NeuLat

A toolbox for Neural samplers in Lattice field theories

Work in collaboration with: Christopher J. **Anders**, Lena **Funcke**, Karl **Jansen**, Shinichi **Nakajima** and Pan J. **Kessel**.

Why Normalizing Flows for LFT?

- Lattice configurations are sampled i.i.d., thus **reducing autocorrelation**.
- Sampling is **embarrassingly parallel**, e.g., faster and more efficient.
- Direct estimation of **thermodynamic observables** (partition function, free energy, etc.).
- **Inductive biases**, e.g., symmetries, are easy to incorporate.
- The trained models can be used for **interpolation** (extrapolation) in parameter space.
- **Transfer** weights of flows trained on smaller systems to train on larger ones.
- …

→ Plenary talk by Gurtej Kanwar (Monday 31st July)

What is NeuLat?

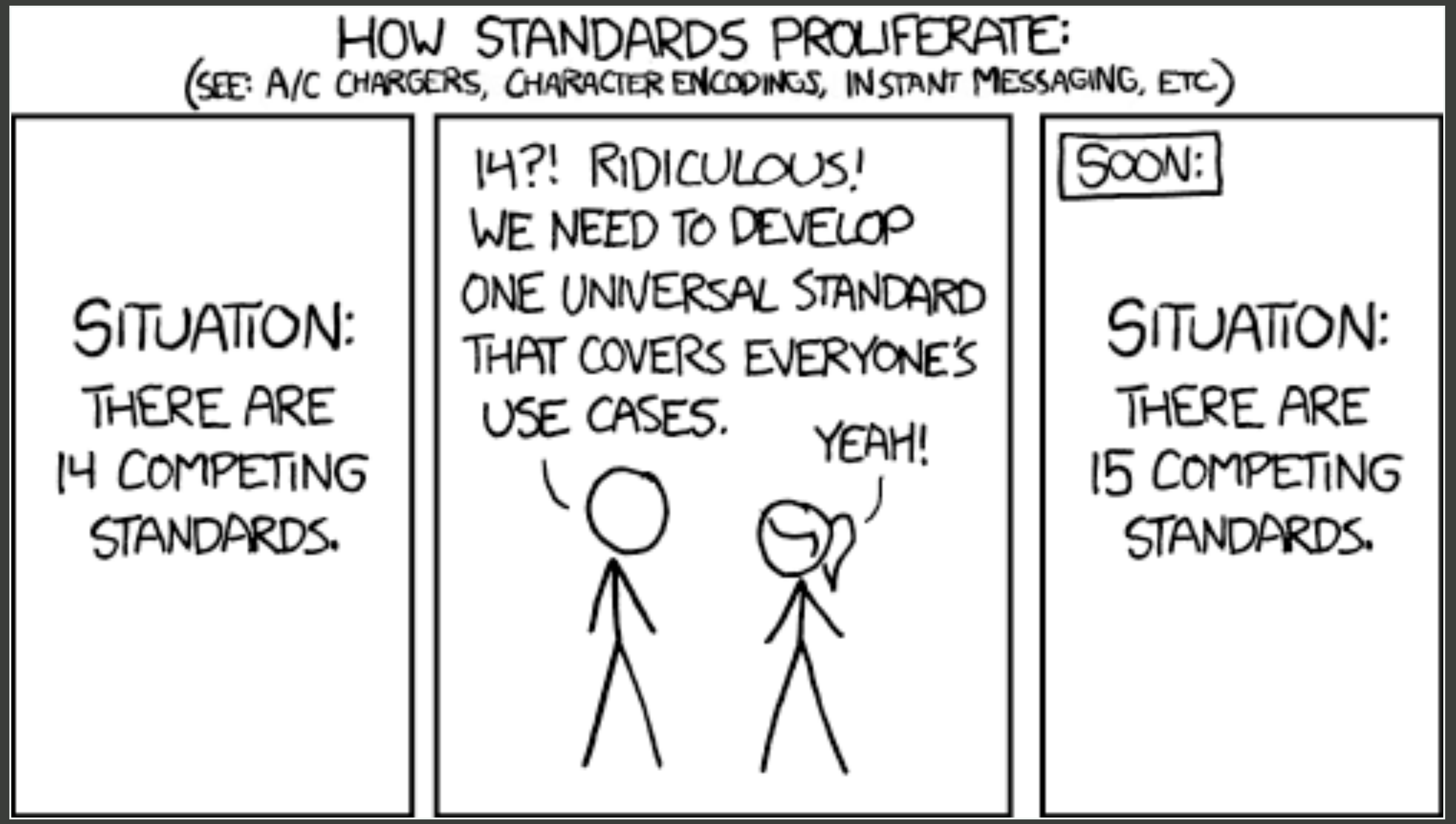
- NeuLat is an ML-based **software package** for benchmarking and test models for LFT e.g.,
  - 1+1D ϕ^4-theory
  - 1+1D $U(1)$ gauge theory
- No such effort was made **yet** to combine existing tools into one software.
- NeuLat is meant to be a **community-wide** effort.
- The **core team** of NeuLat:
  - Expertise in ML **software development**.
  - Expertise in **LFT**.
  - **Various contributions to the field:** asymptotically unbiased estimators (Nicoli K.A. et al.), thermodynamic observables (Nicoli K.A. et al.), mode-dropping estimators (Nicoli K.A. et al.), path gradients (Vaitl L. et al. (2022)), and trivializing maps with flows (Bacchio S. et al. (2023)).

What are the benefits?

- Faster development of **new ideas**.
- Easier to **reproduce** newly published results (in the flow-based sampling community).
- Easier for people to **enter the community** and experiment with state-of-the-art techniques.
- Save the effort of **re-implementing** standard methods (e.g., architecture, estimators, etc.).
- Allow for immediate **extension to other fields** in physics (e.g., condensed matter physics).
- Similar **examples for ML frameworks** in other scientific communities:
    - SchNetPack - Deep Neural Networks for Atomistic Systems → TU berlin
    - BGFlow - Boltzmann Generators (BG) and other sampling methods

Why NeuLat?

- Many tools have been **independently** proposed.
- No **reference implementation** exists.
  - Often needs to reimplement existing code.
  - Different ML libraries.
  - Different code styles and structures.

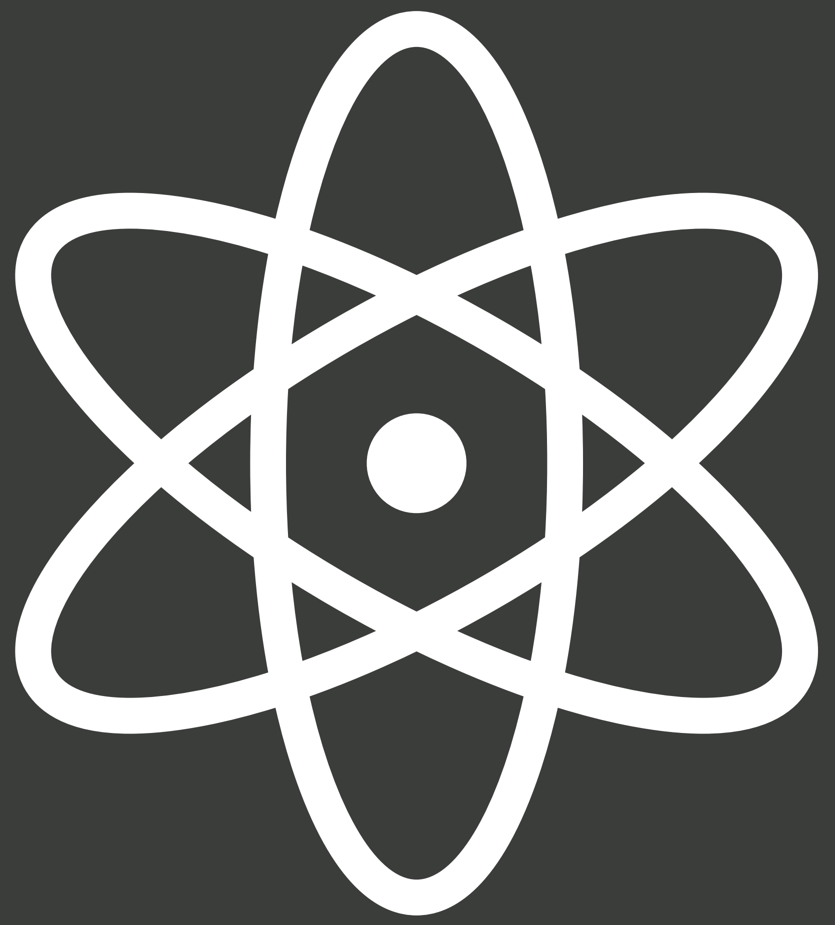


Credits: xkcd.com/927

- Big (unnecessary) **overhead** (often seen also in the ML community).
- Excellent repositories are already available (though limited in scope).
  - fthmc: Field Transformation HMC
  - l2hmc-qcd l2hmc-qcd

  👏 Shout-out to Sam Foreman et al., for the great work!
  - nflows
  - GomalizingFlow 👏 Julia package from A. Tomiya and collaborators!

Normalizing Flows for LFT

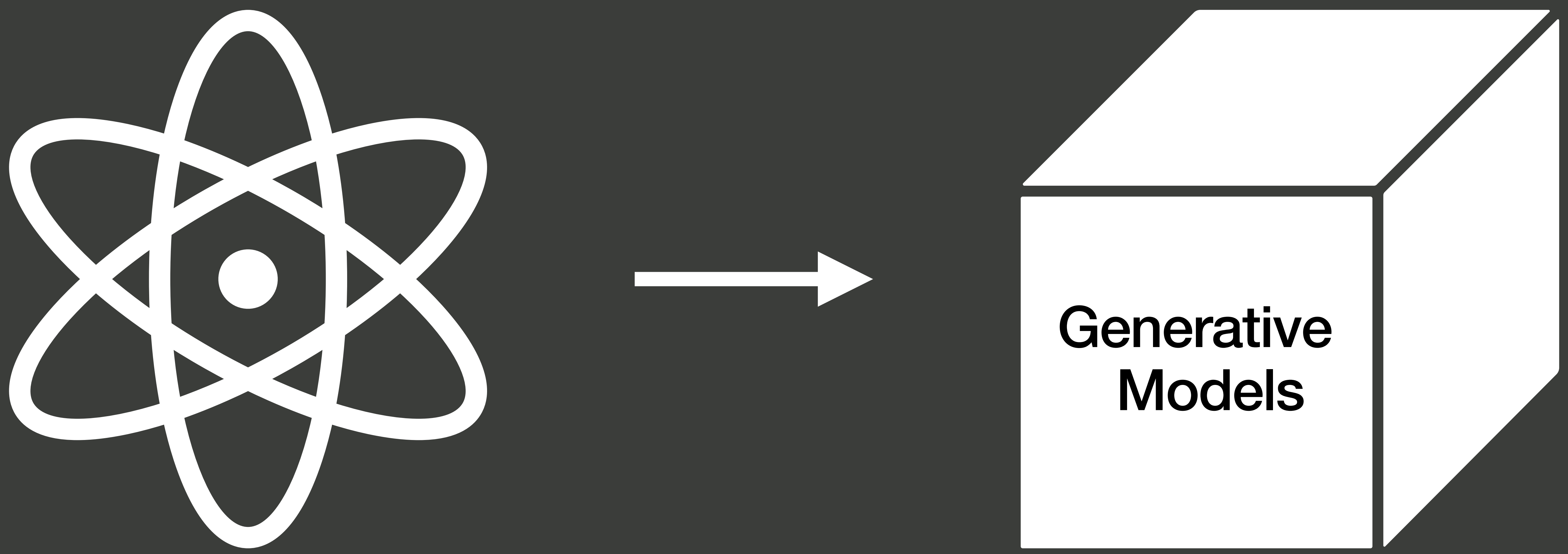


Input:

- Action* $S[U]$ ✅
- Samples (HMC) ⚠️

*Here U should denote generalized field configurations e.g., scalar fields, gauge fields.

Normalizing Flows for LFT



Input:

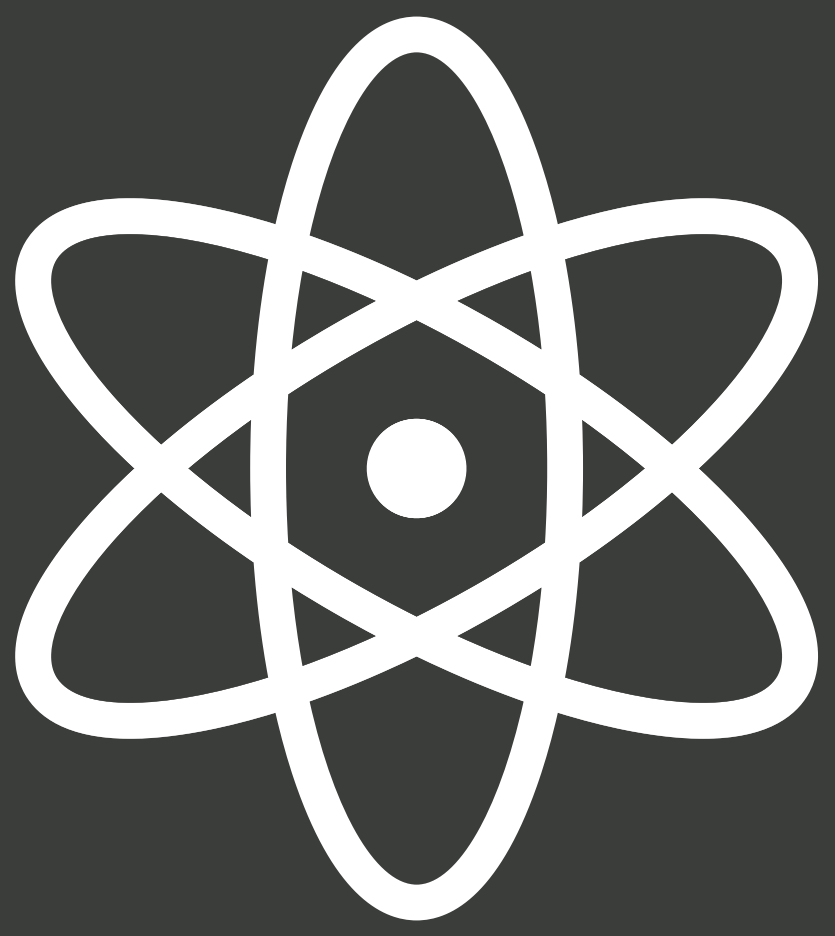
- Action* $S[U]$ ✅
- Samples (HMC) ⚠️

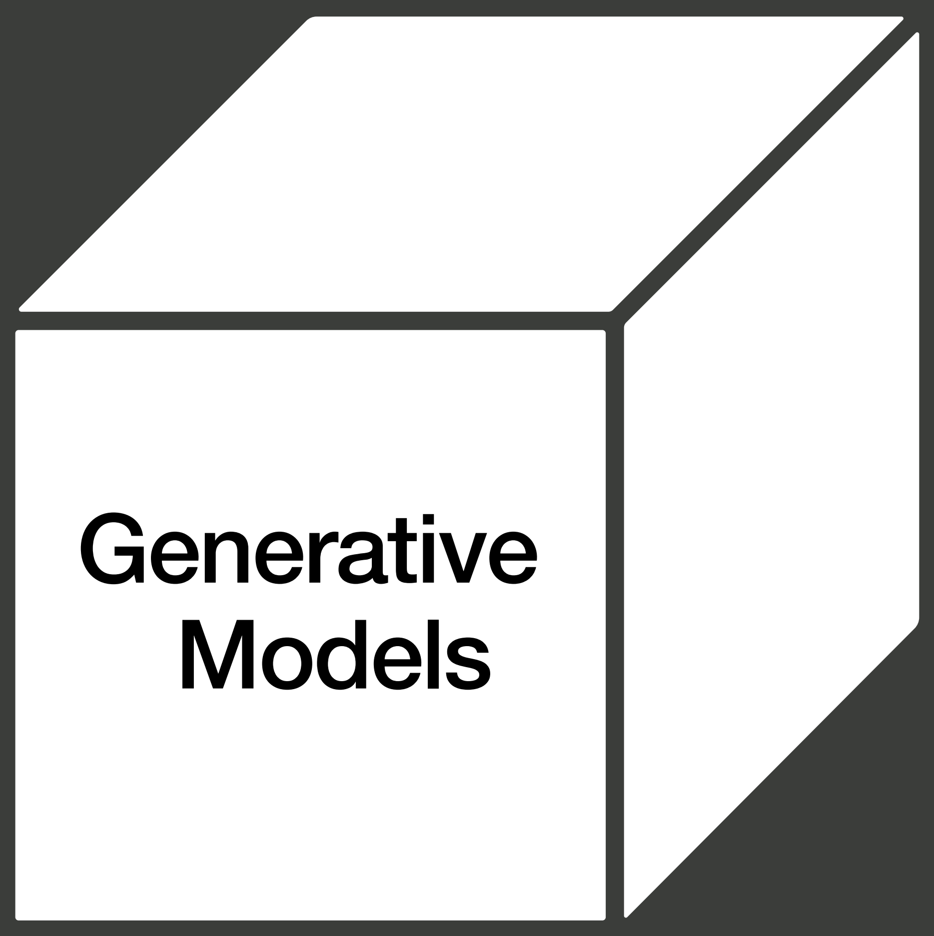
ML black(-box) magic:

- Train generative models
  - **Normalizing Flows**
  - Autoregressive Models
  - Diffusion Models
- Learn normalized densities

*Here U should denote generalized field configurations e.g., scalar fields, gauge fields.

Normalizing Flows for LFT





$$q_\theta(U) \approx \frac{e^{-S[U]}}{Z}$$

Input:

- Action* $S[U]$ ✅
- Samples (HMC) ⚠️

*Here U should denote generalized field configurations e.g., scalar fields, gauge fields.

ML black(-box) magic:

- Train generative models
  - **Normalizing Flows**
  - Autoregressive Models
  - Diffusion Models
- Learn normalized densities

Output:

- Normalized density $q_\theta(U)$
- Approximation of target $p(U)$
- Embarrassingly parallel sampling

⚠️ Not possible with standard HMC

Historical Development of a Promising Avenue

NICE

2014

NICE: NON-LINEAR INDEPENDENT COMPONENTS ESTIMATION

Laurent Dinh David Krueger Yoshua Bengio*
Département d'informatique et de recherche opérationnelle
Université de Montréal
Montréal, QC H3C 3J7

Normalizing Flow for VI

2015

Variational Inference with Normalizing Flows

Danilo Jimenez Rezende DANILOR@GOOGLE.COM
Shakir Mohamed SHAKIR@GOOGLE.COM
Google DeepMind, London

RealNVP

2016

DENSITY ESTIMATION USING REAL NVP

Laurent Dinh*
Montreal Institute for Learning Algorithms
University of Montreal
Montreal, QC H3T1J4

Jascha Sohl-Dickstein
Google Brain

Samy Bengio
Google Brain

Historical Development of a Promising Avenue

Quantum Chemistry

Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning

FRANK NOÉ, SIMON OLSSON, JONAS KÖHLER, AND HAO WU Authors Info & Affiliations

SCIENCE • 6 Sep 2019 • Vol 365, Issue 6457 • DOI: 10.1126/science.aaw1147

Scalar Field Theories

Flow-based generative models for Markov chain Monte Carlo in lattice field theory

M. S. Albergo, G. Kanwar, and P. E. Shanahan
Phys. Rev. D **100**, 034515 – Published 22 August 2019

Statistical Mechanics

Asymptotically unbiased estimation of physical observables with neural samplers

Kim A. Nicoli, Shinichi Nakajima, Nils Strodthoff, Wojciech Samek, Klaus-Robert Müller, and Pan Kessel
Phys. Rev. E **101**, 023304 – Published 10 February 2020

2014 2015 2016

NICE: NON-LINEAR INDEPENDENT COMPONENTS ESTIMATION

Variational Inference with Normalizing Flows

DENSITY ESTIMATION USING REAL NVP

Historical Development of a Promising Avenue

$U(1)$, $SU(N)$ gauge theories

Equivariant Flow-Based Sampling for Lattice Gauge Theory

Gurtej Kanwar, Michael S. Albergo, Denis Boyda, Kyle Cranmer, Daniel C. Hackett, Sébastien Racanière, Danilo Jimenez Rezende, and Phiala E. Shanahan

Phys. Rev. Lett. **125**, 121601 – Published 15 September 2020

Sampling using $\mathrm{SU}(N)$ gauge equivariant flows

Denis Boyda, Gurtej Kanwar, Sébastien Racanière, Danilo Jimenez Rezende, Michael S. Albergo, Kyle Cranmer, Daniel C. Hackett, and Phiala E. Shanahan

Phys. Rev. D **103**, 074504 – Published 20 April 2021

Thermodynamic observables

Estimation of Thermodynamic Observables in Lattice Field Theories with Deep Generative Models

Kim A. Nicoli, Christopher J. Anders, Lena Funcke, Tobias Hartung, Karl Jansen, Pan Kessel, Shinichi Nakajima, and Paolo Stornati

Phys. Rev. Lett. **126**, 032001 – Published 19 January 2021

Pseudofermions in 1+1D

Flow-based sampling for fermionic lattice field theories

Michael S. Albergo, Gurtej Kanwar, Sébastien Racanière, Danilo J. Rezende, Julian M. Urban, Denis Boyda, Kyle Cranmer, Daniel C. Hackett, and Phiala E. Shanahan

Phys. Rev. D **104**, 114507 – Published 15 December 2021

2014 — 2015 — 2016 — 2019

NICE: Non-linear Independent Components Estimation

Variational Inference with Normalizing Flows

Density estimation using Real NVP

Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning

Historical Development of a Promising Avenue

<u>Many</u> great works published between 2021 and 2023 and eventually…

The first proof of principle of sampling $SU(3)$ LGT.

↓

Plenary talk by Gurtej Kanwar (Monday 31st July)

Normalizing flows for lattice gauge theory in arbitrary space-time dimension

Ryan Abbott,[1,2] Michael S. Albergo,[3] Aleksandar Botev,[4] Denis Boyda,[1,2] Kyle Cranmer,[5] Daniel C. Hackett,[1,2] Gurtej Kanwar,[6,1,2] Alexander G.D.G. Matthews,[4] Sébastien Racanière,[4] Ali Razavi,[4] Danilo J. Rezende,[4] Fernando Romero-López,[1,2] Phiala E. Shanahan,[1,2] and Julian M. Urban[1,2]

[1] *Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[2] *The NSF AI Institute for Artificial Intelligence and Fundamental Interactions*
[3] *Center for Cosmology and Particle Physics, New York University, New York, NY 10003, USA*
[4] *DeepMind, London, UK*
[5] *Physics Department, University of Wisconsin-Madison, Madison, WI 53706, USA*
[6] *Albert Einstein Center, Institute for Theoretical Physics, University of Bern, 3012 Bern, Switzerland*

Applications of normalizing flows to the sampling of field configurations in lattice gauge theory have so far been explored almost exclusively in two space-time dimensions. We report new algorithmic developments of gauge-equivariant flow architectures facilitating the generalization to higher-dimensional lattice geometries. Specifically, we discuss masked autoregressive transformations with tractable and unbiased Jacobian determinants, a key ingredient for scalable and asymptotically exact flow-based sampling algorithms. For concreteness, results from a proof-of-principle application to SU(3) lattice gauge theory in four space-time dimensions are reported.

2014 — NICE: Non-linear Independent Components Estimation

2015 — Variational Inference with Normalizing Flows

2016 — Density estimation using Real NVP

2019 — Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning

2020 — Equivariant Flow-Based Sampling for Lattice Gauge Theory
Gurtej Kanwar, Michael S. Albergo, Denis Boyda, Kyle Cranmer, Daniel C. Hackett, Sébastien Racanière, Danilo Jimenez Rezende, and Phiala E. Shanahan
Phys. Rev. Lett. 125, 121601 – Published 15 September 2020

2021 — Flow-based sampling for fermionic lattice field theories
Michael S. Albergo, Gurtej Kanwar, Sébastien Racanière, Danilo J. Rezende, Julian M. Urban, Denis Boyda, Kyle Cranmer, Daniel C. Hackett, and Phiala E. Shanahan
Phys. Rev. D 104, 114507 – Published 15 December 2021

Historical Development of a Promising Avenue

One work, in particular, boosted the development of this new field between 2021 and 2023

Introduction to Normalizing Flows for Lattice Field Theory

Michael S. Albergo,[1,*] Denis Boyda,[2,3,4,†] Daniel C. Hackett,[3,4,‡] Gurtej Kanwar,[3,4,§] Kyle Cranmer,[1] Sébastien Racanière,[5] Danilo Jimenez Rezende,[5] and Phiala E. Shanahan[3,4]

[1] *Center for Cosmology and Particle Physics, New York University, New York, NY 10003, USA*
[2] *Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont IL 60439, USA*
[3] *Center for Theoretical Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA*
[4] *The NSF AI Institute for Artificial Intelligence and Fundamental Interactions*
[5] *DeepMind, London, UK*

(Dated: August 9, 2021)

This notebook tutorial demonstrates a method for sampling Boltzmann distributions of lattice field theories using a class of machine learning models known as normalizing flows. The ideas and approaches proposed in arXiv:1904.12072, arXiv:2002.02428, and arXiv:2003.06413 are reviewed and a concrete implementation of the framework is presented. We apply this framework to a lattice scalar field theory and to U(1) gauge theory, explicitly encoding gauge symmetries in the flow-based approach to the latter. This presentation is intended to be interactive and working with the attached Jupyter notebook is recommended.

2014 — NICE: Non-linear Independent Components Estimation (Laurent Dinh, David Krueger, Yoshua Bengio)

2015 — Variational Inference with Normalizing Flows (Danilo Jimenez Rezende, Shakir Mohamed)

2016 — Density estimation using Real NVP (Laurent Dinh, Jascha Sohl-Dickstein, Samy Bengio)

2019 — Boltzmann generators: Sampling equilibrium states of many-body systems with deep learning

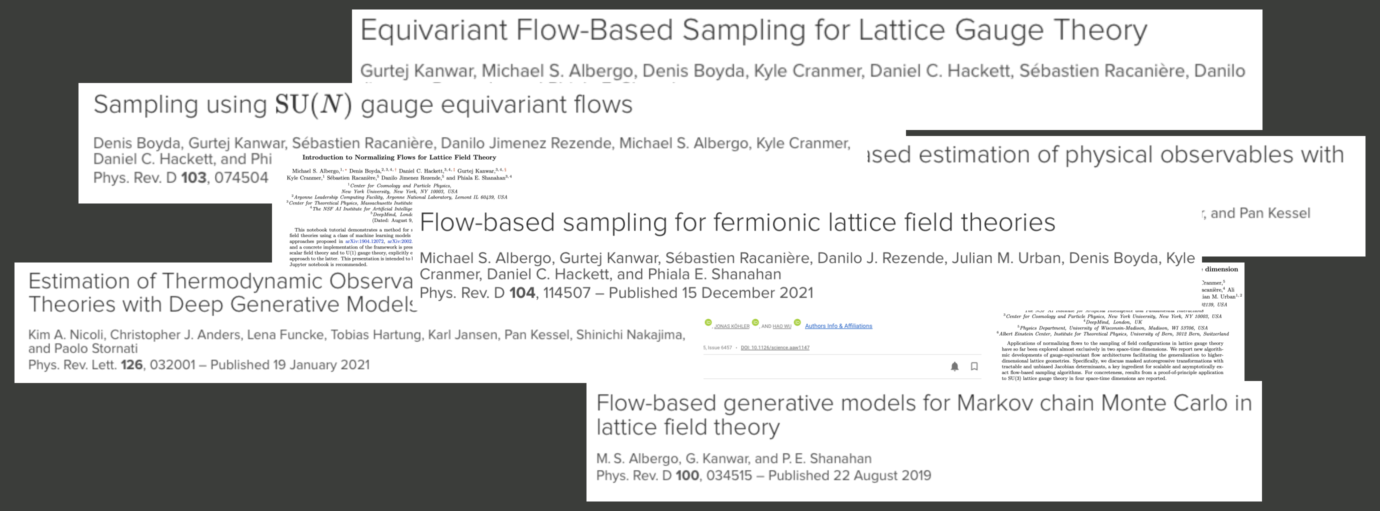
2020 — Equivariant Flow-Based Sampling for Lattice Gauge Theory (Gurtej Kanwar, Michael S. Albergo, Denis Boyda, Kyle Cranmer, Daniel C. Hackett, Sébastien Racanière, Danilo Jimenez Rezende, and Phiala E. Shanahan; Phys. Rev. Lett. **125**, 121601 – Published 15 September 2020)

2021 — Flow-based sampling for fermionic lattice field theories (Michael S. Albergo, Gurtej Kanwar, Sébastien Racanière, Danilo J. Rezende, Julian M. Urban, Denis Boyda, Kyle Cranmer, Daniel C. Hackett, and Phiala E. Shanahan; Phys. Rev. D **104**, 114507 – Published 15 December 2021)

2023 — Normalizing flows for lattice gauge theory in arbitrary space-time dimension

NeuLat

Goal: incorporate as many contributions from 5 years of research progress into a single software framework.

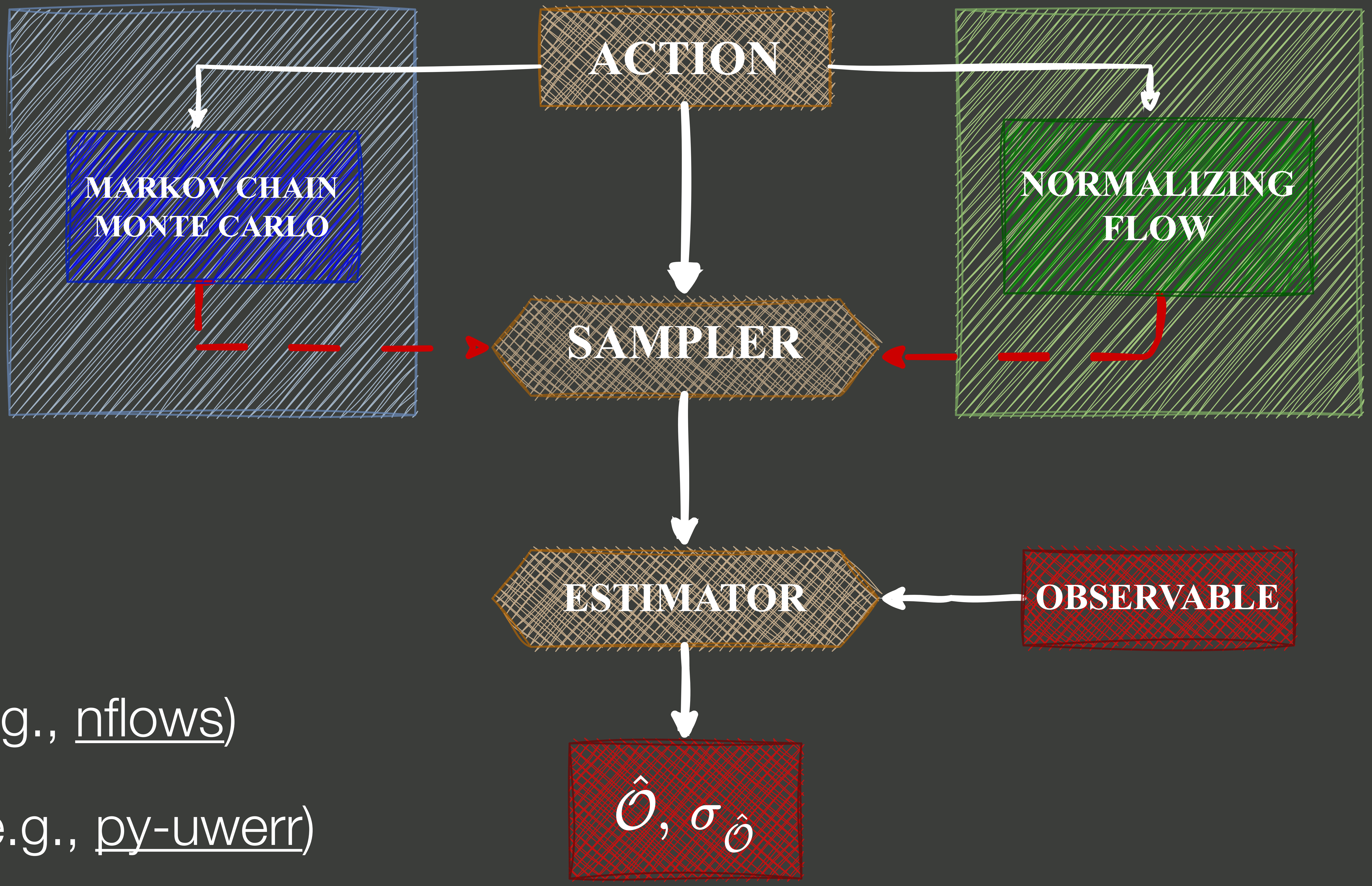


NeuLat

Goal: incorporate as many contributions from 5 years of research progress into a single software framework.

NEULAT

Software Overview



- PyTorch backend
- MCMC-based sampling
- Flow-based sampling (e.g., nflows)
- Observable estimation (e.g., py-uwerr)

Basic Workflow

Step 0: Define the action of the physical system to simulate.

Step 1: Build a Markov chain and a custom normalizing flow model.

Step 2: Specify loss and optimizer and train the flow model.

Step 3: Estimate observables using samples from HMC and trained flow.

```
n_samples, train_steps, batch = 1000, 1000, 500
action = Phi4Action(kappa=0.3, lamb=0.022)

hmc_chain = HMCMarkovChain(action, lat_shape=[16, 16], burn_in=100)
model = Flow(
    lat_shape=[16, 16],
    base_dist=NormalDistribution(),
    coupling=NiceCoupling(),
    n_couplings=6
)

optim = torch.optim.Adam(model.parameters(), lr=learning_rate)
loss_fn = ReverseKLLoss()
for _ in range(train_steps):
    configs, log_probs = model.sample_and_log_prob(batch)
    loss = loss_fn(action(configs), log_probs)
    optim.zero_grad(); loss.backward(); optim.step()

obs = ObservableEstimator(['action', 'absmag'])
flow_obs = obs.evaluate(model.sample(n_samples))
hmc_obs = obs.evaluate(hmc_chain.sample(n_samples))
```

Key Features

- **Density Estimation**: Learn approximations of targeted Boltzmann distributions $q_\theta \approx p$.
- **Sampling:**
  - MCMC implementations (HMC, Cluster algorithms, etc.).
  - Neural Importance Sampling (see Albergo et al. (2019), Kanwar et al. (2020), Nicoli et al. (2021)+ refs. therein).
  - Neural HMC (see same papers referenced above).
- **Estimation**:
  - Asymptotically unbiased estimators for physical observables (see Nicoli et al. (2020)).
  - Direct estimation of thermodynamic observables with flows and HMC (see Nicoli et al. (2021)).
  - Sampling in the presence of mode-collapse (see Nicoli et al. (2023)).
- **Customizable**: Easy to incorporate a new action/theory or customize new, equivariant flow-layers.

… and more!

Future of NeuLat

A working release of the software is planned by the **end of 2023**:

- (1+1) ϕ^4 scalar field theory - Albergo et al. (2019)
- (1+1) U(1) gauge theory - Kanwar et al. (2020)
- Thermodynamic observables - Nicoli et al. (2021)
- Mode-dropping estimators - Nicoli et al. (2023)
- …

Future releases will expand the NeuLat toolbox with important additional features:

- Stochastic normalizing flows - Caselle et al. (2022)
- Conditional normalizing flows - Gerdes et al. (2023)
- Path gradients - Vaitl et al. (2022)
- Hubbard Model - Wynen et al. (2019)
- …

Conclusion

- We presented **NeuLat**, a software for flow-based simulation of LFT.
- The software is meant to be accessible, **modular**, and easy to **extend** and **maintain**.
- This eliminates the **overhead** of re-implementing existing code between different formats.
- The first **release** of the software is planned for the **upcoming months**.
- NeuLat is aimed to be a **community-wide effort**. Get in touch if you would like to contribute.

Thank you for listening!

Get in touch:

@nicoli_kim

knicoli@uni-bonn.de

github.com/nicoliKim

Scan the QR, click here or go to https://forms.gle/LhgNvhHyeHKUUVjv7 if you are interested!