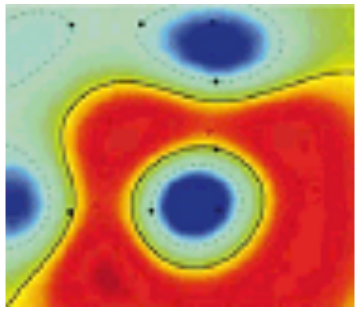

# Machine Learning for Thermodynamic Observables

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**K.A. Nicoli**, C. Anders, L Funcke, T. Hartung, K. Jansen, P. Kessel, S. Nakajima, P. Stornati, Phys. Rev. Lett. 126 (2021) 3, 032001

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# In collaboration with this awesome team…


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**Nicoli**, Anders, Funcke, Hartung, Jansen, Kessel, Nakajima, Stornati, Phys. Rev. Lett. 126 (2021) 3, 032001


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# The curse of MCMC samplers

Even specified MCMC algorithms come at a **cost**

👎 **Sequential Sampling** $\implies$ Can't be parallelized

👎 **Critical Slowing down** $\implies$ Exponential increase of computational cost

👎 **No direct access to** $Z$ $\implies$ Boltzmann distribution known up to normalization

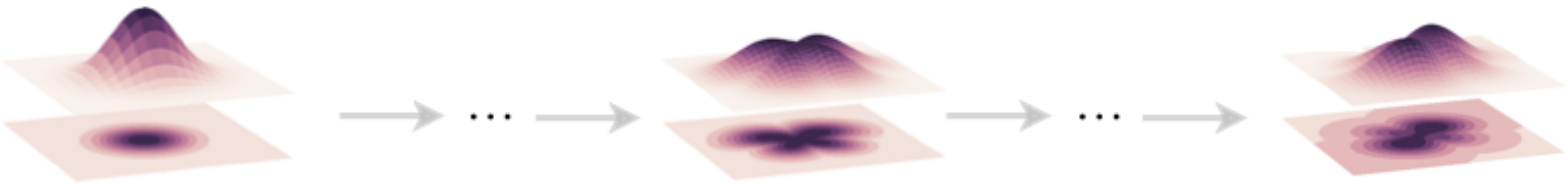
👎 **Integration through phase** $\implies$ **ratios of partition functions** $\frac{Z_t}{Z_0} = \Delta F_t = \mathbb{E}_{p_0}\left[\frac{\exp(S_t)}{\exp(S_0)}\right]$

👎 Stepping through phase space leads to **large statistical errors**

👎 **No direct access to** $F = -T \ln Z$ and thermodynamic observables

# Normalizing Flows

$$z \sim \mathcal{N}(0,\mathrm{I}) \xrightarrow[g_\theta(z) = \left(y^L \circ y^{L-1} \circ \ldots \circ y^1\right)(z)]{} \phi = g_\theta(z)$$



(Albergo, Kanwar, Shananah, 2019)

$$\boxed{q_\theta(\phi) = q_0(g^{-1}(\phi)) \left| \det \left( \frac{\partial g}{\partial z} \right) \right|^{-1}}$$

- Flow trained to **approximate the path integral distribution**
- **Exact density** $q_\theta$ → **variational approximation** with free parameters $\theta$ (NNs)
- $g_\theta$ **: invertible, differentiable, tractable Jacobean**
- Training: minimize **reverse KL** divergence → $KL(q_\theta || p) = \int \mathrm{D}[\phi]\, q_\theta(\phi) \ln \left( \frac{q_\theta(\phi)}{p(\phi)} \right)$

# Estimation of Thermodynamic Observables

$$\hat{\phi} \sim q_\theta \longrightarrow \phi \sim p(\phi)$$

- Exact density $q_\theta$ allows to estimate the partition function by MC sampling:

$$Z = \int \mathrm{D}[\phi]\,\tilde{p}(\phi) = \int \mathrm{D}[\phi]\,q_\theta(\phi)\,\tilde{w}(\phi) \quad \text{where} \quad \tilde{w}(\phi) = \frac{\exp[-S(\phi)]}{q_\theta(\phi)}$$

$$\Big\downarrow\ \hat{\phi}_i \sim q_\theta$$

$$Z \approx \hat{Z} = \frac{1}{N}\sum_{i=1}^{N} \tilde{w}(\hat{\phi}_i) \longrightarrow \hat{F} = -T\ln\hat{Z} \longrightarrow \boxed{\begin{gathered} \hat{p} = -\frac{\hat{F}}{V} \\ \hat{H} = \beta(U - \hat{F}) \end{gathered}}$$

# $\phi^4$ real scalar field theory

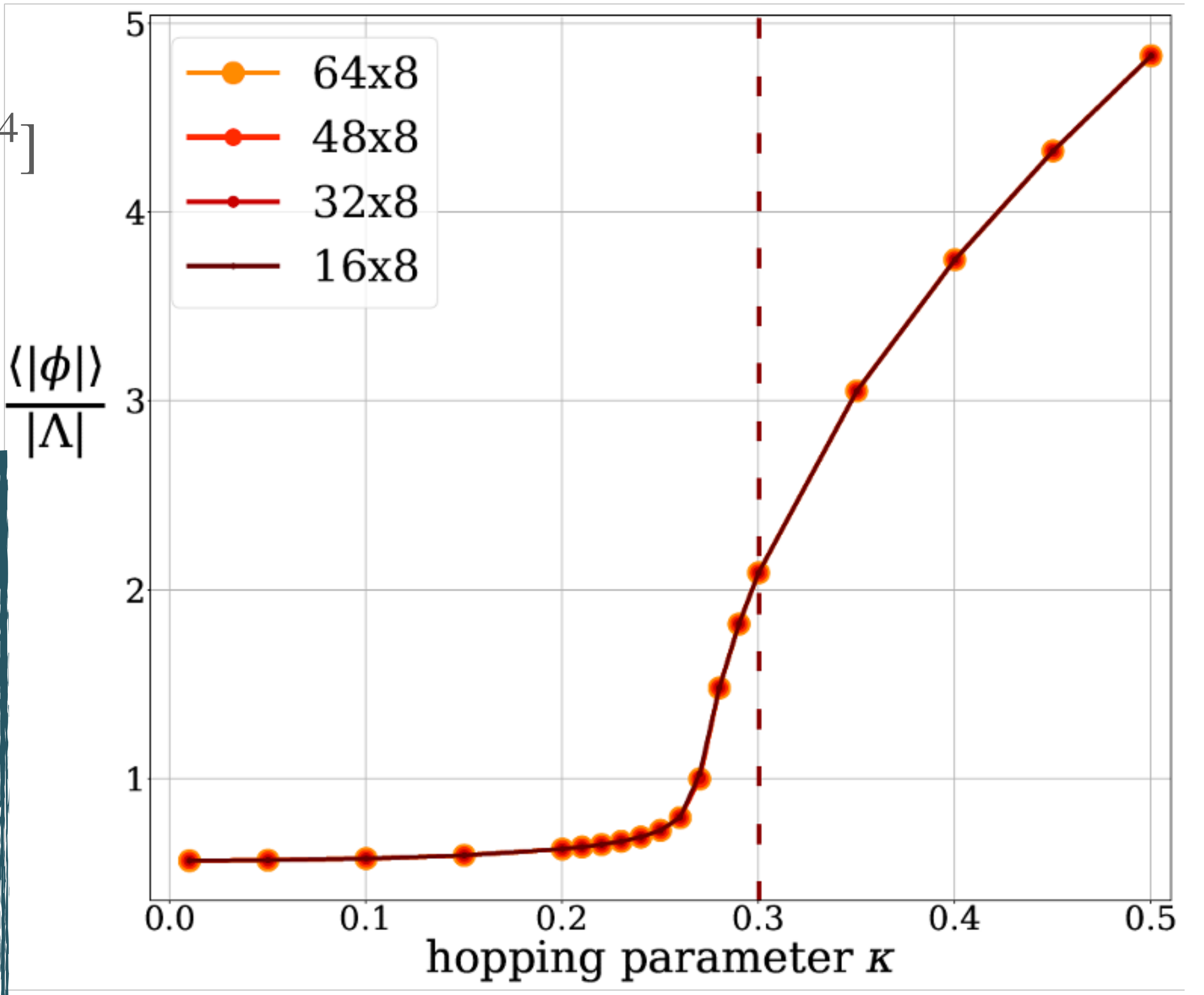
**$\phi^4$ – theory**

$$S = \sum_{x\in\Lambda} [-2\kappa \sum_{\mu=1}^{d} \phi(x)\phi(x+\hat{\mu}) + (1-2\lambda)\phi(x)^2 + \lambda\phi(x)^4]$$

- Need to know $F_0$ to access $F_t$
- No direct estimates of $Z$ and $F_t$
- Only differences $\Delta F_t = F_t - F_0 = -T \ln \frac{Z_t}{Z_0}$
- Integrate a trajectory through phase space

**Source of large statistical errors for MCMC based methods** 👎

Spontaneous Symmetry Breaking

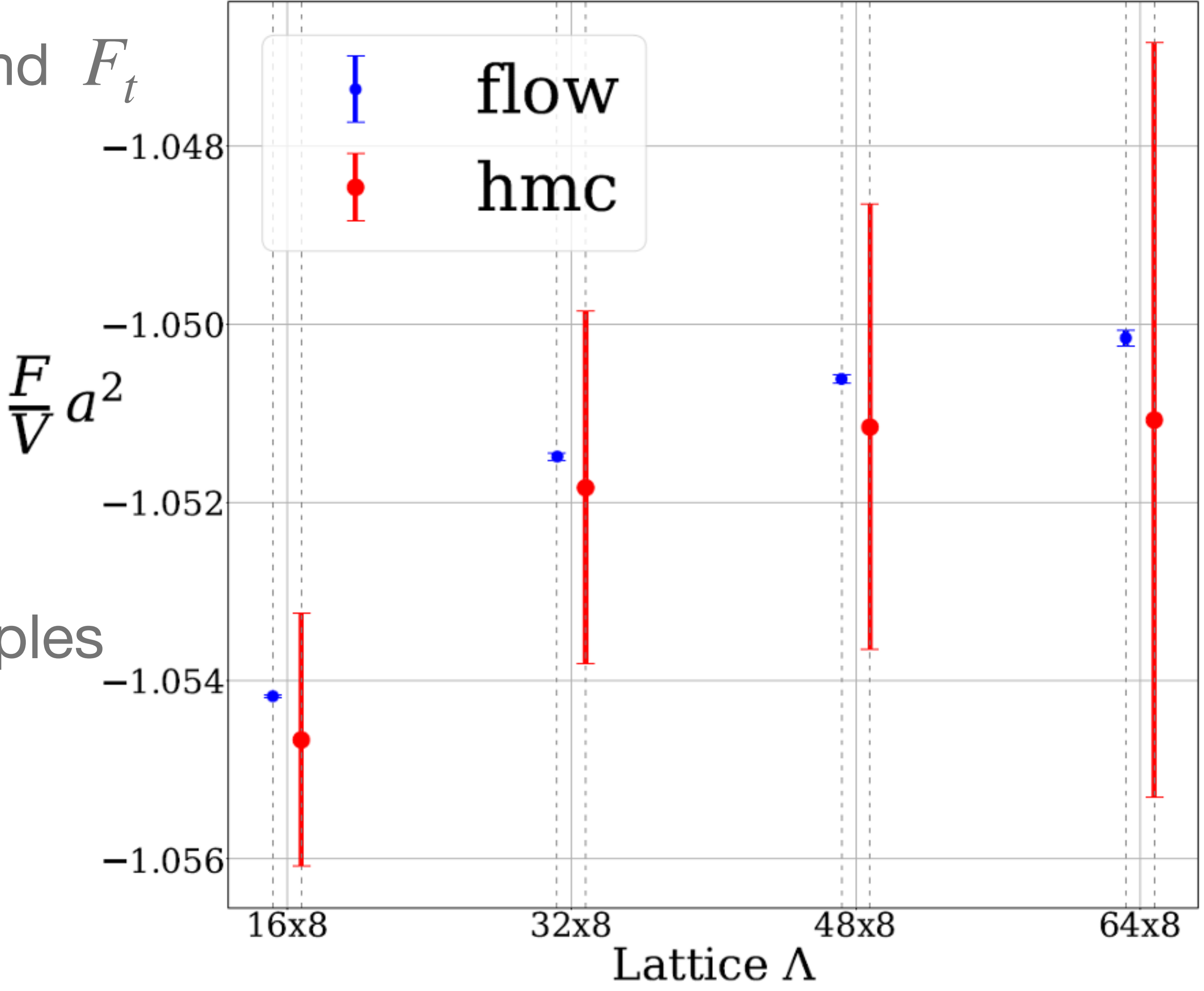


# Broken Phase: $\kappa = 0.3$

- $\kappa = 0.3$
- $\lambda = 0.022$
- Different Volumes $|\Lambda| = N_s \times N_t$

## MCMC:

- Larger statistical errors (phase transition)
- **14** Markov HMC chains between $F_0$ and $F_t$
- **400k** samples per chain



## NFLOW:

- Less sensitive to critical regime
- Importance sampling with 5.6M samples
- Expensive training, cheap sampling

# Why is this advantageous?

1. **Smaller errors** and less sensitivity to the **critical regime**

2. **iid sampling** ($\neq$ for MCMC: sequential sampling)

3. Sampling can efficiently be **parallelized**

4. **Direct, point-wise** estimation of thermodynamic quantities (e.g. $Z, F, H, p$)

    - No need of exact estimation for $F_0$

    - T-QCD application $F_0$ is approximated (not exact) → additional systematic error

## Future Directions

- Scaling to bigger lattices.
- Different theories
    - Boyda, Kanwar, …, Shanahan, 2021 - *SU(N)* Gauge equivariances
    - Albergo, Kanwar, …, Shanahan, 2021 - Fermionic lattice field theories

Thanks for your attention!