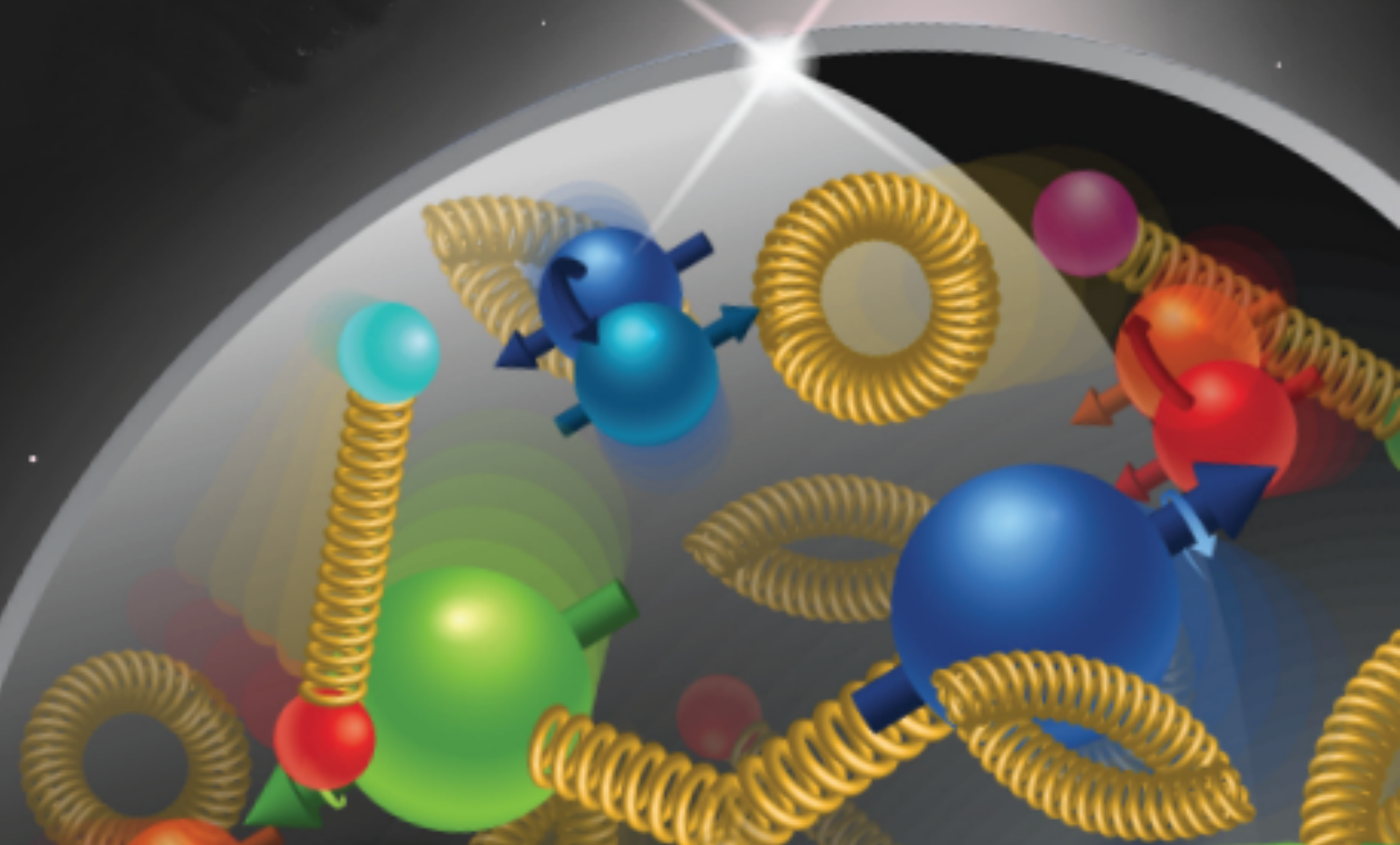
PHIALA SHANAHAN

STATUS UPDATE: FLOW MODELS FOR LATTICE QCD



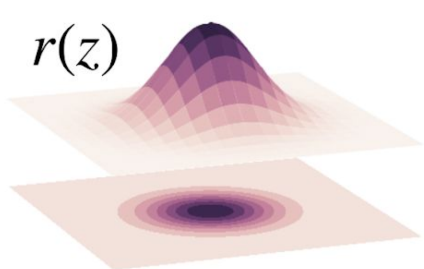
Massachusetts Institute of Technology

Flow models for lattice QCD

Flow models: Machine-learned maps between probability distributions
[Rezende & Mohamed 1505.05770]

z —— $f(z)$ ——→ φ

$r(z)$

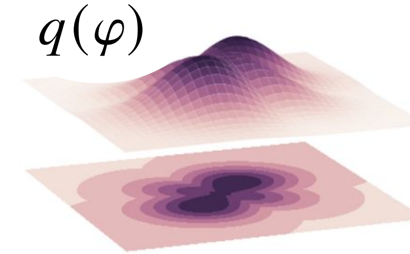


"**Base**" distribution

Flow transformation

- Invertible, tractable Jacobian
- Many free parameters for optimization

$q(\varphi)$



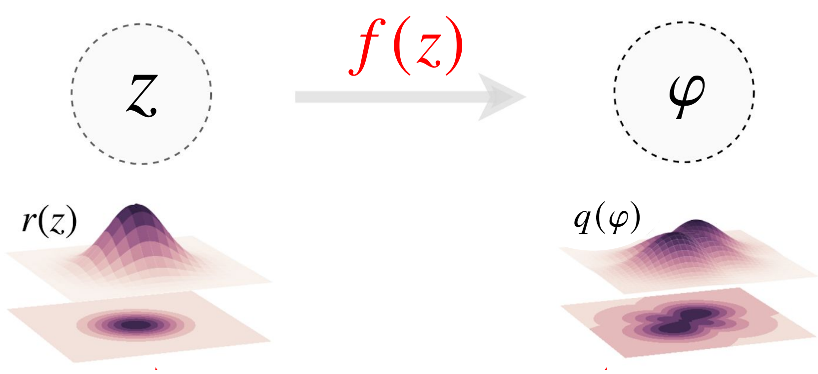
"**Model**" distribution

$q(\varphi) = r(z) |\det \partial f(z)/\partial z|^{-1}$

Fields via flow models

Example application: Embarrassingly parallel direct sampling

Flow model as an approximate trivialising map



"**Base**" distribution:
Efficient to sample
e.g., Haar-uniform

"**Model**" distribution

$$q(\phi) \approx \frac{1}{Z} e^{-S(\phi)}$$

- Independent samples of the base distribution map to independent samples of the model distribution

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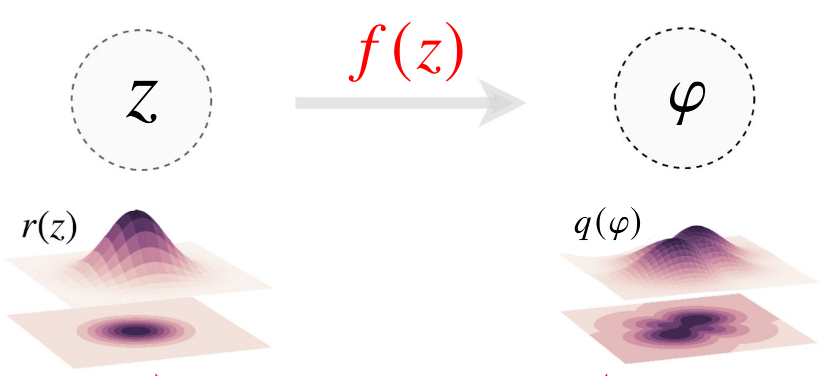

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Efficient to sample
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"Model" distribution
$q(\phi) \approx \frac{1}{Z} e^{-S(\phi)}$

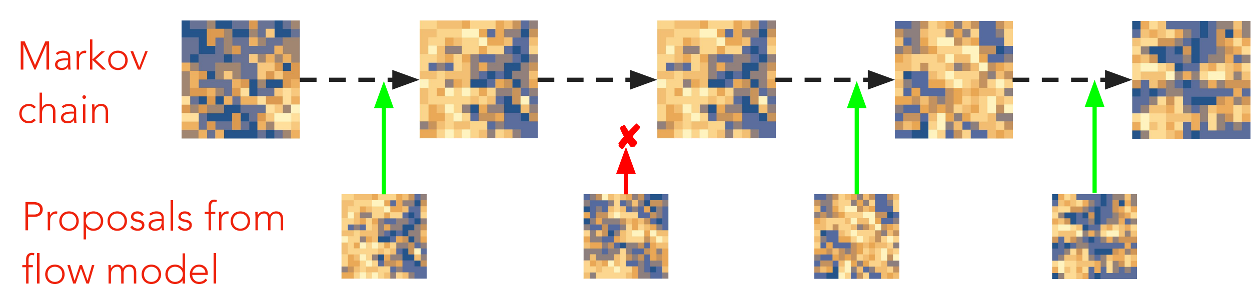
- Independent samples of the base distribution map to independent samples of the model distribution

- **Train the model:**
  Gradient descent to minimise "loss function" with minimum at $q(\phi) = \frac{1}{Z} e^{-S(\phi)}$

$$L(q) = \int d\phi \, q(\phi) [\log q(\phi) + S(\phi)]$$

Estimate stochastically by sampling from the model, i.e., "self training"

- **Guarantee exactness:**
  Reweight or form a Markov chain with Metropolis-Hastings accept/reject step



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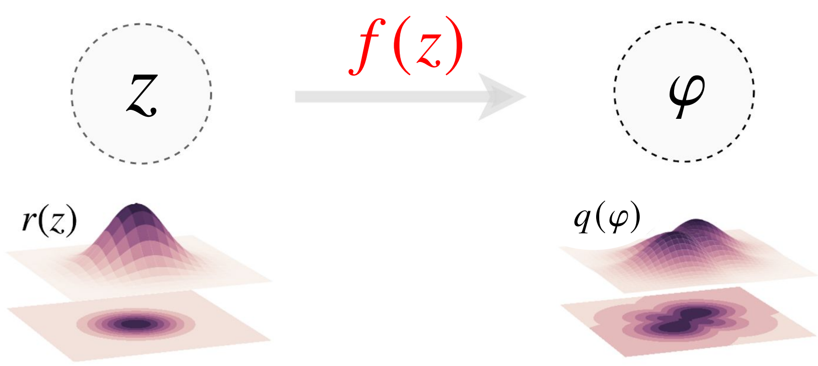

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Proof-of-principle applications to simple lattice field theories reveal many potential advantages c.f. HMC

- Mitigation of **critical slowing-down** and **topological freezing**
- Efficient **parameter-space exploration** (by re-tuning trained models)
- Direct access to the **partition function**

Direct sampling is only one of many approaches to using flow models for lattice QCD!

Flow models for lattice QCD

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[Rezende & Mohamed 1505.05770]

Many possible applications of flow models in lattice QCD

- Direct sampling i.e., $r(z)$ is a trivial distribution and $q(\phi) \approx \frac{1}{Z} e^{-S(\phi)}$
  Generalisation of [Lüscher 0907.5491]
- Hybrid sampling approaches
  e.g.,generalize the proposal distribution in HMC [Foreman et al., 2112.01582]; flows in lattice subdomains [Finkenrath 2201.02216]
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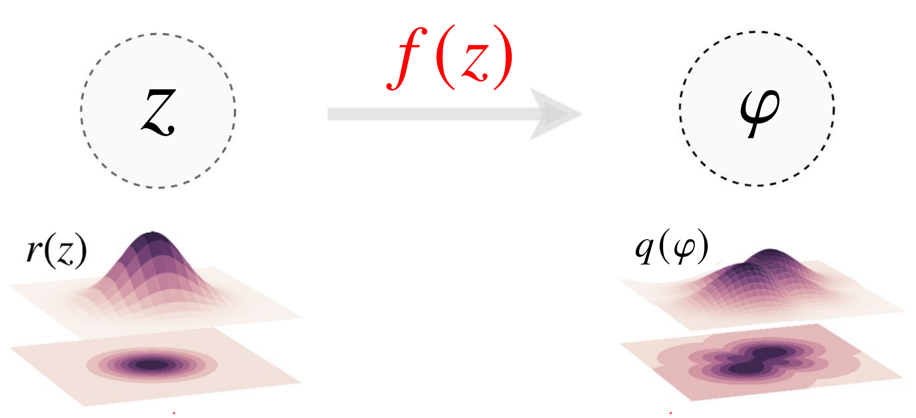

Flow architectures designed for QCD gauge fields can be trained and applied in many different ways!

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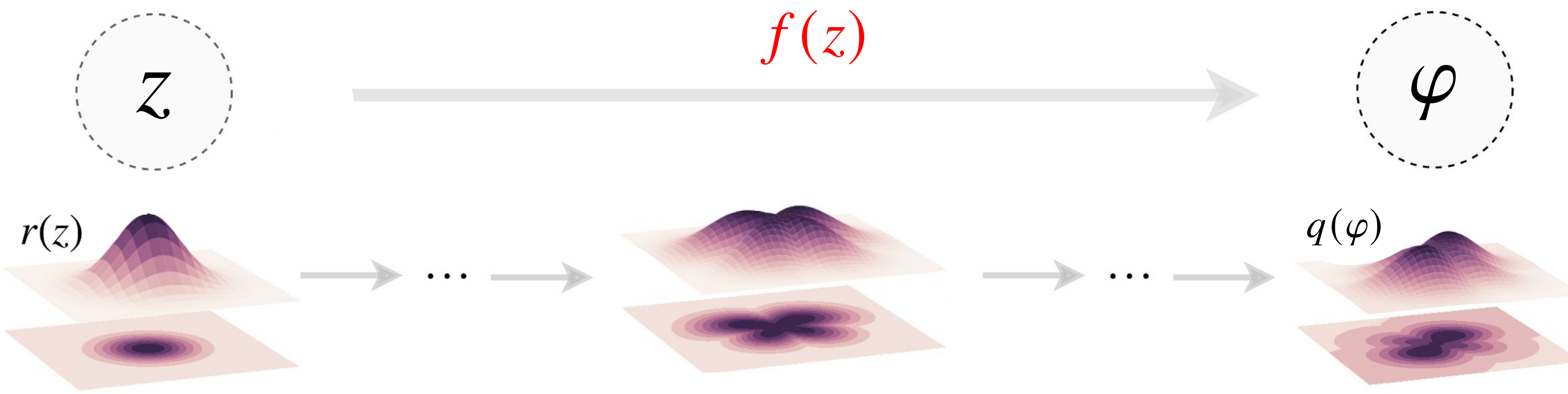
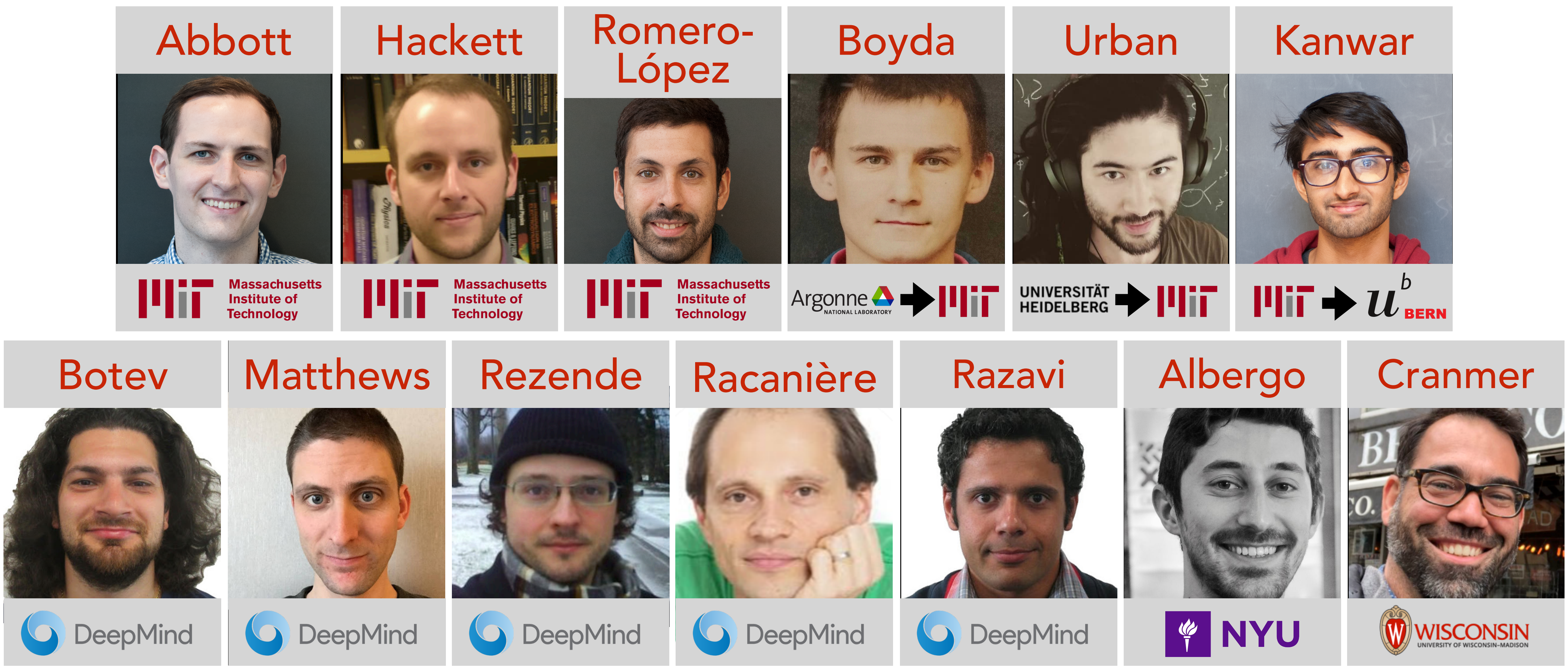


Goal: engineer flow architectures that effectively parameterise transformations of lattice gauge fields

- Diffeomorphisms on lattice field degrees of freedom
- Encode symmetries, e.g., gauge symmetry
- Flexible/expressive/can encode correlations at physically-relevant scale etc

Flow models for lattice QCD

- **MIT-led program** to develop flow model architectures for applications across lattice QCD
- **Ongoing industry collaboration** w/ Google DeepMind



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✓ **Gauge field theories**

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- Architectures for theories with fermions [Albergo et al., 2106.05934]
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✓ **Initial application to QCD in 4D**
[This talk+upcoming manuscripts on scaling and 4D]

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[see also tutorial notebook 2101.08176, work on multimodal distributions 2107.00734]

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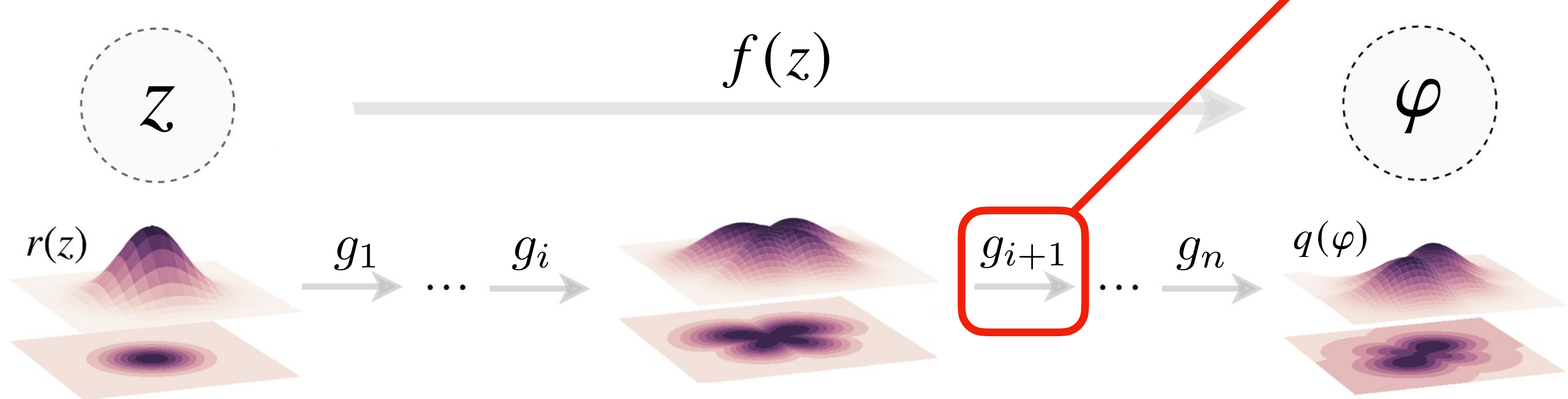
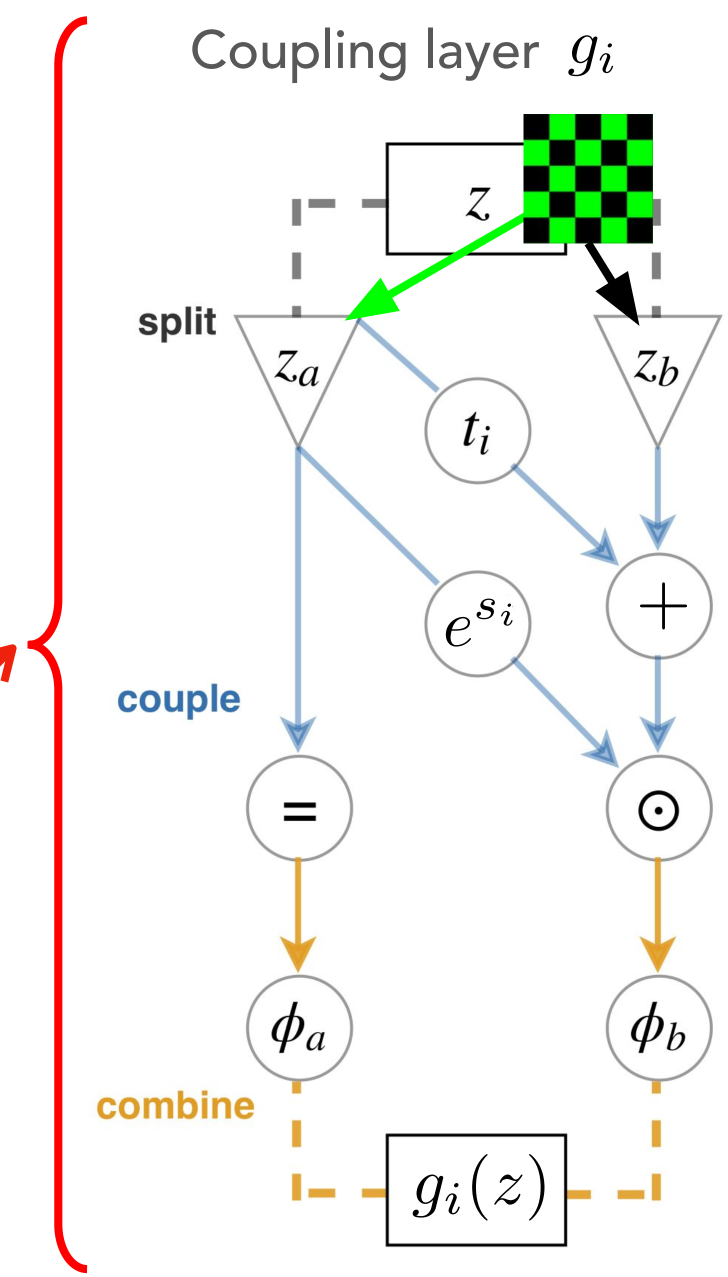
Flow models for scalar fields

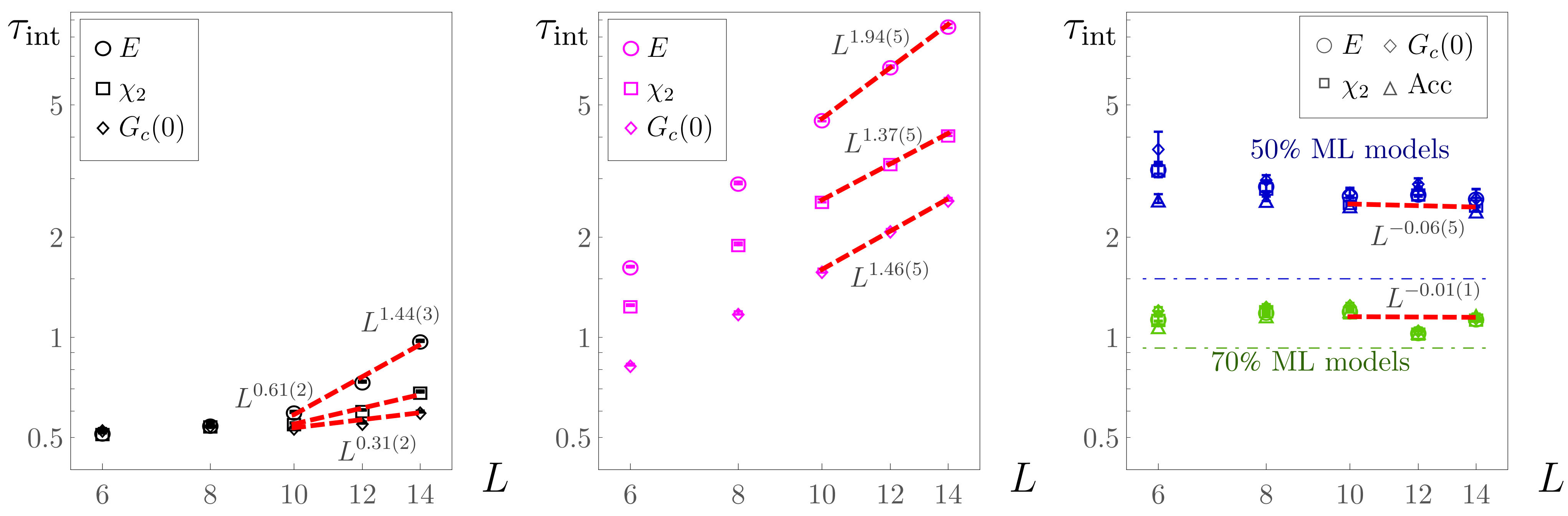
- First demonstration of flows as non-sequential samplers for lattice field theory [Albergo et al., 1904.12072]
- Variation of "**real non-volume-preserving flows**" developed for image generation [Dinh et al., 1605.08803]
  - Update field via sequential "coupling layers" g_i
  - Each layer transforms half of the degrees of freedom conditioned on the other half
    $z_a \to \phi_a = z_a \qquad z_b \to \phi_b = z_b e^{s(z_a)} + t(z_a)$
  - Transformations parameterised by arbitrary neural networks s_i, t_i





Flow models for scalar fields

Demonstration of accelerated sampling at the cost of model engineering and training (ϕ[4] theory, 2D, parameters tuned for constant m_pL) [Albergo et al., 1904.12072]



(a) HMC ensembles (b) Local Metropolis ensembles (c) Flow-based MCMC ensembles

- **Many choices in architecture design**
  (e.g., prior distribution, variable splitting, neural network structure); further work by our group and others [e.g., Nicoli et al., 2007.07115, 2111.11303; Del Debbio et al., 2105.12481; Singha et al., 2207.00980; +…]
- Current best implementations by our group **orders of magnitude more efficient** than 2019 approach! → Architecture development matters

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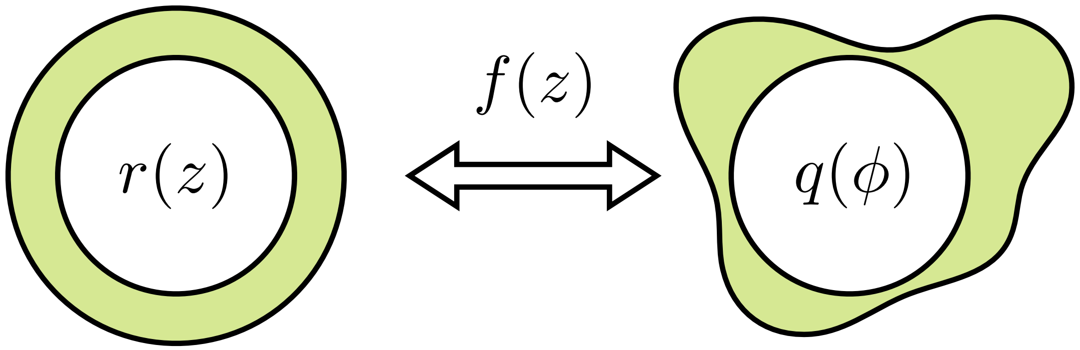
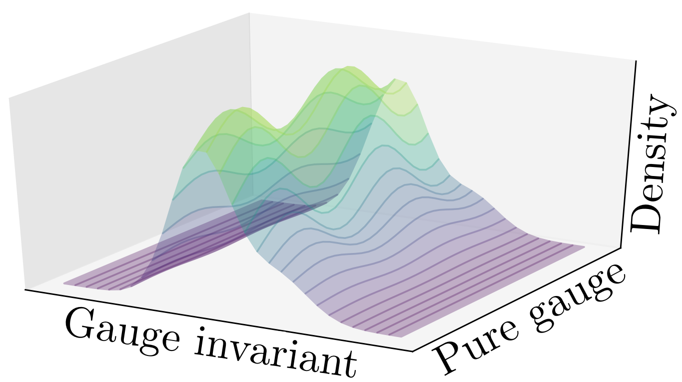
Flow models for gauge field theories

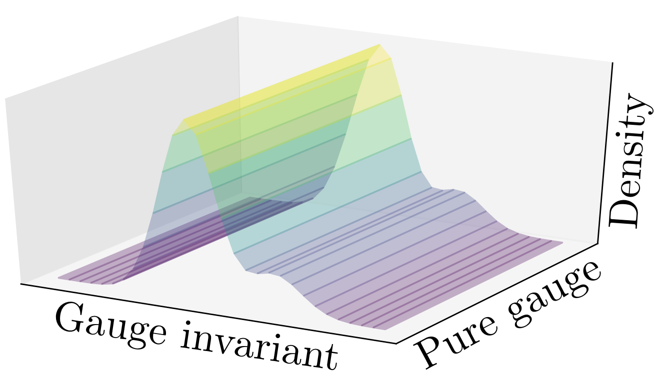
Flow models for gauge field theories require additional developments:

- Definition of flow transformations on **compact connected manifolds** (unlike real transformations relevant for images, scalar field theory) [Rezende et al., 2002.02428]



- Encoding complex **symmetries** of probability distribution (spatial, gauge, …) [Kanwar et al., 2003.06413, Boyda et al., 2008.05456; Related ideas in Favoni et al., 2012.12901,2111.04389; Luo et al., 2012.05232]
  - Not essential for correctness
  - Crucial for practical training of high-dimensional models with high-dimensional symmetries

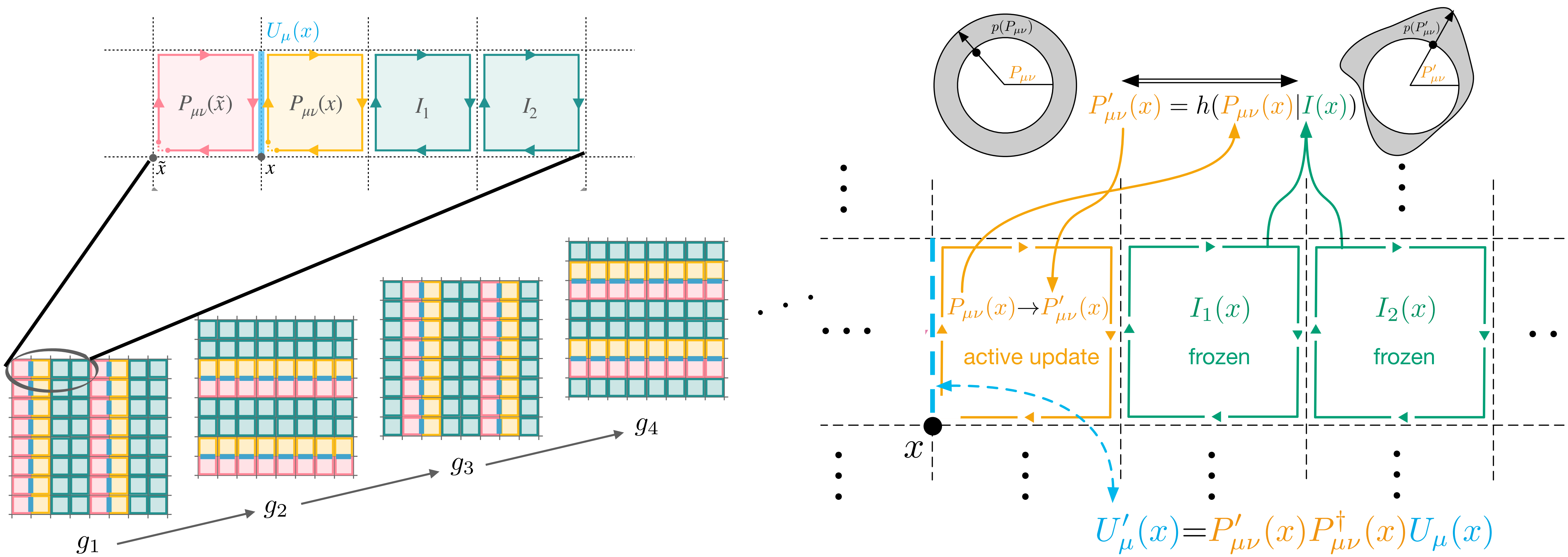




Flow models for gauge field theories

Development of gauge-equivariant flow models for Abelian and non-Abelian theories [Kanwar et al., 2003.06413, Boyda et al., 2008.05456; Favoni et al., 2012.12901,2111.04389; Luo et al., 2012.05232]

- Transform subset of links conditioned on the remaining subset
- Create gauge-equivariant layers by acting via transformations of (untraced) loops



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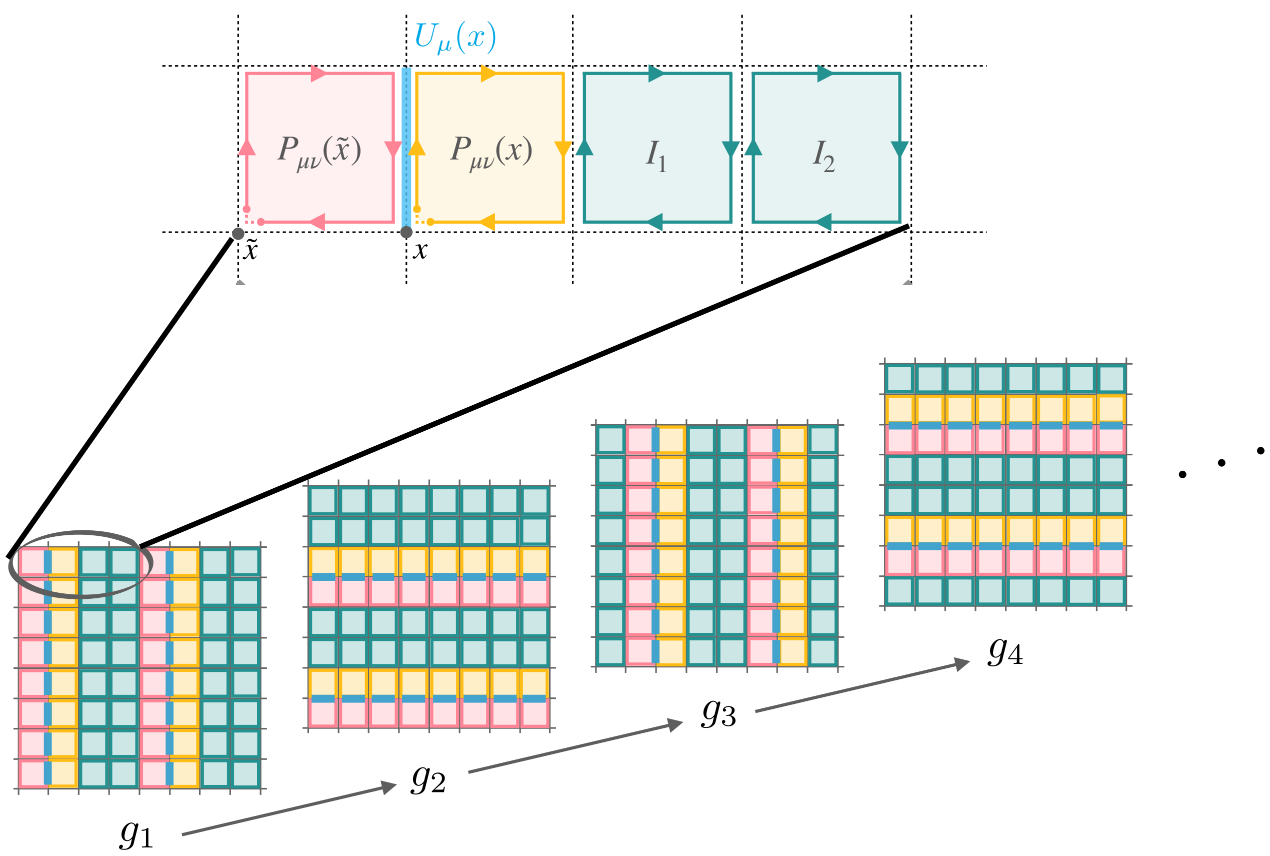
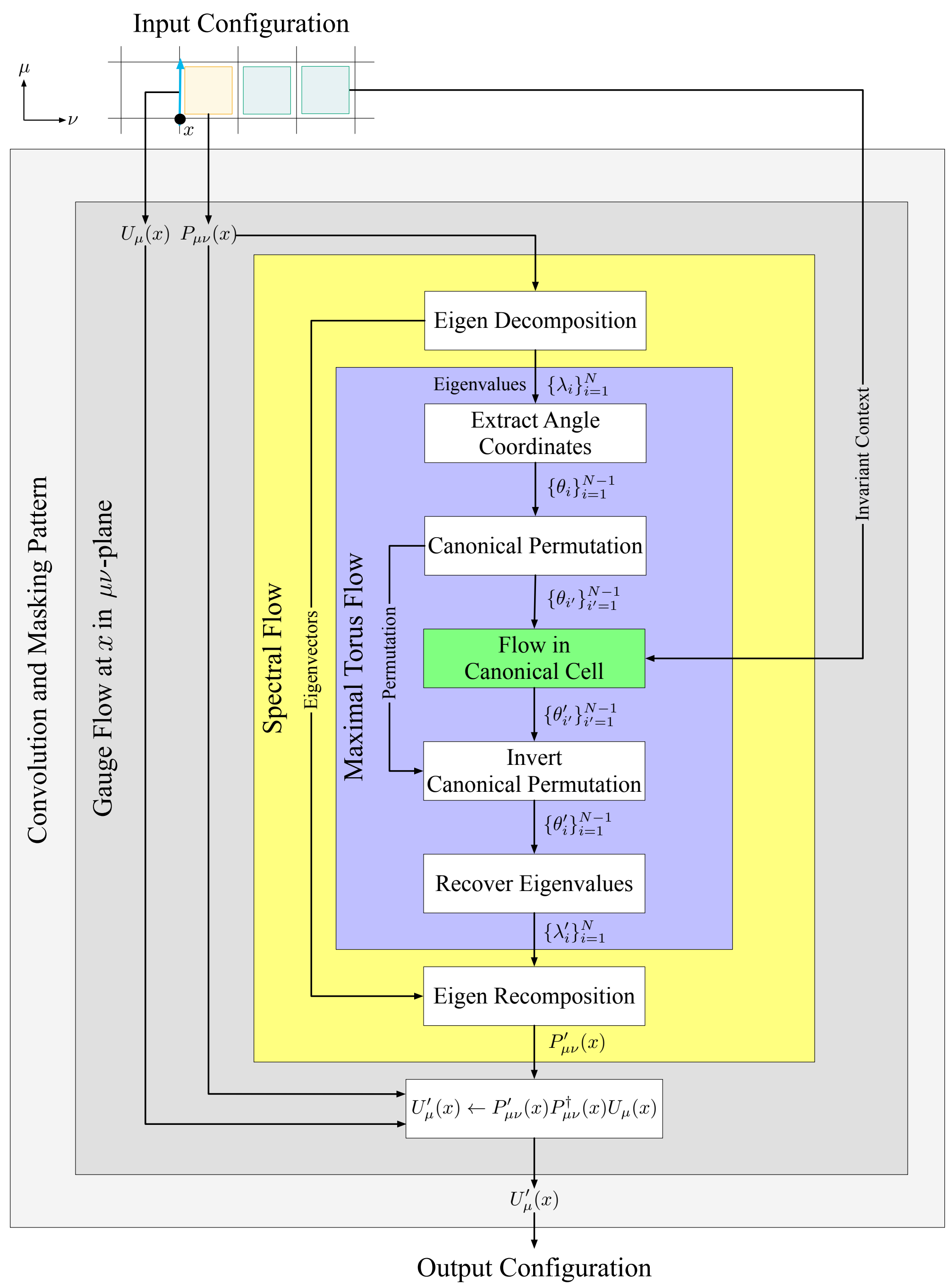
- Gauge-equivariant layers for Non-Abelian theories by stepping via eigendecomposition of (untraced) loops





Flow models for gauge field theories

Demonstration of accelerated sampling in U(1) field theory

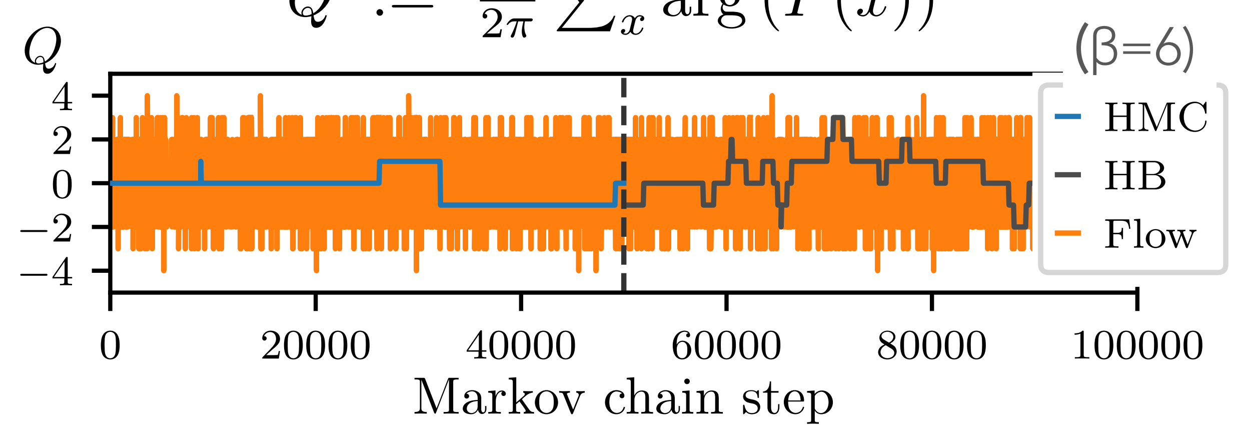
(2D, L=16) [Kanwar et al., 2003.06413]

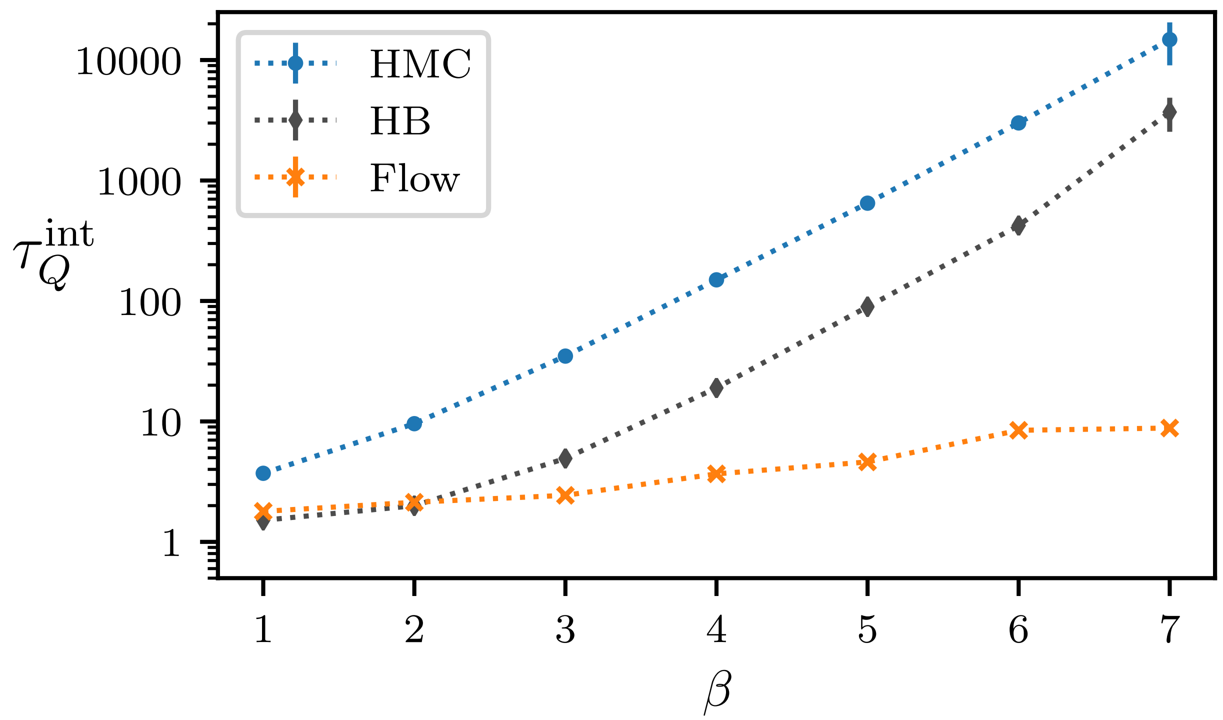
$$S(U) := -\beta \sum_x \mathrm{Re}\, P(x)$$

- **Efficient sampling of different topological sectors**
- Cost of sample from flow model ~ cost of HMC trajectory i.e., **flow model orders of magnitude more efficient at large coupling**
- Increase in autocorrelation time in flow samples at large coupling resulting from lower model quality

➡ illustrates trade-off between sampling cost and model development/training

$$Q := \frac{1}{2\pi} \sum_x \arg\left(P(x)\right)$$





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Fernando Romero-López's talk in previous session

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Flow models for lattice QCD

2-slide recap of Fernando Romero-López's talk in this session

Flows for fermonic gauge theories

- Straightforward approach consists on integrating out fermions:

$$\int \mathcal{D}[U]\mathcal{D}[\psi,\bar{\psi}]e^{-S_{\text{gauge}}(U)}\boxed{e^{-S_{\text{ferm}}(\psi,\bar{\psi},U)}} \longrightarrow \boxed{\int \mathcal{D}[\psi,\bar{\psi}]e^{-S_{\text{ferm}}(\psi,\bar{\psi},U)} = \prod_{f=1}^{N_f} \det D_f(U)}$$

- Full action can be expressed only in terms of gauge variables:

$$S_E(U) = -\beta \sum \mathrm{Re}\, P(x) - \log\det D[U]^\dagger D[U]$$ "exact determinant"

- One can use gauge-equivariant architectures from pure gauge models:

[Kanwar, Albergo, Boyda, Cranmer, Hackett, Racanière, Rezende, Shanahan 2003.06413]
[Boyda, Kanwar, Racanière, Rezende, Albergo, Cranmer, Hackett, Shanahan 2008.05456]

6 /15 Fernando Romero-López, MIT

Flow models for lattice QCD

2-slide recap of Fernando Romero-López's talk in this session

(2D, N_f=2, β=2, L=16, κ=0.276)

Flows for fermionic gauge theories

- Straightfor
  $\int \mathcal{D}[U]\mathcal{D}[\psi,$
- Full action
  $S_E(U) = -$
- One can us
  [Kanwar, Alber
  [Boyda, Kanwa

The Schwinger model at criticality

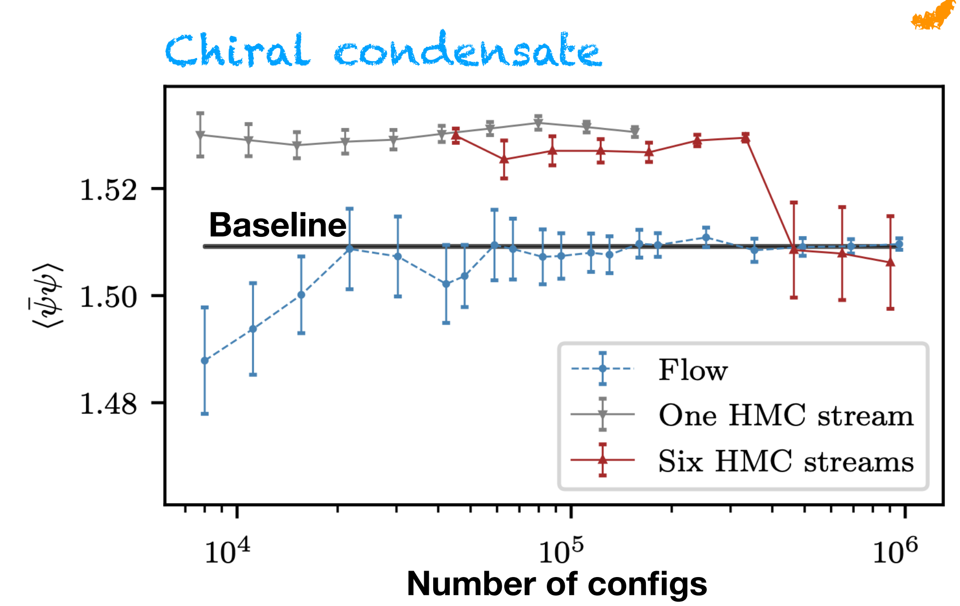
Critical parameters:

- Vanishing fermion mass
- Diverging correlation length

! Hardest to simulate in HMC

✗ HMC shows biased results with underestimated errors

✓ Flow-based sampling provides correct results



[Albergo, Boyda, Cranmer, Hackett, Kanwar, Racanière, Rezende, FRL, Shanahan, Urban 2202.11712]

! Evaluation of the fermion determinant is expensive.

$$S_E(U) = -\beta \sum_x \mathrm{Re}\, P(x) - \log\det D[U]^\dagger D[U]$$

Not feasible for QCD-scale calculations!

- Scalable approach: use stochastic determinant estimators!

→ Pseudofermions!

7 /15

Pseudofermion architectures defined in the rest of Fernando's talk

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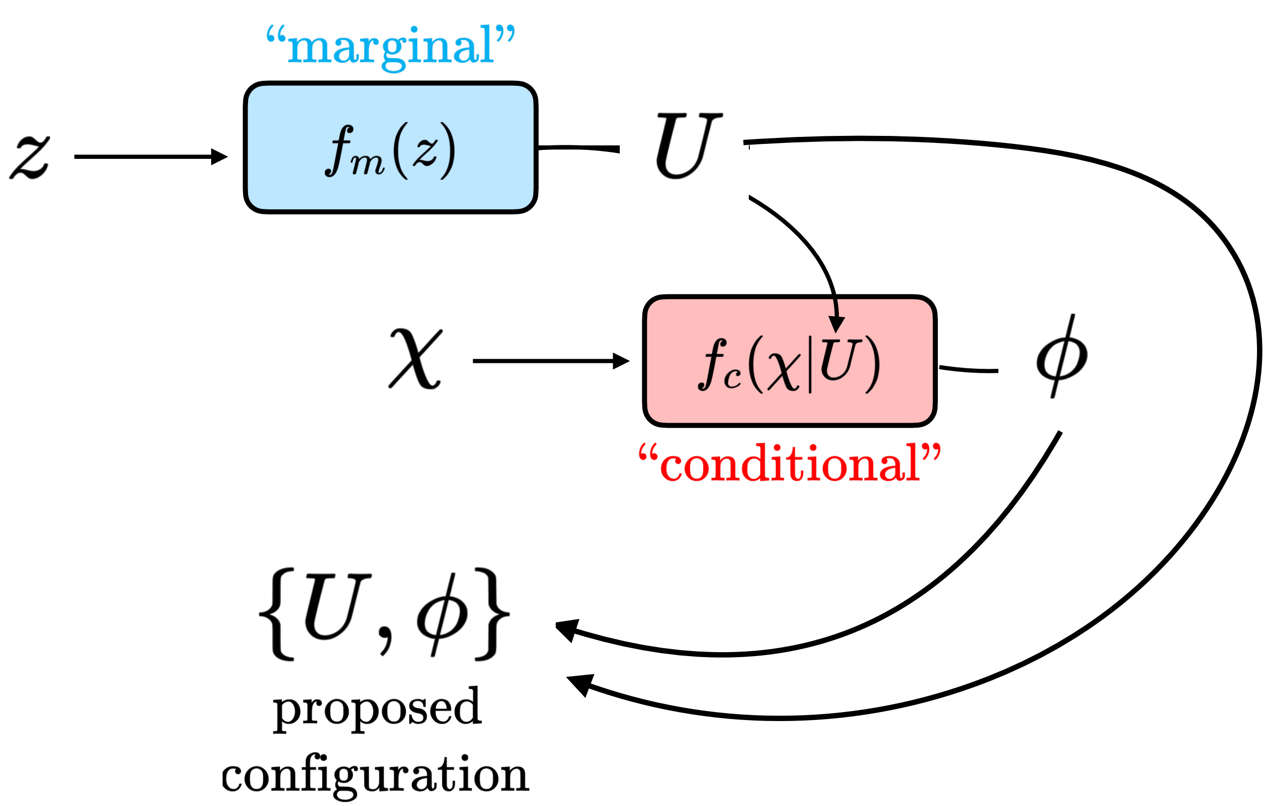
- Direct combination of published results on gauge-equivariant flows and pseudofermions [Boyda et al., 2008.05456, Abbott et al., 2207.08945]
- Illustration at straightforward parameters $V=4^4$, $N_f=2$, $\beta=1$, $\kappa=0.1$
- Observables from flow ensemble in precise agreement with HMC at high statistics (65k samples)
- Development and scaling of QCD-specific architectures in full swing — stay tuned!



Marginal:

- Haar-uniform base distribution
- 48 gauge-equivariant spline coupling layers
- Spatially separated convolutions in spectral flow to define spline parameters

Conditional:

- Gaussian base distribution
- 36 pseudofermion coupling layers built from parallel transport convolutional networks
- Alternating spin and spatial masking pattern

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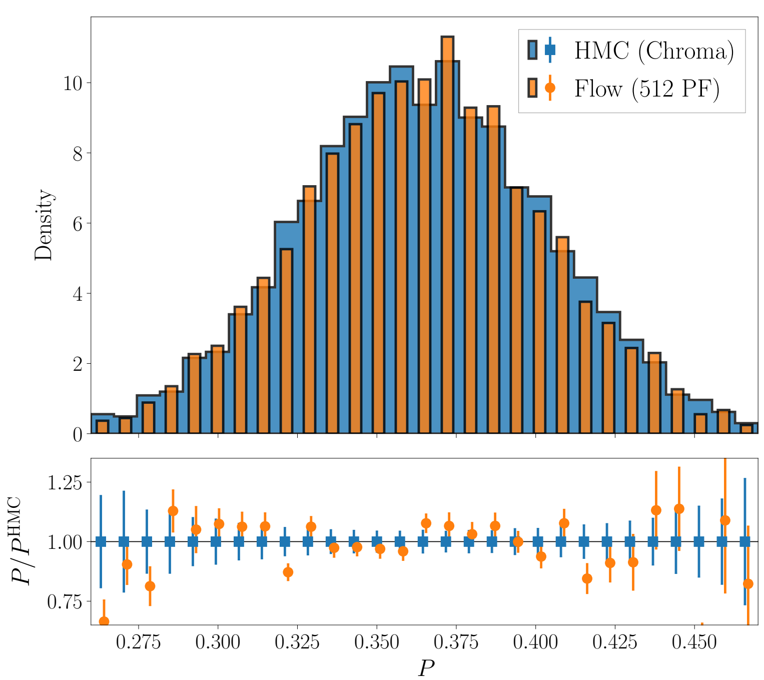
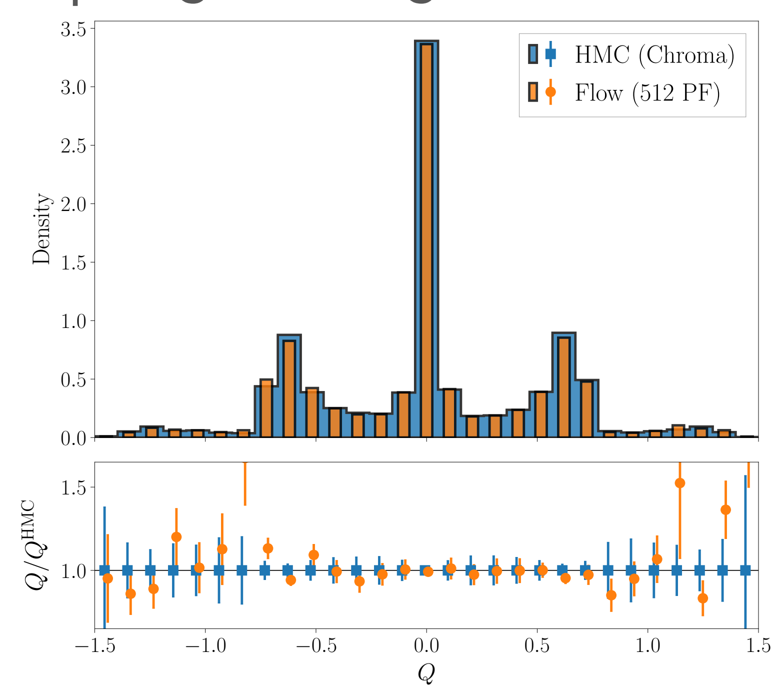
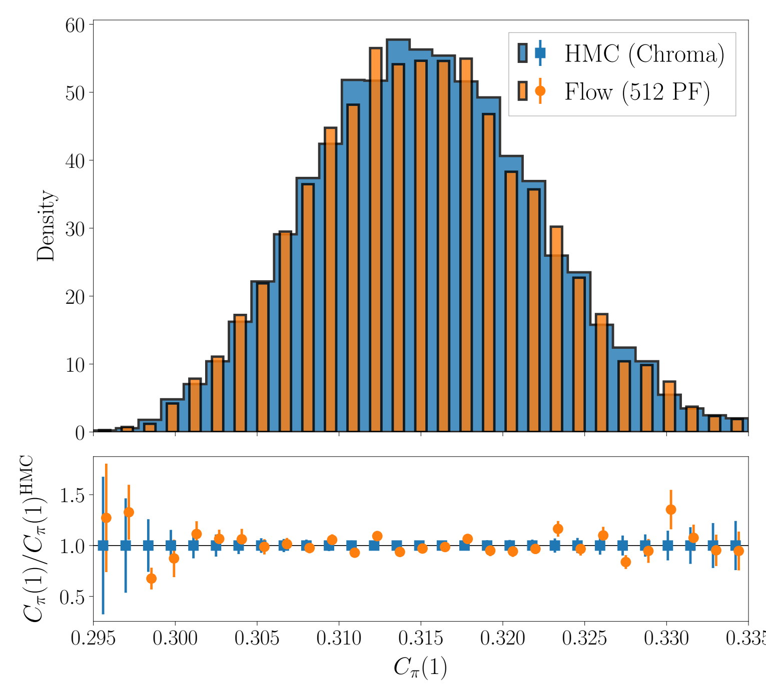
Plaquette



Topological charge (Wilson flowed)



Pion correlation function (t=1)

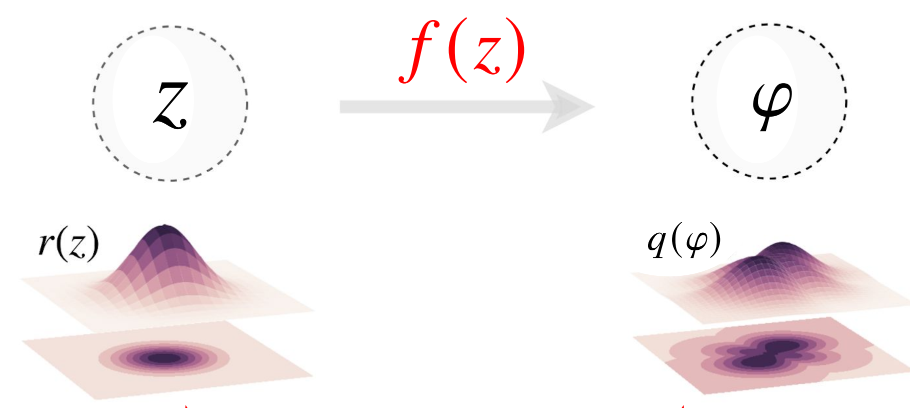


Outlook: Flow models for lattice QCD

All fundamental components in place to begin exploration of flow models for lattice QCD!

Significant efforts still required to exploit potential of flow models for lattice QCD

- QCD-specific engineering and development only just beginning
- Scaling to state-of-the-art requires engineering custom ML architectures to similar scale as largest industrial ML models



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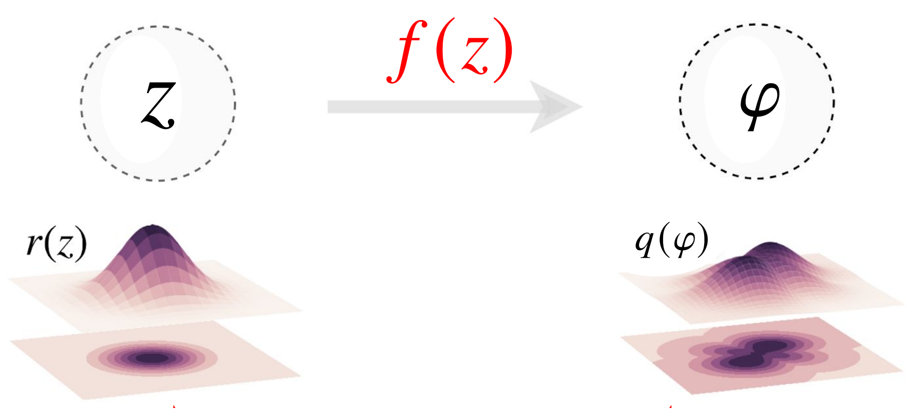

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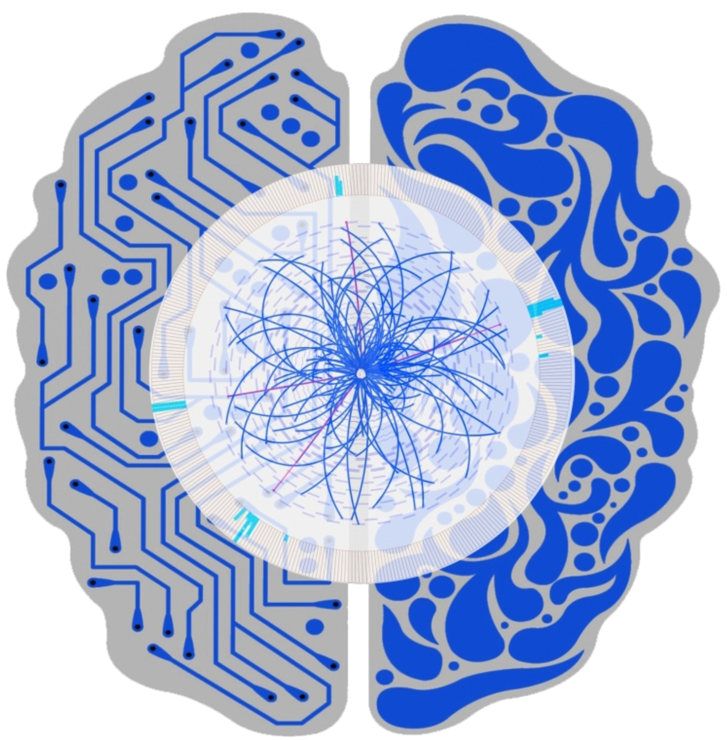
The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI /aɪ-faɪ/ iaifi.org)



Develop artificial intelligence based on physics principles “Ab-Initio AI”

Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality, unitarity, gauge invariance, entropy, least action, factorization, unit tests, exactness, systematic uncertainties, reproducibility, verifiability, …

Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation

26

The NSF AI Institute for Artificial Intelligence and Fundamental Interactions (IAIFI /aɪ-faɪ/ iaifi.org)

Develop artificial intelligence
based on physics principles
"Ab Initio AI"

…haviors,
factorizatio…
reproducibility, verifia…

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Advance physics knowledge — from the smallest building blocks of nature to the largest structures in the universe — and galvanize AI research innovation