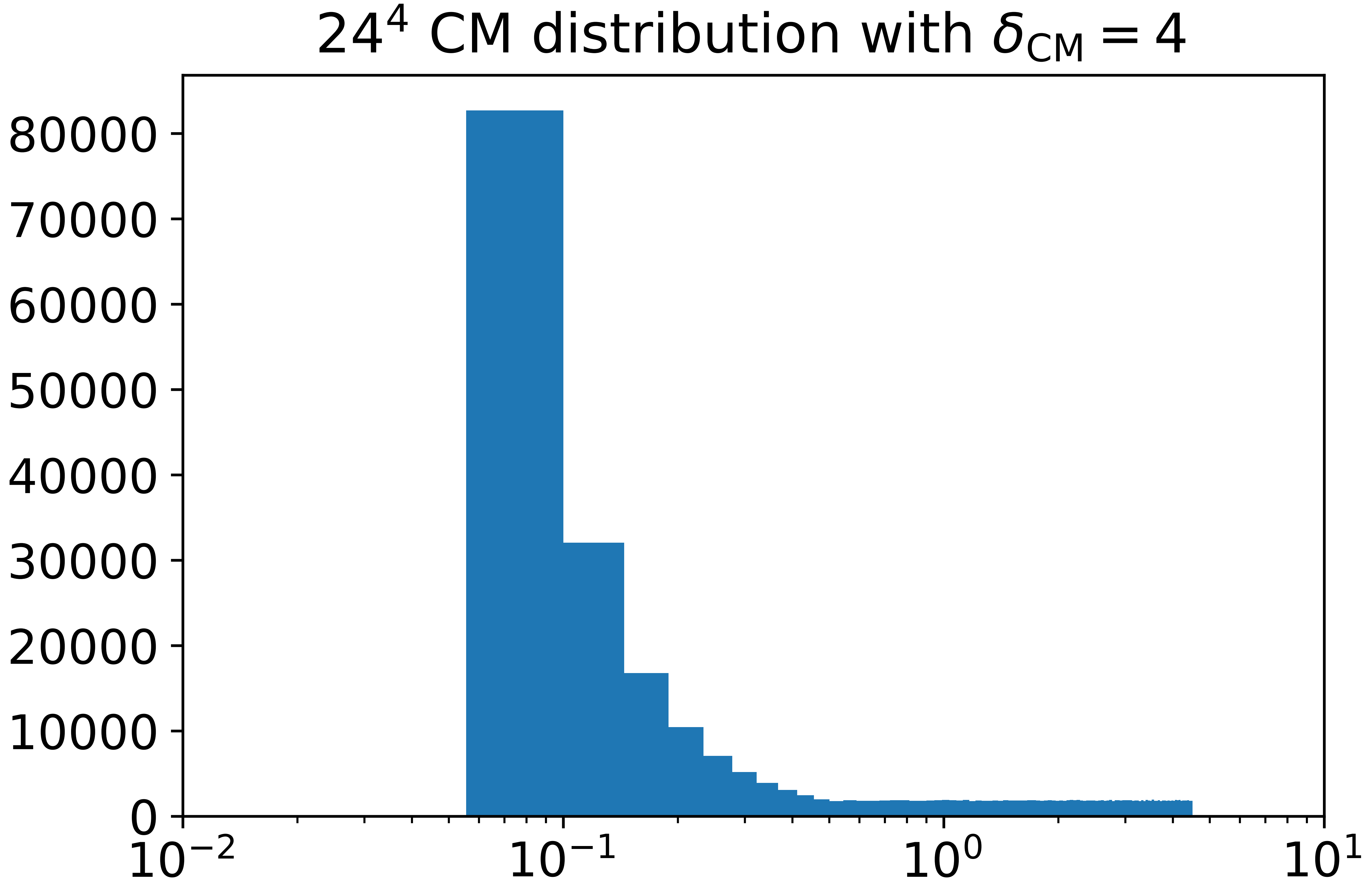
- Modify distribution of conjugate momenta to have different widths, $w_{j,\mu,a}$ which may depend on lattice site, link and/or color
- Draw $h_{j,\mu,a}$ from $\int [dh_{j,\mu,a}] \ \exp\left(-\sum_{j,\mu,a} 2w_{j,\mu,a} h^2_{j,\mu,a}\right)$
- $w_{j,\mu,a} = 1/2$ is normal HMC
- Keep $\Pi_{j,\mu,a} w_{j,\mu,a} = (1/2)^{32N^4}$ for N^4 lattice by choosing weights from $w = 1/2 + \delta_{\mathrm{CM}} \cdot r$ where r is uniformly distributed and $r \in [0,1)$ and then choosing another weight, randomly, equal to $1/w$
- What effect does variable width have on HMC?

Distributions of conjugate momenta

$\delta_{\mathrm{CM}} = 1$



$\delta_{\mathrm{CM}} = 4$



No large effect on HMC from variable width conjugate momenta

Spatially non-local conjugate momentum modes

1. Consider an orthogonal transformation from position space to another basis: $\tilde{\phi} = J\phi$
2. Draw $\tilde{h}$ from $\int [d\tilde{h}_i] \ \exp\left(-\sum_i 2w_i \tilde{h}_i^2\right)$
3. Then in original basis have $\int [dh_i] \ \exp\left(-\sum_{ij} h_i K_{i,j} h_j\right)$ where $K_{i,j} = \sum_m J^{\mathrm{T}}_{i,m} 2w_m J_{m,k}$
4. Index can label lattice site and/or link and/or color
5. $H = \frac{1}{2} \sum_{x,x',\mu',\mu,a,a'} h_{x,\mu,a} K_{x,\mu,a;x',\mu',a'} h_{x',\mu',a'} - S_{\mathrm{W}}$
6. Calculation of K is an $O(N^3)$ calculation

Changes to HMC

1. Initial conjugate momenta chosen as $h_i = \sum_j (J^{-1})_{i,j} \frac{r_j}{\sqrt{2w_j}}$ where r is a random variable chosen from e^{-r^2}

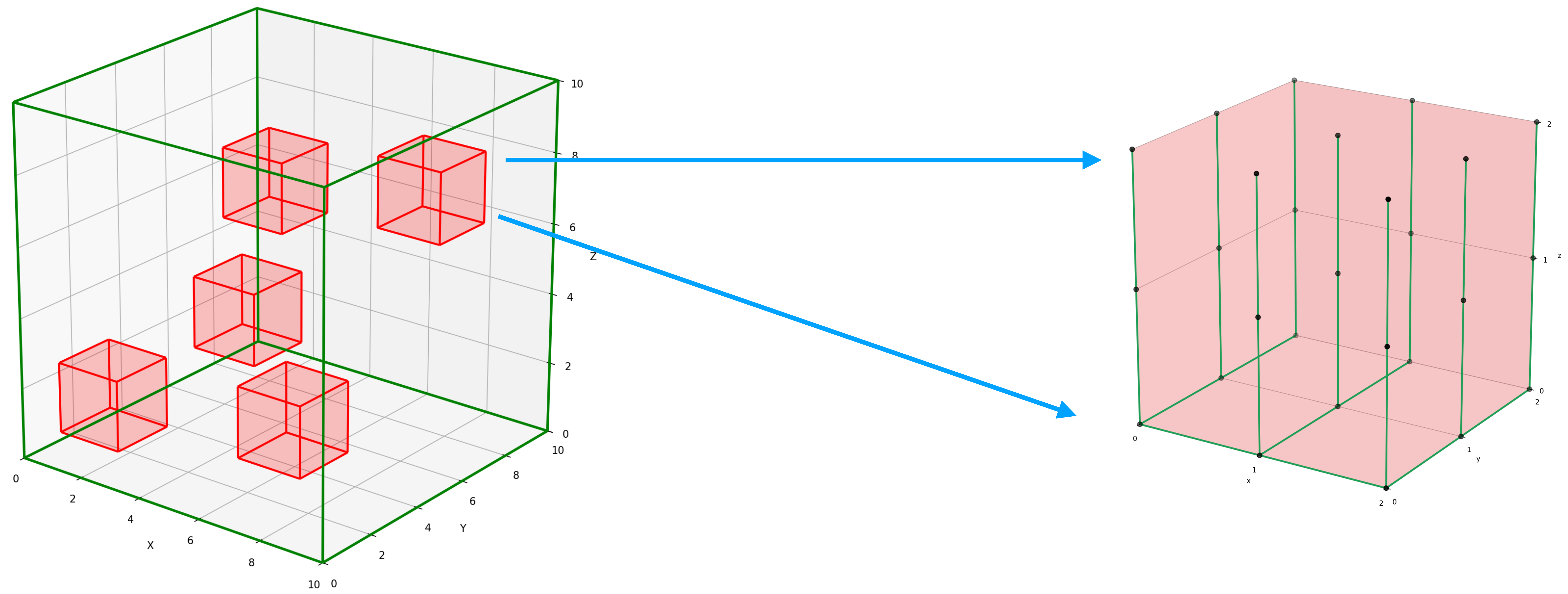
2. Conjugate momentum update for a particular d.o.f. includes non-local terms from forces for other d.o.f: $\dot{h}_i = (K^{-1})_{i,j} F_j$

3. Need to do this in a region of lattice that is in a fixed gauge.

Axial Gauge Evolution

- All d.o.f in a subvolume that are not gauge fixed are put into a lexicographic ordering and a 1-d Fourier transform is done over that ordering to create a non-local basis.

- The ordering has not been chosen with any particular insight



24^4 lattice, $\beta = 6.0$

Variable conjugate momentum width	local	Traj. length	steps	dt	Total traj.	acc.	Integrated autocorrelation time in trajectories	Integrated autocorrelation time in MD time units	plaquette
0	yes	1/2	64	0.0078125	216k	0.81	12.0(1.8)	6.0(0.9)	0.593686(2.4)
0	yes	1	20	0.04	109k	0.90	6.5(8)	6.5(8)	0.593685(2.6)
4.0	10, 3^3 subV	1/2	100	0.005	20k	0.77	5.5(1.0)	2.5(0.5)	0.593683(5)
4.0	12, 4^4 subV	1/2	100	0.005	10.8k	0.77	7.9(1.6)	4.0(0.8)	0.593689(9)

Last 2 rows use Fourier Transform to make spatial CM correlated.

Gauge Fixed Subvolumes

- The calculation of the kernel, $K_{i,j} = \sum_m J^{\mathrm{T}}_{i,m}\, 2w_m\, J_{m,k}$, needs to be done at the start of every trajectory. This is an M^3 calculation, where M is the number of active modes in the sub volume, including color d.o.f
- Using Apple's MLX routines, these dense matrix multiplies can be done on an M4 chip, for example, at more than 10 TFflops. CPU using Eigen sustains ~50 Gflops
- MLX has convenient, easy to use C++ syntax to load and return Eigen C++ matrices.

N^4 is the sub volume size

M is the number of non-gauge fixed d.o.f

N	3	4	5	6	7	8
M	1088	4104	11008	24200	46656	81928

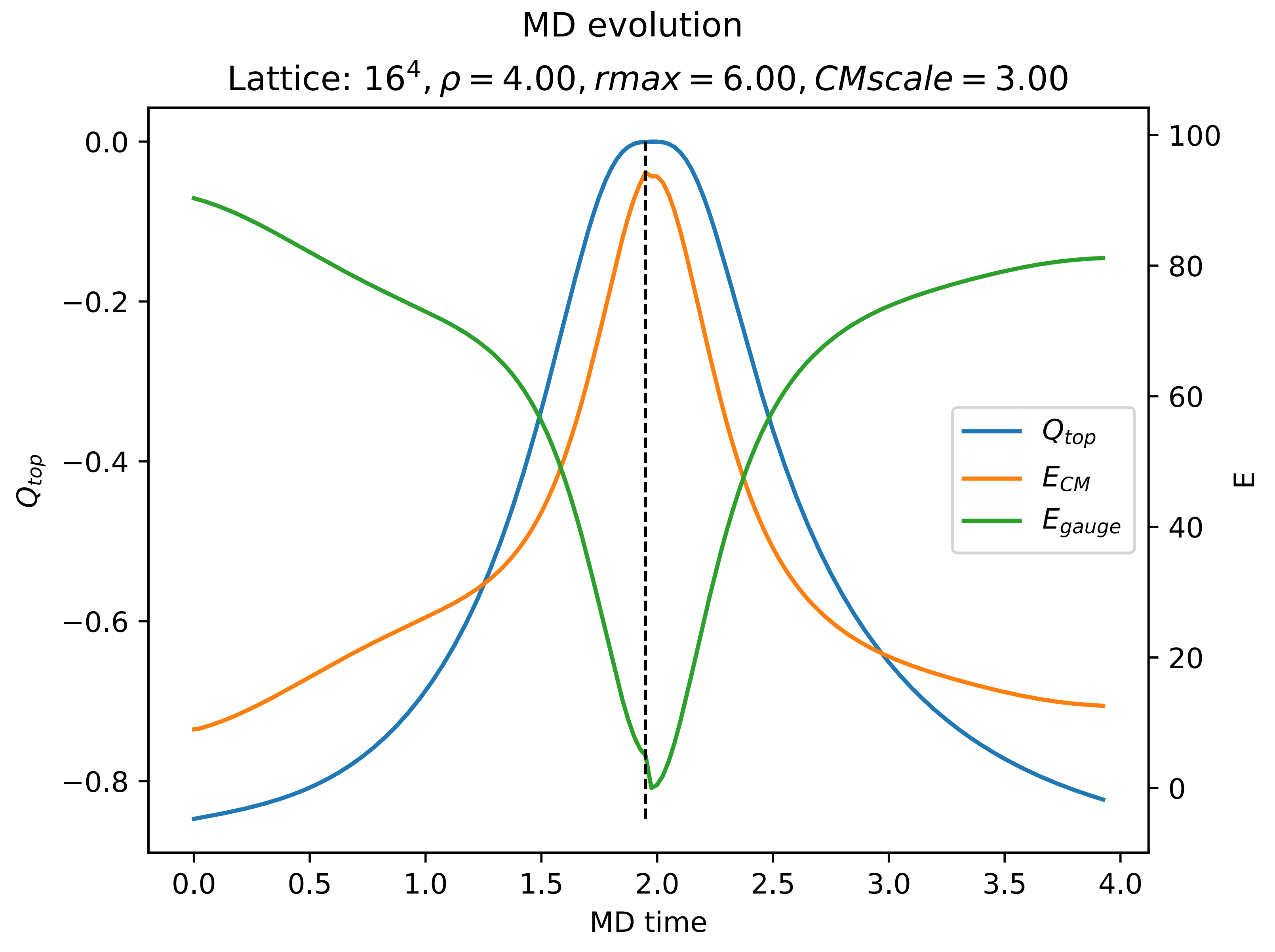
Choosing Coherent Conjugate Momentum Modes

- Have code which allows multiple, gauge fixed subvolumes to be defined and evolved.
- Within the subvolume, an orthonormal basis can be chosen with the goal of promoting better sampling of phase space
- Topology change is an obvious goal
- AI/ML opportunity to help with this
- Starting initial idea, use coherent conjugate momenta that favor topology change in a unit link background gauge field
- Gauge fixing and small subvolumes help keep links close the the identity.

Truncated Instantons and Axial Gauge

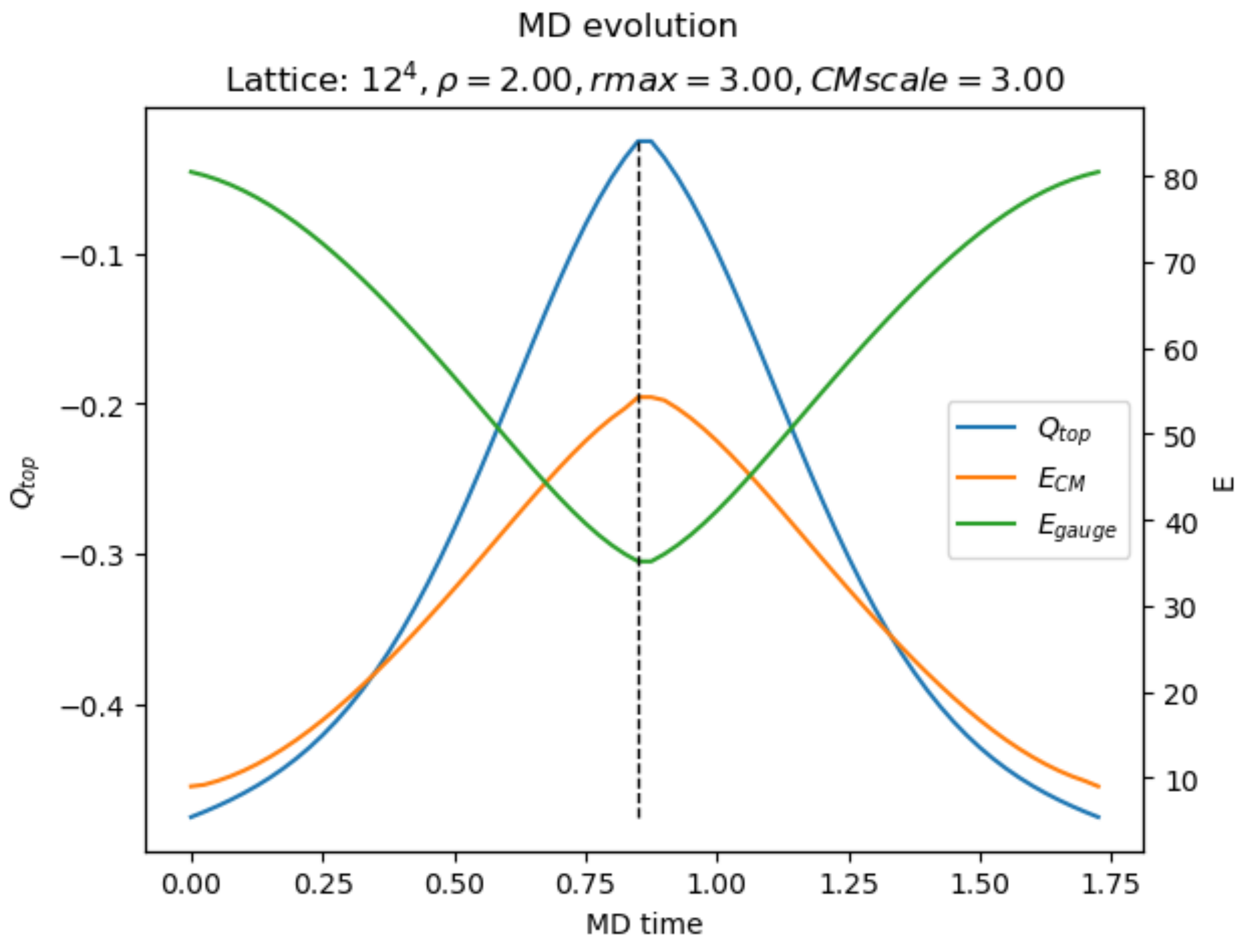
- From a lattice instanton of size ρ and a second instanton of size $\rho - \epsilon$, can get initial conjugate momenta that will shrink the instanton through MD evolution.
- When gauge action is its smallest, set all links to identity and flip sign of conjugate momenta.

Singular gauge



These are not gauge transforms of each other, because different gauge transformations put $I(\rho)$ and $I(\rho - \epsilon)$ into axial gauge.

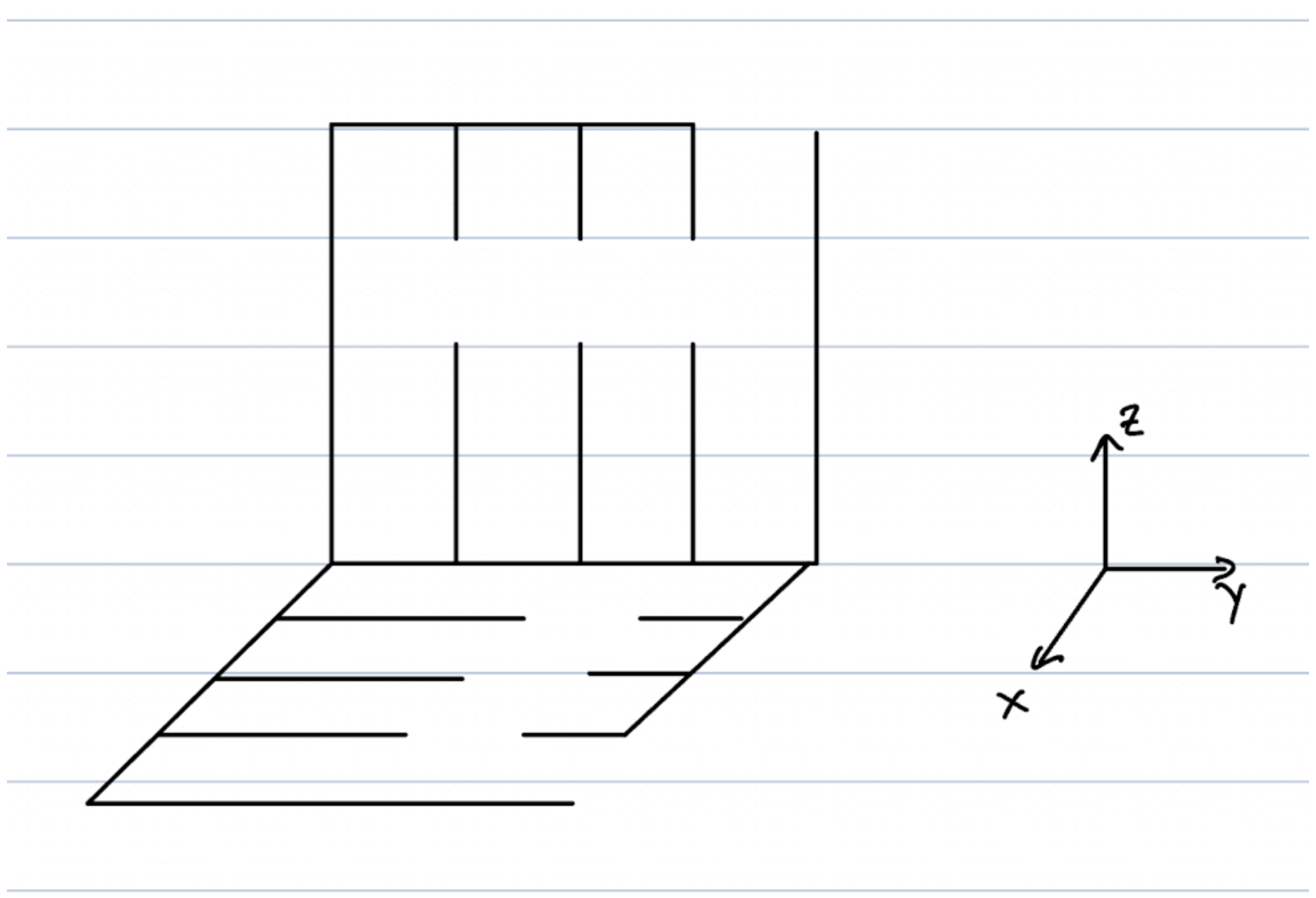
Axial gauge



Truncated Instantons and Internal Gauge

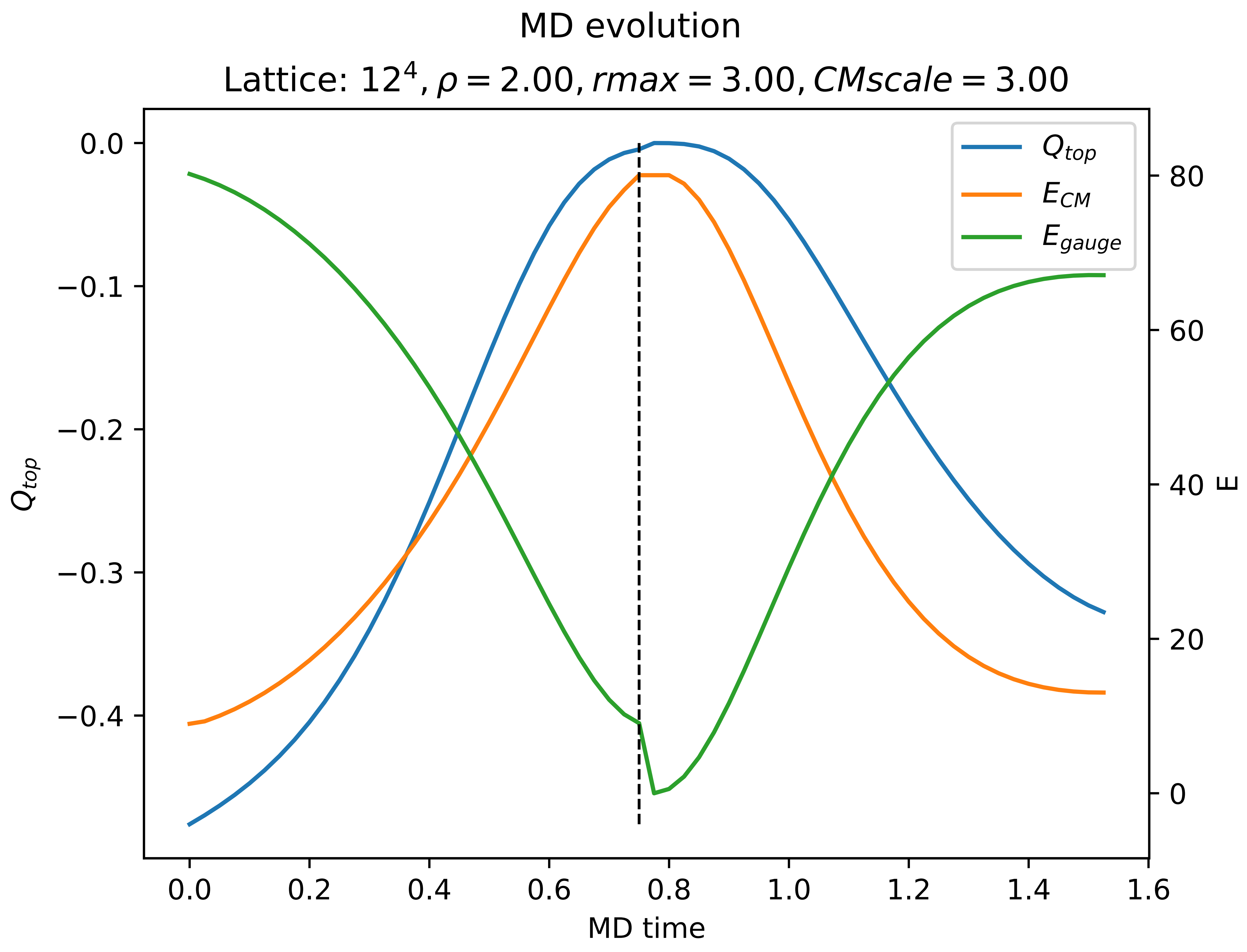
- Axial gauge has gauge fixing matrices far from the identity on the boundaries of the subvolume for the truncated instanton

- Define an internal maximal tree gauge which does not have gauge fixing matrices far from the identity on the boundary



Truncated Instanton Evolution in Internal Gauge

- Now, in a 7^4 subvolume, can start with a truncated instanton and choose initial conjugate momenta to make it shrink
- Evolving with MD, one gets a configuration with $Q_{\text{top}} = 0$ and almost no action in the gauge fields.
- Reversing the conjugate momenta produces a configuration with about 2/3 of the initial value of Q_{top}



Conclusions

- Accurate autocorrelation times are difficult to measure and can impact error on something as simple and local as the plaquette.

- HMC evolutions with coherent conjugate momenta in gauge fixed subvolumes give correct results and more running is needed to see if there is any impact on autocorrelation times.

- Ready to try particular non-local conjugate momentum modes, including ones that drive topology change for lattices with links equal to unity

- There are other ways to imagine choosing coherent conjugate momenta, including having AI train on the many small subvolumes of a large lattice.