Localized machine learned flow maps to accelerate Markov Chain Monte Carlo simulations

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Berlin - Activate Workshop

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Motivation

- Standart Model of Particle Physics
- Monte Carlo simulation of lattice gauge theories

Gauge equivariant/normalizing flows

J. F., arXiv:2201.02216

- Proposal via flows
- Domain Decomposition
- Applications in 2D

Fine graining flows in 2D

J. F., arXiv:2402.12176

- Maps and training
- Tunneling rate

Global corrections with the fermion determinant

- Domain decomposition of fermions
- Towards high acceptances

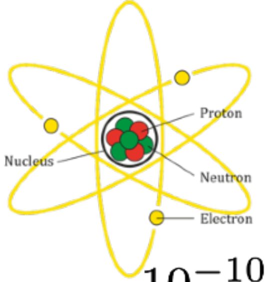
Motivation

The length scale of our known world

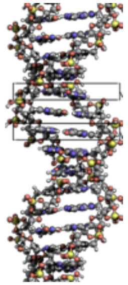
Planck scale

Standard Model of particle physics

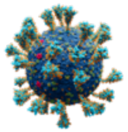
Atom



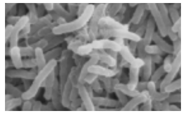
DNA



Coronavirus

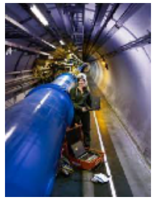


Bakteria



Ant

Large Hadron Collider

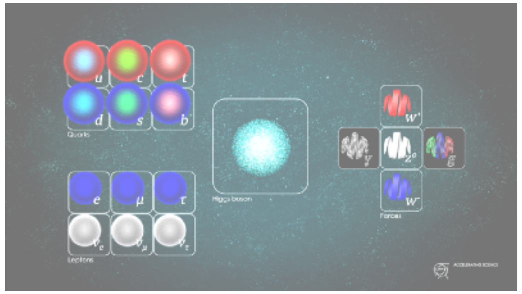


Sun

Universe

10^{-35} 10^{-20} 10^{-15} femto meter 10^{-10} angstrom 10^{-9} nano meter 10^{-8} 10^{-7} 10^{-6} micro meter 10^{-5} 10^{-3} milli meter 1 meter 10^{3} kilo meter 10^{9} 10^{26}

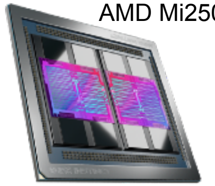
scale in meter



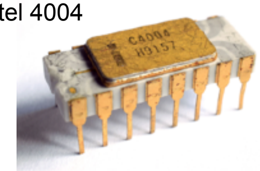
metal–oxide–semiconductor field-effect transistor scaling

2024 ?	2016	2003	1984	1971
$2\ nm$	$10\ nm$	$90\ nm$	$1\ \mu m$	$10\ \mu m$

AMD Mi250X



Intel 4004



Standard Model

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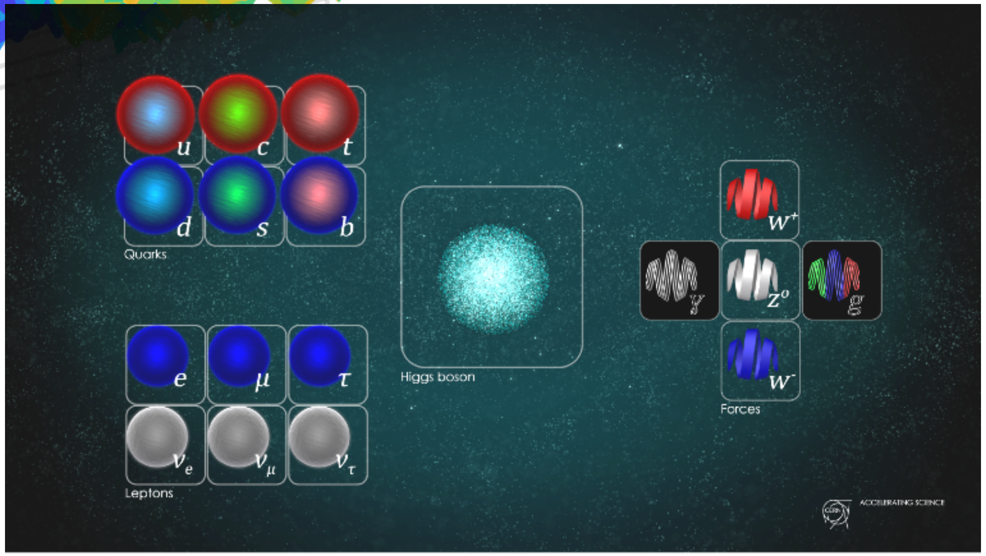

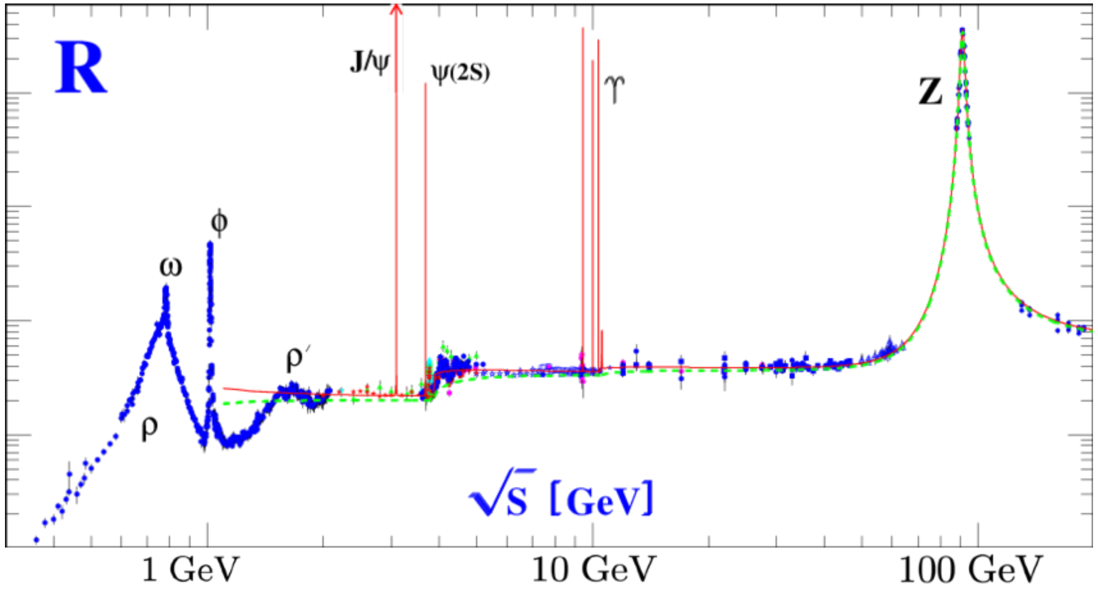

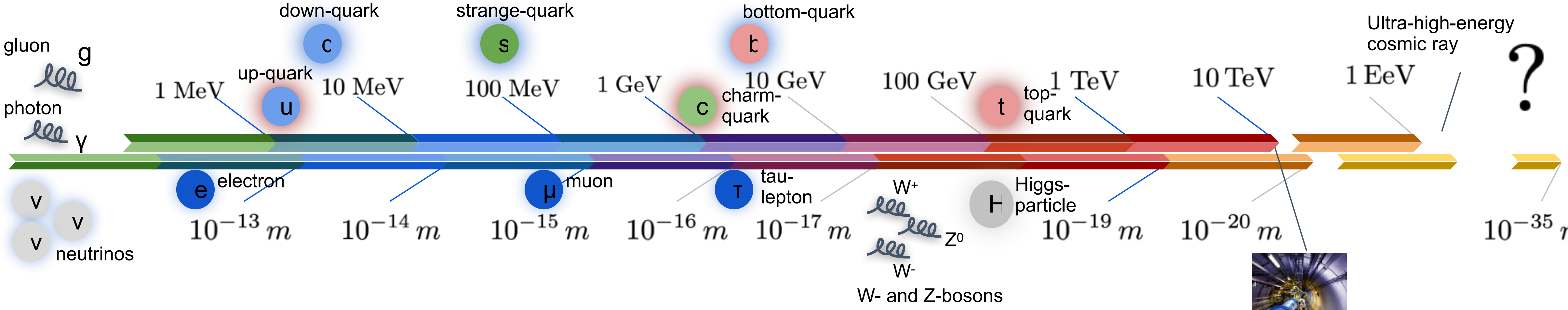

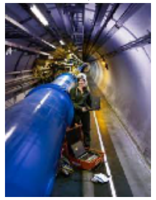

Collision energy
Large Hadron Collider

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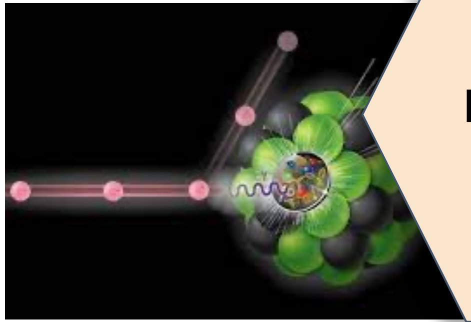
Standard model

Understanding the building blocks of our world

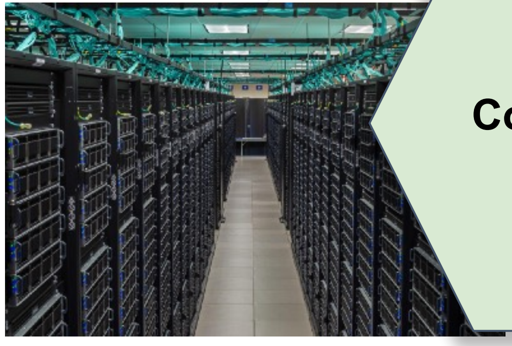
Particle Collider: like LHC or future EIC



Experiment

Theory

Computation

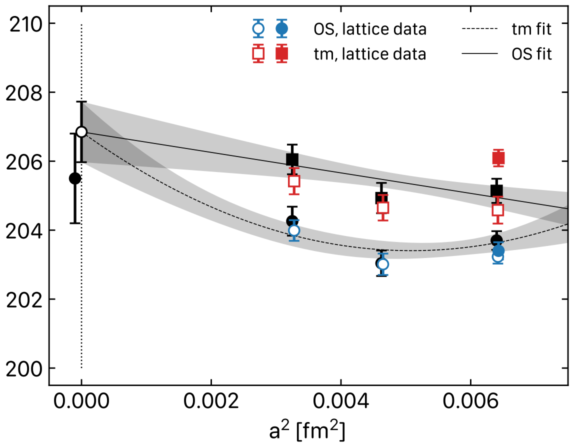


Lagrangian of Standard model - QED, QCD, Weak Interactions - solvable via perturbation theory at high energy

$$
\begin{aligned}
\mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\
& + i \bar{\Psi} \not{D} \psi \\
& + D_\mu \Phi^\dagger D^\mu \Phi - V(\Phi) \\
& + \bar{\Psi}_L \hat{Y} \Phi \Psi_R + h.c.
\end{aligned}
$$

At low energies QCD is non-perturbative
⇨ Lattice QCD only known ab initio method to predict

- Constituents of matter
- Zoo of baryonic states

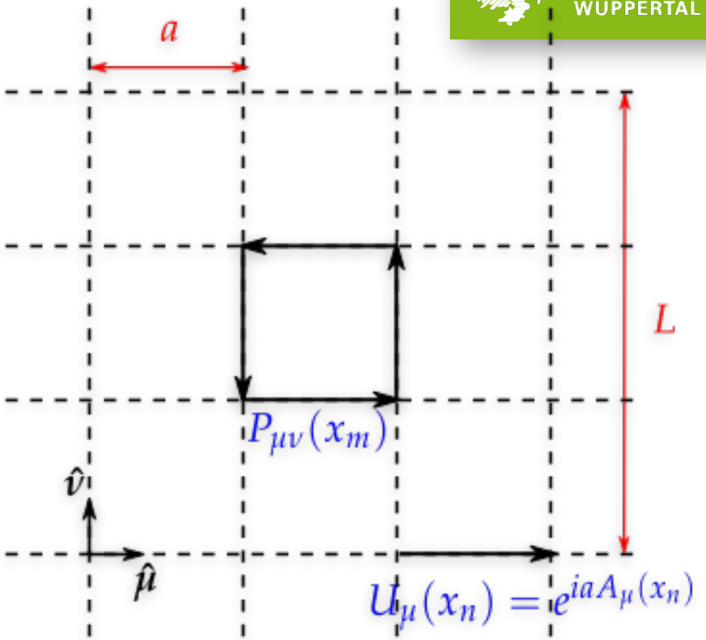


Simulation at the Precision Frontier:
Markov chain Monte Carlo

$$\langle \mathcal{O} \rangle = \int D[U,\phi]\ \mathcal{O}(U) \cdot \rho(U)$$

where

$$\rho(U) = Z^{-1} \left(\prod_j^{N_f} \det D_j(U) \right) e^{-\beta_g(U)}$$



Lattice QCD:
❖ 4 dimensional lattice: V=L x L x L x T
❖ State of the art   V = 2* (96^3) points

❖ physical degrees of freedoms:
SU(3) matrices, 8 real numbers per matrix

❖ SU(3) matrices are acting as parallel transporter between points:
-> 4*V links

High dimensional integral
❖ possible to solve via Markov chain Monte Carlo methods

here, we will mainly use:

We will discuss mainly the 2D-Schwinger model with U(1) links

Generic models are only applied to *pure gauge weight*

$$\rho_{PG} \propto \exp\{-\beta S_g(U)\}$$

And fermions are treated via correction steps

$$\rho_f \propto \prod_j^{N_f} \det D_j(U)$$

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Critical slowing down

here: 2D Schwinger Model

Markov chain Monte Carlo algorithm

Standard large scale MCMC method:

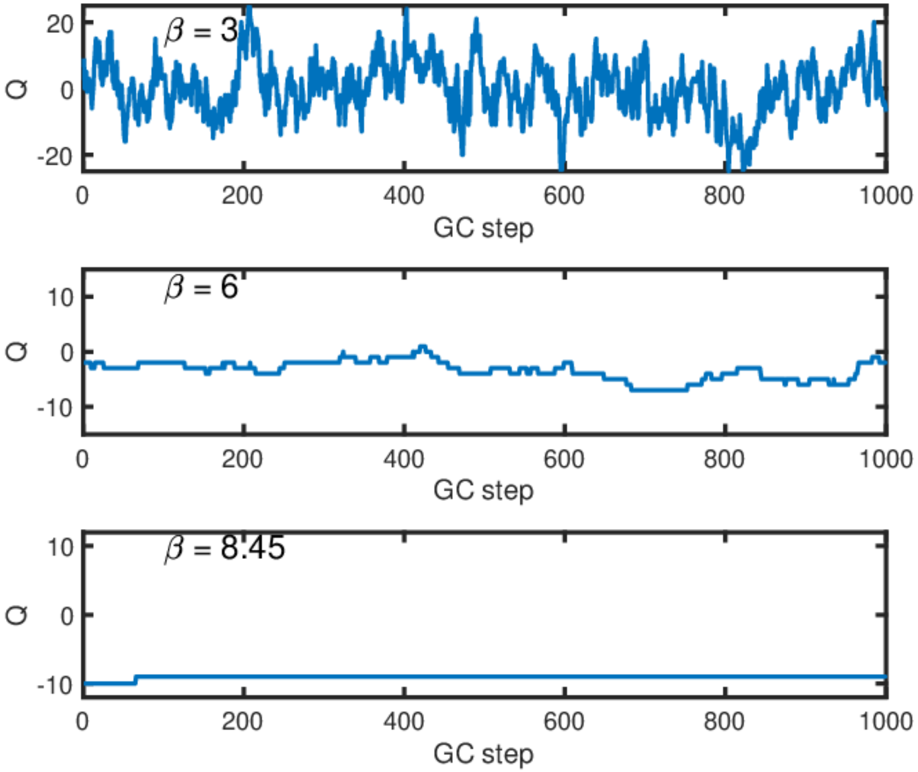
- Hybrid Monte Carlo (HMC) algorithm
  - based on molecular dynamics

$$\dot{P} = -\frac{\partial H}{\partial U} \quad \text{and} \quad \dot{U} = \frac{\partial H}{\partial P}$$

❖can be integrated using numerical integrators
❖Sampling configuration in field space

❖Ensemble average over these configurations:

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_i \mathcal{O}(U_i) + \sqrt{\frac{2\tau_{int}\sigma^2}{N}}$$



❖ for very fine lattice spacings a<0.05 fm sampling of independent configuration becomes hard $\tau_{int} \gg 1$
❖ the HMC algorithm freezes out a topological sector

severe critical slowing down

- Efficient algorithm in QCD missing (openBC would be a possibility)

S. Schaefer et al., Null. Phys. B 845 (2011) 93-119

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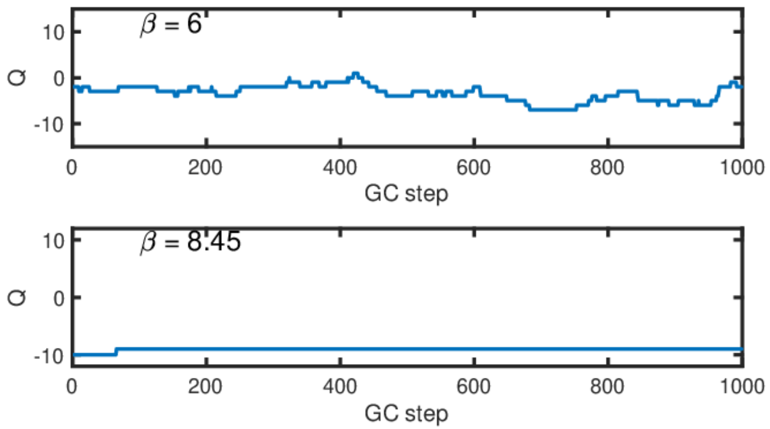
General structure of a MCMC algorithm:

1. Propose U' according to $T_0(U \to U')$
2. Correct with $P_{acc}(U \to U') = \min\left[1, \frac{\tilde{\rho}(U)\rho(U')}{\rho(U)\tilde{\rho}(U')}\right]$



MCMC samples sufficient if:

❖ Proposal can efficiently propose independent configurations
❖ Correction steps has a good acceptance rate

Sampling via HMC simulations are suffering from point 1.)
❖ integrating Molecular Dynamics induces only small changes in the fields

❖ **How to improve that ?**

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Idea: Sampling from an independent distribution

Idea: starting from a unitary distribution and map into target space

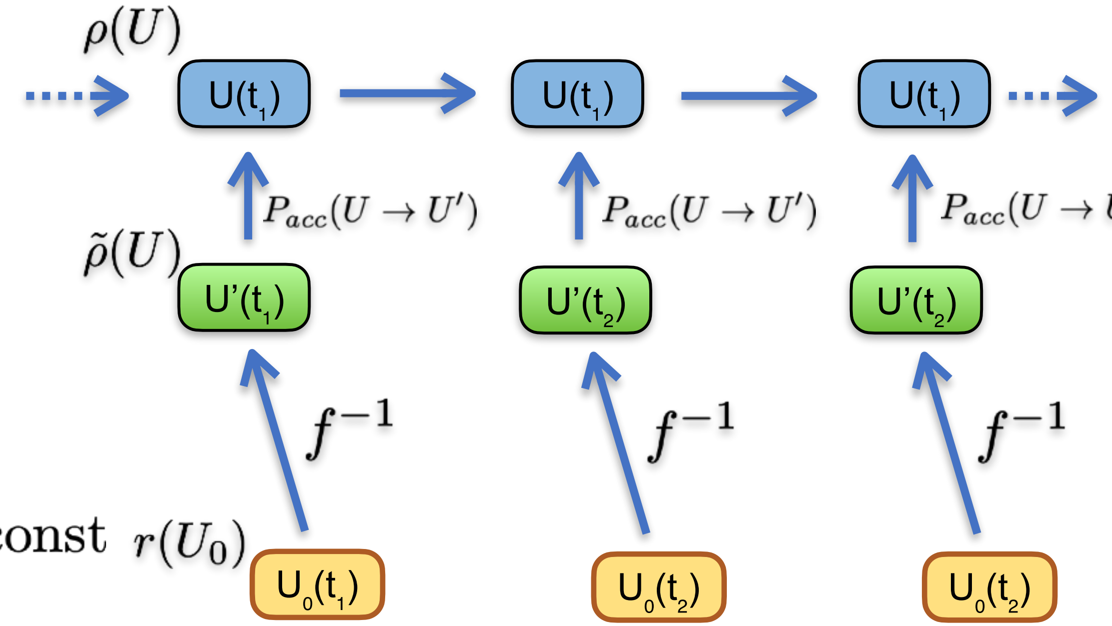
★**Trivialising maps**: Luescher, Commun.Math.Phys. 293 (2010)

- start from a trivial distribution $r(U_0)$
- construct field transformation towards target distribution $f^{-1}(U_0) \to U$

Flow distribution is given then by the Jacobian of the transformation

$$\tilde{\rho}(U) = r(f(U)) \cdot \left|\det \frac{\partial f(U)}{\partial U}\right|$$

Trivialising Map: $$\ln(\tilde{\rho}(f^{-1}(U_0))/\rho(f^{-1}(U_0))) = \text{const}$$



Maps can be parametrised and learned:

- ✦ Continuous flows — Bacchio et al., arXiv:2212.08469
- ✦ Equivariant flows using neural networks
  Here, we will use

Albergo et al., Phys.Rev.D 100 (2019) 3, 034515

Kanwar et al., Phys.Rev.Lett.125 (2020) 12, 121601

Boyda et al., Phys.Rev.D 103 (2021) 7, 074504

Albergo et al., arXiv:2101.08176

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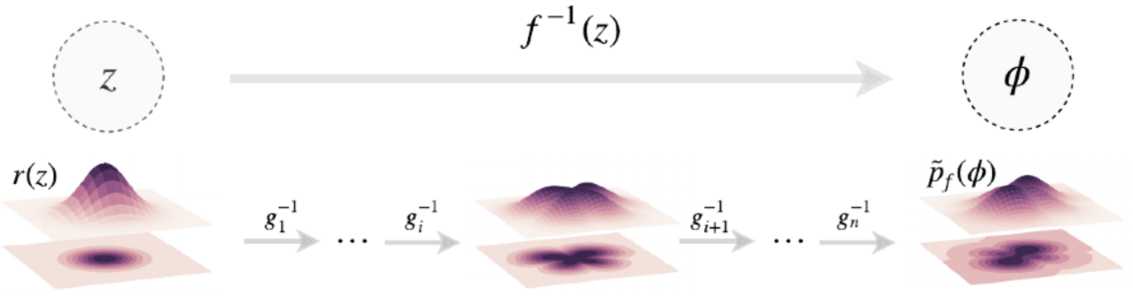
Generative model

Generative model in ϕ^4 - model (U(1)) with normalising (gauge invariant) flow

Albergo et al., Phys.Rev.D 100 (2019) 3, 034515



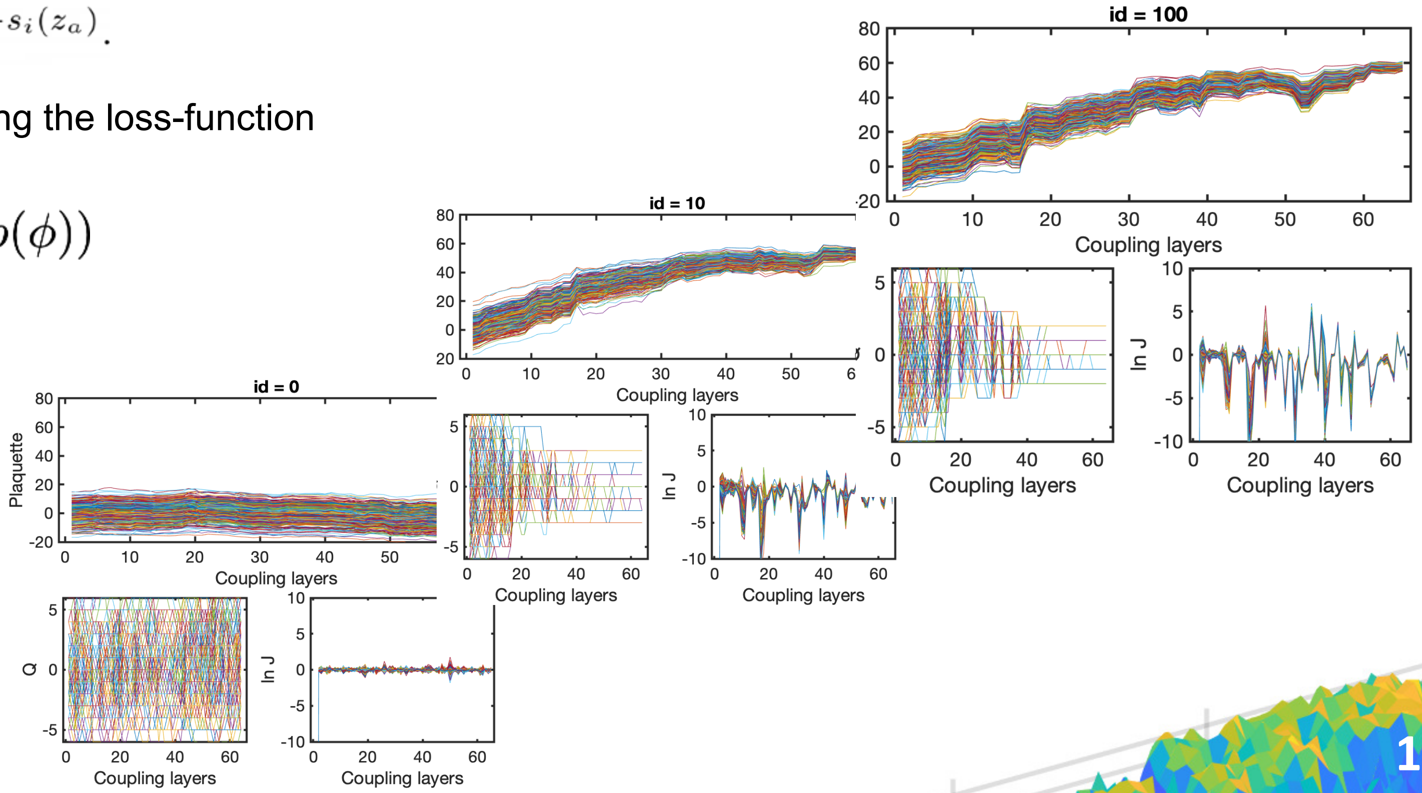
$$\tilde{\rho}(U) = r(f(\phi)) \prod_j \det J(g_j^{-1}(\phi^{(i)}, s_i, t_i))$$

- introduce coupling layers with

$$g_i^{-1}(z) := \begin{cases} \phi_a = z_a \\ \phi_b = (z_b - t_i(z_a)) \odot e^{-s_i(z_a)}. \end{cases}$$

- train the coupling layers t_i and s_i by minimizing the loss-function

$$L(\tilde{\rho}) = \int \prod \phi_j \, \tilde{\rho}(\phi) \ln(\tilde{\rho}(\phi)/\rho(\phi))$$



Construction the layer such that

- Forwards and backward map easily to compute
- Alternating freezing and unfreezing variable to get block diagonal Jacobians

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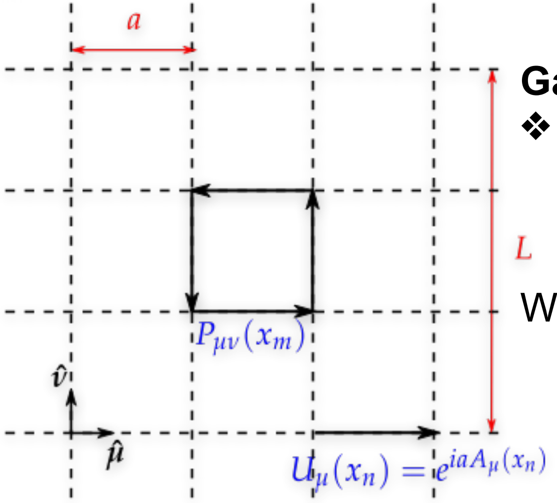
Application to gauge theories:

Kanwar et al., Phys.Rev.Lett.125 (2020) 12, 121601

Boyda et al., Phys.Rev.D 103 (2021) 7, 074504

Albergo et al., arXiv:2101.08176



Gauge invariant maps

❖ Lattice actions are gauge invariant under

$$U_\mu(x) \to g(x)^\dagger U_\mu(x) g(x+\hat{\mu})$$

Wilson pure gauge action given by sum over plaquettes:

$$S_g(U) = 1 - \frac{1}{2N} \mathrm{ReTr} \sum_{x,\mu>\nu} P_{\mu,\nu}(x)$$

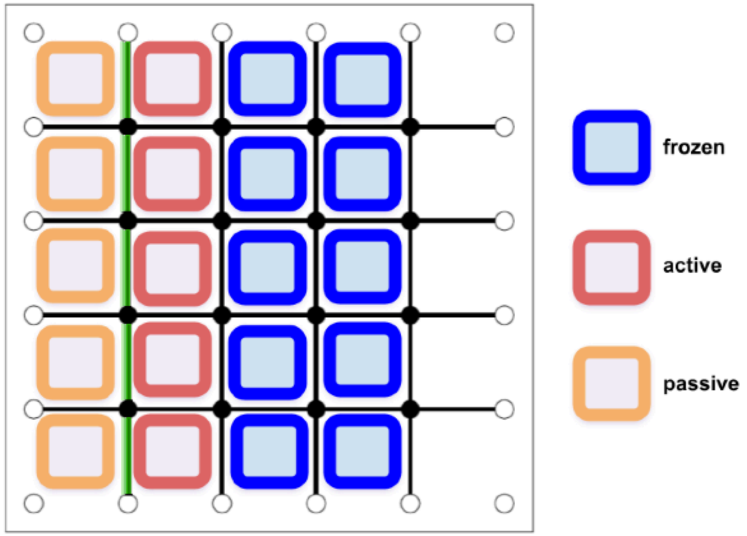
With $P_{\mu,\nu}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x)$
Which is gauge invariant

Idea: update gauge invariant object, plaquettes
And propagate update to the links via

- however this change also neighbour plaquettes

Maps are changing:

❖ *Active* : are updated
❖ *Passive* : are not touched
❖ *Frozen* : can be use to feed the networks



❖ Note: Links and plaquette needs to stay in the group
❖ Coupling layers/parameterization needs to account for that
 ❖ See for details

Boyda et al., Phys.Rev.D 103 (2021) 7, 074504

R. Abbott et al., arXiv:2401.10874

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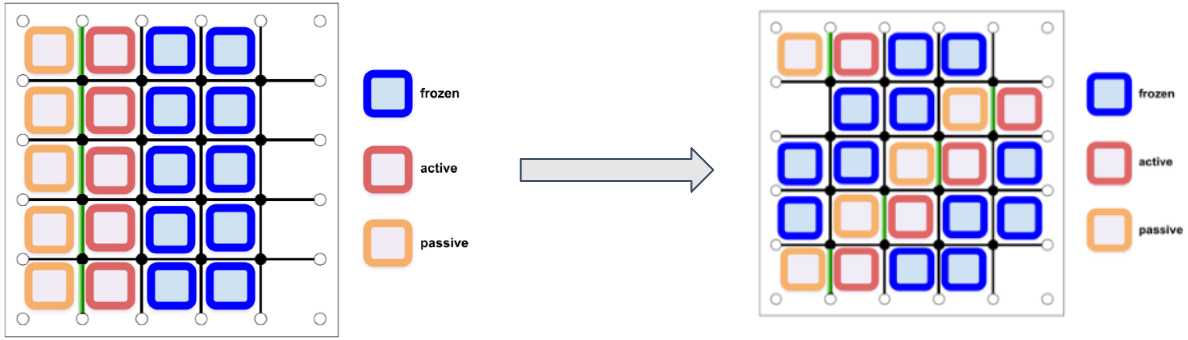
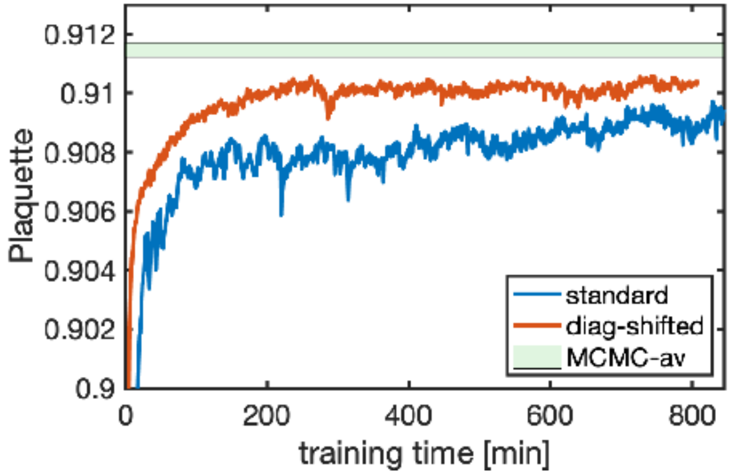
Some insides into gauge invariant flows

How to design coupling layers:



- Mapping can be optimized by including symmetries
  - Partially translation invariant by convolutional networks

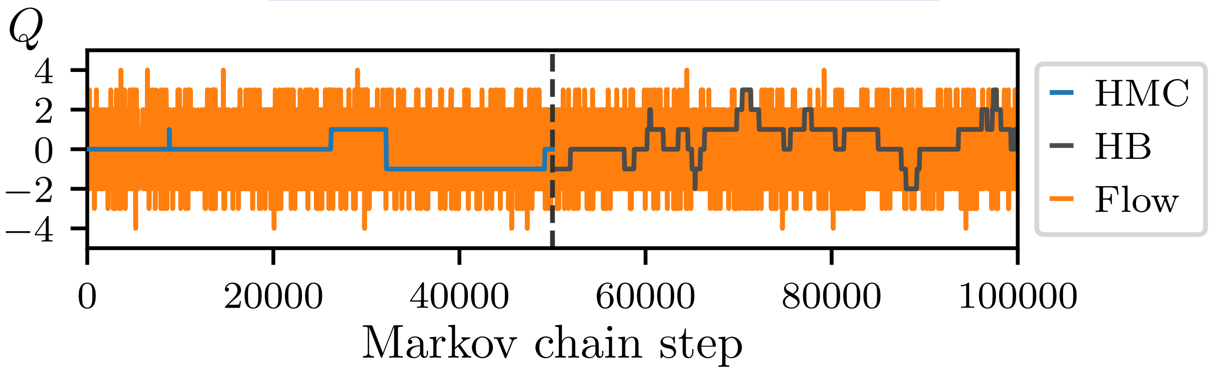
Structure of networks
- convolutional kernels with size 3
  - note that only frozen plaquettes are used as input values
- with hidden layers (here default 2 with 8 nodes)
- 8 coupling layers corresponds to a full update



Updating masks improve convergence rate and acceptance from 30% to 50%

Decoupling of topological sectors:

Kanwar et al., Phys.Rev.Lett.125 (2020) 12, 121601



- Gauge proposal can indeed solve topological freezing

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Lets take a look to the second step:

1. Propose U' according to $T_0(U \to U')$
2. Correct with $P_{acc}(U \to U') = \min\left[1, \frac{\tilde{\rho}(U)\rho(U')}{\rho(U)\tilde{\rho}(U')}\right]$

We have a proposal which generates independent configurations with weight:

$$\tilde{\rho}(U) = r(f(U)) \cdot \left|\det \frac{\partial f(U)}{\partial U}\right|$$

Need correction steps to correct towards the right weight: $\rho_{PG} \propto \exp\{-\beta S_g(U)\}$

Acceptance rate:

In case ratio of distributions $(\tilde{\rho}(U)\rho(U'))/(\rho(U)\tilde{\rho}(U'))$ is log-normal distributed.

- for the acceptance rate follows

Creutz, Phys. Rev. D38 (1988) 1228–1238

$$P_{acc} = \mathrm{erfc}\{\sqrt{\sigma^2(\Delta S)/8}\}$$

with $\Delta S = \ln\{\rho(U')\} - \ln\{\rho(U)\} + \ln\{\tilde{\rho}(U)\} - \ln\{\tilde{\rho}(U')\}$

Scaling of normalizing flows

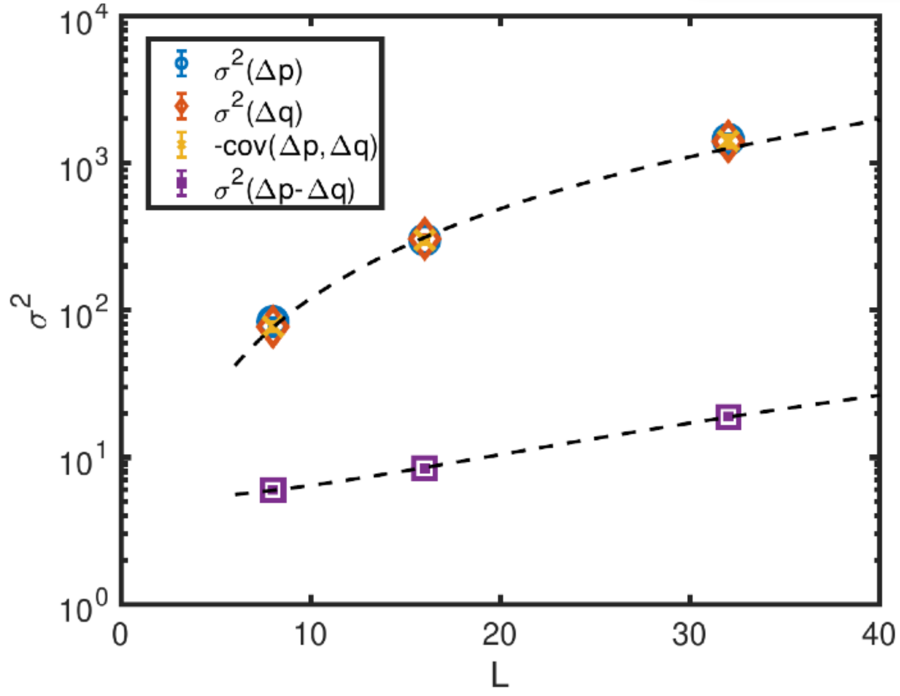
Del Debbio, Phys. Rev. D 104, 094507

Fine tuning problem:
How the variance scales $\sigma^2(\Delta S)$

Covariances of distributions scales like variances

$$\mathrm{var}(\Delta\rho) + \mathrm{var}(\Delta\tilde{\rho}) \approx -2 \cdot \mathrm{cov}(\Delta\rho, \Delta\tilde{\rho})$$

But $\sigma^2 = \mathrm{var}(\Delta\rho) + \mathrm{var}(\Delta\tilde{\rho}) - 2 \cdot \mathrm{cov}(\Delta\rho, \Delta\tilde{\rho})$
still grows with the volume



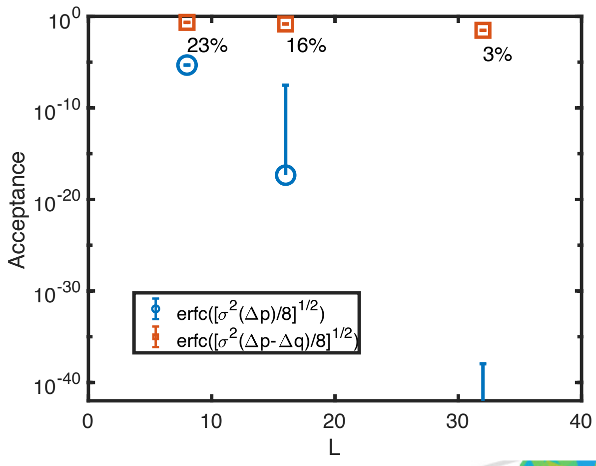
Volume fluctuations

❖ Localized models:

$$\sigma^2(S) = \langle S^2 \rangle - \langle S \rangle^2 \quad = V(a_0 + a_1 e^{-d} + a_2 e^{-\sqrt{2}d} + \ldots)$$

❖ Variance scales with the volume, acceptance rate is rapidly 0

❖ Requires modifications for larger volumes



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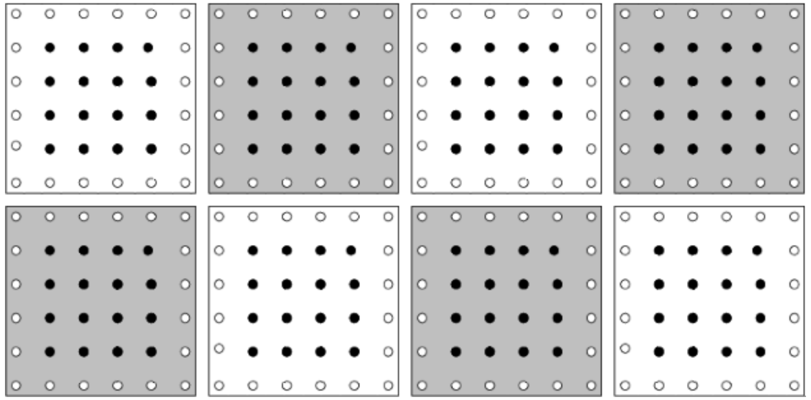
Domain Decomposition

Idea: Decomposition of lattice into domain

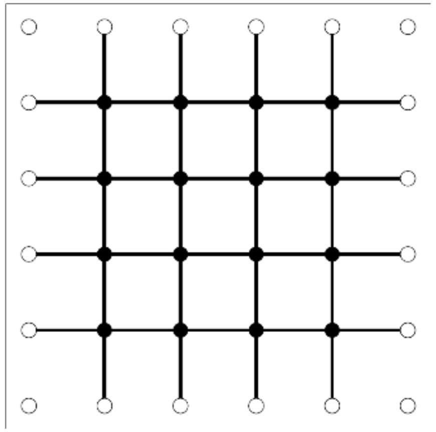


Separate action into:

$$S_{global} = \sum_{blk} S_{local} + I(S_{global}, S_{local})$$

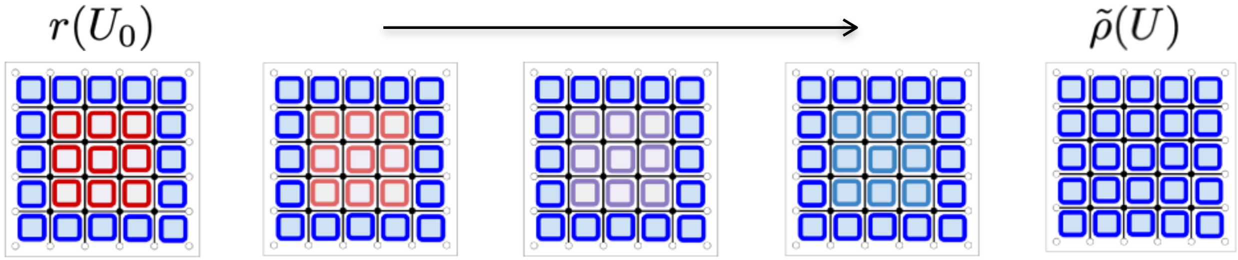
Decomposition straightforward for ultra local lattice actions
- ϕ^4 - model
- Pure gauge theories

This becomes harder if fermions are included



Domain Decomposition of normalizing flow
- update only links/variables inside blocks by creating maps of active links within each block

Training: (one possibility)
- using different boundaries for each sample in the batch
- increase iteration before boundaries updated to 1000



Taken from: M. Luscher, CPC 165 (2005) 199-220

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Test in the ϕ^4 Model

Lets test domain decomposition in the ϕ^4 - model:

$$S(\phi) = \beta \sum_x \phi(x)\phi(x+\hat{\mu}) + \phi^2(x) + \lambda(\phi^2(x) - 1)^2$$

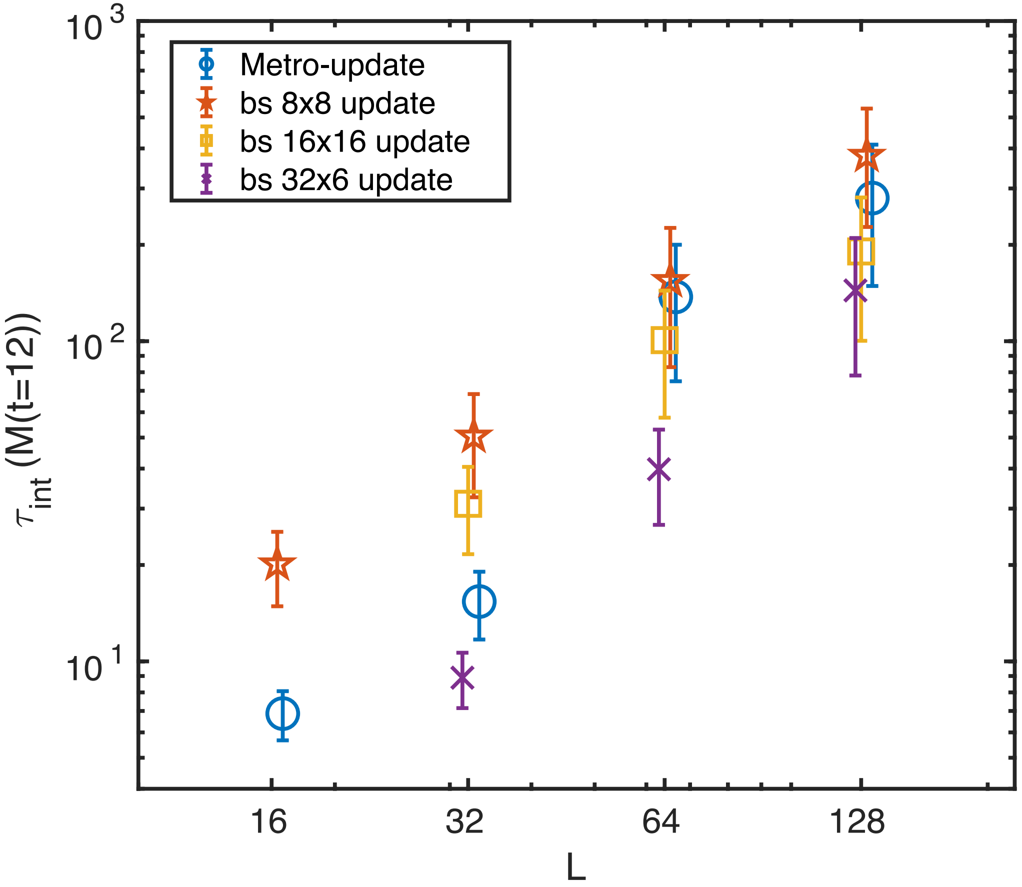
Acceptance rate for flow model become tiny for L> 32
Close to phase transition, model becomes critical.

❖ Order parameter is related to the magnetiziation:

$$M = \frac{1}{V} \sum_x \phi(x)$$

At 2D parameter set taken from

Korzec et al. Comput.Phys.Commun. 182 (2011)



Autocorrelation of magnetisation shows no improvements if domain size is fixed but lattice size is scaled

Test in the ϕ^4 Model

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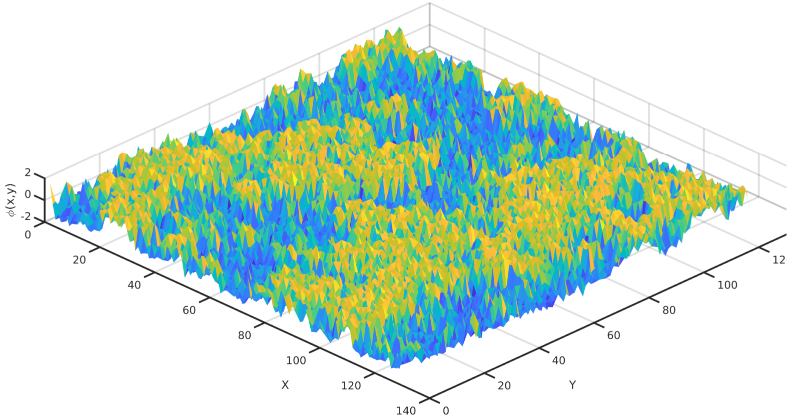
Close to criticality:

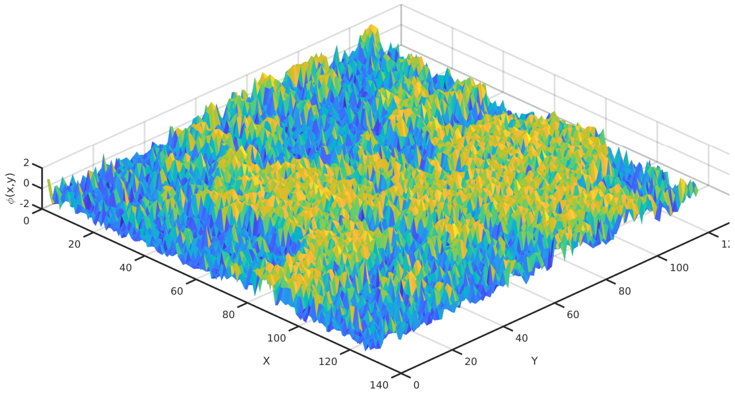
Correlation length increases with lattice size:

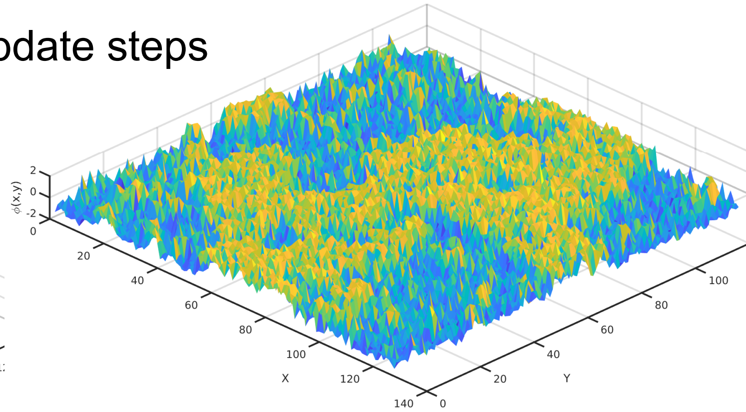
$$\xi \propto L$$

If domain size is smaller < L
the MC-time for de-correlation increases

Here, the magnetisation close to criticality is shown
- using L = 128 and separated by 40k metropolis update steps







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Domain decomposition in the Schwinger Model

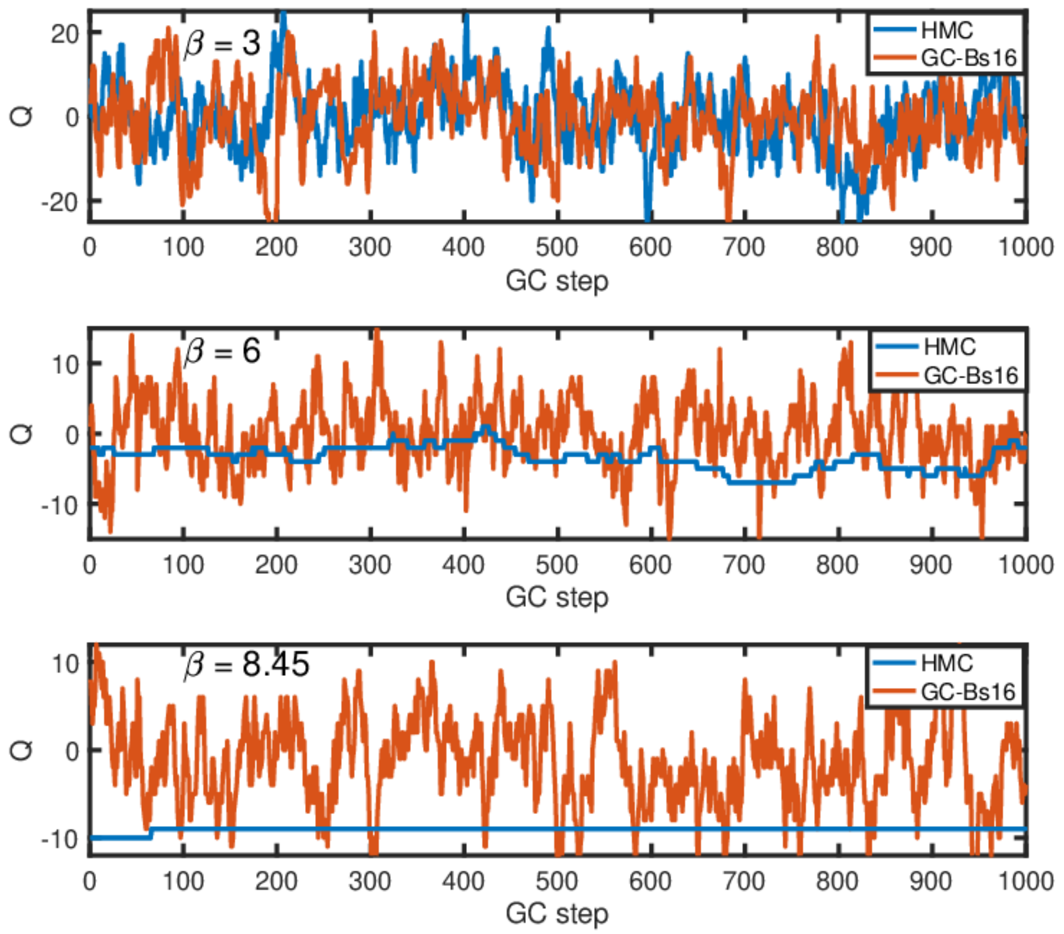
Lets take a look to 2D - U(1) gauge model

$$S_g(U) = \beta \sum_{x,\mu} \mathrm{Re}\left(1 - U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)\right)$$

Train with fixed boundary conditions using L = 8

❖ reduced acceptance rate compare to periodic case (40% to 25%)
❖ Scaling towards large lattice sizes is trivial

Effect on observables:
❖ using L=8 domain updates:
  ✦ Samples topological sectors
  ✦ For $\beta > 5$ outperforms HMC



Domain decomposition works because topological charges are localised

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Towards more Complex models

Works well for L=8, **however**: becomes difficult for larger volumes (needed in 4D-SU(3))

J.F., arXiv:2201.02216

For 4D - SU(3)

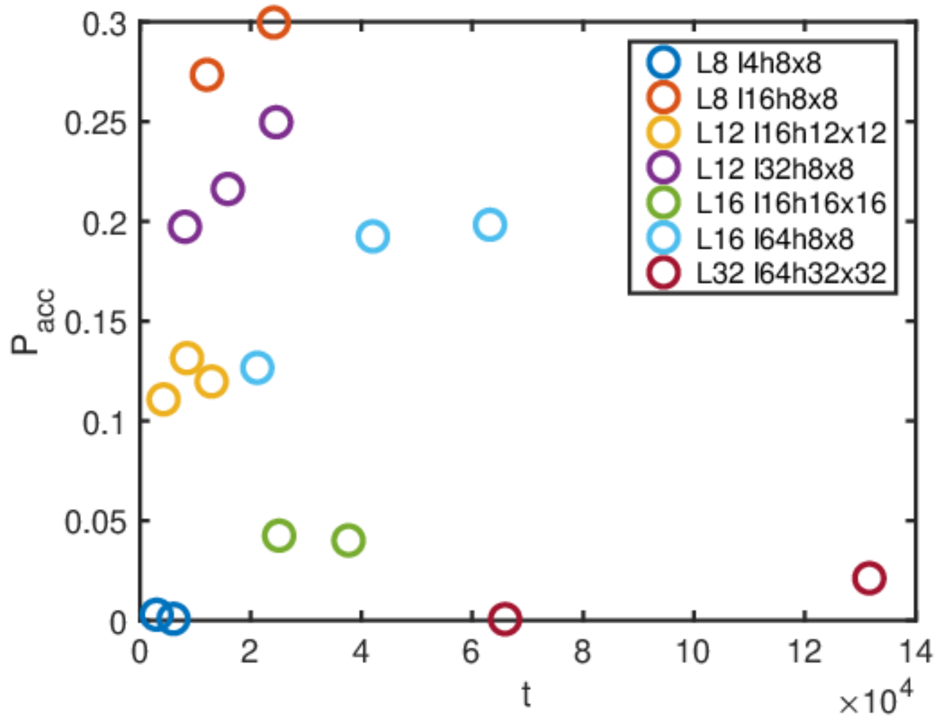
- Block size has to be > 0.4 fm to change topology

For a=0.05, its requires a block of length Lb = 8
- For the physical degrees of freedoms follows:
  - 6*8*(8)^4 = 200k

Thats more **dof** than for the 2D-U(1) with L=128
- thats out of reach with the current flow models
- Acceptance rate is zero

New approaches needed:
- include additional symmetries
- Adapt flow maps

Bacchio et al., arXiv:2212.08469



Here: using flows to fine grain updates

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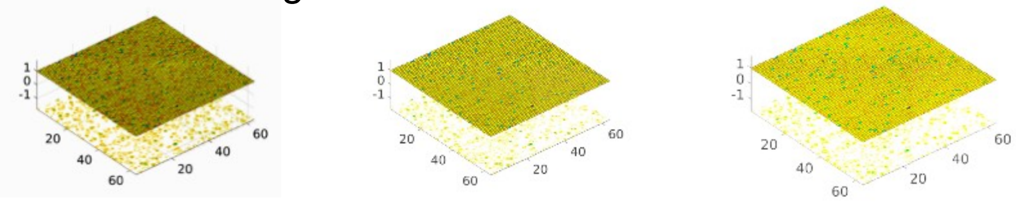
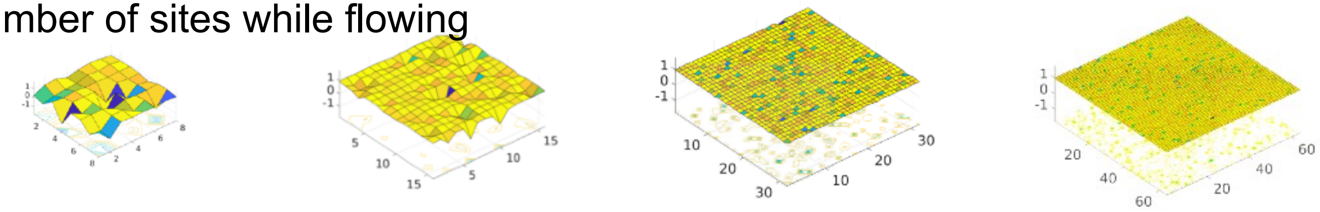
Fine graining flows

Flow maps:

Standard Map: Keep L/a fixed
❖ Physical lattice size is decreasing



Natural Projection: Keep physical box size fixed
❖ extend number of sites while flowing

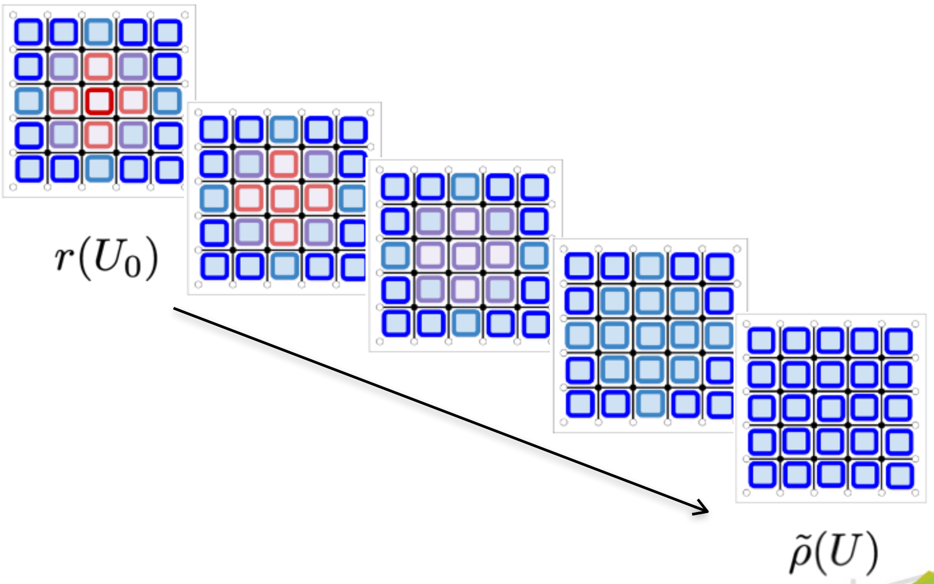


Idea: Effective coarse to fine graining

Introduce a smoothing mapping within a larger lattice
❖ place local defect and smooth out

- like multi-tempering approaches
  - successfully applied in 4D-SU(N)

C. Bonati et al., PRD 99, 054503 (2019)



Here: use local flow transformations
❖ needs adjustments/modifications
  ✤ Maps: localization of updates
  ✤ Training conditions / loss function
✤ Train for topological tunneling

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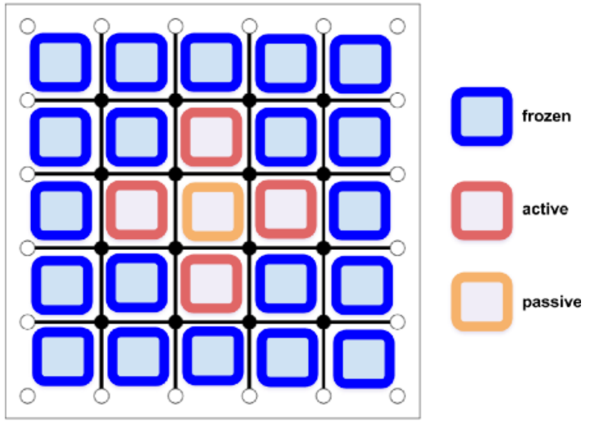
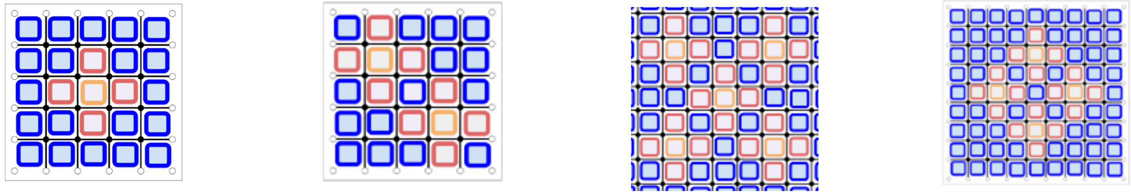
Training techniques



Localized update:
Center symmetric update
❖ only randomise all 4 links of center plaquette
❖ in 2D use a max. compact map
  ✦ active to passive ratio = 4:1

Kernel 0 Kernel 1 Kernel 2 Kernel 3

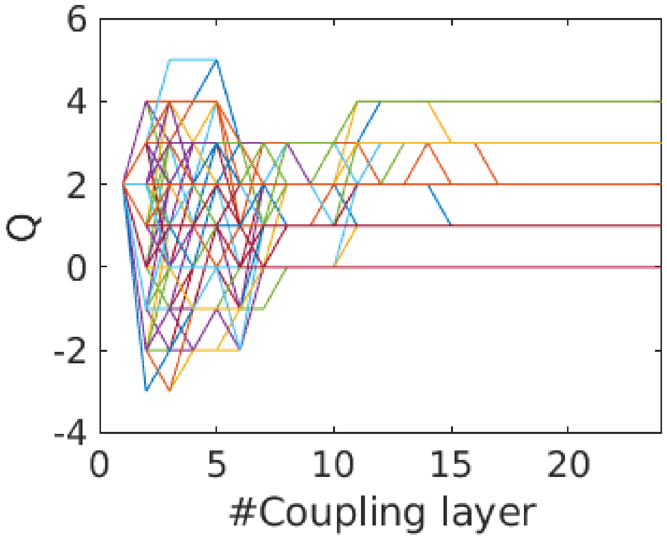


In line with Kanwar et al., Phys.Rev.Lett.125 (2020) 12, 121601

Modification of the loss-function:
Training for topological transitions
❖ by modification of the loss-function

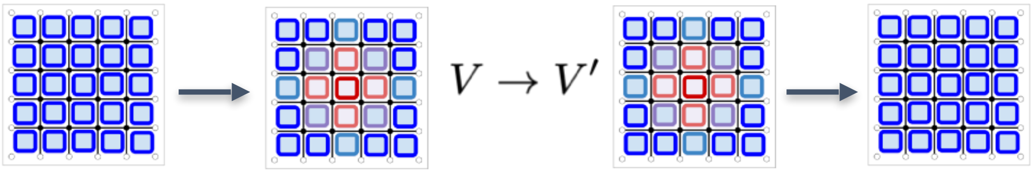
$$L = \ln(\tilde{\rho}(U')/\rho(U')) \cdot |Q(U') - Q(U)|$$

Train transitions using only four uniformed links
❖ Correlations need to be smeared out
❖ otherwise fancy plaquette update



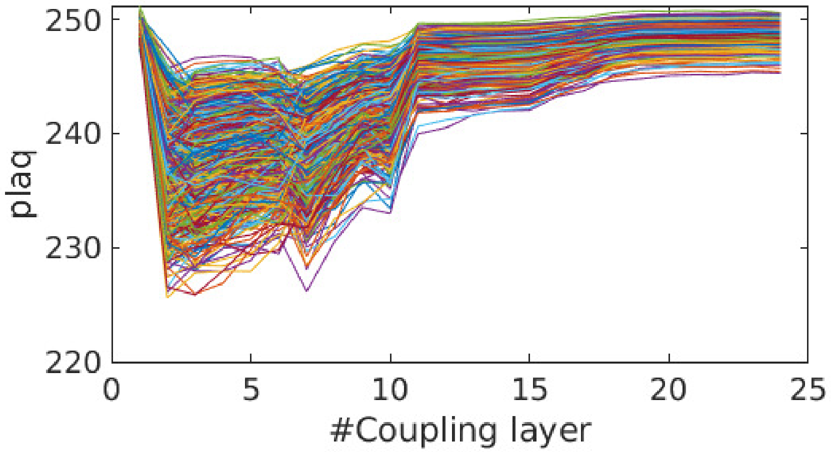
Grinding the fine graining

$f(U) = V$ $\quad$ $f^{-1}(V') = U'$



Graining needs change of update procedure:
Requires back transformation before the update
- ❖ Currently: for training fix backward transformation and update occasionally
- ❖ Allows for new loss-function
  - ❖ Works in combination with topo. loss and fixed backward transformation

$$L = \ln\{\rho(U')\} - \ln\{\rho(U)\} + \ln\{\tilde{\rho}_{fixed}(U)\} - \ln\{\tilde{\rho}_{train}(U')\}$$



Grinding training:
Current training setup: relative long training chain

Pre-train on L=8 with pBC

Retrain on L=16 with fixed $\tilde{\rho}$

Build up chain via intermediate loss

Fine tune with updated $\tilde{\rho}$

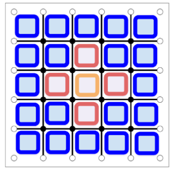
Use HMC generated configs

Fine Graining Flows

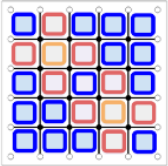
Test fine graining updates

- Updates at $\beta = 11.25$
- Kernel 1-3 used
  Use 3x[1, 3, 2] + 2 with shifts

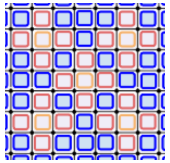
Kernel 0



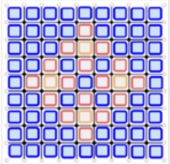
Kernel 1

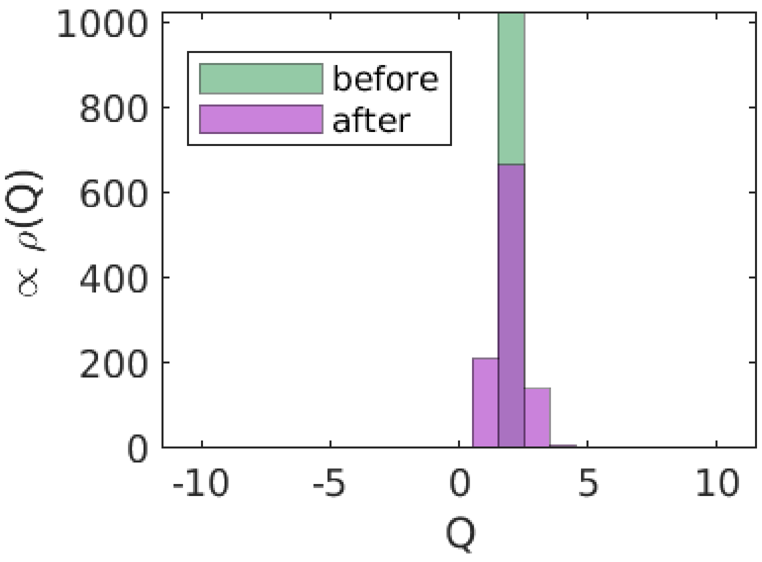


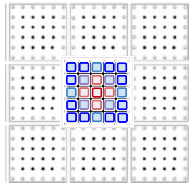
Kernel 2



Kernel 3

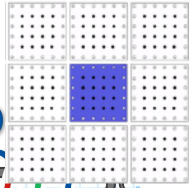






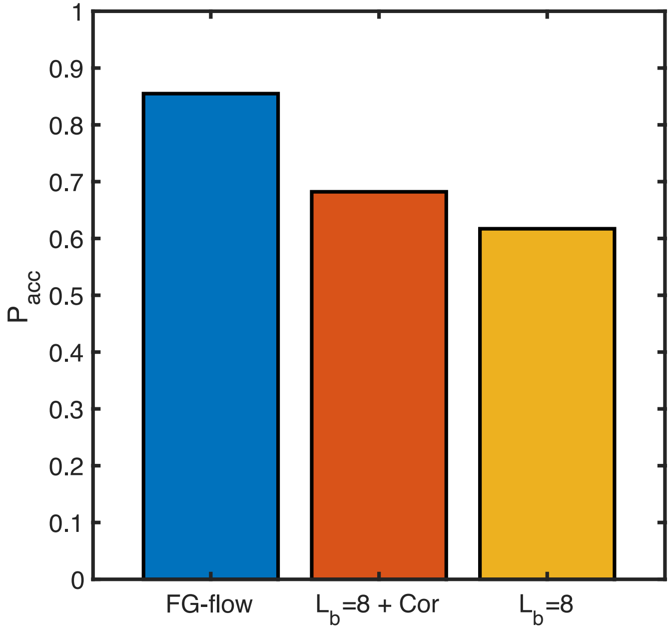
Local updates also increase block determinants acceptance rate

$$P^{(b)}_{acc}(U \to U') = \min\left[1, \frac{\det(D^b(U'))^2}{\det(D^b(U))^2}\right]$$



- Using an Fine Grain - flow update within a L=16 box
  - Acceptance rates of Pacc ~ 0.85 can be reached

- Flow updates within L=8 box is reaching Pacc ~ 0.6 %



Results: Tunneling rate

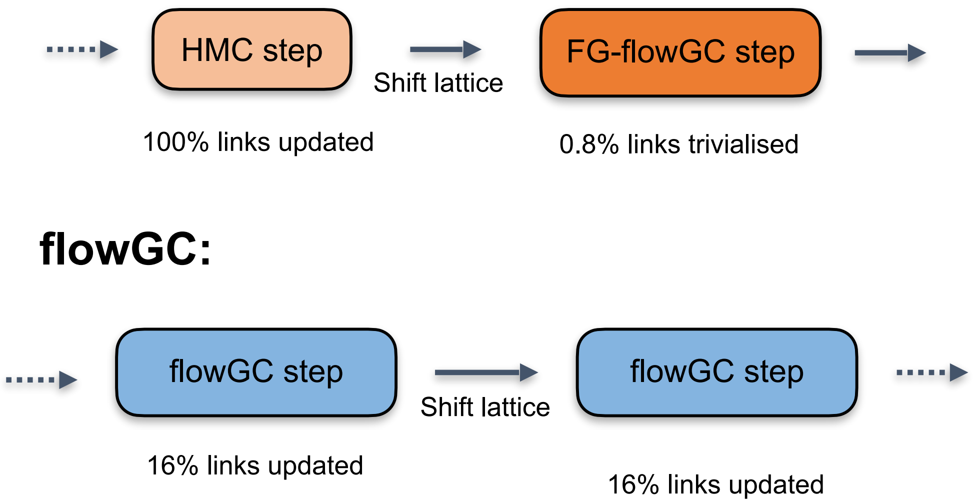
Tunneling rate:

$$T(Q) = \langle |Q_i - Q_{i+1}| \rangle$$

Flow enables simulations beyond beta > 6.0

FG-flowGC:

flowGC:



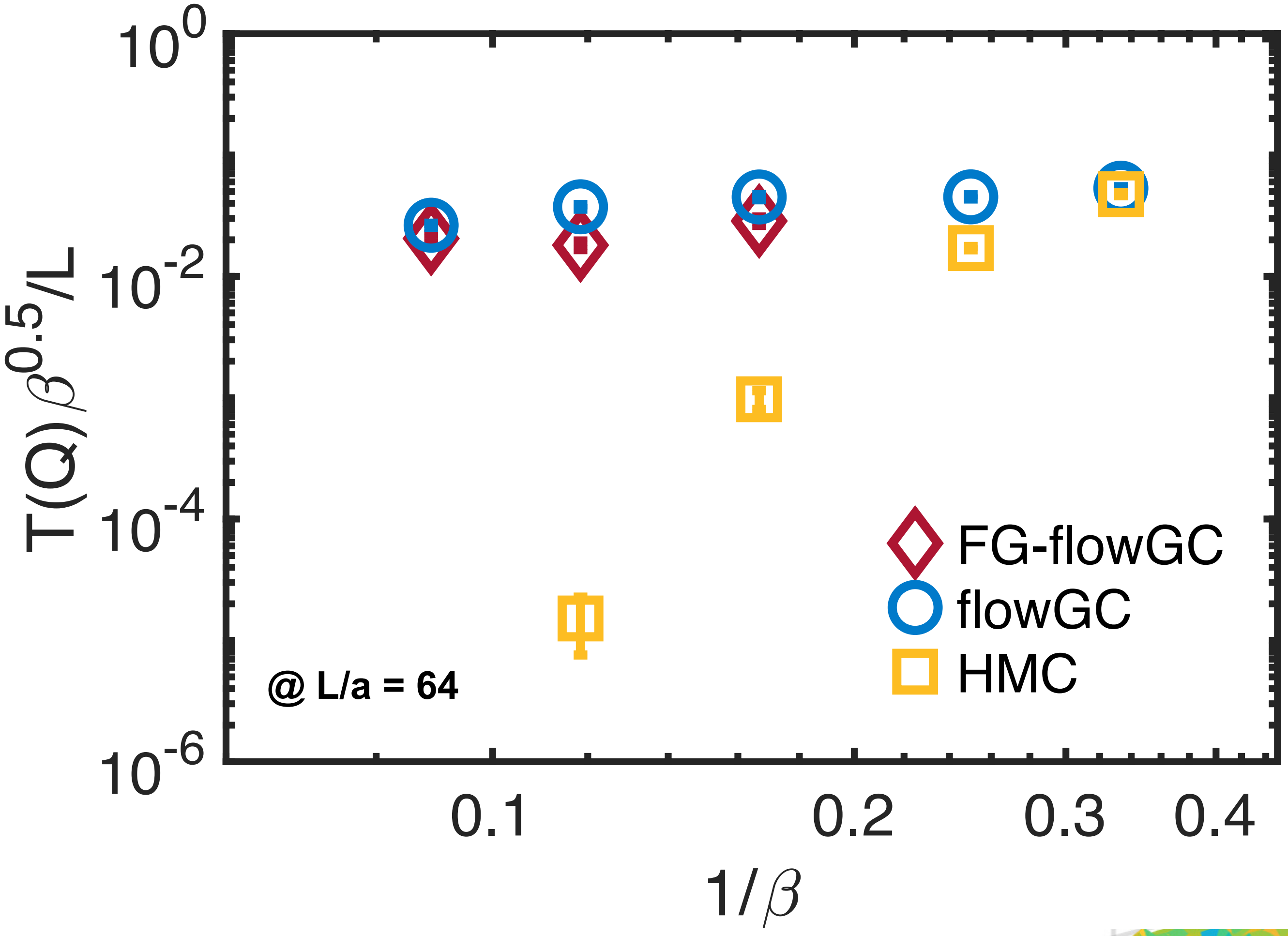


Table of Content

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- Simulations at the precision frontier
- Monte Carlo simulation

Gauge equivariant/normalizing flows
J. F., arXiv:2201.02216
- Introduction
- Domain Decomposition
- Applications in 2D

Fine graining flows in 2D
J. F., arXiv:2201.02216
- Maps and training
- Tunneling rate

Global corrections with the fermion determinant
- Domain decomposition of fermions
- Towards high acceptances

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Recursive Domain Decomposition

Action with fermions:

$$\rho(U) = Z^{-1}\left(\prod_{j}^{N_f} \det D_j(U)\right) e^{-\beta_g(U)}$$

with $\det D(U)$ is a *localised* action

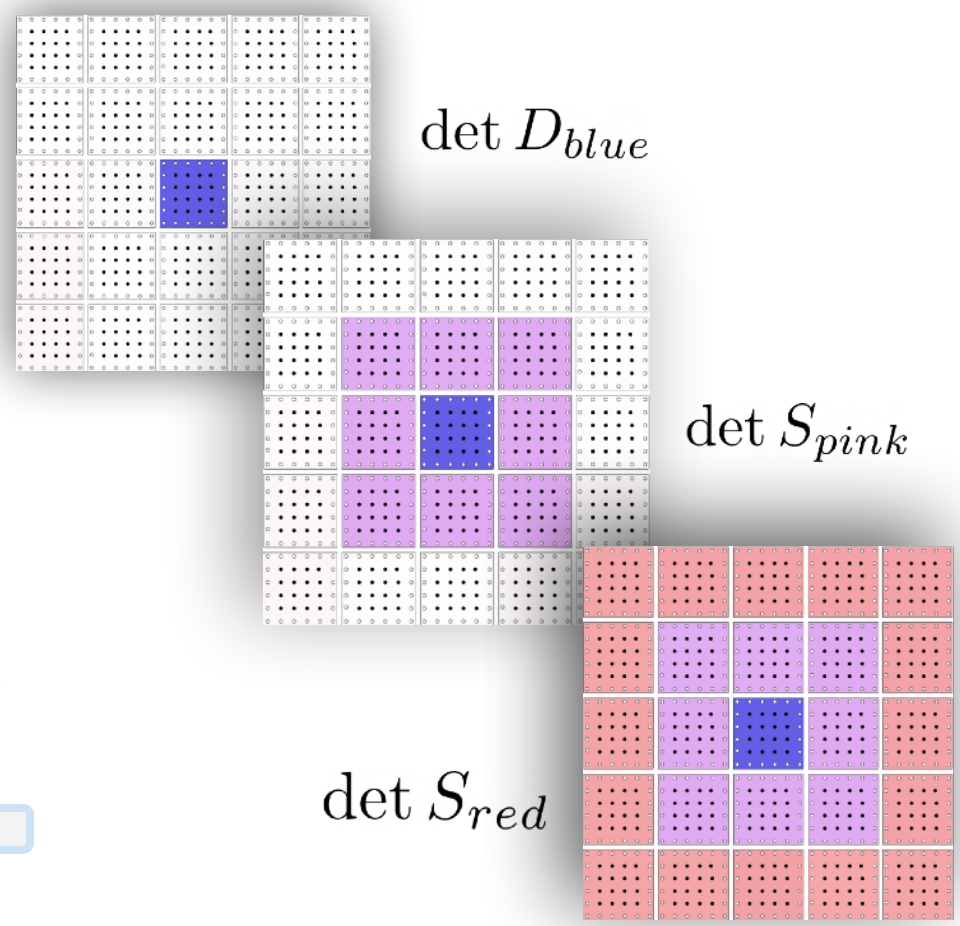
- distance interaction decays with

$$cov(x,y) \propto \exp\{-m_{PS}|x-y|\}$$

Idea: using exact decomposition of fermion action:

$$\det D = \det S_{red} \cdot \det S_{pink} \cdot \det D_{blue}$$

effective long range decomposition of the fermion determinant



M. Luscher, CPC 165 (2005) 199-220

J.F. et al., CPC 184 (2013) 1522-1534

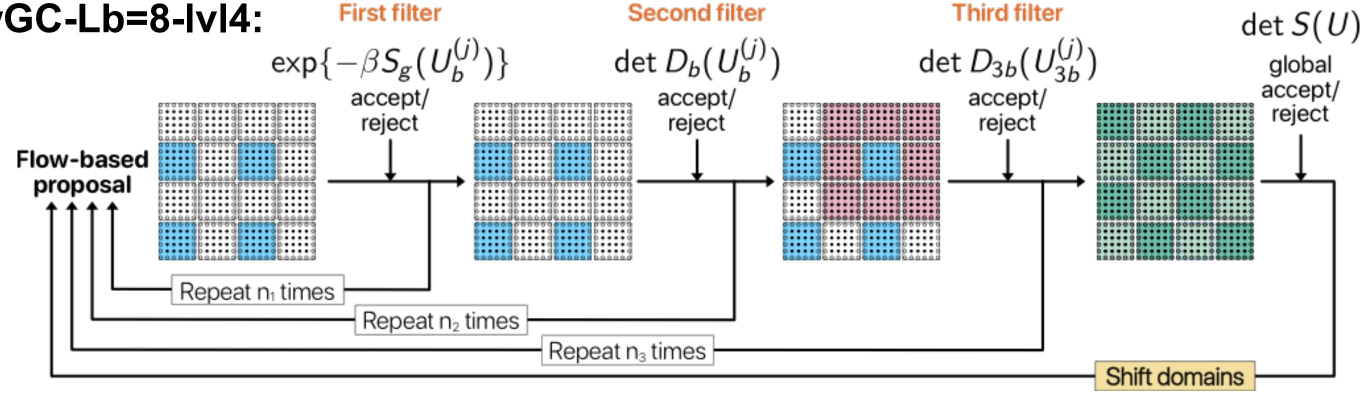
M. Cè et al., Phys.Rev.D 93 (2016) 9, 094507

M. Cè et al., Phys.Rev.D 95 (2017) 3, 034503

Correction steps With Fermions

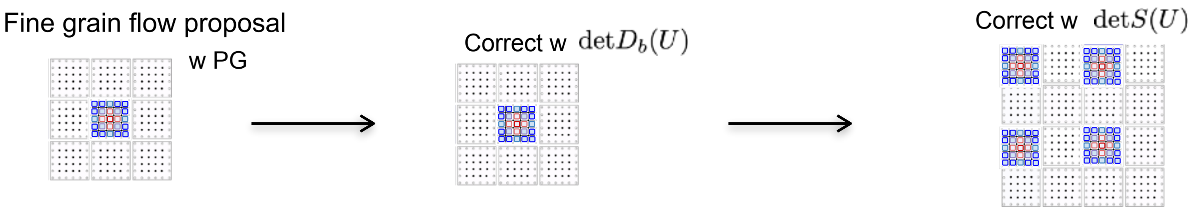
Fermion Corrections via hierarchical Filter and flow-based pure gauge updates

flowGC-Lb=8-lvl4:

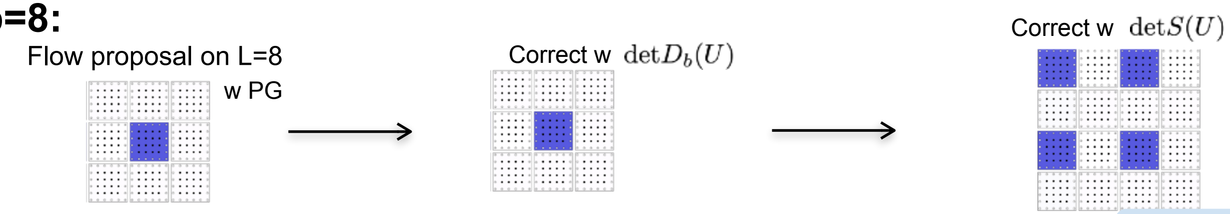


GC-bare:

FG-flowGC:

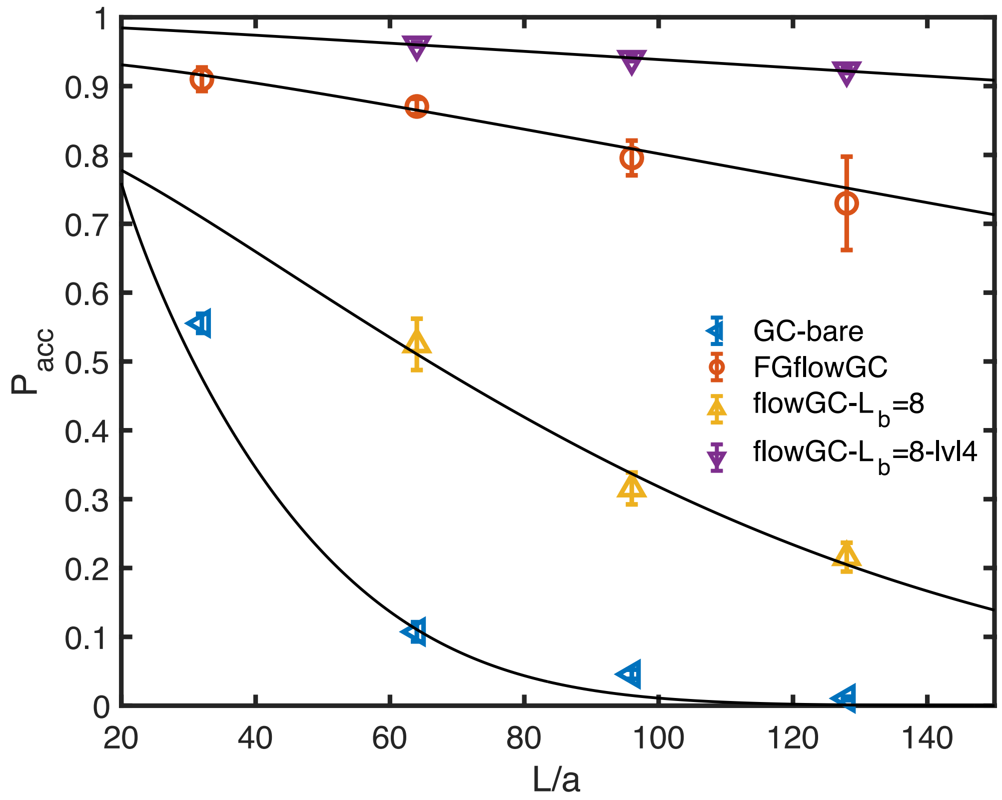


flowGC-Lb=8:



J.F., arXiv:2201.02216

2D - Schwinger Model Global acceptance rate



$\beta = 6.0$ **@ z = 0.2**

N. Christian et al., Nucl.Phys.B 736 (2006)

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Combination with HMC

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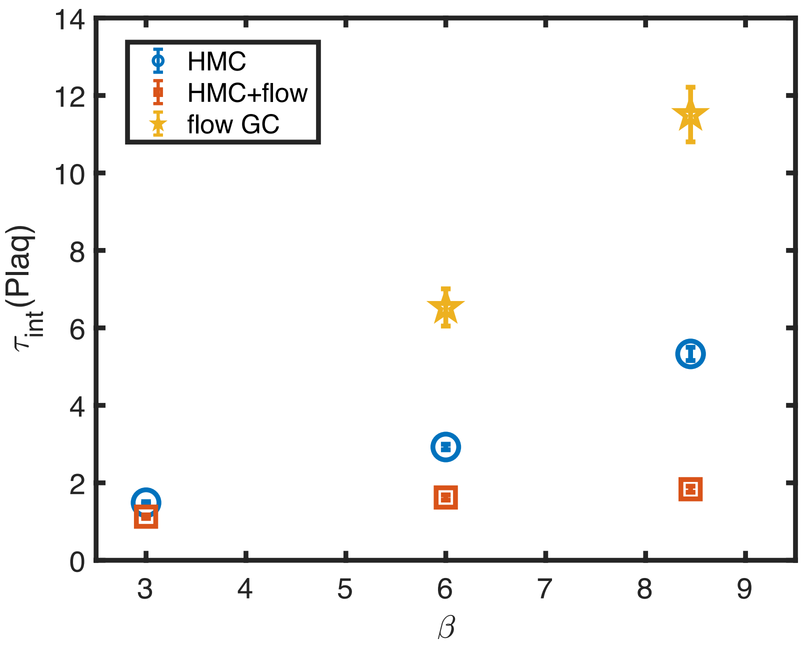
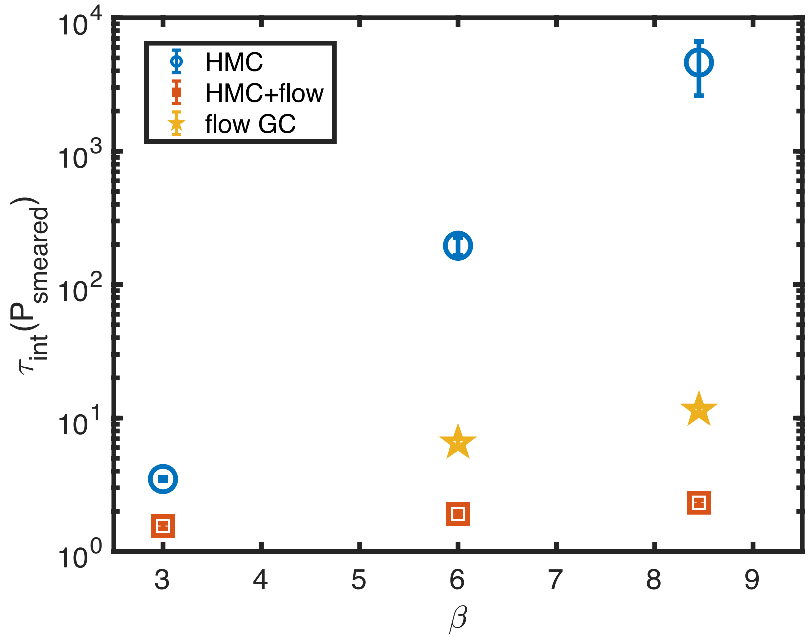
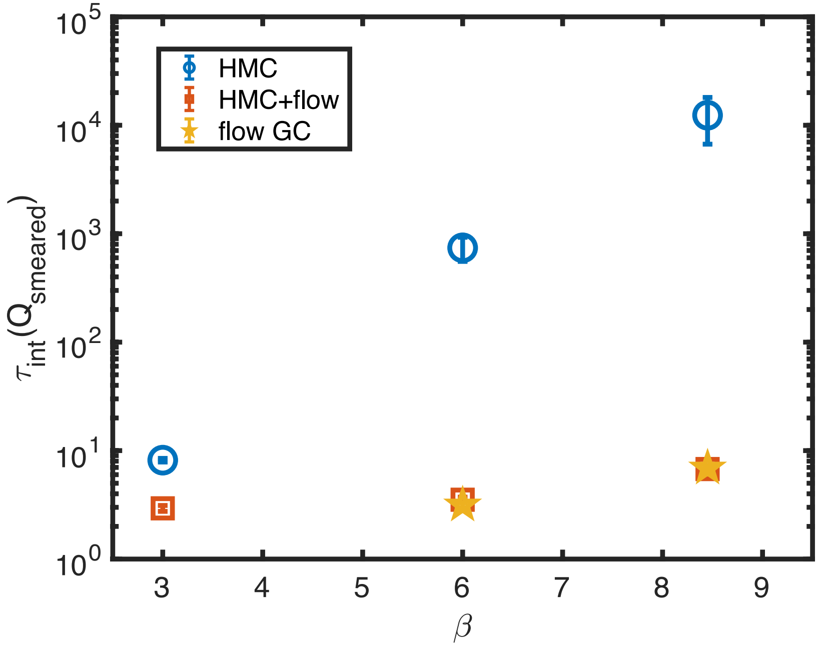
High statistic runs (at fixed L=32):
Analyse autocorrelation

Similar to
D. Albandea et al., Eur.Phys.J.C 81 (2021) 10, 873







HMC+flow:
Outperforming other. methods

⋯→ HMC step → Flow GC step → HMC step ⋯→

Conclusion

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Addressing scalability

❖ using domain decomposition — J. F., arXiv:2201.02216

- ❖ Works as long as domain size is larger than *correlation length* of the critical observable
  - ❖ Works to sample different topological sectors in gauge models (here U(1))

Modification of updates — J. F., arXiv:2402.12176

❖ fine graining local updates

❖ Topological transition can be trained in 2D-U(1)

Next steps towards 4D SU(3)

❖ Complexity increases, more degrees of freedom and topological charge is not an exact integer

❖ Using flows within multi-tempering approaches looks promising

- ❖ Flow distance shorter, project from near

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Thank you

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Appendix

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Motivation: Lattice QCD at the Precision Frontier

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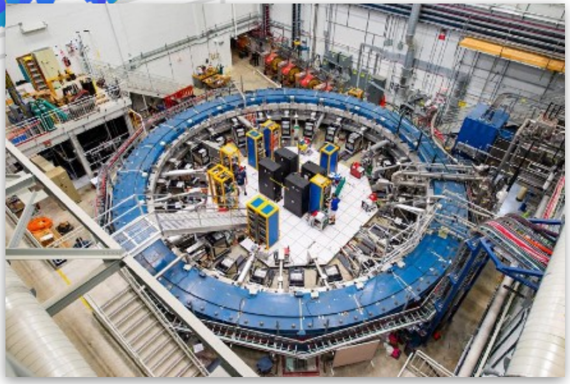
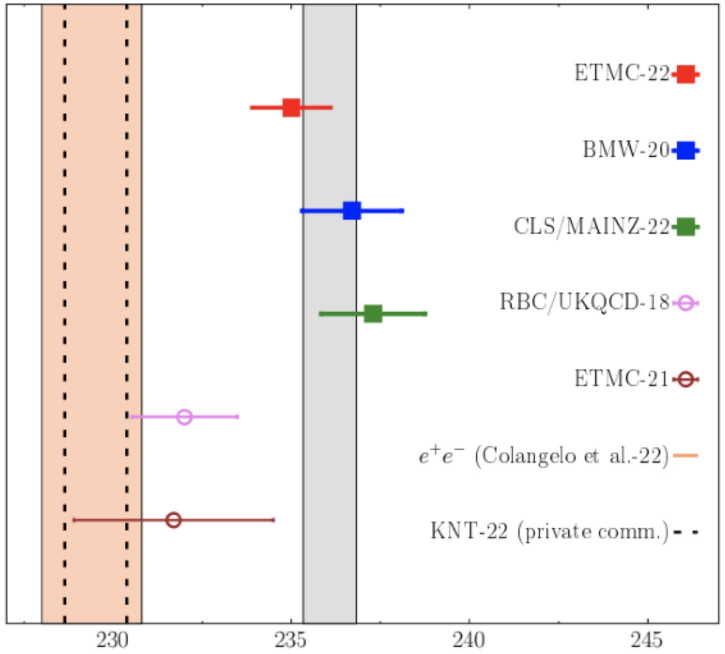
Lattice Quantum Chromodynamics
At the precision frontier

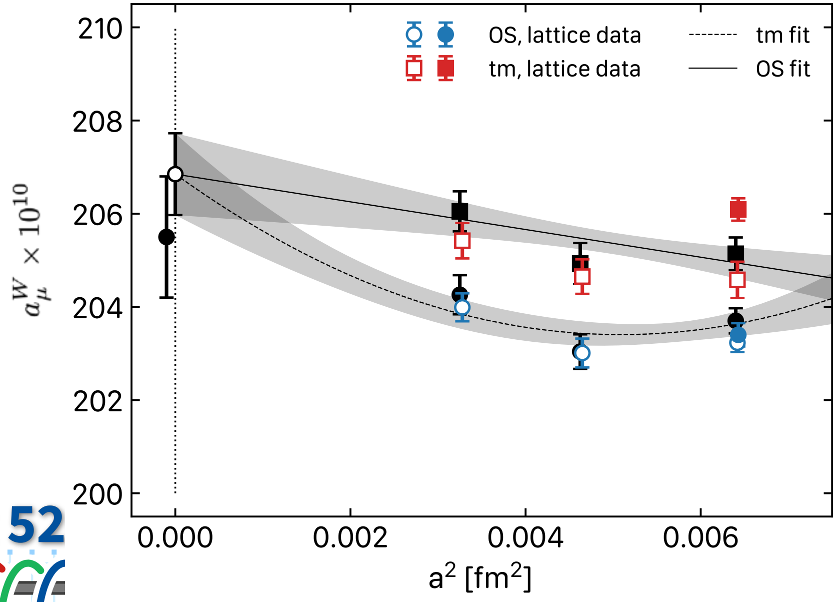


Muon and Flavor Physics
are indicating New Physics;
ab initio LQCD calculations are needed

Search for new physics in the precision frontier by
- ❖ high precision measurements
- ❖ theoretical prediction

deviations are signs for new physics





Anomalous magnetic moment of muon:
Muon g-2 Experiment at FermiLab increased precision
- ❖ > 5σ deviation between experiment and data-driven approach
- ❖ 4σ deviation between lattice and data-driven approach

To resolve this puzzle:

Precision Measurement of Lattice QCD are needed

❖ finer lattice spacings needed to match future experiments precision

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Details on normalizing flows

Let's defined our minimization condition:

The loss function:

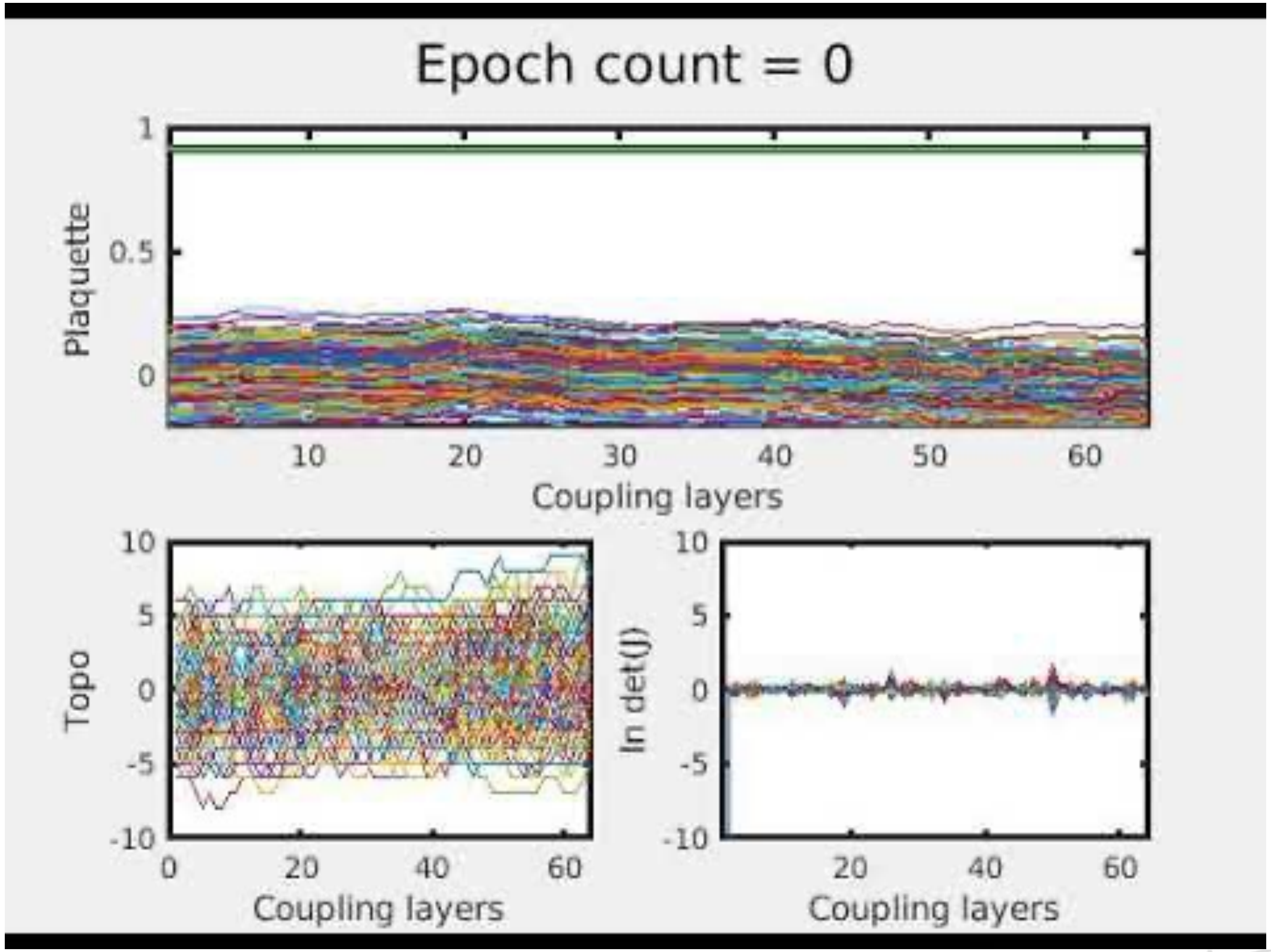
$$L(\tilde{P}) \;:=\; D_{KL}(\tilde{P}||p) - \log Z$$
$$= \int \prod_j d\phi_j \, \tilde{P}(\phi)(\log \tilde{P}(\phi) + S(\phi)).$$

- with ultra-local plaquette action:

$$\ln(\rho(U)) = -\beta \sum_x P_{12}(U)$$

- and flow distribution:

$$\tilde{\rho}(U) = \rho_{trival}(m^{-1}(U)) \prod_j \det J(g_j^{-1}(\alpha_{i,j}^{(0)}))$$



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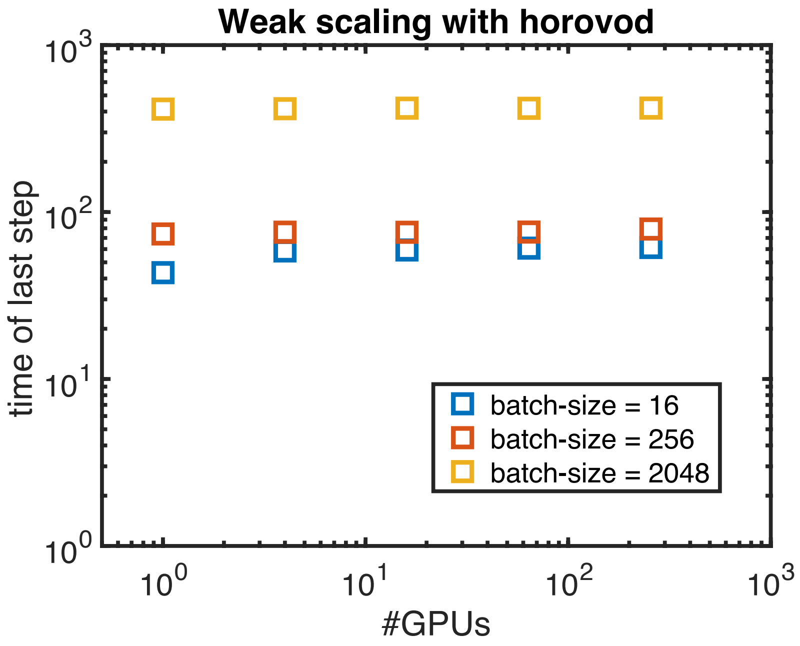
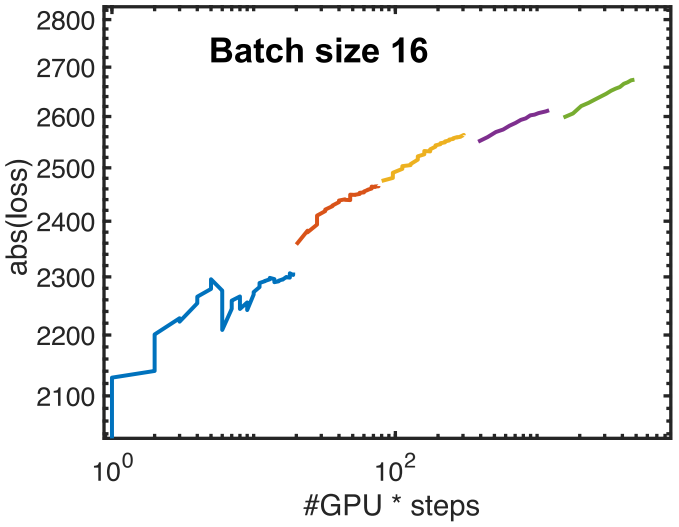
How to scale up:

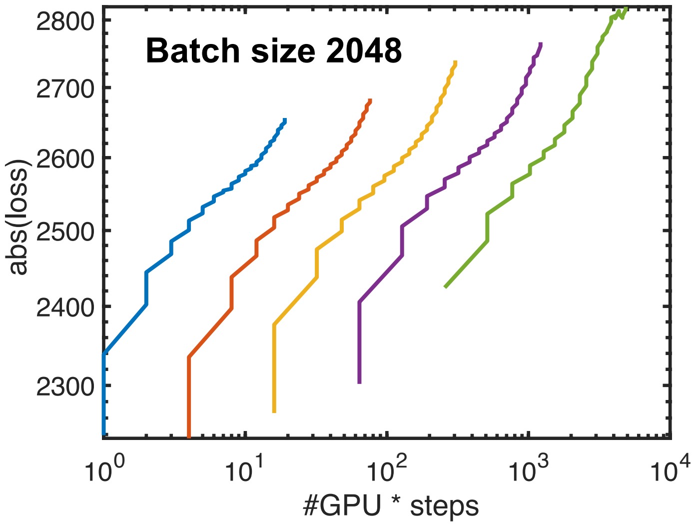
Exercise with horovod

- Simple to implement but needs fine tuning
- adds new batch to each additional GPU
  - Total batch-size = #GPUs x local batch-size

Modifications:
  - Switch to double precision
  - Use horovod.Adasum
  - Use schedular for stepsize decay







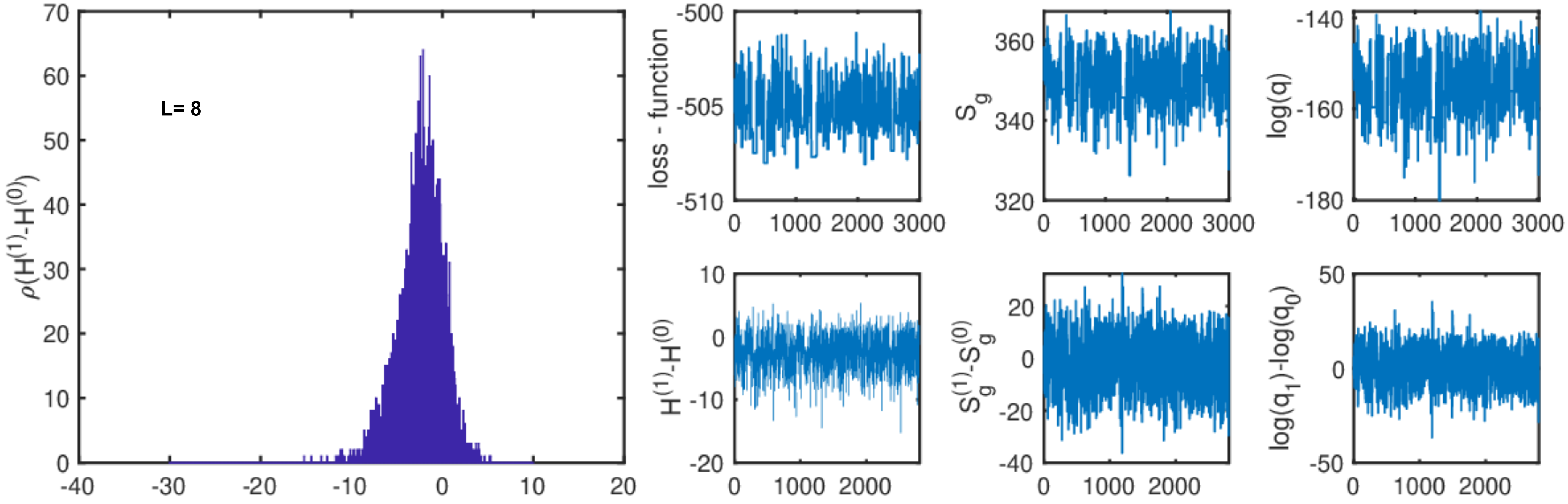
Benchmark runs on JUWELS-BOOSTER

- Loosely coupled scales weakly perfect
- For smaller batch-sizes works fine
- For larger batch-sizes convergence deteriorates

Some insides on normalising flows

Correlations of distribution $\tilde{\rho}$ and ρ

- covariance need to be of $\mathrm{cov}(\tilde{\rho}, \rho) \propto \mathcal{O}(V)$ to compensate extensive variances $\sigma^2 \propto \mathcal{O}(V)$



Works for L=8 → L=16

Some insides on normalising flows

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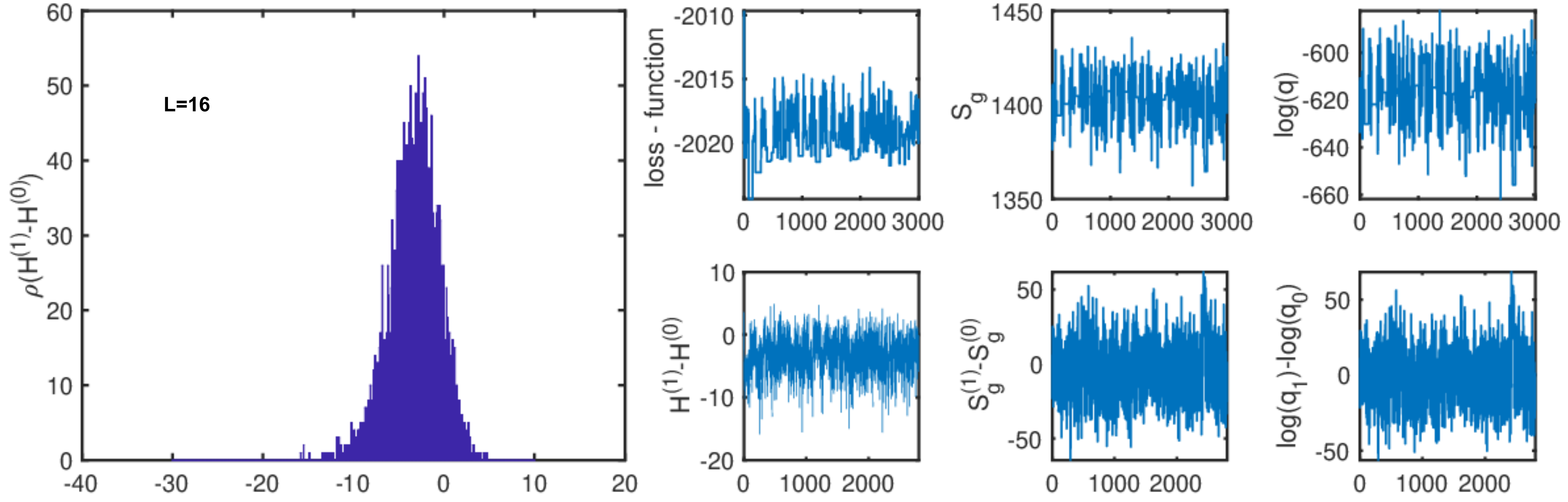

Works for L=8 → L=16

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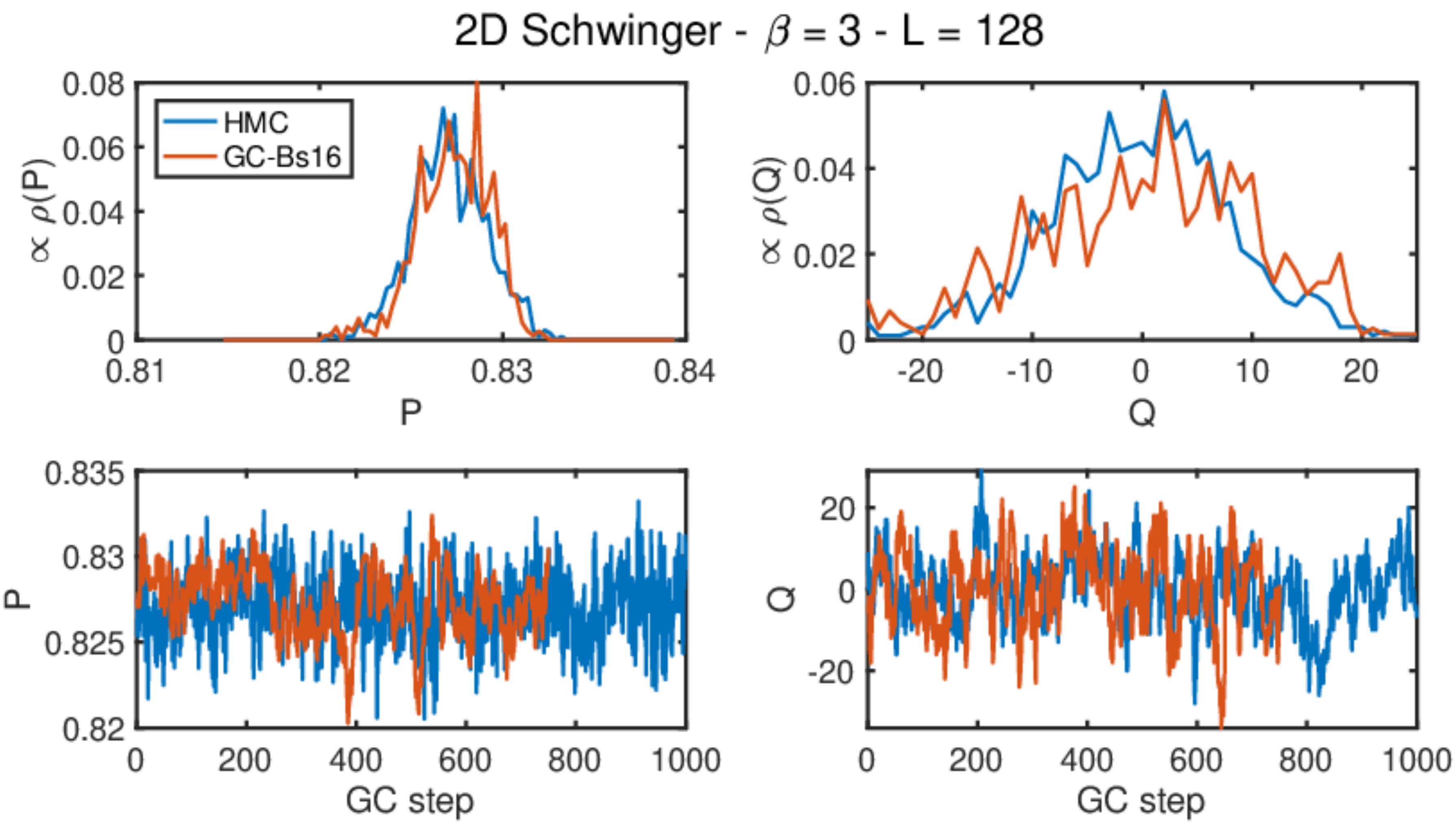
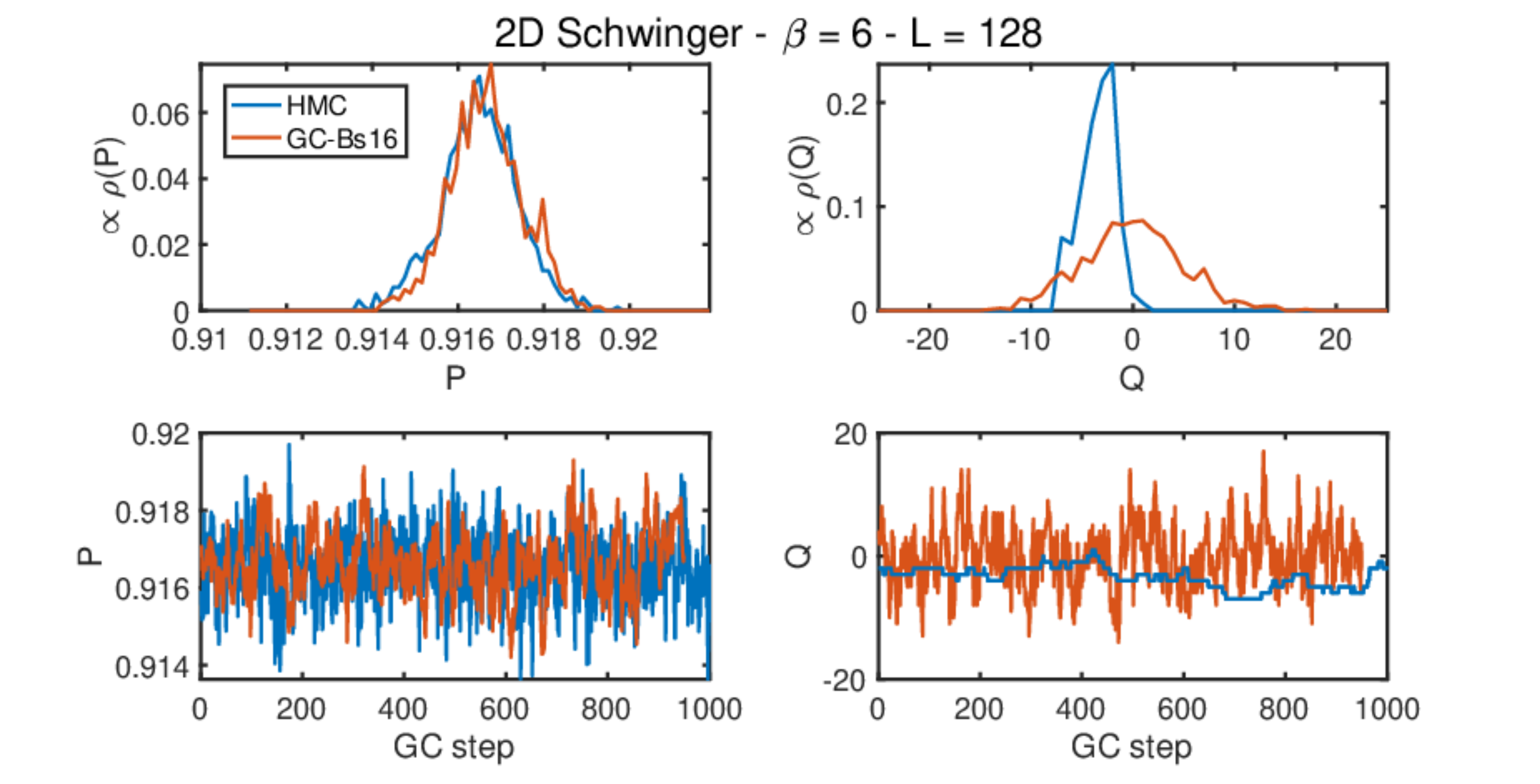
Run statistic

- L = 128
- beta = 3.0
- m = -0.082626



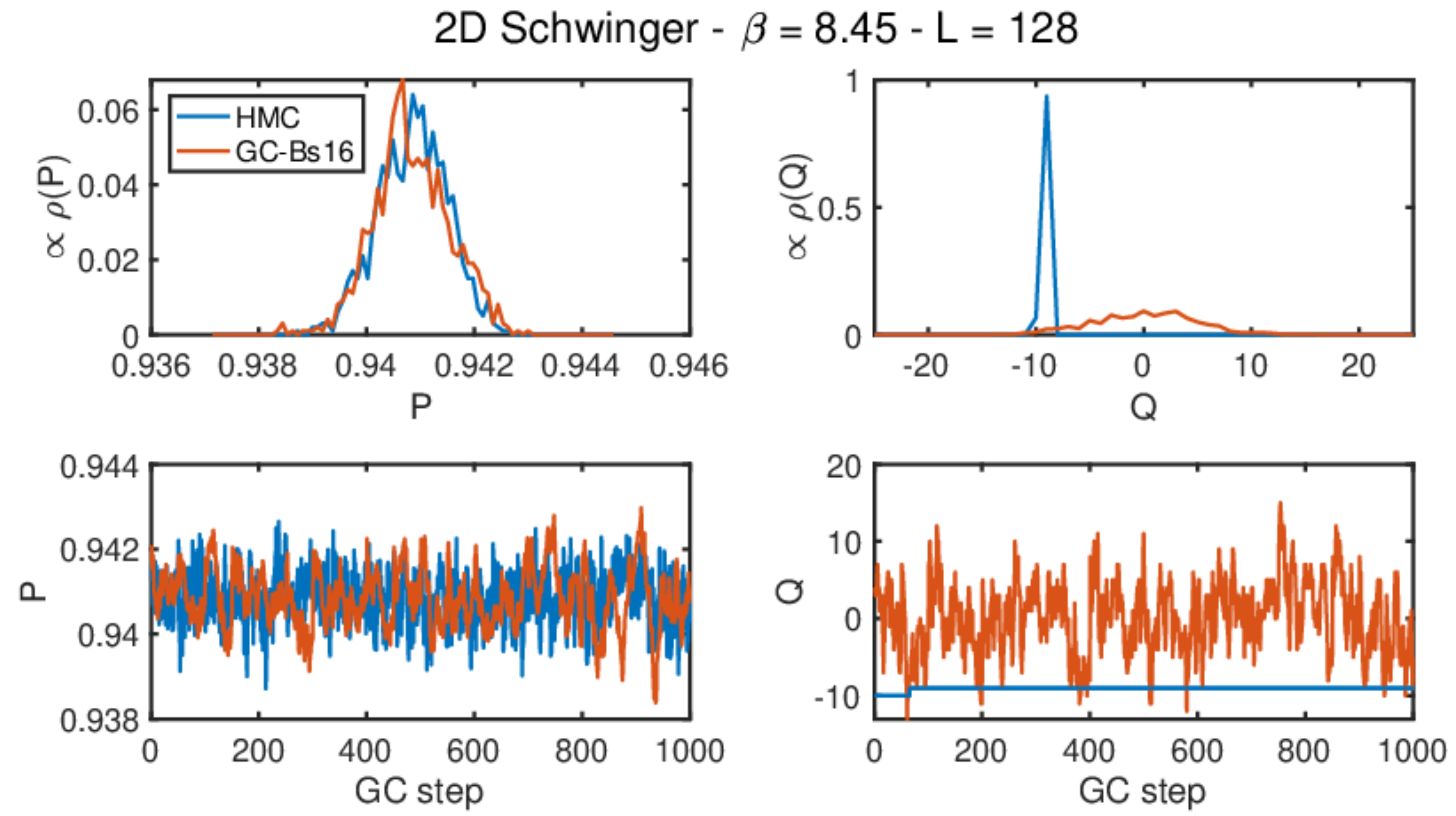
Run statistic

- L = 128
- beta = 6.0
- m = -0.0342



Run statistic

- L = 128
- beta = 8.45
- m = 0.0



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Hierachical Filter Steps

How to control $\sigma^2(\Delta S)$

1. by using correlations between ρ and $\tilde{\rho}$
2. by reduction of degrees of freedom of ρ and $\tilde{\rho}$

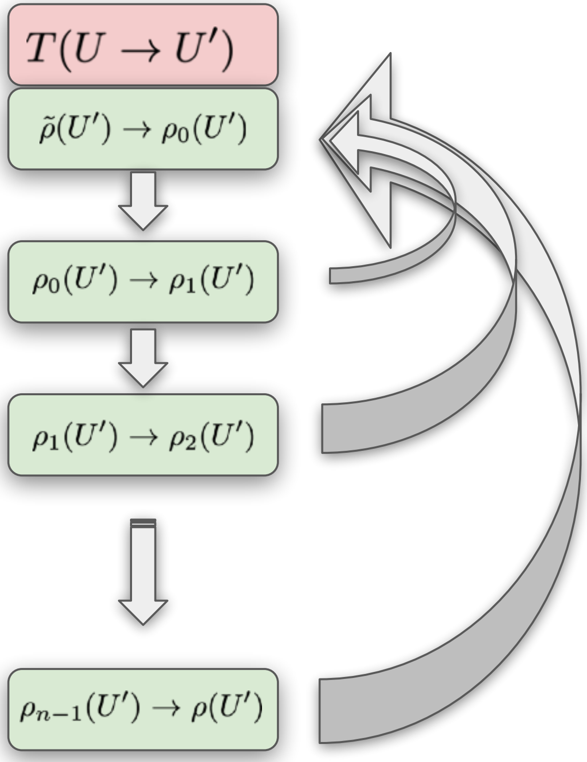
Generalization leads to factorization with parametrization of ρ via

$$\rho_n(U) = P_0(U,\alpha_i^{(0)})\, P_1(U,\alpha_i^{(1)})\ \dots P_n(U,\alpha_i^{(n)})$$

and GC step is spliting up into *n* successive steps

$$P^i_{acc}(U \to U') = \min\left[1, \frac{\rho_{j-1}(U,\alpha_i^{(j-1)})\rho_j(U',,\alpha_i^{(j)})}{\rho_j(U,,\alpha_i^{(j)})\rho_{j-1}(U',\alpha_i^{(j-1)})}\right]$$

- Iterate each step to filter out local fluctuations

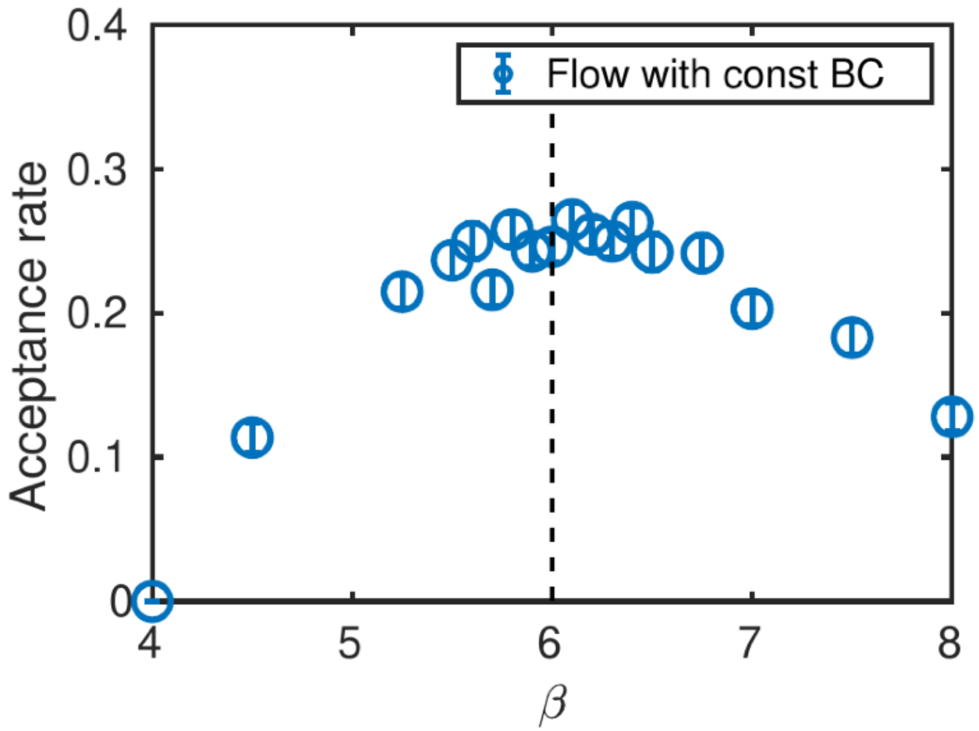


Training with fix boundaries

Adaptation of training procedure

By:

- Using the periodic trained model to generate boundaries or starting from random and shift lattice after each epoch
- Using different boundaries for each batch with total batch size 4096
- Increase iteration before boundaries updated to 1000
- Using diagonal masks to increase overlap with frozen plaquettes (faster convergence)



Acceptance rate of fixed boundaries drops down to ~25% with L = 8 (from 50% periodic case)

- due to the ultra locality of gauge action: larger volumes are trivial to generate

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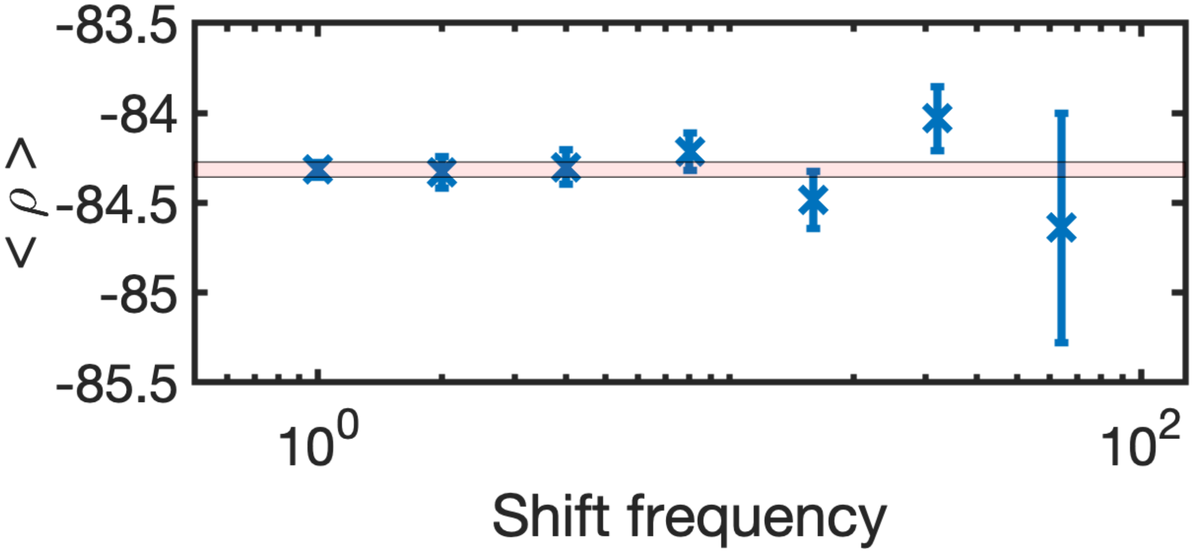
Training with fix boundaries

A priori unknown: Maps under shifts of the lattice

$$T_{\vec{x}} : \vec{x_0} \to \vec{x_0} + \vec{x}$$

Lattice action is invariant but maps *a priori* not

$$\langle \tilde{\rho}(U) \rangle \neq \langle \tilde{\rho}(T_{\vec{x}}(U)) \rangle$$



Idea: check numerical if one can detect deviations

- check if the inverse map maps into the trivial space

$$m^{-1} : T(U) \to T(U_{trivial}) \in \rho_{trivial}?$$

- check if observables are sampled correctly via histograms and via mean values

no numerical indication that shift is violating sampling

- ideally do several iterations of flow updates after a shift

(would eliminate any violation via thermalization)

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Topological sampling in case of the Dirac Index

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Topological tunneling requires energy

The Index theorem gives some illustrative insides:

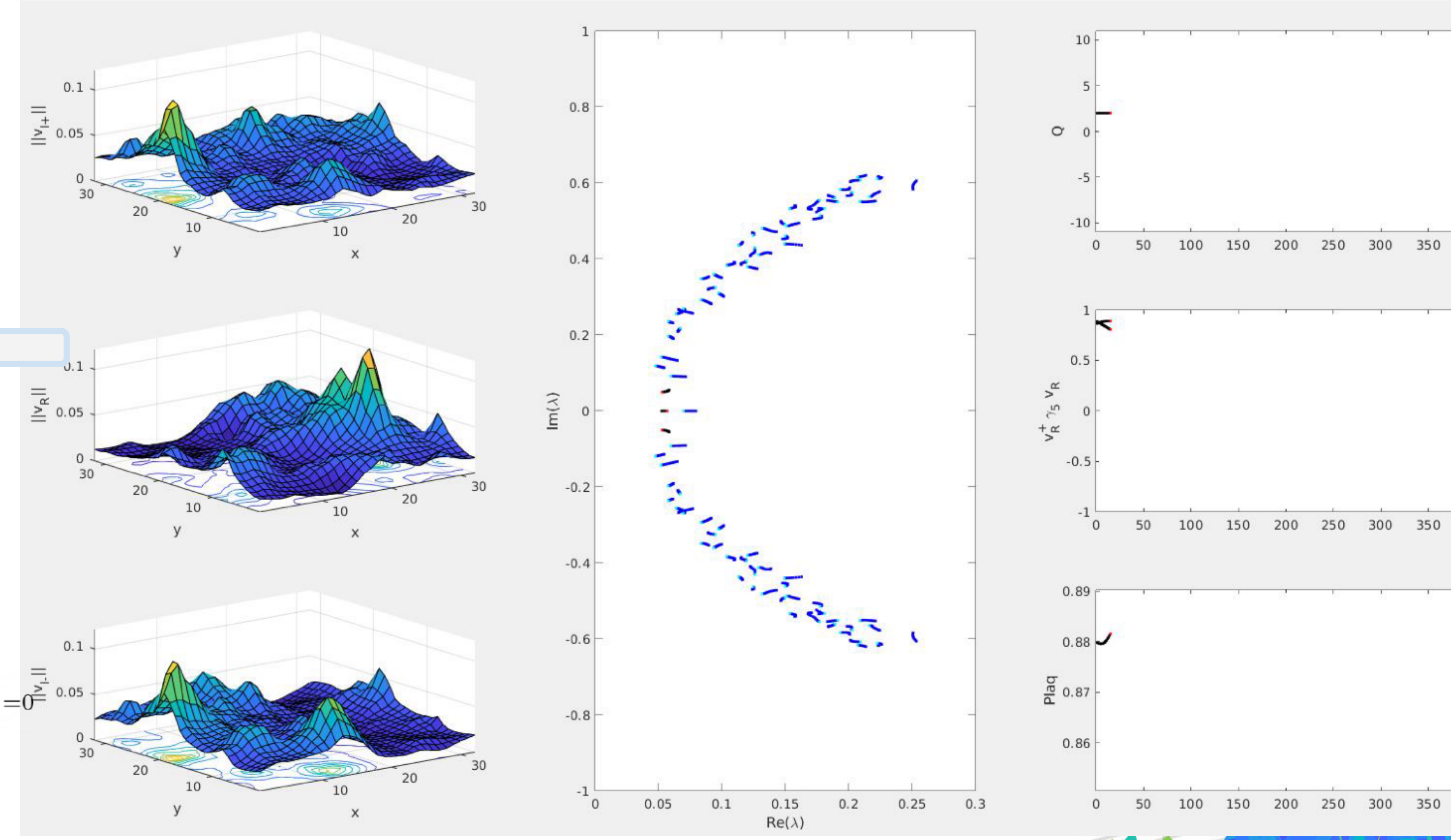
$$N_R - N_L = Q^{geo}$$

Atiyah and Singer, 1963

with the geometric definition:

and $$Q^{geo} = \frac{1}{2\pi} \sum_x \theta_{12}(x)$$

$$\mathrm{Index}(D) = N_R - N_L = \sum_i \chi_i |_{\lambda(D)=0}$$



Modes are localized

❖ **update 8x8 block can flip charge**

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Topological sampling in case of the Dirac Index

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Atiyah and Singer, 1963

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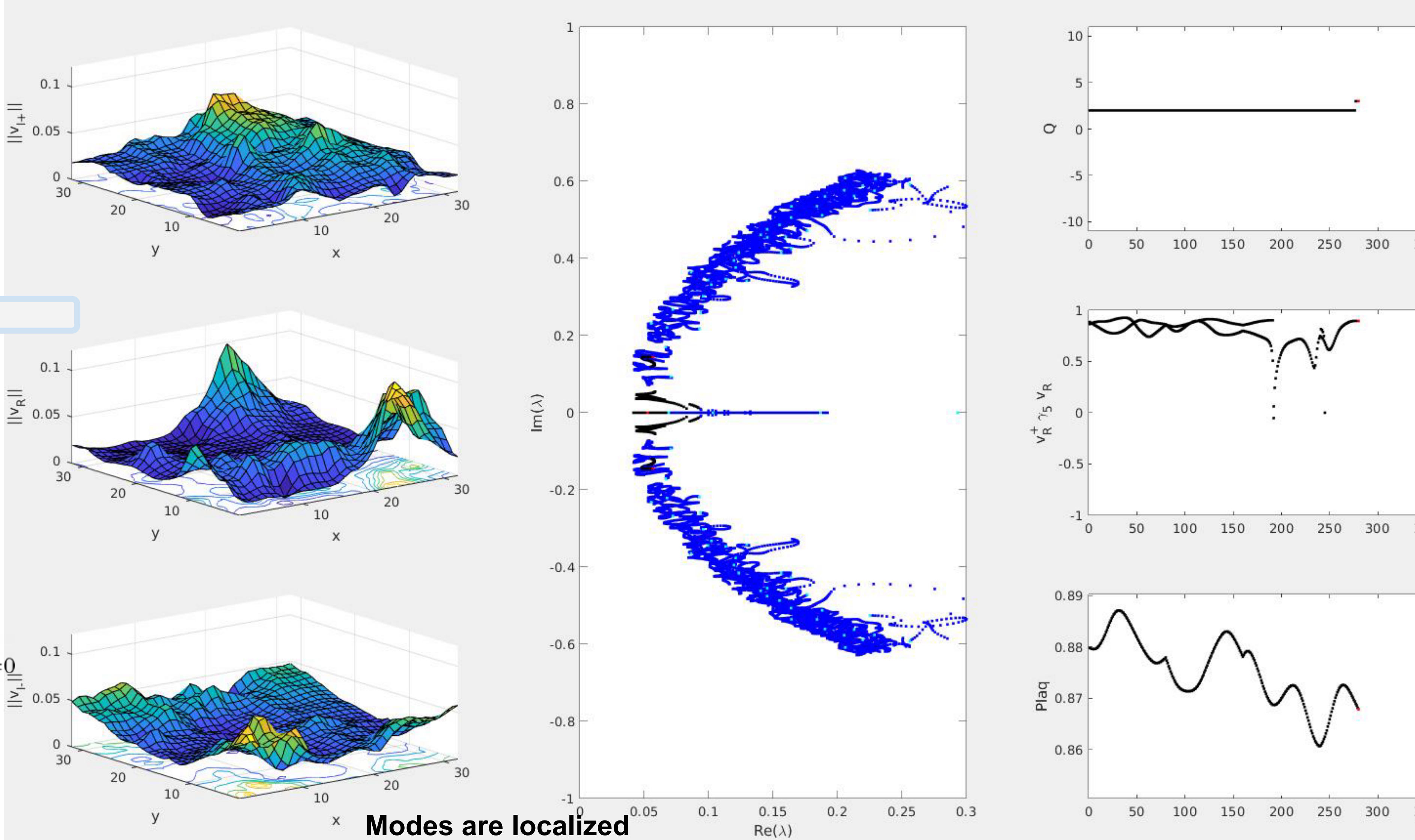

Modes are localized

❖ **update 8x8 block can flip charge**

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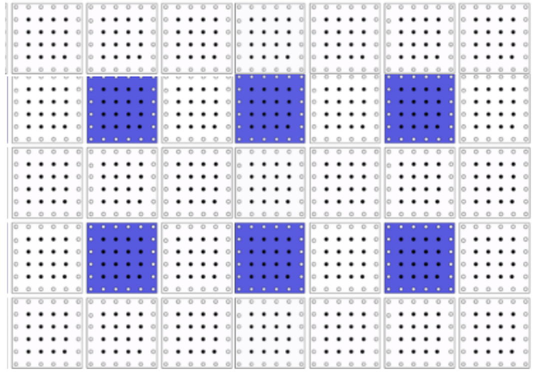
Towards high acceptance



Acceptance rate:

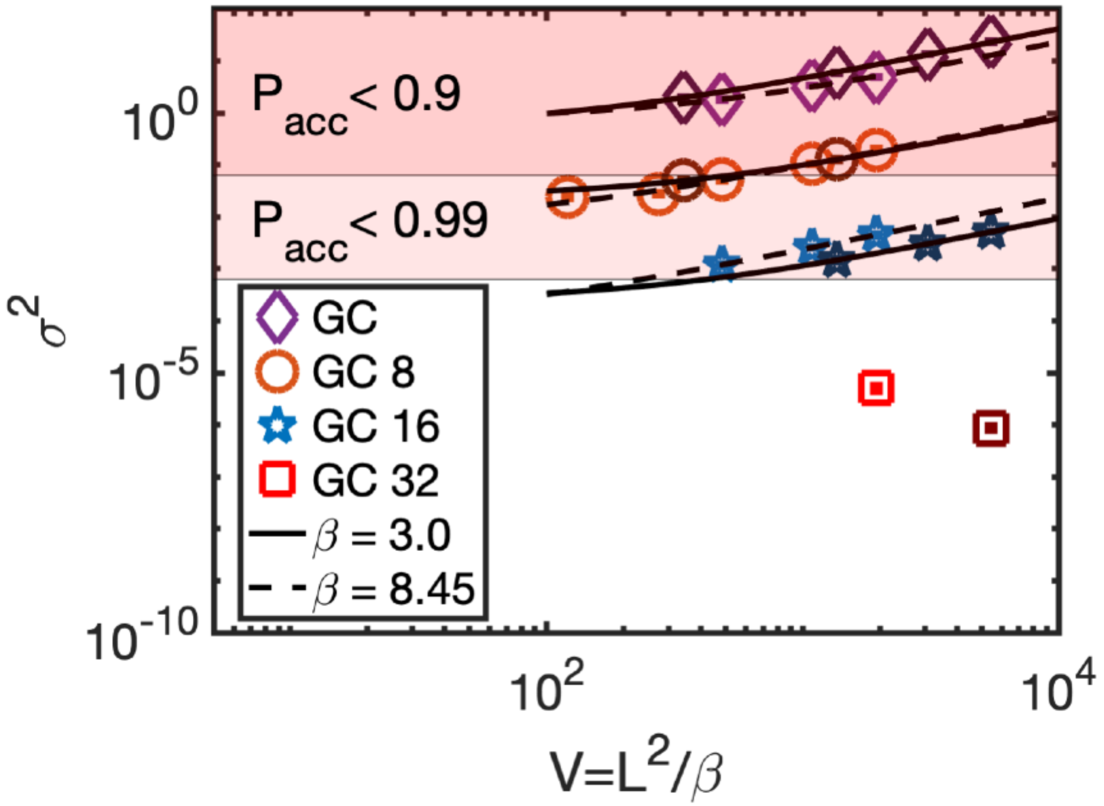
- select L=8 flow proposals
- updating every 4th block, which introduces a distance between active blocks by d = Lbs
  which results into 16% of links updated per step

(independent of global volume!)

runs for different Lbs = 8, 16, 32 with 4 lvl filter steps

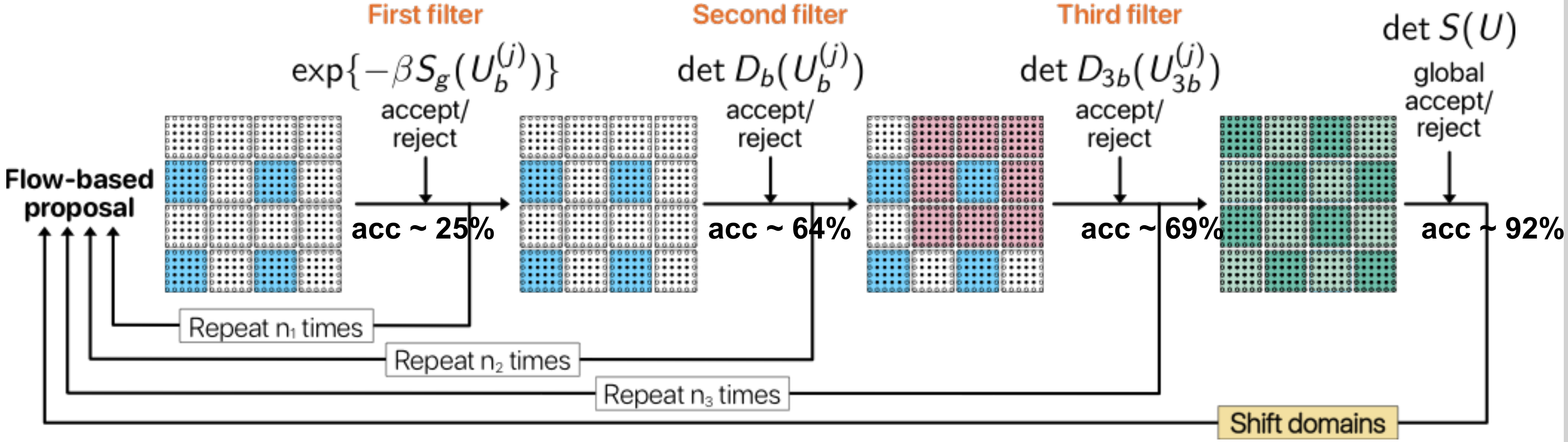
- variance is very efficient reduced for larger Lbs
- volume scaling remains

How only 16% active links influence sampling rates ?



Towards high acceptance

Global Correction Monte Carlo algorithms with equivariant flows:



$$\rho(U) = \det D^2(U)\, e^{-\beta S_g(U)} = e^{-\beta S_g(U)} \prod_b \det D_b^2(U_b) \cdot \det S^2(U)$$

Multilevel hierarchical filter steps with 4 levels

Enhancing acceptance rate by

- ❖ within level 1, 2, 3 each active block can be updated independently from each other
- ❖ use correlation between actions via parameterization,
  - ✦ Using gauge coupling constant $\beta = \beta_0 + \beta_1 + \dots$

β	3.0	6.0	8.45
5 level flowGC with $d = 16$:			
Level 4			
with σ^2	0.0052	0.0369	0.0046
and P_{acc}	0.9713	0.9235	0.9727
$\delta\beta_4^{(3)}$	-2.0037	-2.0182	-2.0087
$\delta\beta_4^{(2)}$	1.0027	1.0061	1.0083
$\delta\beta_4^{(1)}$	-0.0003	0.0008	0.0004
Level 3	$n_1 = 2$		
with σ^2	0.6688	0.6190	0.1546
and P_{acc}	0.6826	0.6940	0.8441
$\delta\beta_3^{(2)}$	-1.1730	-1.3635	-1.3534
$\delta\beta_3^{(1)}$	-0.0006	0.0149	0.0125
Level 2	$n_2 = 4$		
with σ^2	1.4384	0.8325	0.1857
and P_{acc}	0.5487	0.6482	0.8294
$\delta\beta_2^{(1)}$	-0.2482	-0.3082	-0.2863
Level 1	$n_1 = 100$		
with P_{acc}	0.5669	0.2501	0.2794
2 level GC:			
with σ^2	12.3774	9.7119	3.7260
and P_{acc}	0.0786	0.1192	0.3345

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