Simulating the string formulation of SU(3) lattice gauge theory

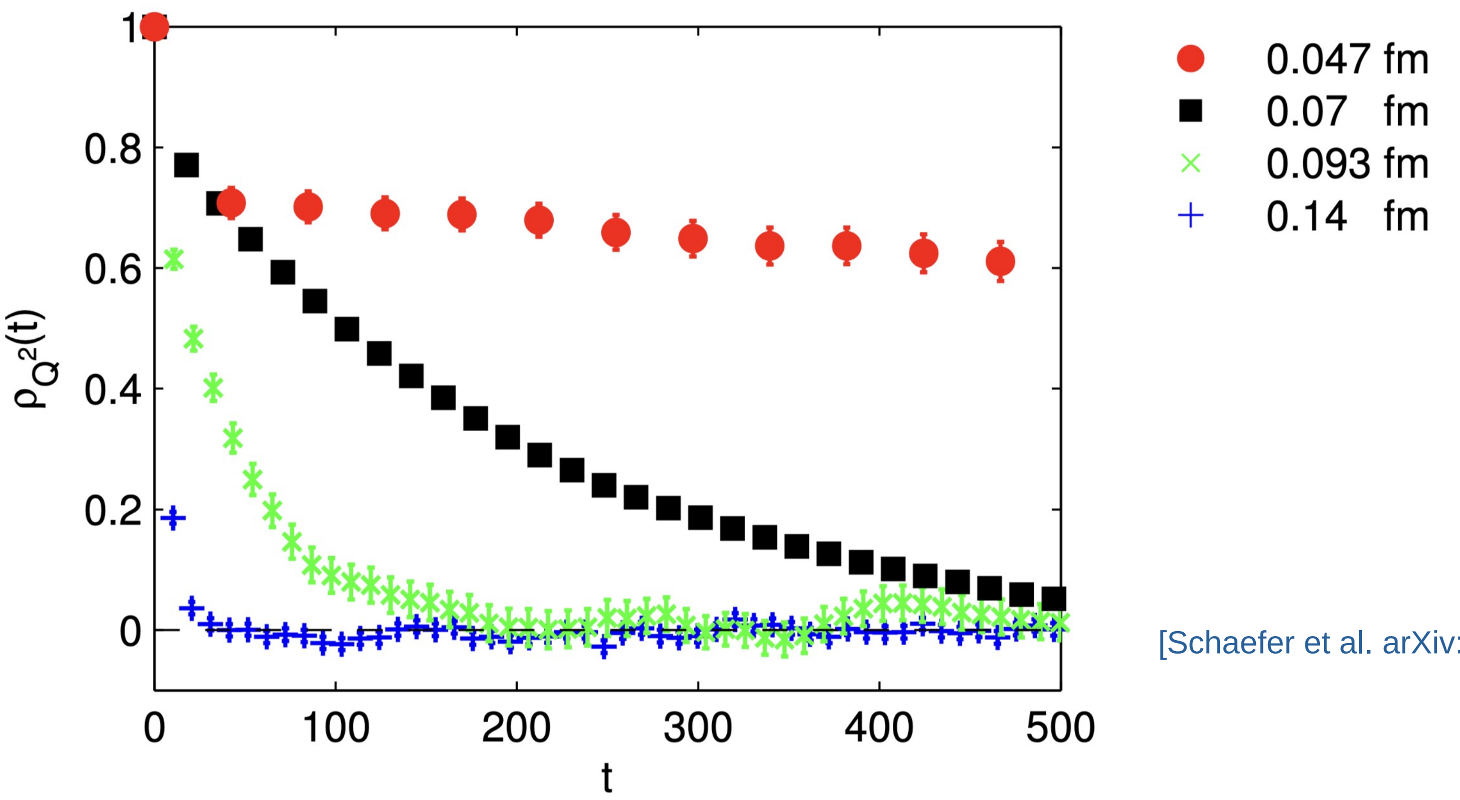
Benjamin Izett

ETH zürich

Overview

Critical slowing down

Increase in cost beyond the naive scaling with the number of sites $\tau_{int} \sim a^{-z}$



[Schaefer et al. arXiv:1009.5228]

If some autocorrelations are longer than the total simulation run then they cannot be detected

Fourier acceleration might help [Batrouni, Phys. Rev. D 32 (1985)] [Davies et al. Phys. Rev. D 37 (1988)] [Horsley et al. arXiv:2308.14628] [Nguygen et al. arXiv:2112.04556] [Duane et al. Phys. Lett. B 176 (1986)] [Davies et al. Phys. Rev. D 41 (1990)] [Christ et al. arXiv:1812.05281]

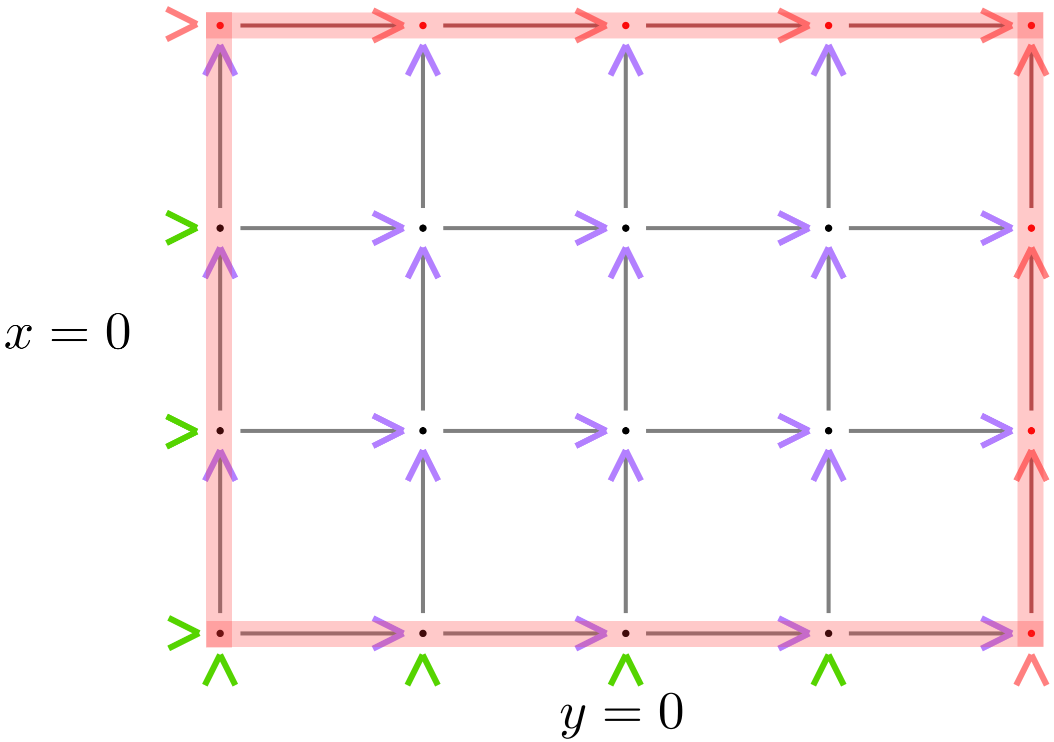
What is the string formulation?

[Batrouni and Halpern, Phys. Rev. D 30 (1984)]

While the usual link variables connect two neighboring sites,

$$V_\mu(x_\mu, x_\perp) = V_\mu(0, x_\perp) \prod_{x'_\mu=0}^{x_\mu-1} U_\mu(x'_\mu, x_\perp)$$

The string variables are Wilson lines along straight paths starting from $(0, x_\perp)$ to $(x_\mu, x_\perp)$

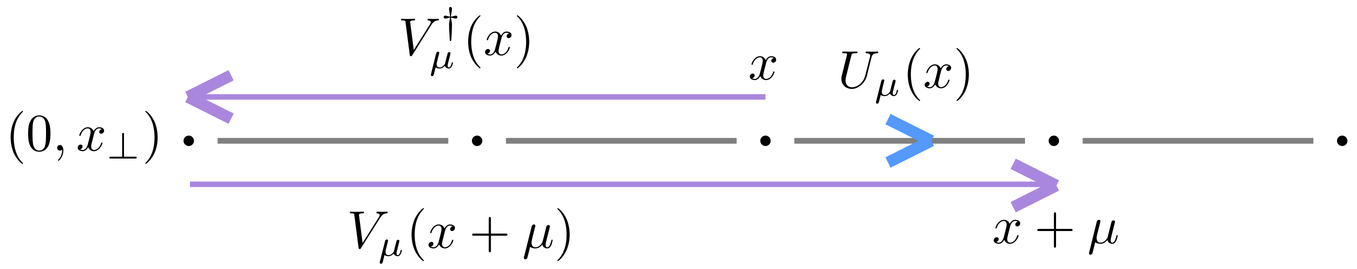


What is the string formulation?

[Batrouni and Halpern, Phys. Rev. D 30 (1984)]

Reconstructing link variables is straightforward

$$U_\mu(x) = V_\mu^\dagger(x) V_\mu(x+\mu)$$



This will be useful when we sample with HMC

We can sample using HMC

[Duane et al, Phys. Lett. B 195 (1987)]

Unit Jacobian and the action remains local in the string variables

[Batrouni and Halpern, Phys. Rev. D 30 (1984)]

$$
\begin{aligned}
Z^U &= \int dV_\mu(0, x_\perp) \int DU \exp\left(-\frac{\beta}{N} \sum_{x,\mu<\nu} \mathrm{Re}\ \mathrm{tr}(1 - P^U_{\mu\nu}(x))\right) \\
&= \int DV \exp\left(-\frac{\beta}{N} \sum_{x,\mu<\nu} \mathrm{Re}\ \mathrm{tr}(1 - P^V_{\mu\nu}(x))\right)
\end{aligned}
$$

$$
\begin{aligned}
P^V_{\mu\nu}(x) =& V^\dagger_\mu(x) V_\mu(x+\mu) V^\dagger_\nu(x+\mu) V_\nu(x+\mu+\nu) \\
& V^\dagger_\mu(x+\mu+\nu) V_\mu(x+\nu) V^\dagger_\nu(x+\nu) V_\nu(x)
\end{aligned}
$$

Can use Hybrid Monte Carlo (HMC) to sample!

HMC for the string formulation

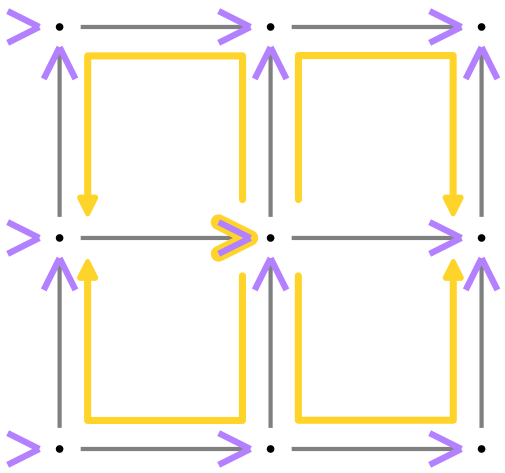
[Duane et al, Phys. Lett. B 195 (1987)]

Introduce conjugate momenta, construct a Hamiltonian and integrate Hamilton's equations of motion

$$H(V,P) = S(V) + T(P) \qquad T = \frac{1}{2}\langle P, P\rangle \qquad P \sim e^{-T(P)}$$

$$\dot{V}_\mu(x) = P_\mu(x) V_\mu(x)$$

$$\dot{P}_\mu(x) = -\partial_{\mu,x} S(V) \equiv F_\mu^V(x)$$



Accept new configuration with probability $\min\left\{1, e^{-\Delta H(V,P)}\right\}$

Need to compute **action** and **molecular dynamics force**

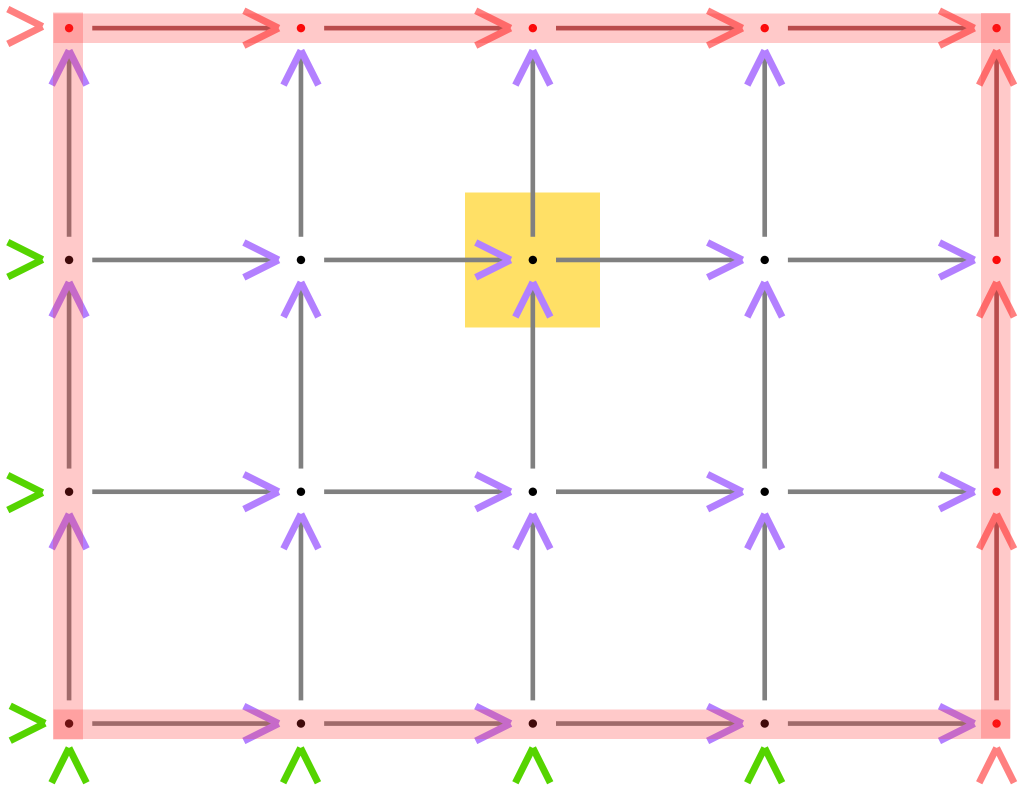
General property:

$$F_\mu^V(x) = V_\mu(x-\mu) F_\mu^U(x-\mu) V_\mu^\dagger(x-\mu) - V_\mu(x) F_\mu^U(x) V_\mu^\dagger(x)$$

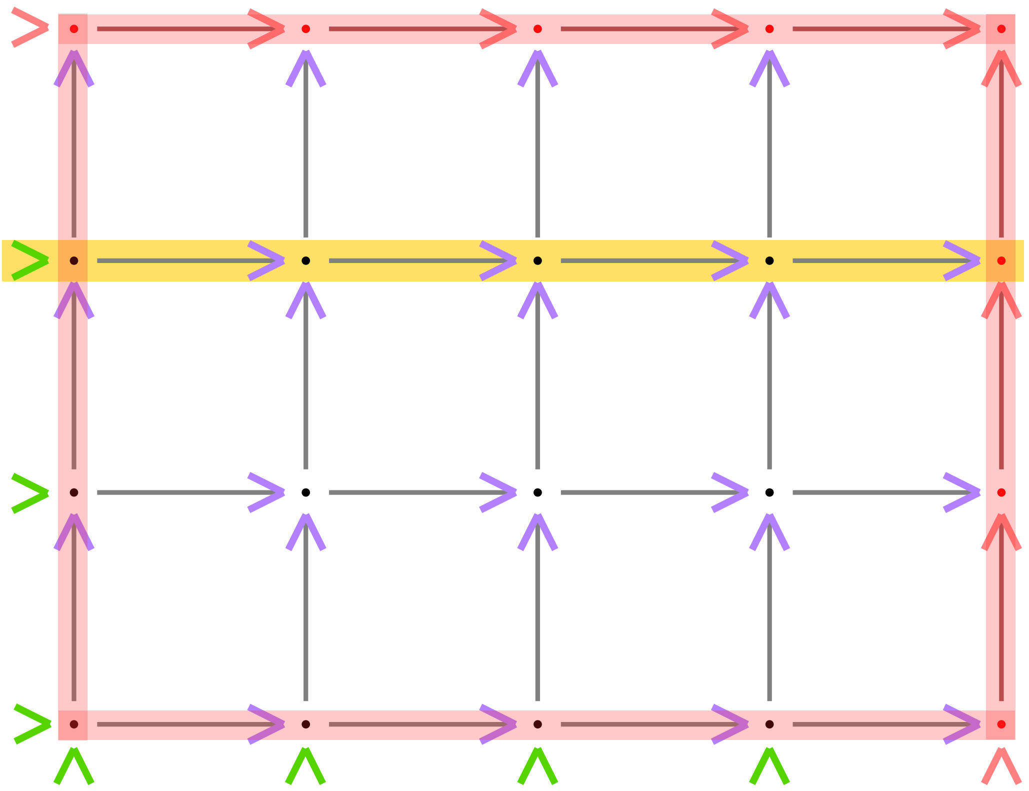
Gauge transformations for string variables

[Batrouni and Halpern, Phys. Rev. D 30 (1984)]

$$V_\mu(x) \to V_\mu(x)\Omega^\dagger(x)$$



$$V_\mu(x) \to G_\mu(x_\perp)V_\mu(x)$$



The MD force transforms differently under gauge symmetry

Under the general transformation

$$U_\mu(x) \to \Omega(x) U_\mu(x) \Omega^\dagger(x+\mu)$$
$$F^U_\mu(x) \to \Omega(x) F^U_\mu(x) \Omega^\dagger(x)$$

In contrast, under

$$V_\mu(x) \to G_\mu(x_\perp) V_\mu(x) \Omega^\dagger(x)$$

We find that

$$\boxed{F^V_\mu(x) \to G_\mu(x_\perp) F^V_\mu(x) G^\dagger_\mu(x_\perp)}$$

Original local gauge symmetry does not appear

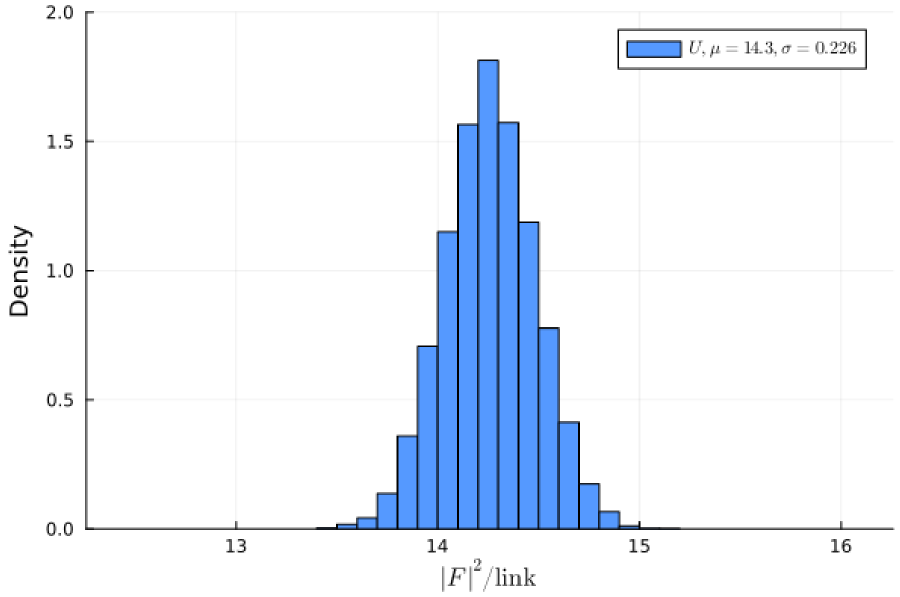
Useful for Fourier acceleration?

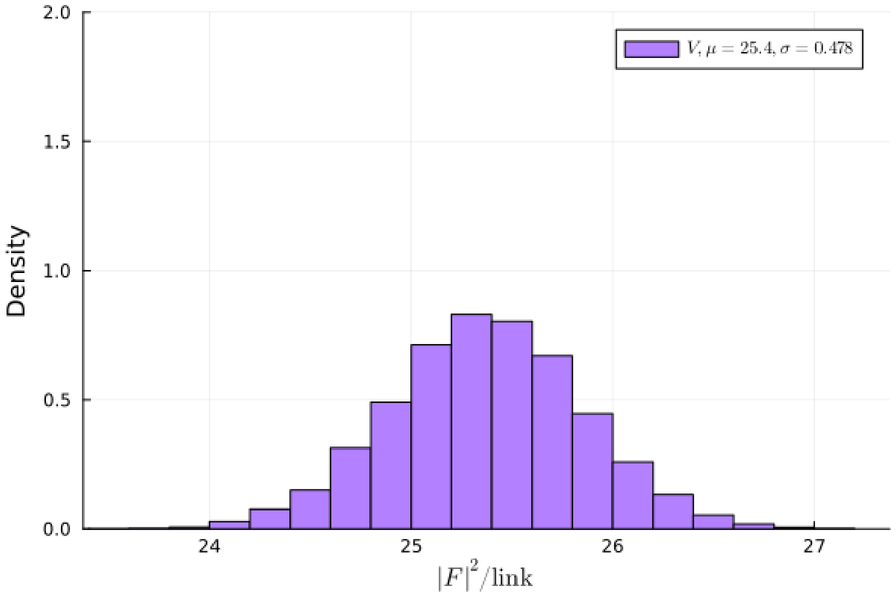
HMC for the string formulation

Compared runs to Wilson formulation SU(3) 4D

Consistent observables (plaquette, Wilson loops) and $\langle e^{-\Delta H} \rangle = 1$

Distribution of the norm of the force on 8^4, $\beta = 6$, with 48 leapfrog steps (Wilson: left, string: right)





Must use smaller integration steps [Schaefer, arXiv:1211.5069]

Fourier acceleration solves free scalar Critical Slowing Down

[Batrouni, Katz, Kronfeld, Lepage, Svetitsky, Wilson]

[Batrouni, Phys. Rev. D 32 (1985)]
[Duane et al, Phys. Lett. B 176 (1986)]
[Davies et al, Phys. Rev. D 37 (1988)]
[Davies et al, Phys. Rev. D 41 (1990)]

Consider free scalar theory $H = \frac{1}{2}\pi^2 + \frac{1}{2}\phi(m^2 - \partial^2)\phi$

Look at evolution in HMC time τ

$$\ddot{\phi}(\tau, x) = -(m^2 - \partial^2)\phi(\tau, x)$$

$$\omega^2(k) = m^2 + k^2 \qquad \tau \overset{\mathcal{F}}{\leftrightarrow} \omega \quad x \overset{\mathcal{F}}{\leftrightarrow} k$$

Modify kinetic term $\frac{1}{2}\pi(1 - \kappa + \kappa\partial^2)^{-1}\pi$ with acceleration parameter $\kappa \in (0, 1)$

$$\ddot{\phi}(\tau, x) = -(1 - \kappa + \kappa\partial^2)^{-1}(m^2 - \partial^2)\phi(\tau, x) \implies \omega^2(k) = \frac{m^2 + k^2}{1 - \kappa + \kappa k^2}$$

Want evolution of modes to be independent of momentum $\kappa = \frac{1}{1 + m^2}$

Modified dynamics cheap using FFTs $\mathcal{O}(N \log N)$

Issues with non abelian Fourier acceleration

The conjugate momenta transform like the molecular dynamics force

$$P_\mu^U(x) \to \Omega(x) P_\mu^U(x) \Omega^\dagger(x)$$

Including ∂_μ in the kinetic term breaks gauge covariance of equations of motion

Two solutions identified:

$\partial_\mu \to D_\mu$ must invert gauge field and can no longer use FFTs

Or gauge fix, recently soft gauge fixing tried but needs costly inner Monte Carlo

[Davies et al. Phys. Rev. D 37 (1988)]
[Duane et al. Phys. Lett. B 176 (1986)]
[Duane et al. Phys. Lett. B 206 (1988)]
[Girolami et al. Stat. Methodology B (2011)]
[Sheta et al. arXiv:2108.05486]
[Nguyen et al. arXiv:2112.04556]
[Jung et al. arXiv:2401.13226]

String formulation may provide an alternative

Keep equations of motion covariant, continue using ∂_μ and FFTs without fixing local gauge symmetry

Paper with string formulation was already referenced in early FA literature but this referred to a corner variables [Batrouni, Phys. Rev. D 32 (1985)]

Fourier acceleration with string variables

The momenta conjugate to the string variables transform as

$$P^V_\mu(x_\mu, x_\perp) \to G_\mu(x_\perp) P^V_\mu(x_\mu, x_\perp) G^\dagger_\mu(x_\perp)$$

Notice that without any changes we can try

$$T_{\text{FA}} = \frac{1}{2} \sum_{x,\mu} \langle P_\mu(x), (K_\mu^{-1} P_\mu)(x) \rangle \qquad P_\mu(x) \sim (K_\mu^{1/2} \xi)(x)$$

$$K_\mu^{-1} = \frac{1}{1 - \kappa + \kappa \partial_\mu^2}$$

Good first step, must remove line redundancy next

Fourier acceleration with string variables

What should we expect from the partial acceleration

Consider free limit $\beta \to \infty$

$$U_\mu(x) = \exp(iaA_\mu(x))$$

$$V_\mu(x) = \exp(ia\phi_\mu(x))$$

$$\ddot{A}_\mu(k) = -\sum_\nu M_{\mu\nu}(k) A_\nu(k)$$

$$U_\mu(x) = V_\mu^\dagger(x) V_\mu(x+\mu)$$

$$M_{\mu\nu}(k) = k^2 \delta_{\mu\nu} - k_\mu k_\nu$$

$$A_\mu(x) = \phi_\mu(x+\mu) - \phi_\mu(x) = \partial_\mu \phi_\mu(x)$$

$$\omega_U^2(k) \sim k^2$$

$$\omega_V^2(k) \sim k^4$$

[Duane et al, Phys. Lett. B 176 (1986)]

Critical slowing down is worse with the string formulation!

Fourier acceleration with string variables

Compute the integrated autocorrelation times for the flowed energy density

Large flow times show dependence on longer modes [Lüscher, arXiv:1006.4518] [Christ et al, PoS LATTICE2024 466 (2025)]

$$L = 12^4 \qquad \beta = 6, 7, 10$$

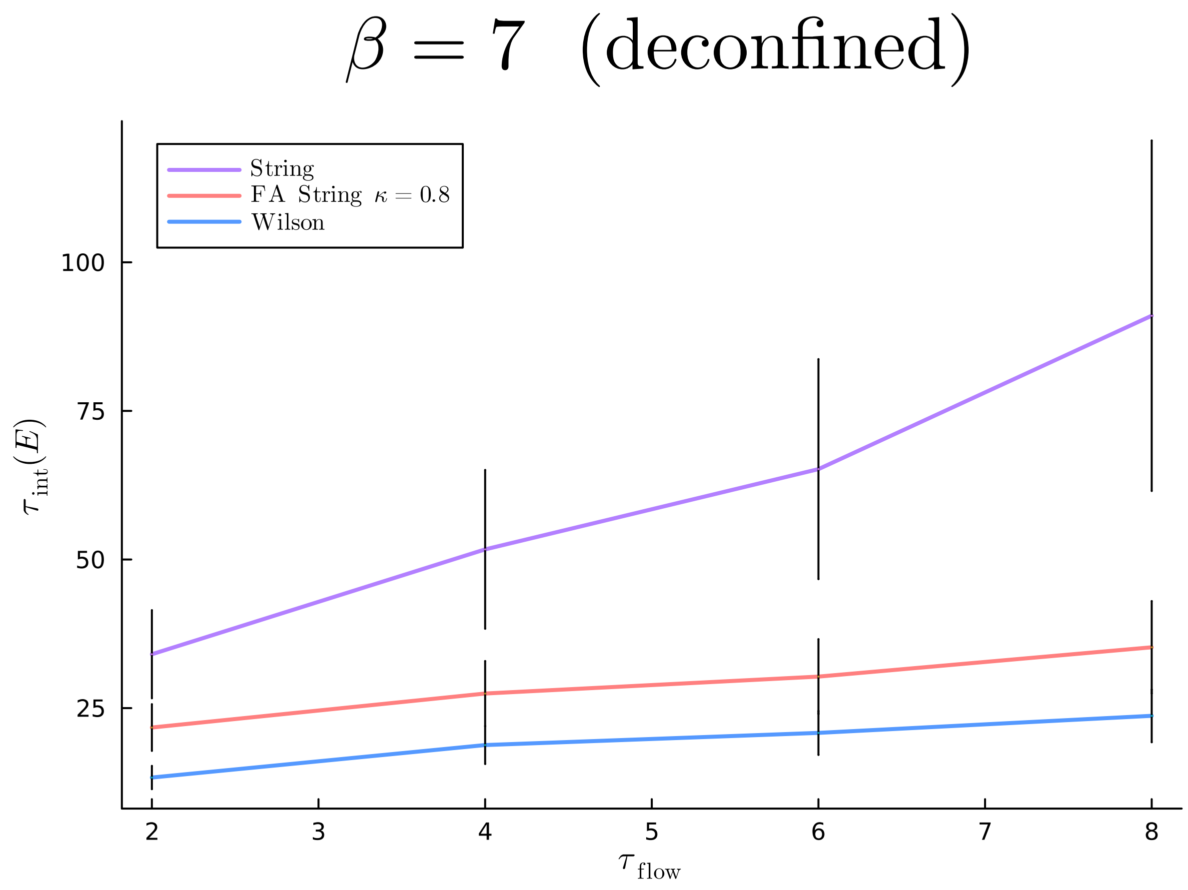
Sample 20000 trajectories, acceptance rate ~ 90%

Acceleration parameter $\kappa = 0.8$

$$\Delta\tau^{FA} \approx 1.5\Delta\tau$$

Fourier acceleration results

Integrated autocorrelation time of flowed energy density against flow time

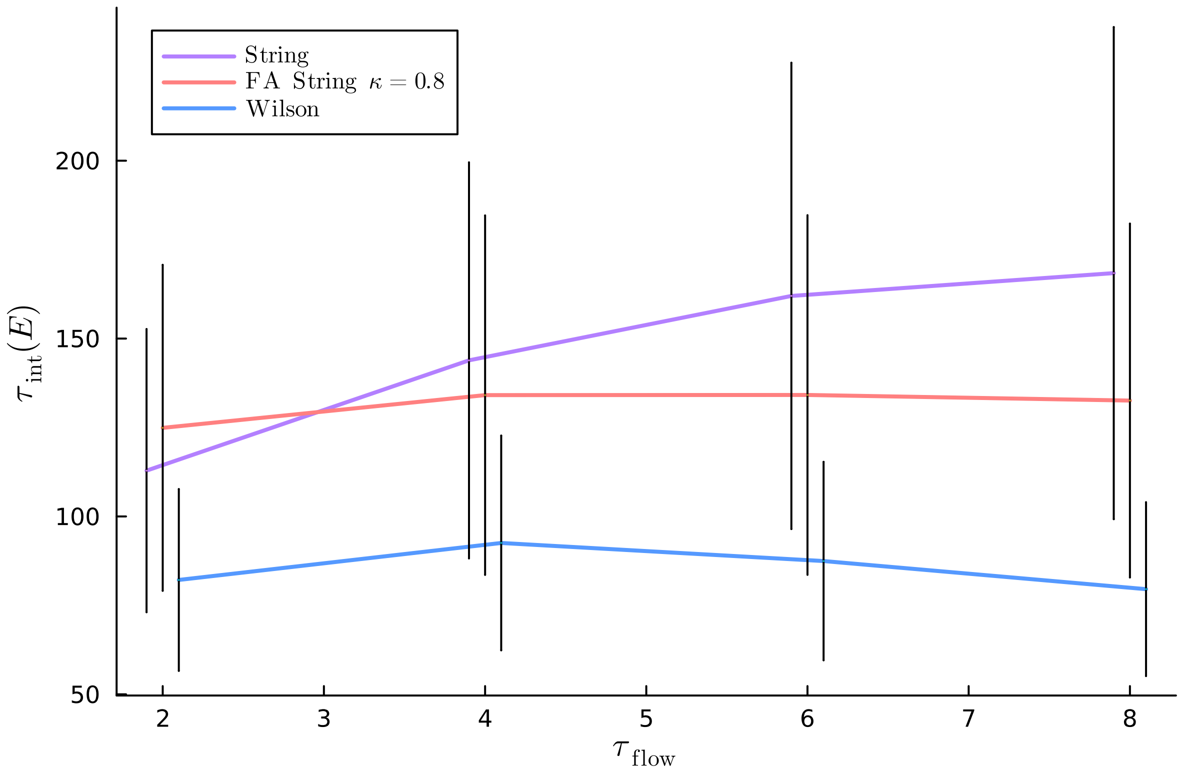


FA is working!

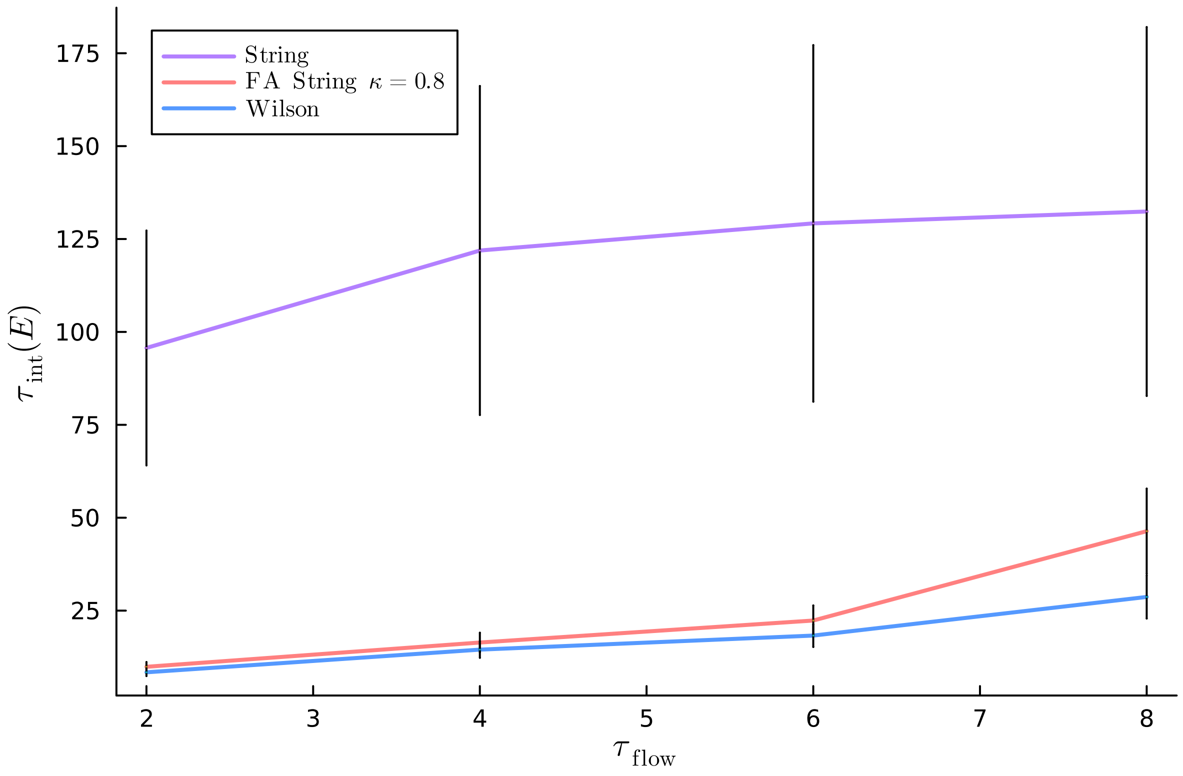
Fourier acceleration results

Integrated autocorrelation time of flowed energy density against flow time

$$\beta = 6 \quad \text{(confined)}$$



$$\beta = 10 \quad \text{(deconfined)}$$



Outlook

Reviewed the string formulation of lattice gauge theory

Simulations can be done using HMC, action and force are straightforward to compute, but needs smaller integration step size

Different gauge transformation properties allow for partial acceleration with regular derivative and without gauge fixing

Alone this is not better than the usual Wilson formulation

Next step is to remove line redundancy, some possibilities are

Use in DD-HMC, define strings relative to inactive sites [Lüscher, arXiv:hep-lat/0409106]

Change formulation such that all lines are connected to origin

Further autocorrelation studies must be done with more observables and larger lattices

Need to tune acceleration parameter and trajectory length

The High Performance Computation Physics Group at ETH