Applications of machine-learned flows to lattice QCD

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Probing the Frontiers of Nuclear Physics with AI at the EIC

Stony Brook / CFNS

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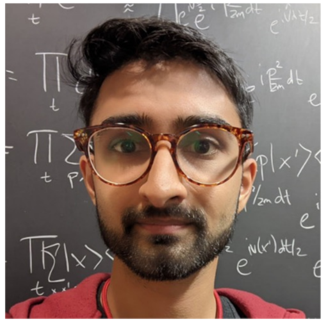
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Quantum Chromodynamics (QCD)

Part of the Standard Model of particle physics

QFT that describes the strong force

- Dynamics of quarks & gluons
- $SU(3)$ gauge theory

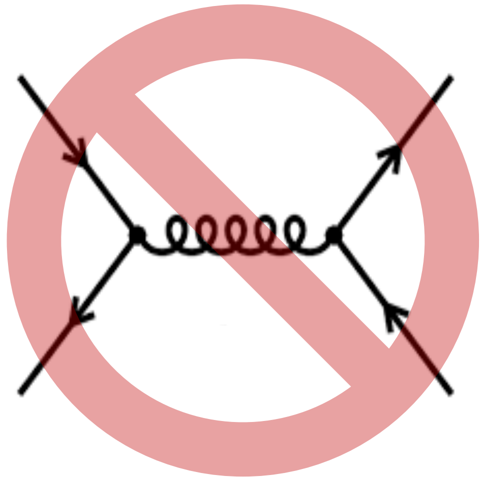
Pen-and-paper calculations don't work

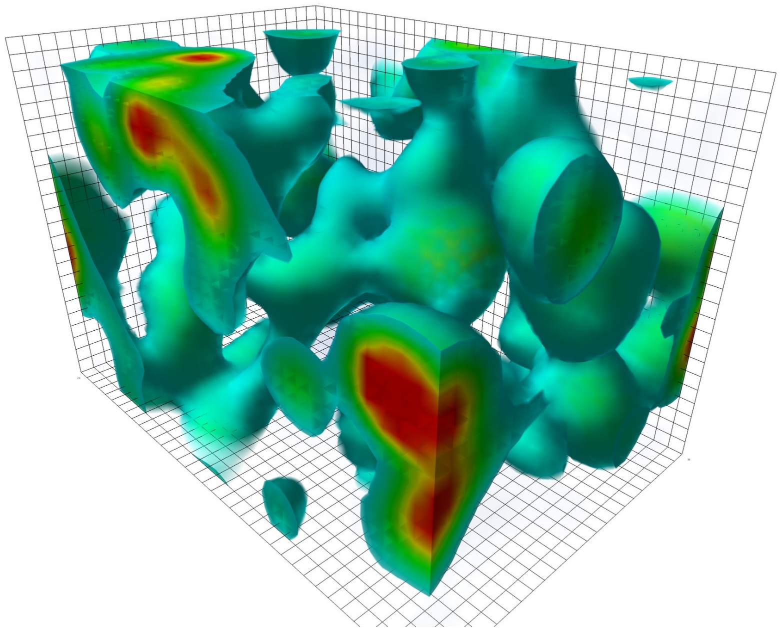
- Strongly interacting QFT
- Non-perturbative dynamics

Instead: lattice QCD!

- Evaluate discretized QCD path integral w/ (MC)MC

Integral part of nuclear/particle theory toolkit

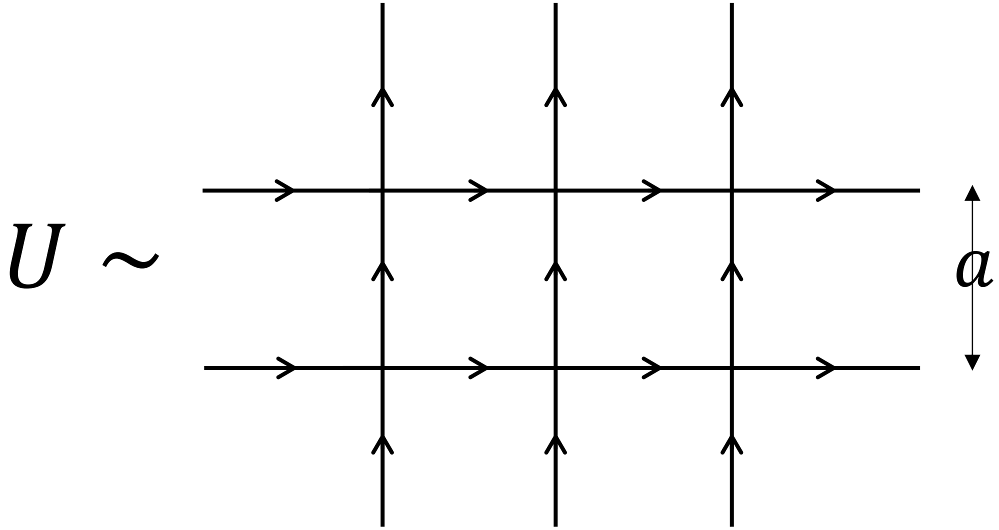




Visualizations of Quantum Chromodynamics

Lattice QCD

Discretized gluon (gauge) field



Setup:

- (3+1)d QFT ⇒ 4d Stat Mech
- Restrict to finite volume
- Discretize spacetime

Use Monte Carlo to (path) integrate over discretized fields:

$$\langle \mathcal{O} \rangle = \int d[U] \frac{1}{Z} e^{-S[U]} \mathcal{O}(U) \equiv \int d[U]\, p(U)\, \mathcal{O}(U) \approx \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(U_i)$$

→ Numerical QFT on supercomputers!

Workflow of a lattice calculation

1. Configuration generation

   Sample ensembles of gauge fields w/ MCMC

   …for different lattice spacings, m_q, V

2. Observable measurements

   Evaluate n-point functions on e/a config

   → compute expectations

3. Analysis

   Extract hadronic properties (masses, matrix elements, etc)

   Extrapolate to physical limit

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Expensive! (items 1–2)

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Accelerate with ML?

Expensive!

Topological freezing

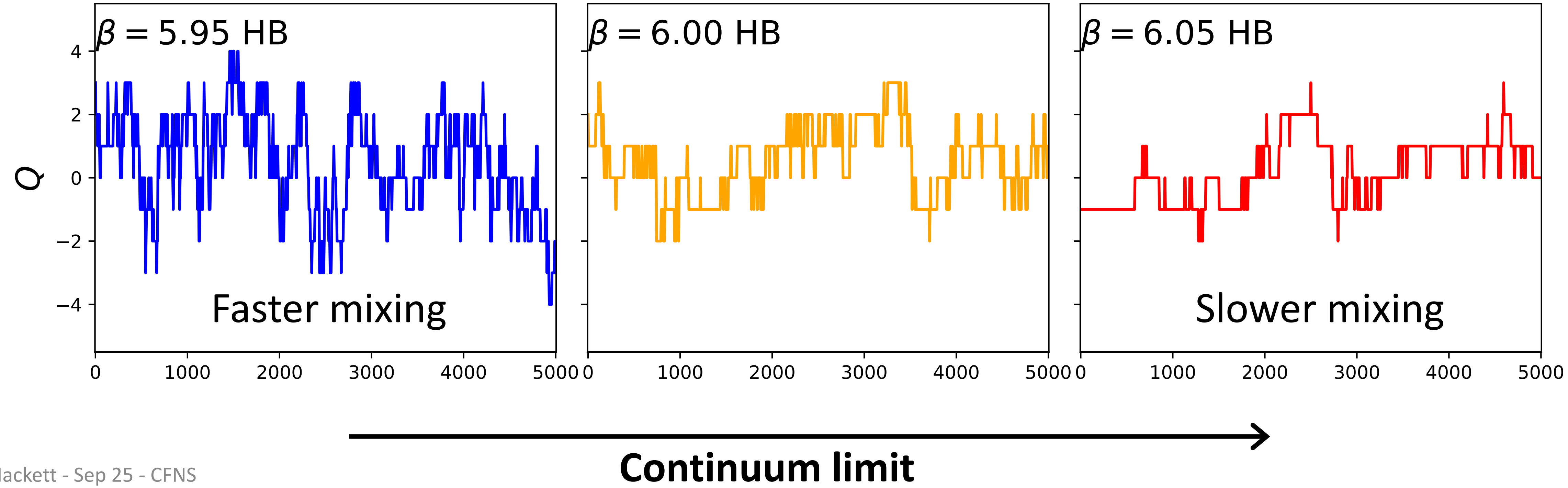
Problem: gauge field distribution is multimodal

Must sample different **topological sectors**

Exponential slowdown of tunneling between sectors w/ standard MCMC algos

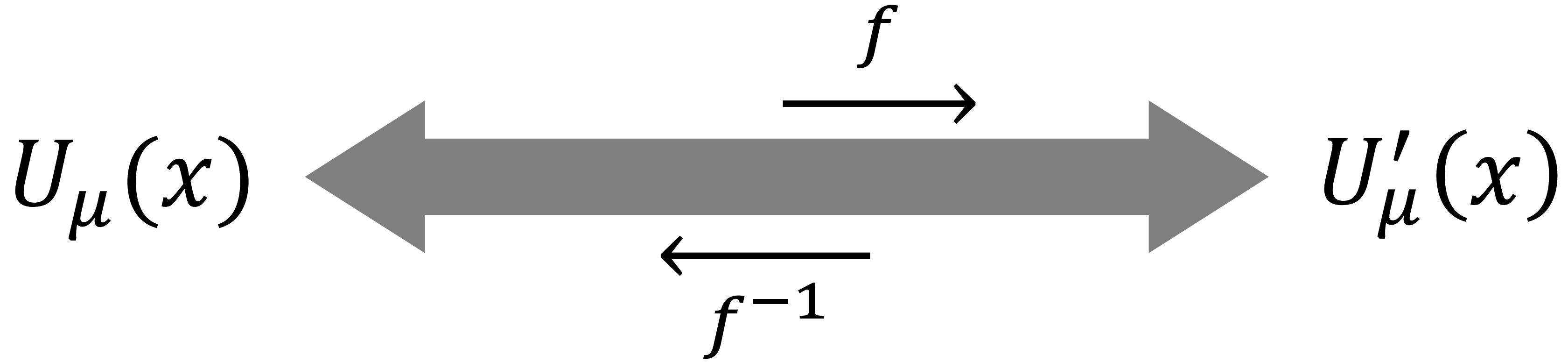
Can result in *effective* loss of ergodicity [2202.1172]

→ Apparent convergence to wrong answers at achievable sample sizes



A New Tool: Machine-learned Flows

f: learned, invertible (diffeomorphic) map between gauge field configs



…with many tunable parameters → ML

…maybe equivariant w/r/t symmetries g of interest $f\big(g(U)\big) = g(f(U))$

…with a tractable Jacobian determinant $J_f(U) = \left|\det \frac{\partial f(U)}{\partial U}\right|$

A New Tool: Machine-learned Flows

Flows are “bridges” between different distributions/theories/actions

$$r(U) = \frac{e^{-S_r(U)}}{Z_r} \quad \underset{f^{-1}}{\overset{f}{\rightleftarrows}} \quad q(U') = \frac{r(U)}{J_f(U)}$$

Exact bridge between r and q

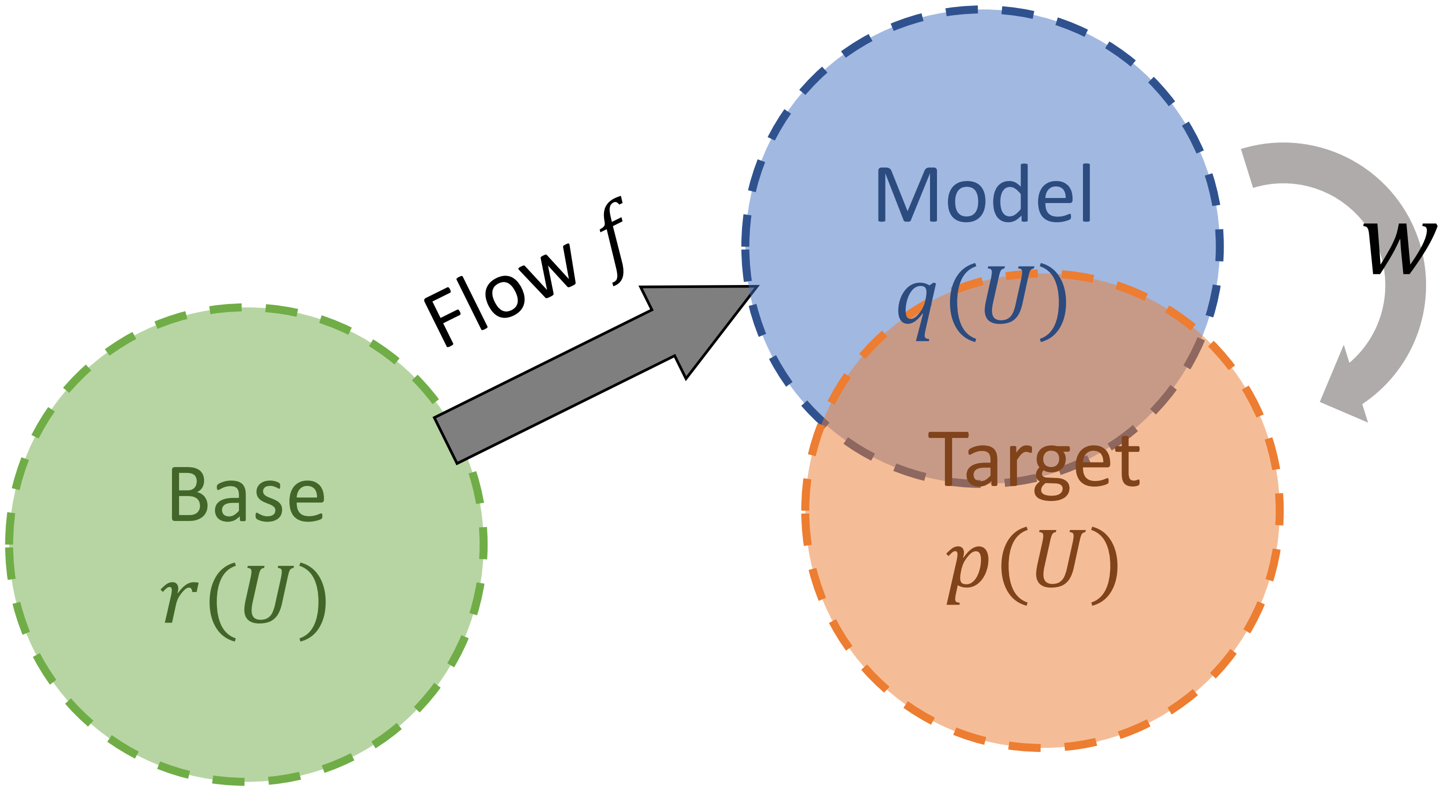
Choose r, but flow induces q

For sampling applications: variationally optimize f so $q \approx p \propto e^{-S_p}$

→ *Approximate* bridge between r and p

(Approximate) direct sampling with flows

Apply f to Haar uniform to get model q, tune f so $q \approx p \propto e^{-S_{\text{target}}}$



Reweight from $q \to p$

$w(U) = p(U) \,/\, q(U)$

$\langle O \rangle_p = \langle wO \rangle_q$

Or, ~ equivalently, Metropolize

→ Flow-based MCMC

a.k.a. neural MCMC

a.k.a. …

Progress so far

Flows for LQFT (scalar field theories)

[1904.12072] [2107.00734] [2211.07541]

Gauge-equivariant flows

U(1) [2003.06413]

SU(N) [2003.06413] [2305.0242]

Flows for fermionic theories

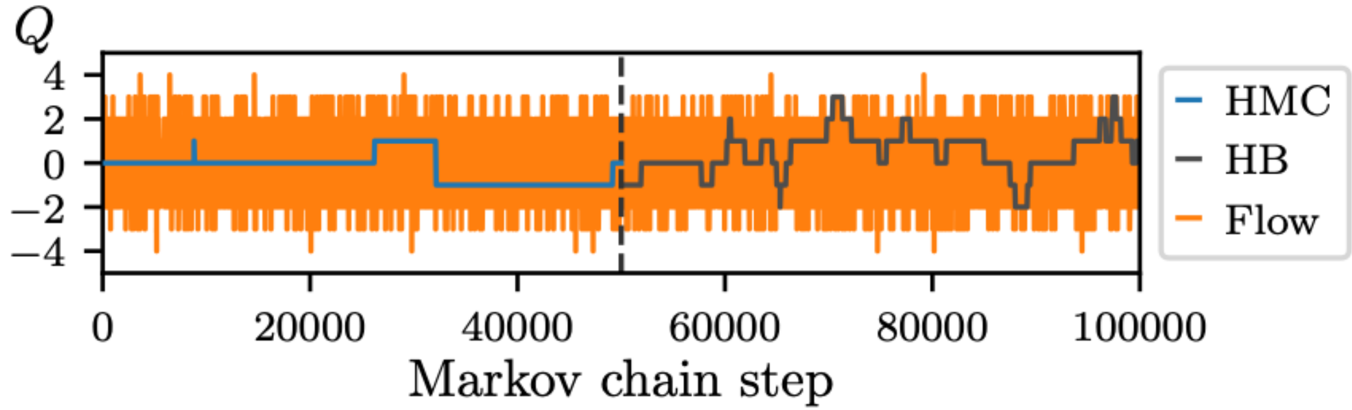
Yukawa model [2106.05934]

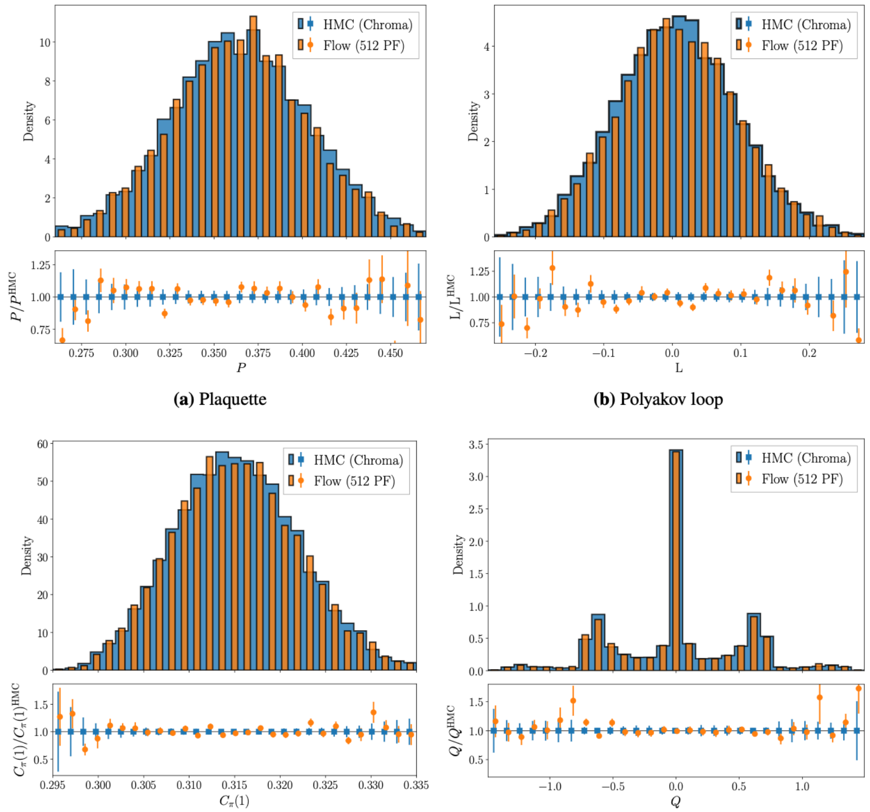
Schwinger model [2202.11712]

Stochastic methods for fermions [2207.08945]

→ First demonstration for QCD! [2208.03832]

Result: Improved sampling in (1+1)d U(1) gauge theory





(a) Plaquette

(b) Polyakov loop

(c) Pion correlation function at $x_0 = 1$

(d) Topological charge at $t/a^2 = 4$

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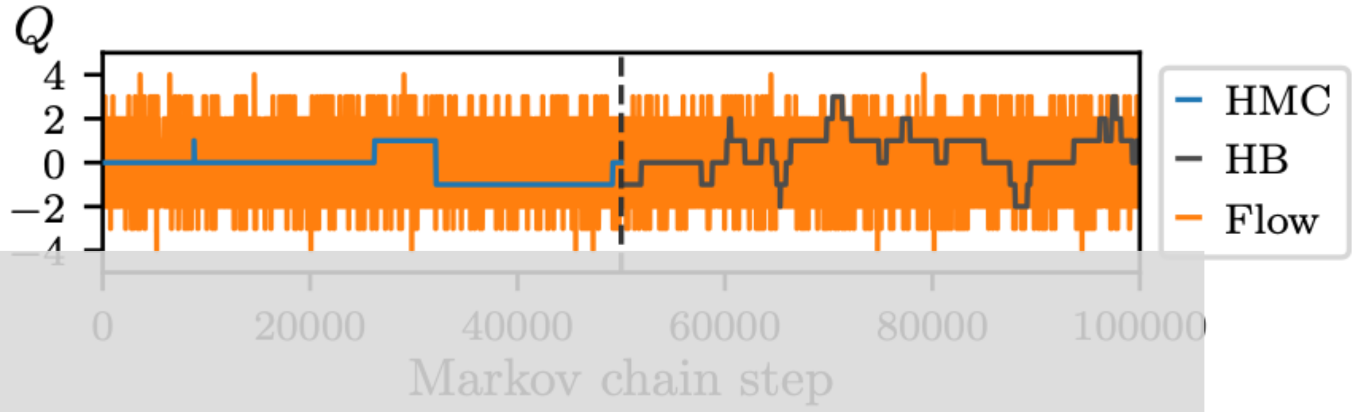

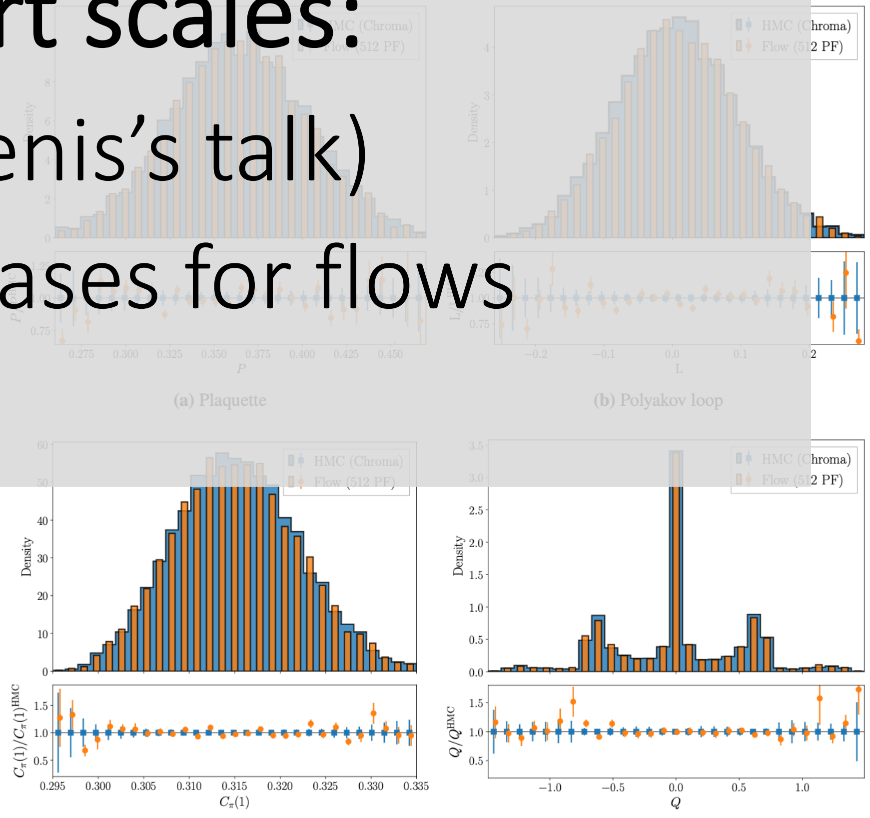

(c) Pion correlation function at $x_0 = 1$

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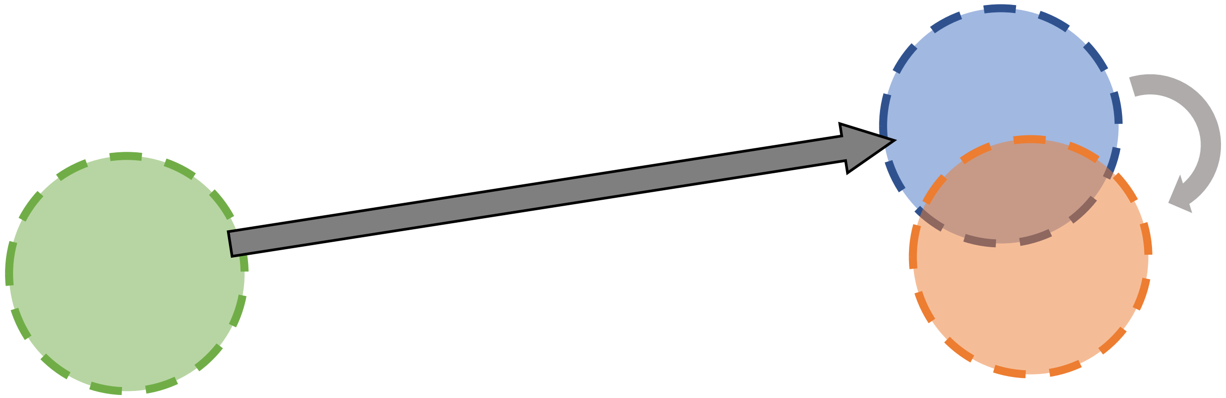
Towards state-of-the-art scales:

1. Better QCD models (Denis's talk)
2. Different algorithmic use cases for flows

Applications



Basic idea: don't flow as far

→ 3x demos

Target theory: $\mathrm{SU}(3)$ gluodynamics

Avoid fermionic complications (for now)

Sample w/ heatbath (HB) + overrelaxation (OR)

"Residual flows" [2305.02402]

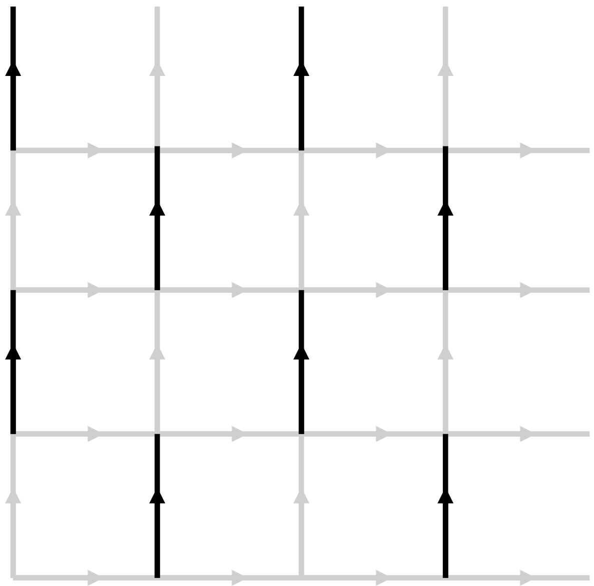
~ ODE flow + variable partitioning (cf. coupling layers)

→ tractable/inexpensive exact Jacobian

Features:

Gauge equivariant flows

Translationally invariant ↔ volume transferrable



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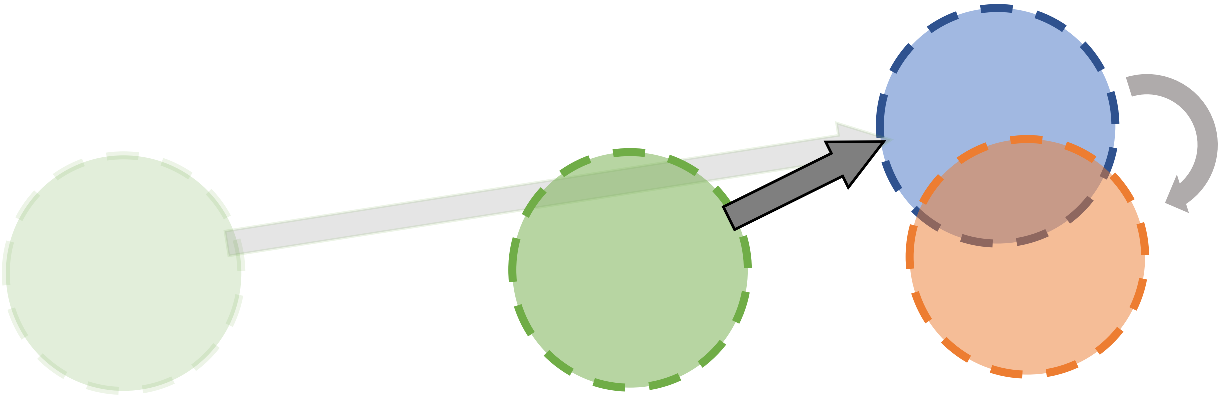

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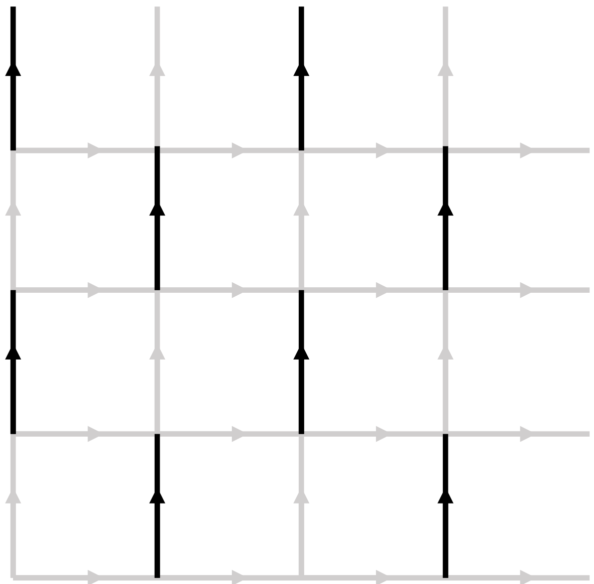


App 1: Correlated ensembles

Flow an ensemble

$\rightarrow$ $\{U\}$ and $\{f(U)\}$ are correlated

This is useful!

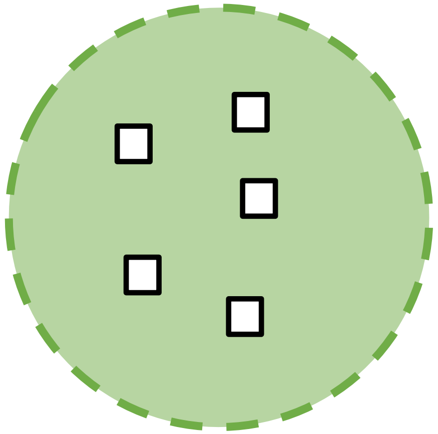
e.g. for noise cancellation in differences

$$\langle O \rangle_p - \langle O \rangle_r$$

$$= \langle wO \rangle_q - \langle O \rangle_r$$

$$= \big\langle w\big(f(U)\big)\, O\big(f(U)\big) - O(U) \big\rangle_{U\sim r}$$

$\{U\} \sim r$



Application: Feynman-Hellmann $\quad S \rightarrow S + \lambda\, O \quad \left.\frac{\partial E_h}{\partial \lambda}\right|_{\lambda=0} \sim \langle h|O|h\rangle$

(Complication: involves fits for E_h, but same idea)

See also [Bacchio 2305.07932]

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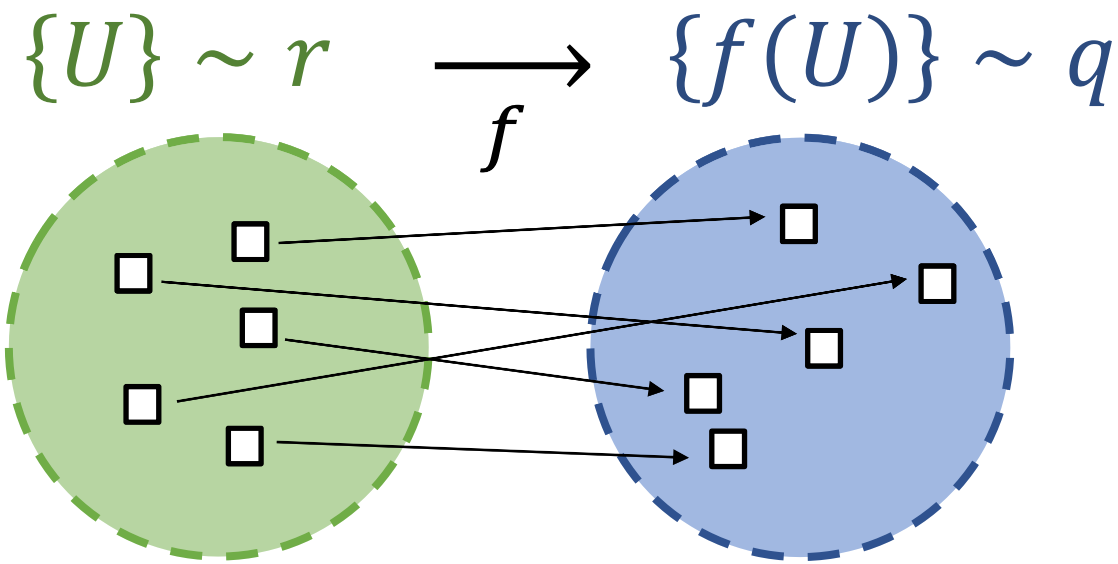

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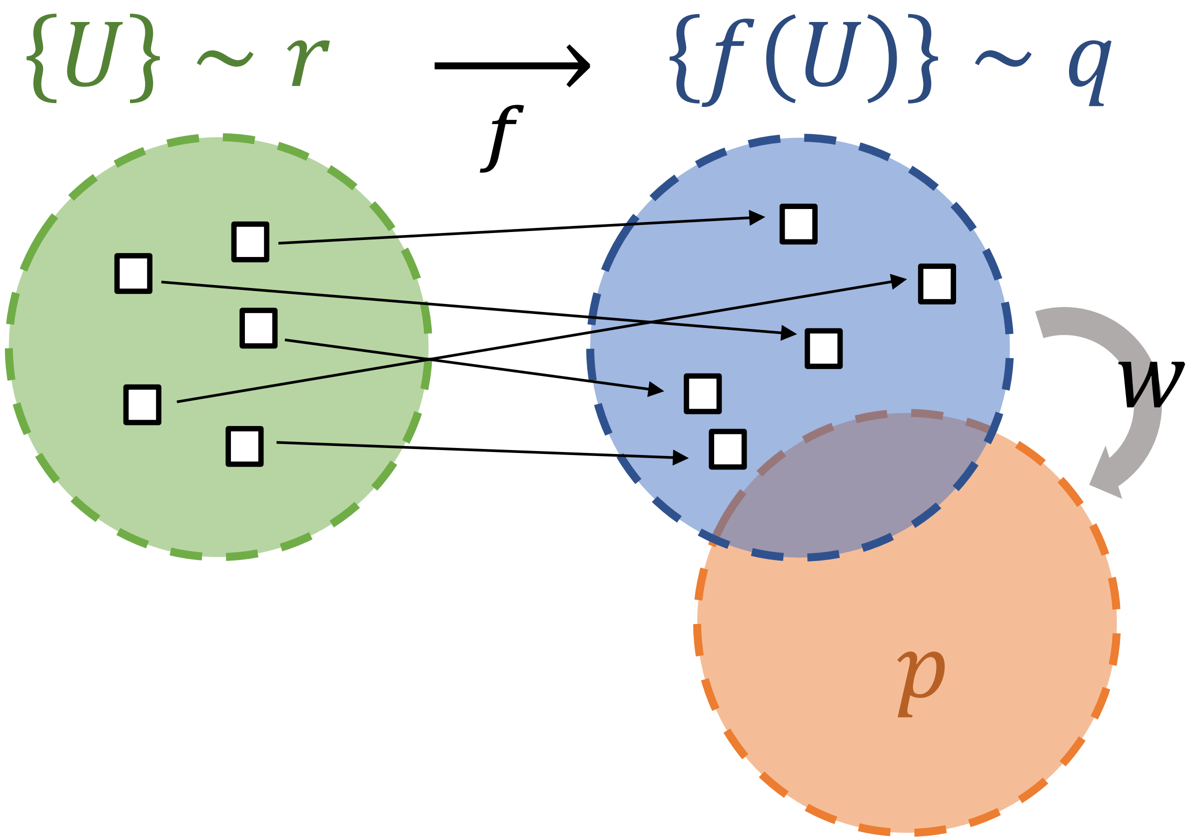

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[QCDSF-UKQCD 1205.6410]

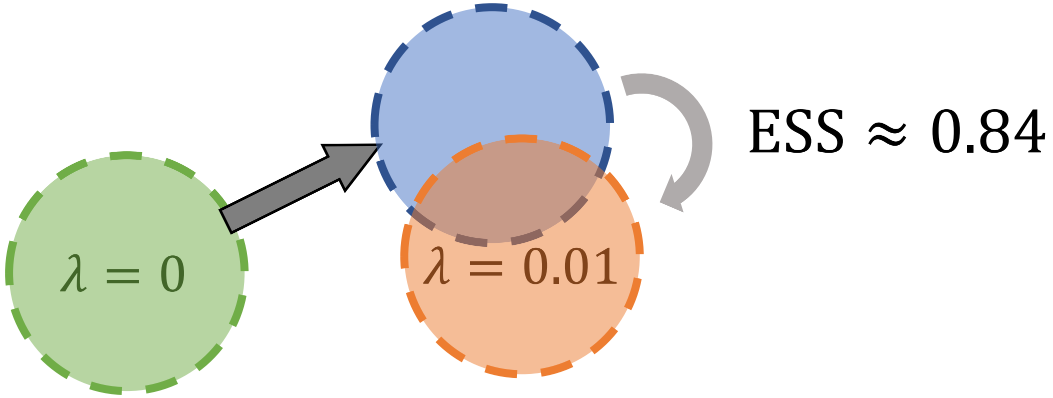
Spatial-temporal anisotropy: $\delta S = -\lambda \frac{\beta}{N_c} \left[\sum_i P_{ti} - \sum_{i<j} P_{ij} \right]$

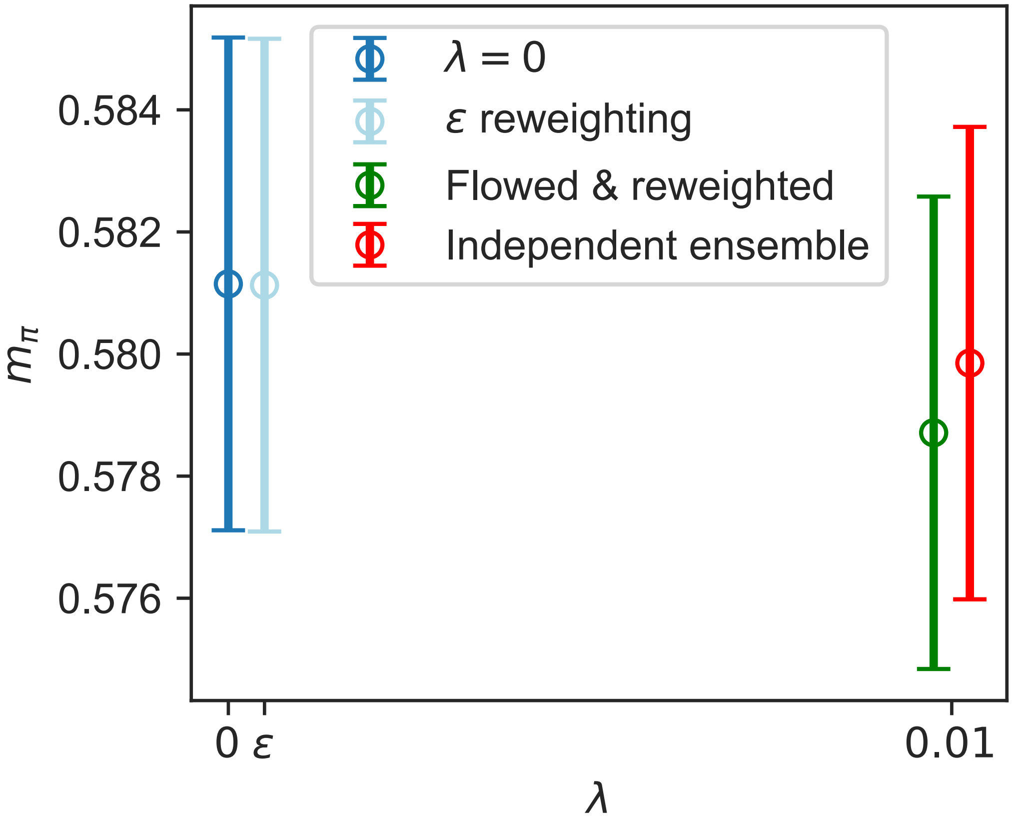
$$\langle x \rangle_g^{\text{lat}} = -\frac{2}{3m} \frac{\partial m}{\partial \lambda}\Big|_{\lambda=0} \approx -\frac{2}{3m} \frac{1}{\lambda} [m(\lambda) - m(0)]$$

Parameters:

$8^3{\times}16 \quad \beta = 6 \quad \kappa = 0.132$ (quenched)

Flow:





Compute $m(\lambda)$ from $\langle w\, C^{2\text{pt}} \rangle_q$

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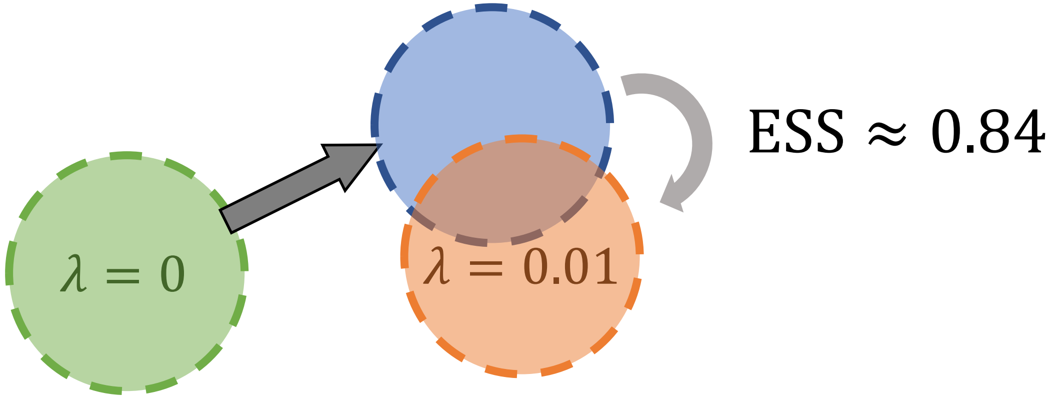

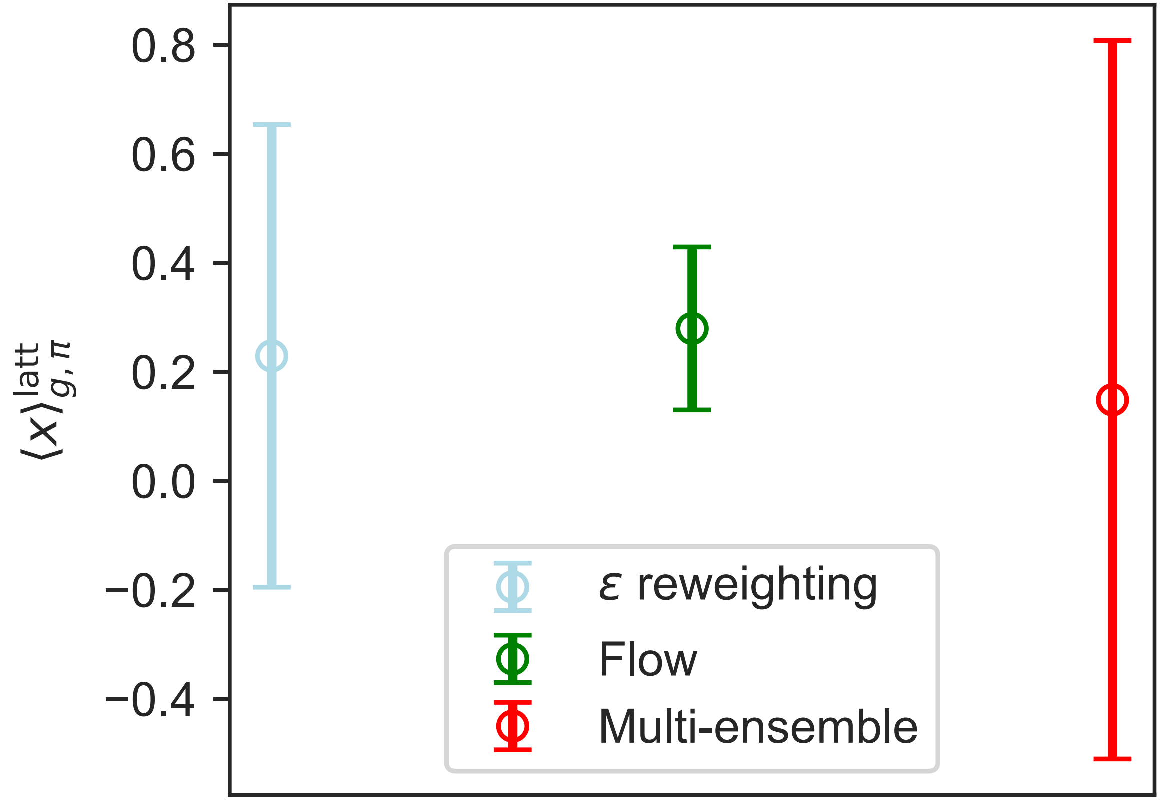

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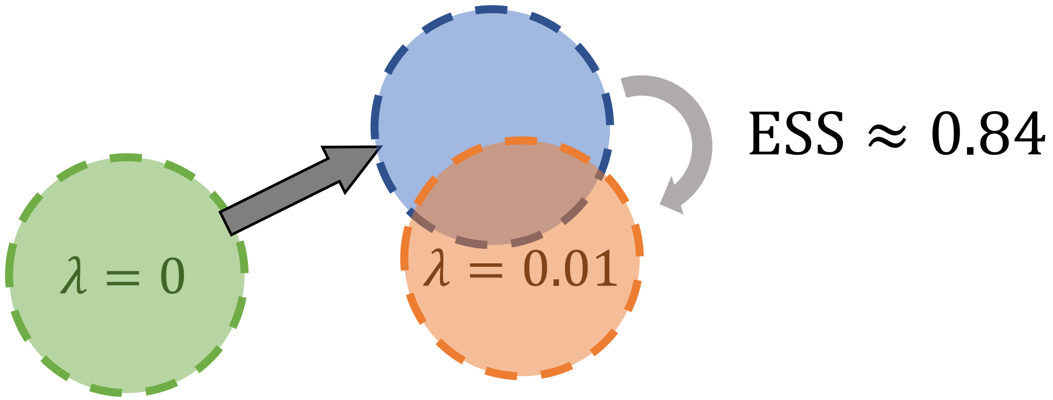
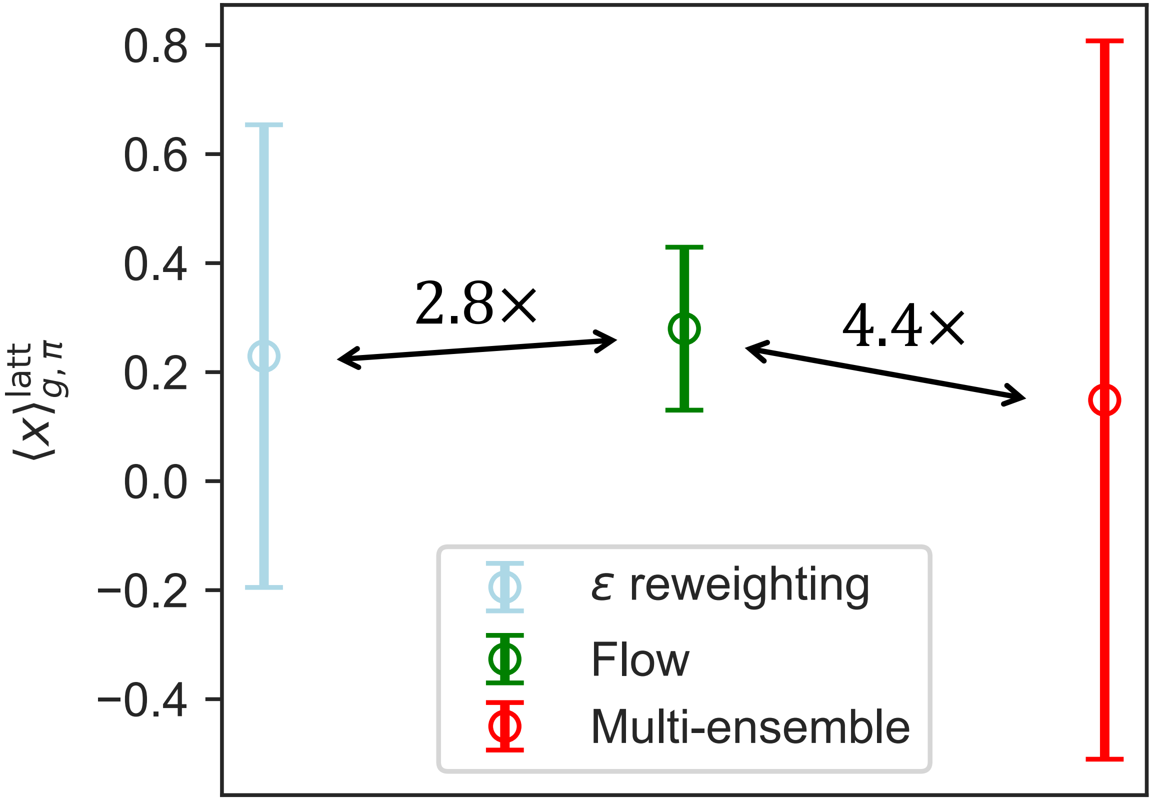


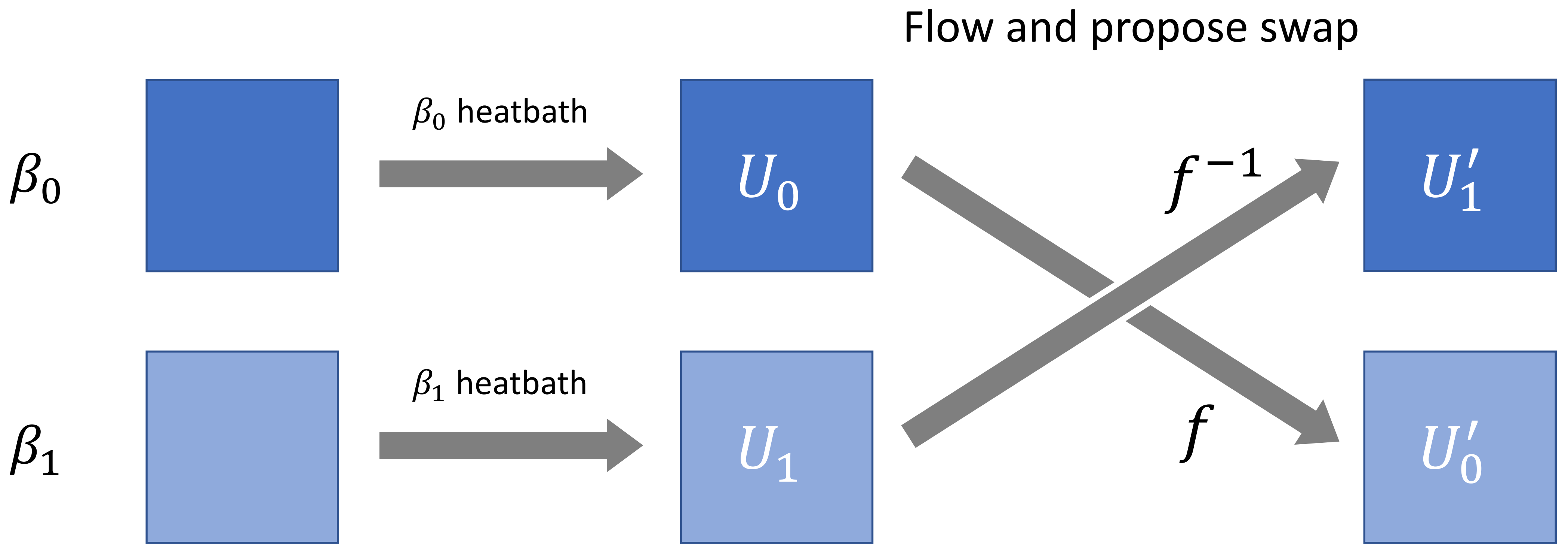


Compute $m(\lambda)$ from $\langle w\, C^{\text{2pt}} \rangle_q$

App 2: Transformed Replica EXchange (T-REX)

(REX a.k.a. parallel tempering) [Invernizzi Krämer Clemente Noé 2210.14104]

Simultaneously sample chains for different targets



$$p_{\mathrm{acc}} = \min\left[1, \frac{p_0(U_1')\, p_1(U_0')}{p_0(U_0)\, p_1(U_1)}\; J_f(U_0)\, J_{f^{-1}}(U_1)\right]$$

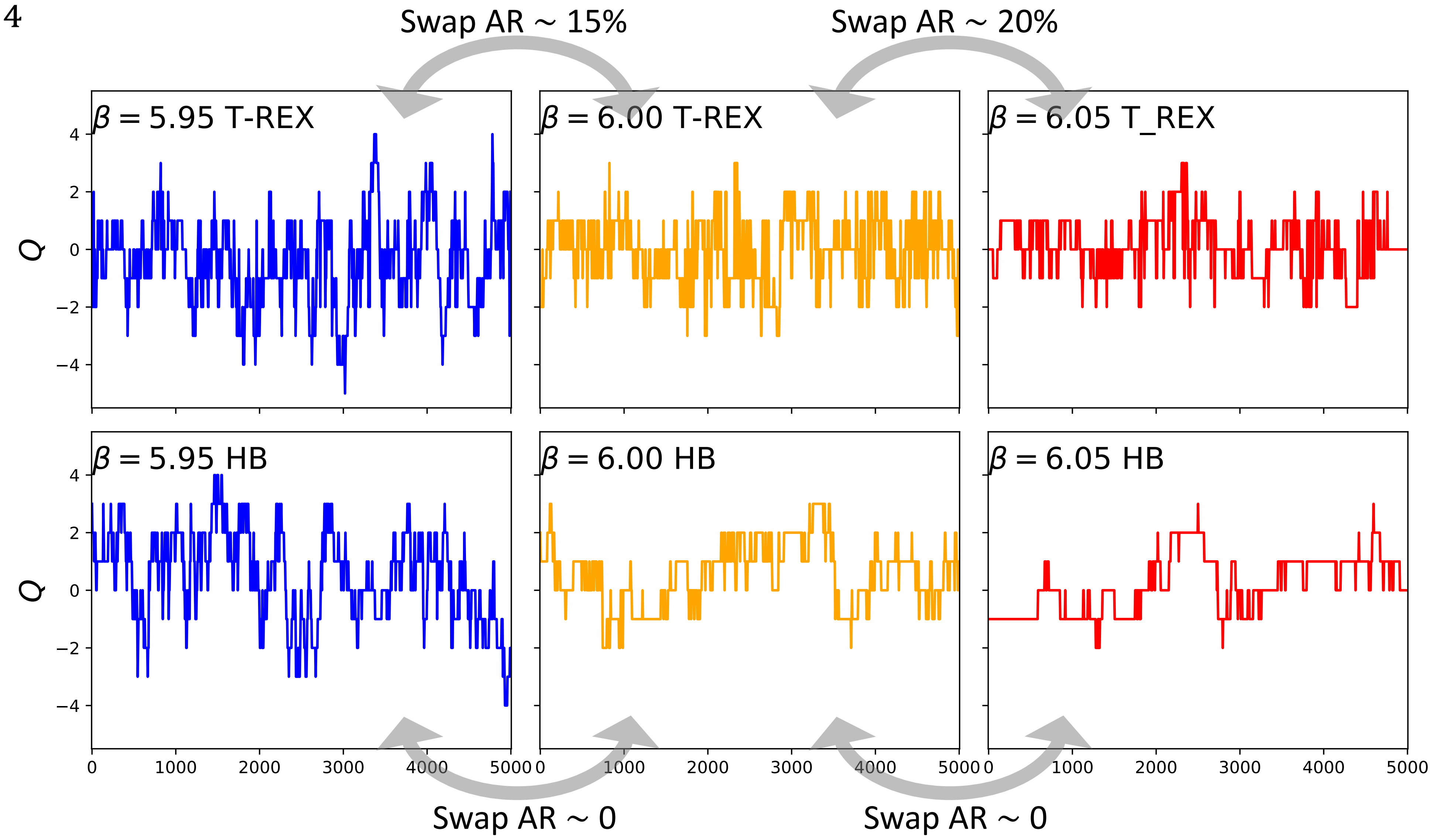
App 2: T-REX Results

Three target βs on 12^4

Two different flows

$5.95 \leftrightarrow 6$

$6 \leftrightarrow 6.05$



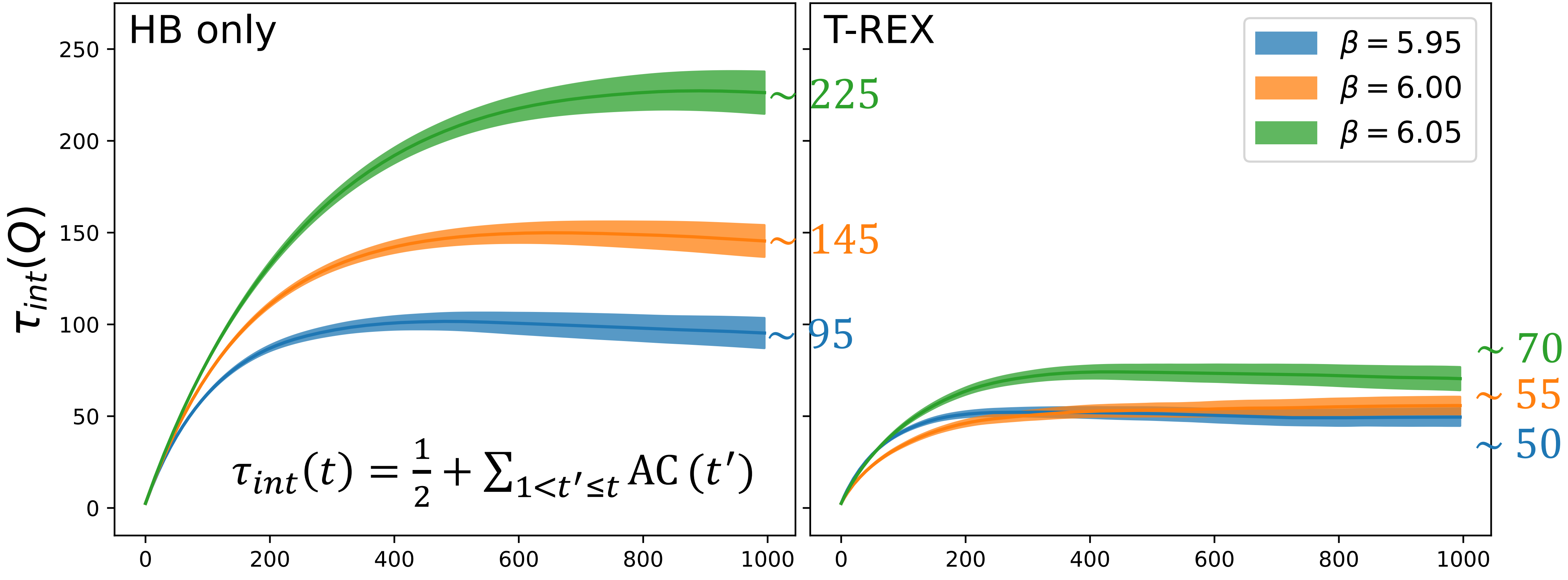
1 step = 5 HB + 2 OR, propose swaps every 5 steps

App 2: T-REX Results

Speed-up for multi-ensemble calculation

T-REX streams correlated (useful!)

Neglecting flow costs!



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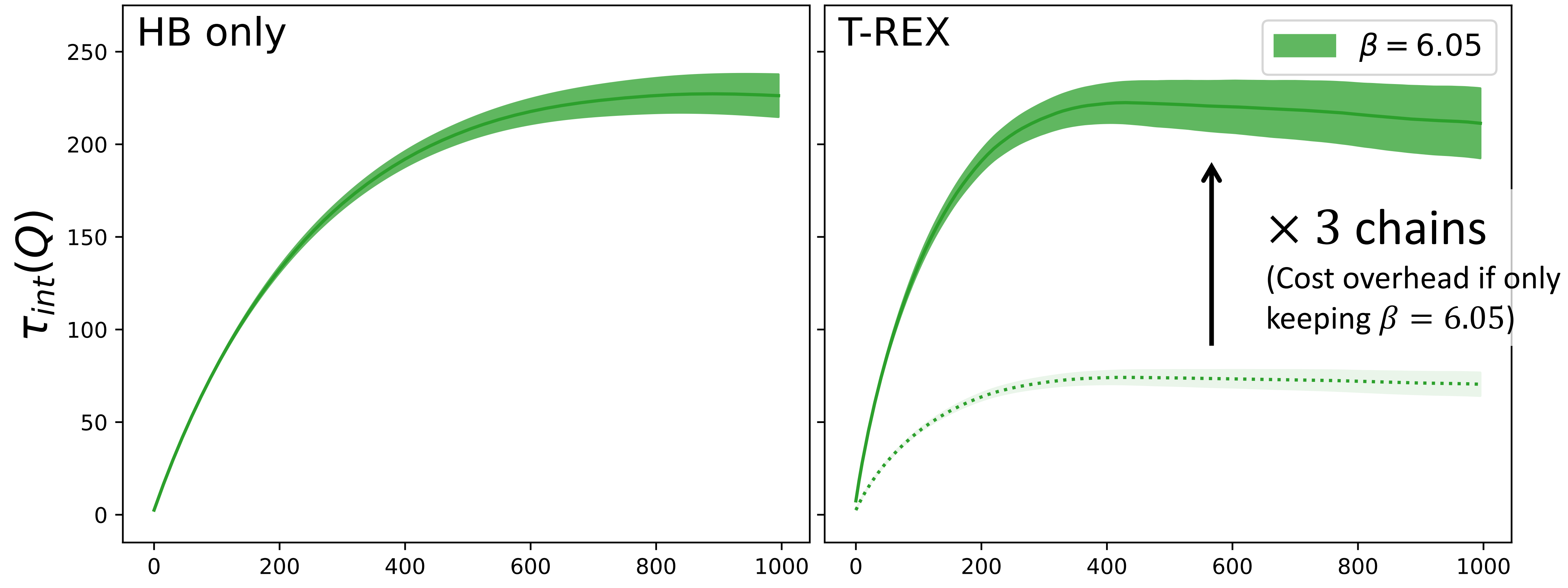
Speed-up for multi-ensemble calculation

T-REX streams correlated (useful!)

Break-even for sampling $\beta = 6.05$

} Neglecting flow costs!



App 3: Parallel Tempering on Boundary Conditions (PTBC)

[Hasenbusch 1706.04443]

[Bonnano Bonati D'Elia 2012.14000]

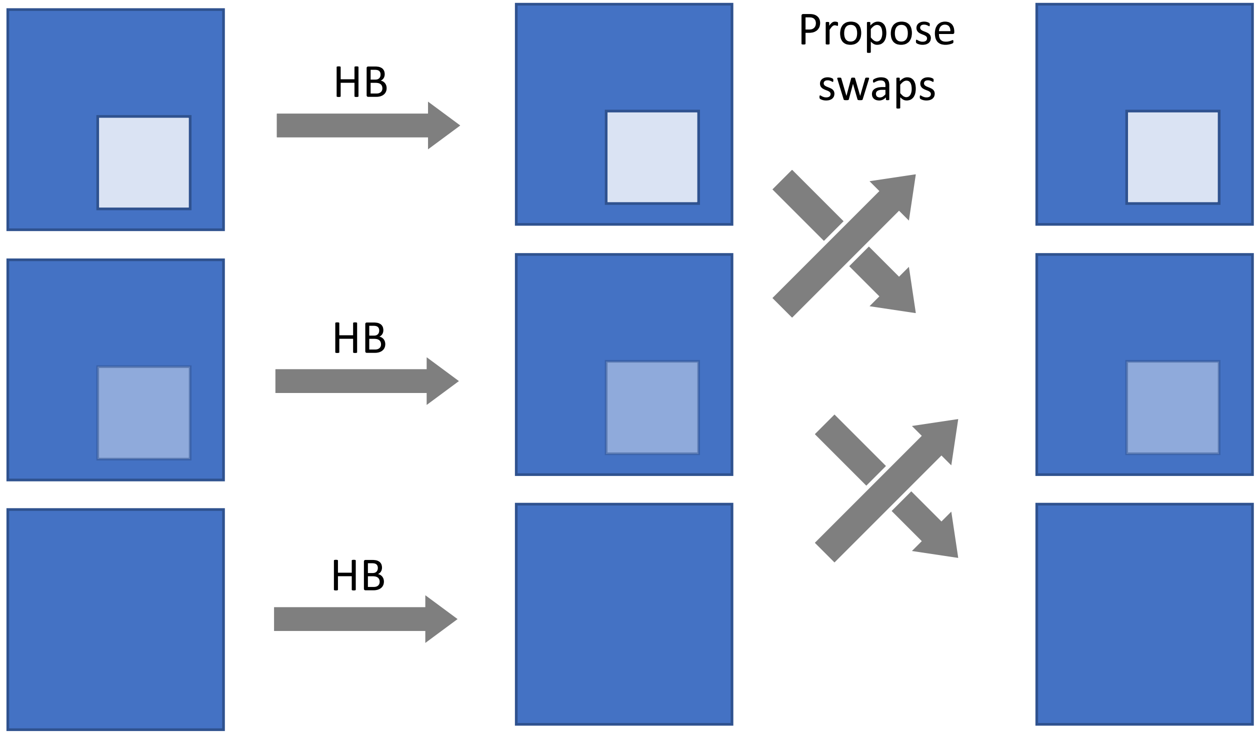
Introduce localized defect

$\beta_{\mathbf{defect}} < \beta_{\mathbf{target}}$

"Poke a hole in the boundary"

→ Faster topological mixing

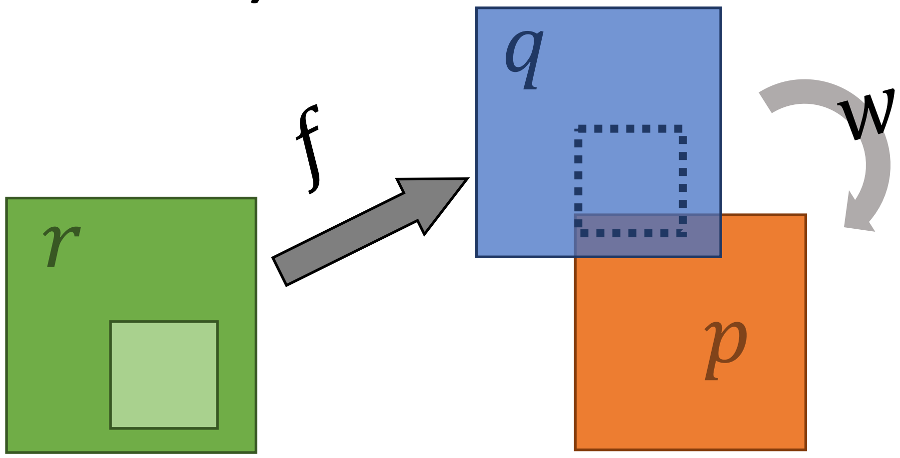
Remove defect w/ REX



App 3: Defect Repair Replica EXchange (DR-REX)

Train flow to repair defect

(Or, multiple flows for several steps of partial repair)

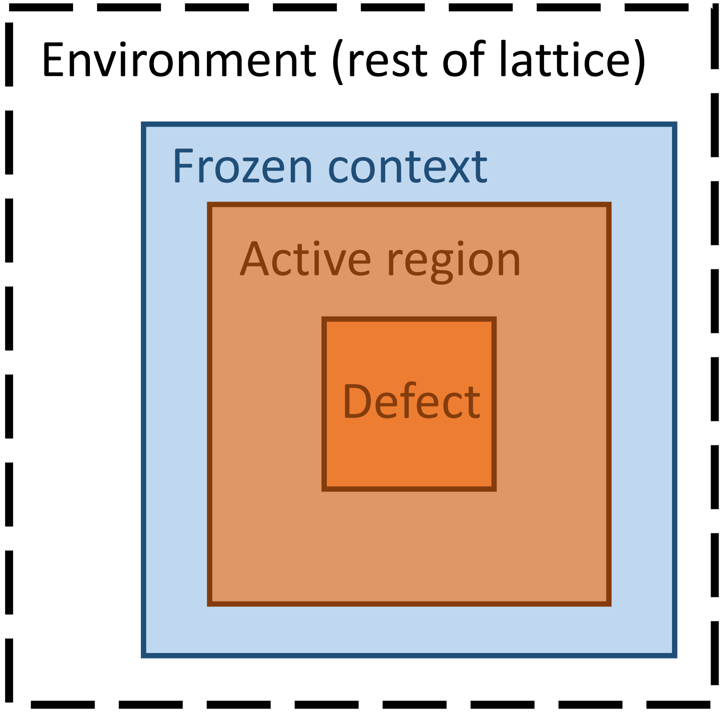


Defect has localized physical effects

Flow acts on subvolume

→ No ESS volume scaling

→ Volume-independent computational cost



App 3: DR-REX Results

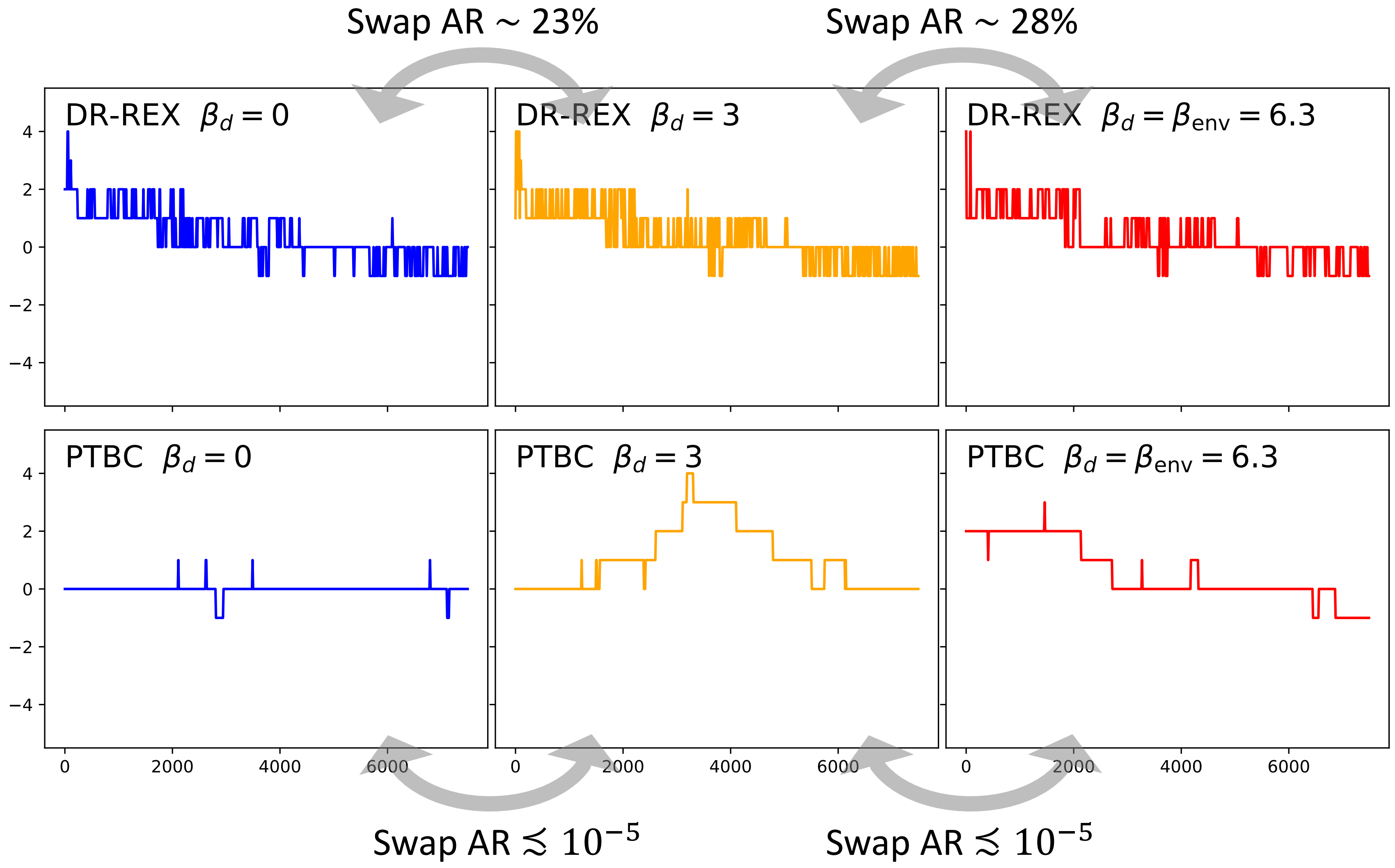
Target: $\beta = 6.3$ on 16^4

2^3 OBC defect

Two flows to repair

$$\beta_d = 0 \rightarrow 3 \rightarrow 6.3$$

Flows act on 8^4 subvolume



Similar swap AR w/o flows requires 7-8 chains

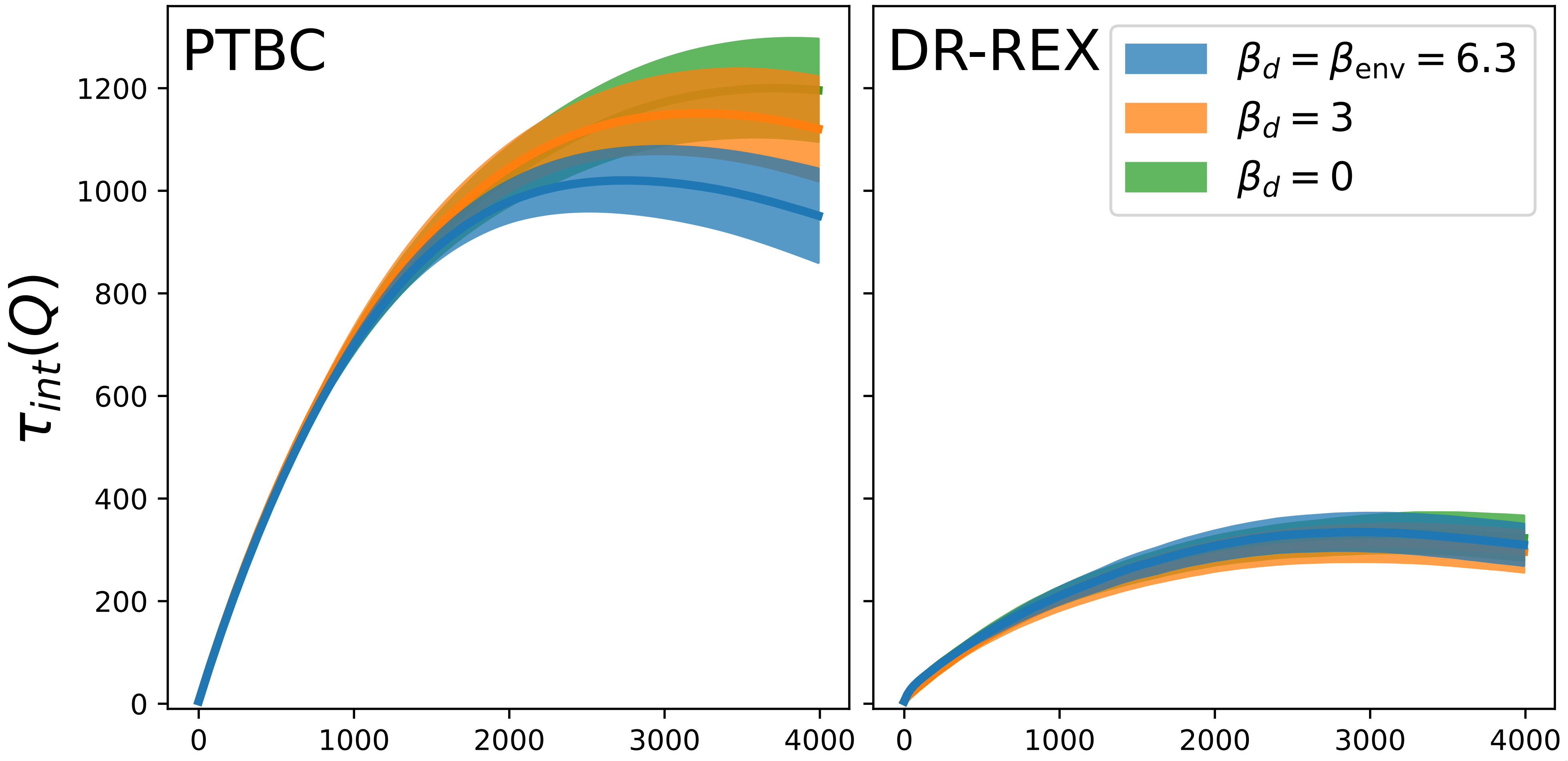
1 step = 1 HB + 5 OR, propose swaps every 10 steps

App 3: DR-REX Results

Target: $\beta = 6.3$ on 16^4

Two flows to repair a 2^3 OBC defect $\beta_d = 0 \rightarrow 3 \rightarrow 6.3$

Flows act on 8^4 subvolume



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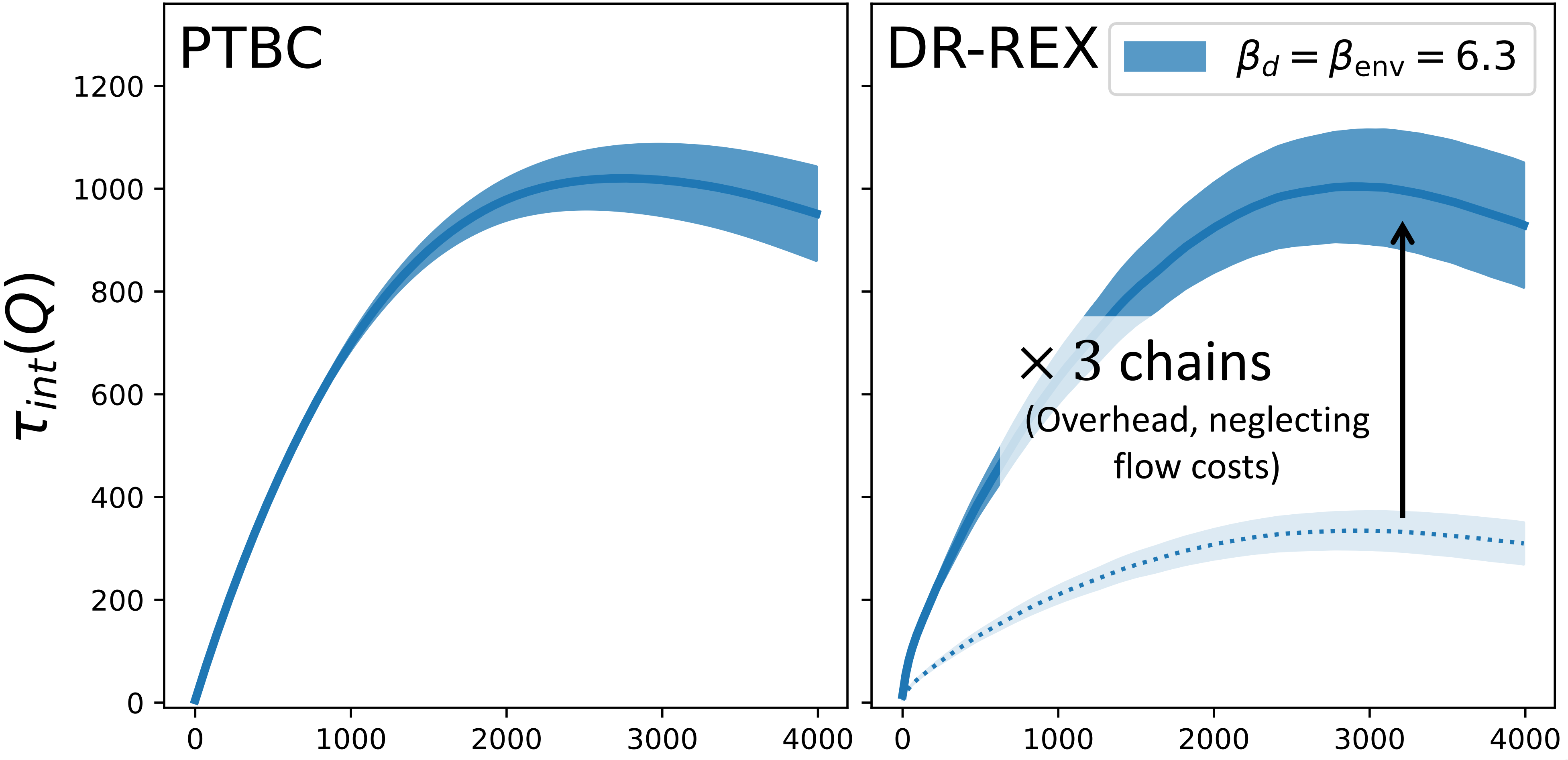

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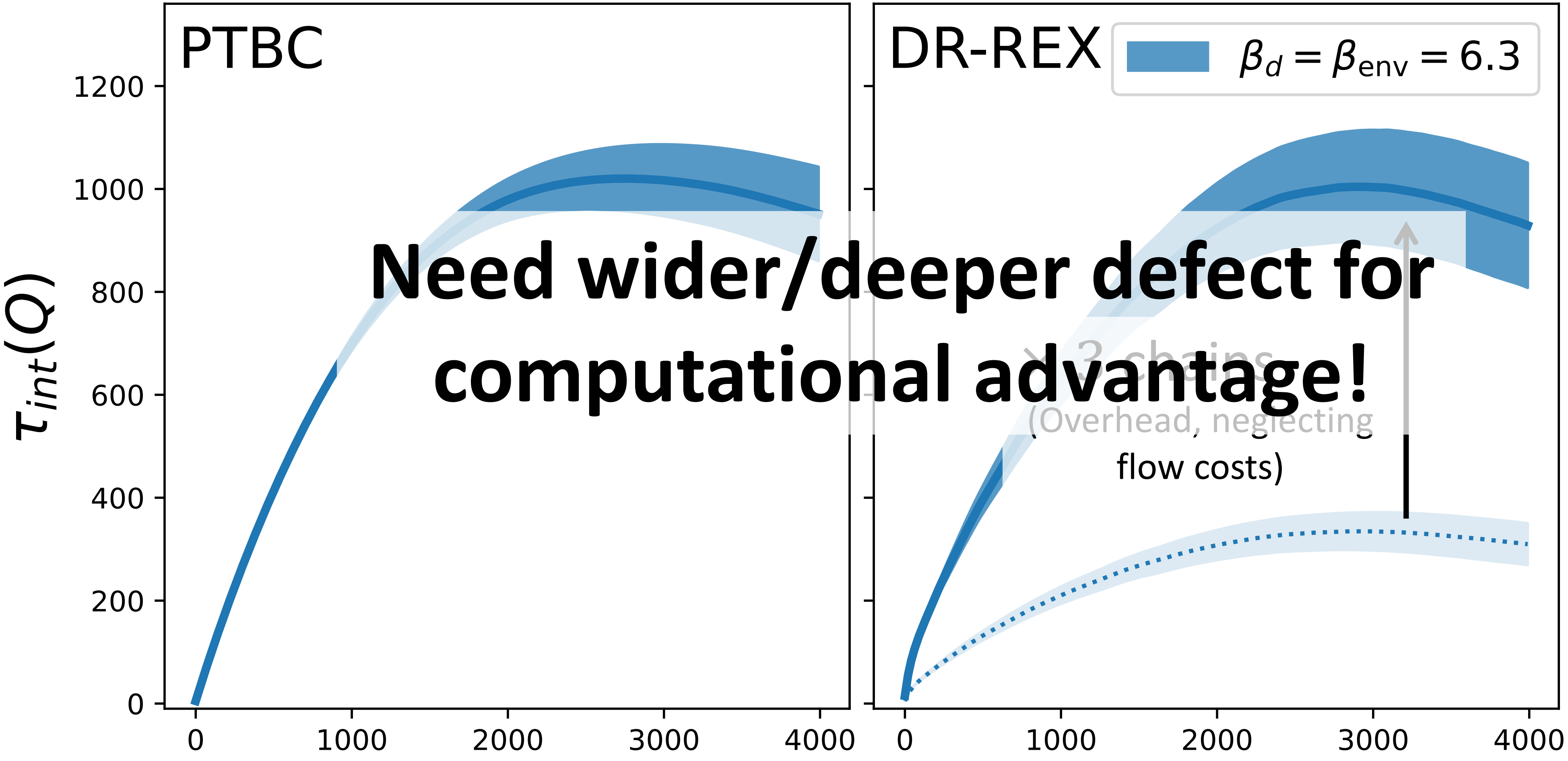

Need wider/deeper defect for computational advantage!

Outlook

Great potential for ML acceleration of lattice QCD calcs

Opportunities for useful applications before full generative modeling

REX makes natural use of flows

- Limiting case: direct sampling
  - See also: CRAFT [Matthews Arbel Rezende Doucet 2201.13117] → SNFs [Nada M 14:30]

Correlated ensembles / T-REX generally applicable in MC calcs

Straightforward generalizations to (pseudo)fermions / QCD

- Flows for fermions [2106.05934] PFs for gauge fields [2207.08945] QCD [2207.08945]

PTBC → DR-REX: very promising