Machine learning for first-principles theory calculations

Phiala Shanahan, MIT

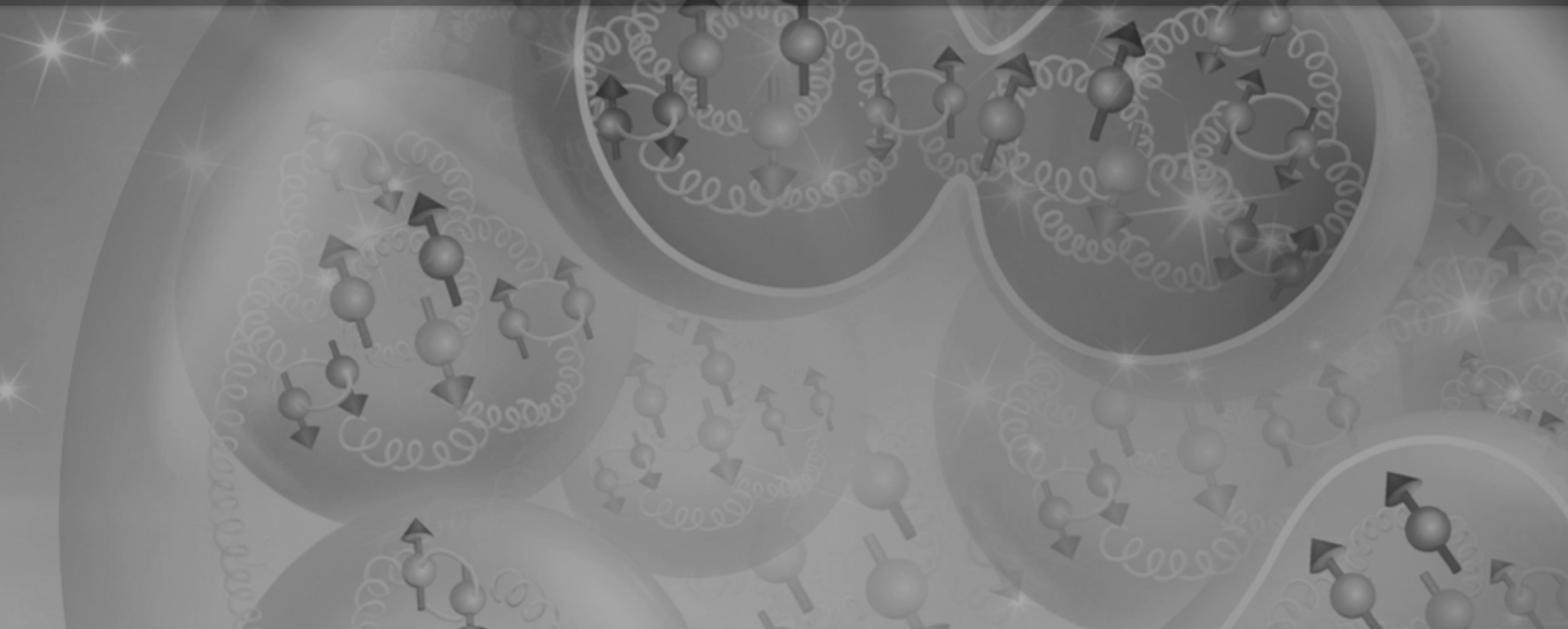


Image Credit: 2018 EIC User's Group Meeting

Massachusetts Institute of Technology

Machine learning for first-principles theory calculations

Phiala Shanahan, MIT

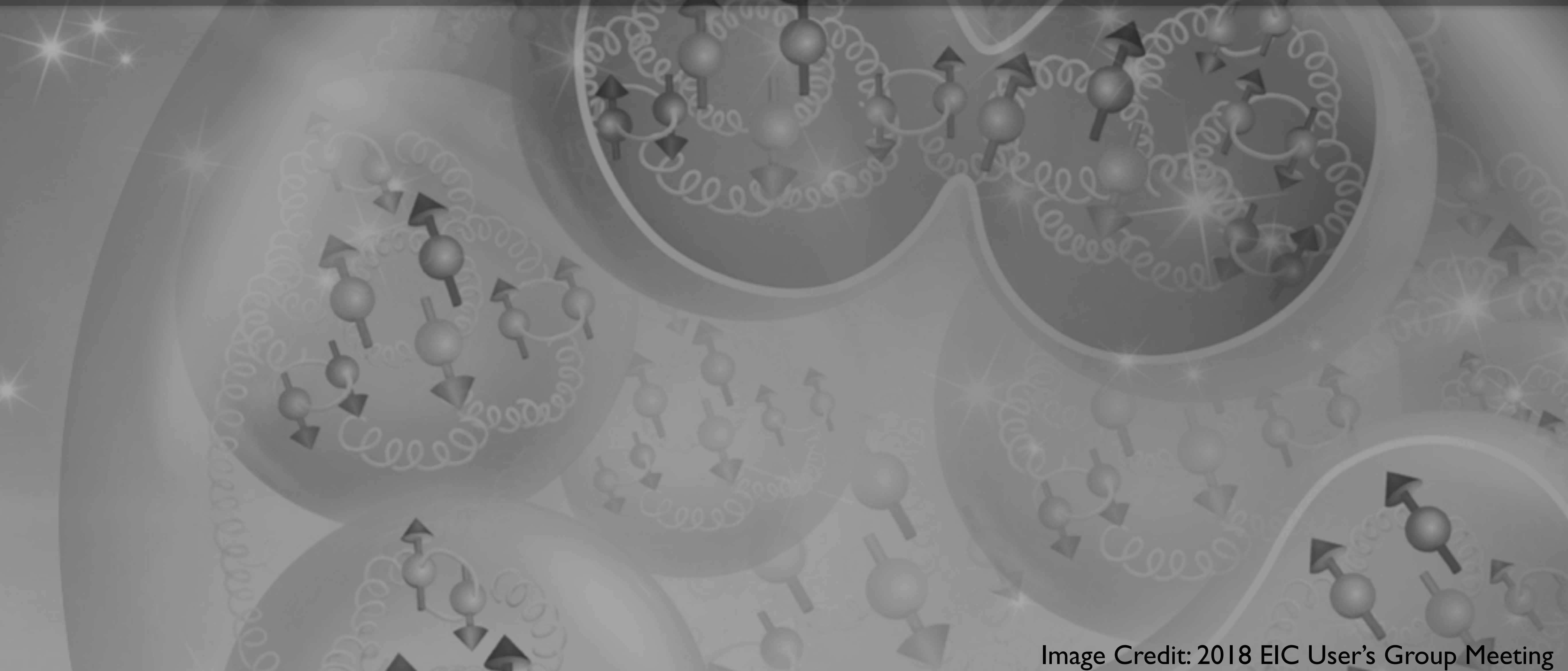


Image Credit: 2018 EIC User's Group Meeting

Machine learning for first-principles theory

Compute **exact** results from known theory
Use AI/ML to do it **faster**

e.g., calculations of the Standard Model, BSM model, EFT, …

Require **mathematical guarantees of exactness** to preserve rigour of first-principles calculations

No room for approximations, errors, modelling, or any uncertainties which cannot be systematically improved

AI/ML algorithm poorly trained → Results correct, but slower

AI/ML algorithm well trained → Results correct, but faster

Machine learning for first-principles theory

Compute **exact** results from known theory
Use AI/ML to do it **faster**

1. Do the calculation the "same way" but faster

e.g., Tune parameters of existing algorithm using AI

[Free parameters of algebraic multigrid for solving linear systems, automatic differentiation rather than stochastic optimisation]

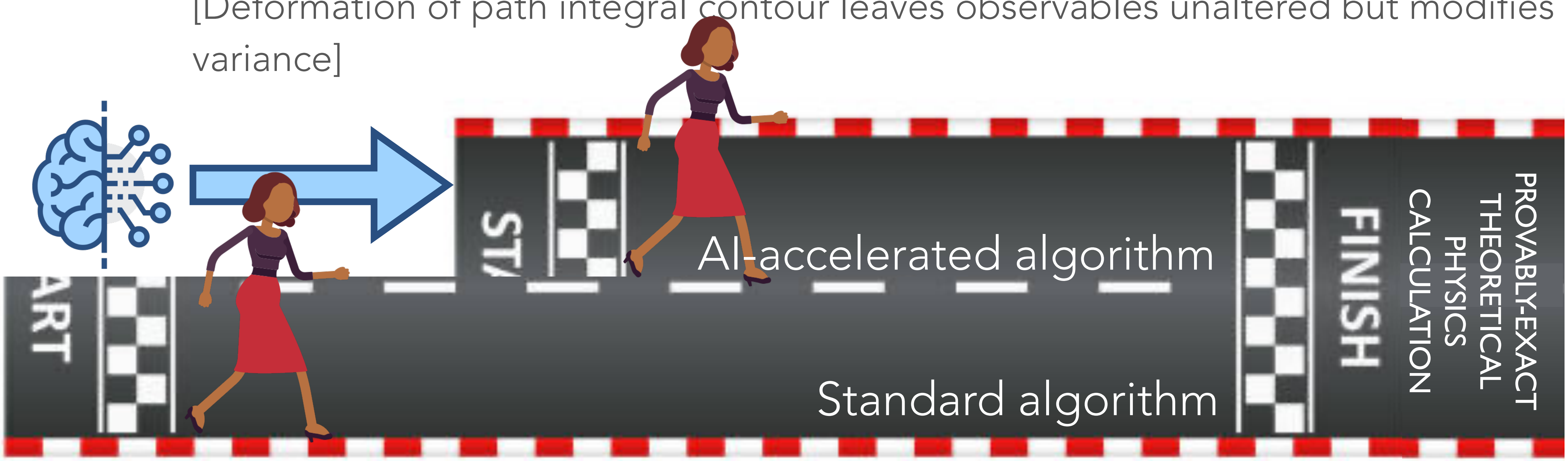
Machine learning for first-principles theory

```
Compute exact results from known theory
Use AI/ML to do it faster
```

2. Transform the problem into a different one with better properties (computationally easier) but same solution

e.g., Preconditioning of any type
[Numerical solver e.g., matrix inversion, faster convergence after preconditioning]

e.g. Change-of-variables
[Deformation of path integral contour leaves observables unaltered but modifies variance]

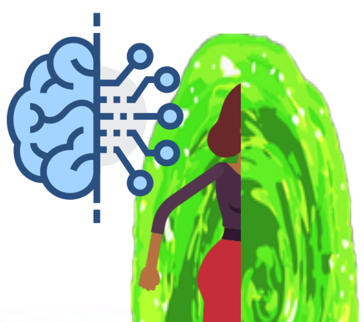


Machine learning for first-principles theory

```
Compute exact results from known theory
Use AI/ML to do it faster
```

3. Solve a different problem, apply a known correction

e.g., Learn a map from one observable to another, bias-correct
[Sloppy and high-precision solutions of linear systems]



e.g. Sample nearby probability distribution,
reweight/resample

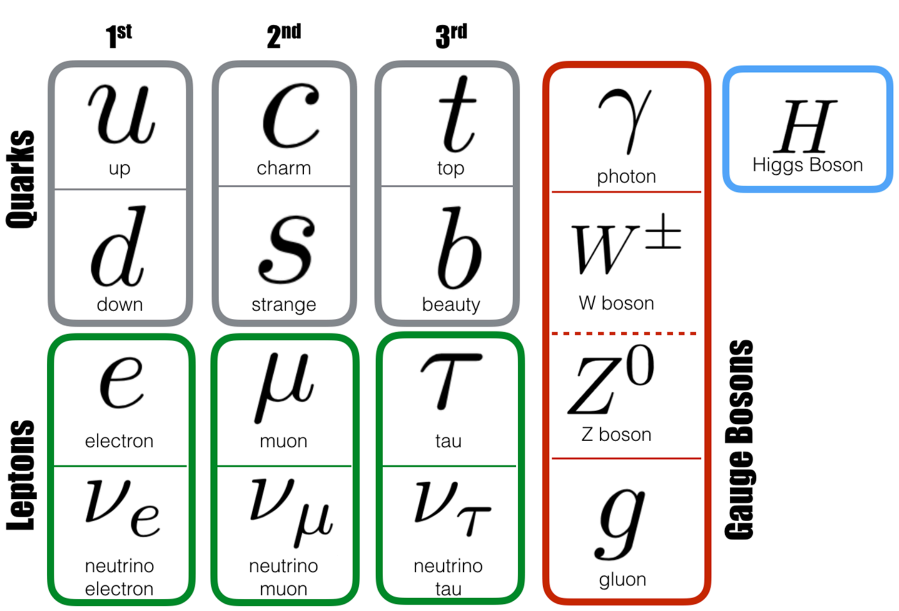
Phiala Shanahan, MIT

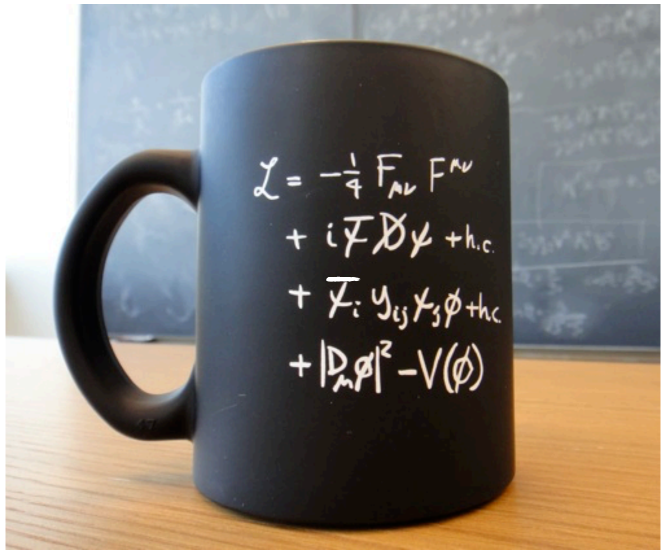
Machine learning for first-principles theory

Compute **exact** results from known theory
Use AI/ML to do it **faster**

3. Solve a different problem, apply a known correction

Now: Details of one example of this approach for lattice QCD calculations of the Standard Model

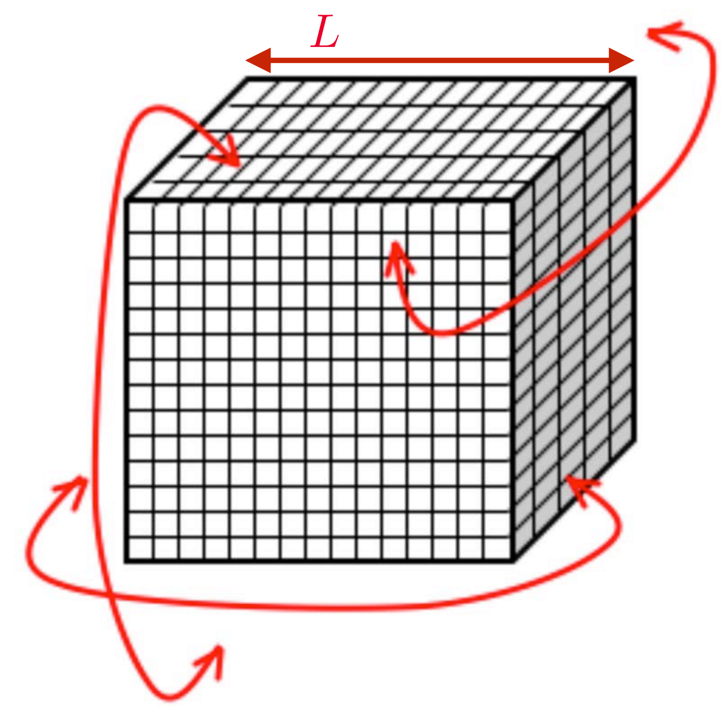




Lattice QCD

Numerical first-principles approach to non-perturbative QCD

- Euclidean space-time
  - Non-zero lattice spacing
  - Finite volume
- Some calculations use larger-than-physical quark masses (cheaper)



Approximate the QCD path integral by **Monte Carlo**

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}A \mathcal{D}\overline{\psi} \mathcal{D}\psi \mathcal{O}[A, \overline{\psi}\psi] e^{-S[A,\overline{\psi}\psi]} \rightarrow \langle \mathcal{O} \rangle \simeq \frac{1}{N_{\mathrm{conf}}} \sum_i^{N_{\mathrm{conf}}} \mathcal{O}([U^i])$$

with field configurations U^i distributed according to $e^{-S[U]}$

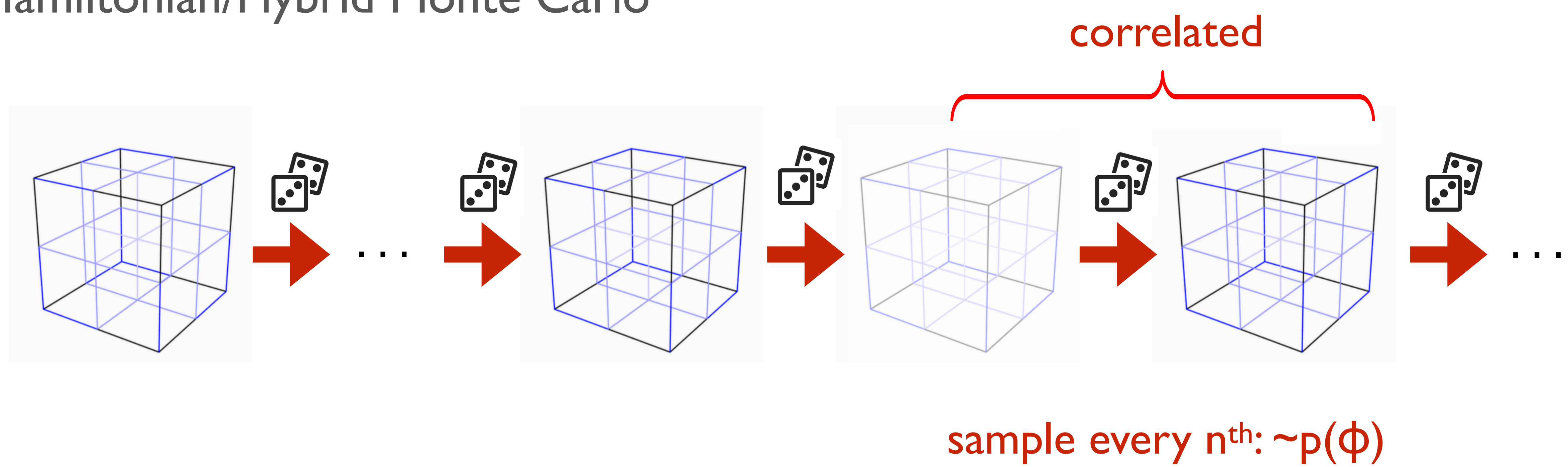
Phiala Shanahan, MIT

Generate QCD gauge fields

Generate field configurations $\phi(x)$ with probability

$$P[\phi(x)] \sim e^{-S[\phi(x)]}$$

Hamiltonian/Hybrid Monte Carlo

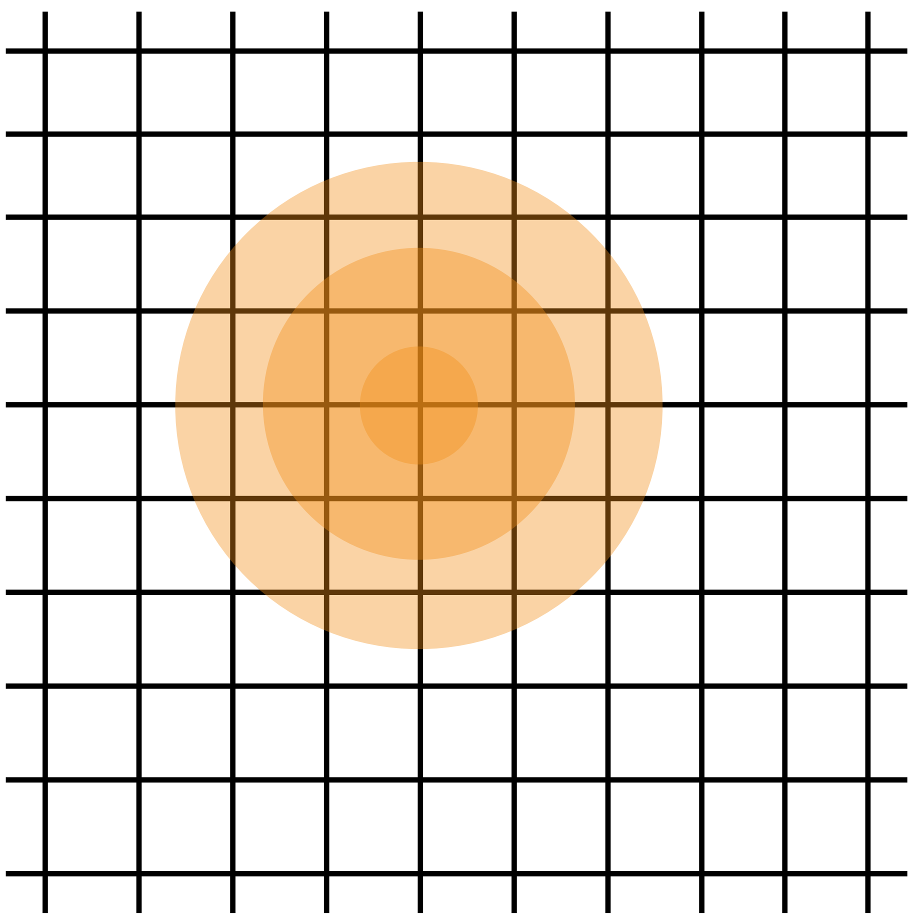


Correlation length dictated by Markov chain '**auto-correlation time**': shorter autocorrelation time implies less computational cost

Generate QCD gauge fields

QCD gauge field configurations sampled via

Hamiltonian dynamics + Markov Chain Monte Carlo



Updates diffusive

Lattice spacing → 0

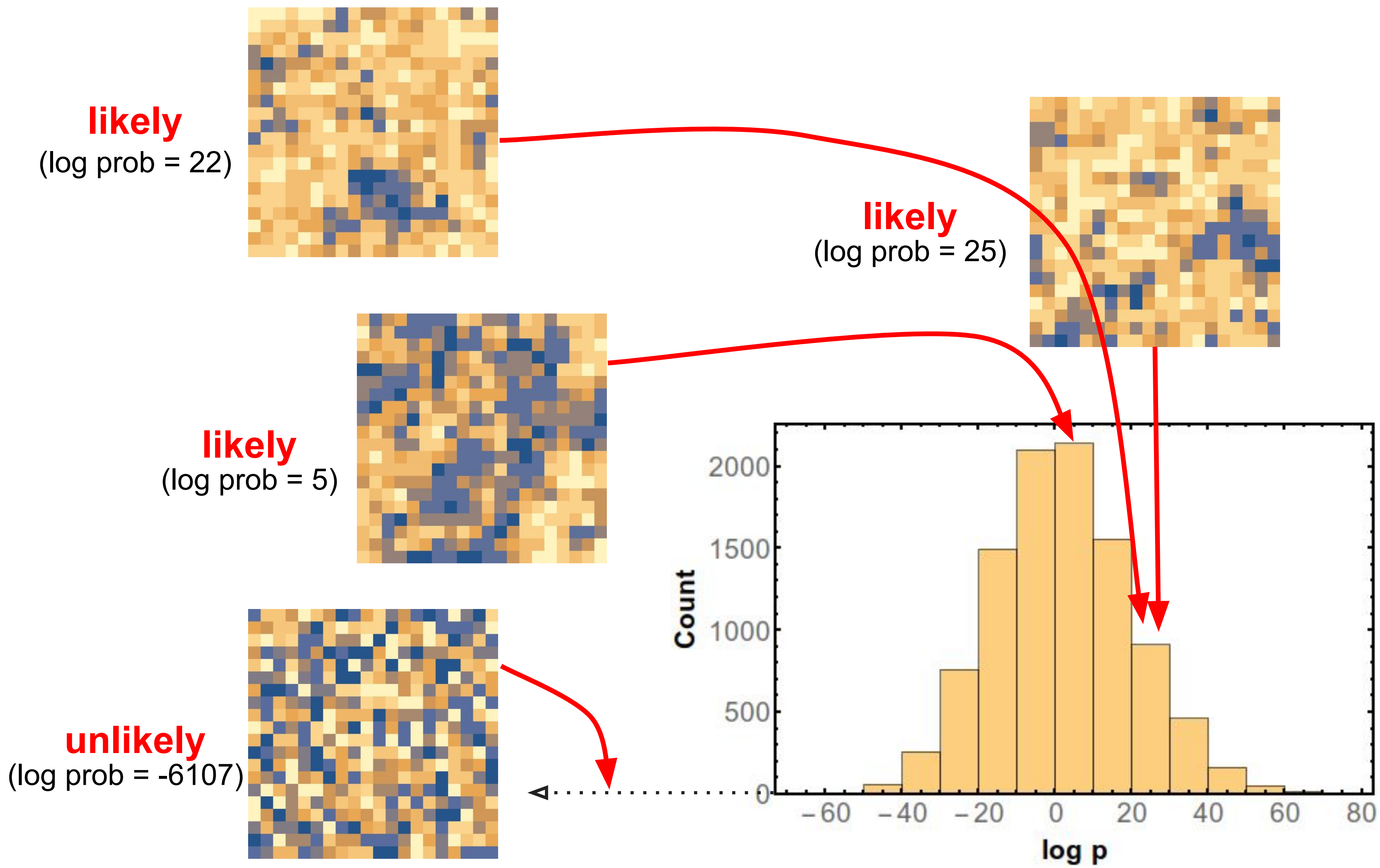
Number of updates to change fixed physical length scale → ∞

"Critical slowing-down" of generation of uncorrelated samples

Generate QCD gauge fields

Generate field configurations $\phi(x)$ with probability

$$P[\phi(x)] \sim e^{-S[\phi(x)]}$$



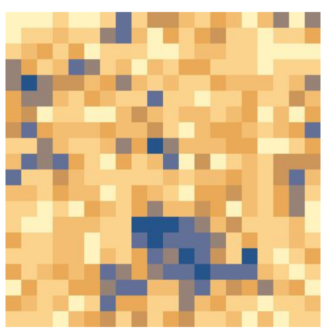
Generate QCD gauge fields

Generate field configurations $\phi(x)$ with probability

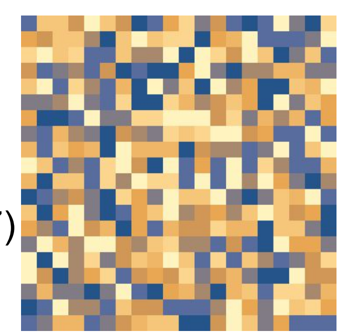
$$P[\phi(x)] \sim e^{-S[\phi(x)]}$$

Parallels with image generation problem

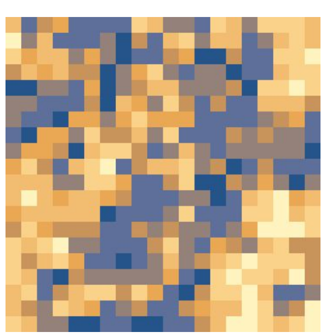
likely
(log prob = 22)



unlikely
(log prob = -6107)



likely
(log prob = 5)

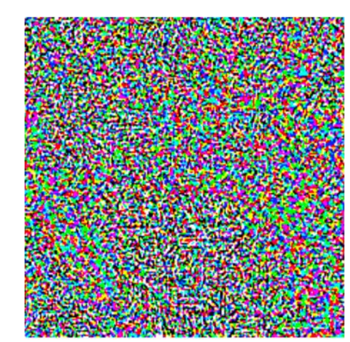


likely

[Karras, Lane, Aila / NVIDIA 1812.04948]

likely

unlikely



thispersondoesnotexist.com

Machine learning QCD

Ensemble of lattice QCD gauge fields

- Ensemble of gauge fields has meaning
- $64^3 \times 128 \times 4 \times 9 \times 2$ $\simeq 10^9$ numbers
- ~1000 samples
- Long-distance correlations are important
- Gauge and translation-invariant with periodic boundaries

CIFAR benchmark image set for machine learning

- Each image has meaning
- 32 x 32 pixels x 3 cols $\simeq$3000 numbers
- 60000 samples
- Local structures are important
- Translation-invariance within frame

Machine learning QCD

Ensemble of lattice QCD gauge fields

- ...f gauge fields has
- ...important
- Gauge and translation-invariant with periodic boundaries

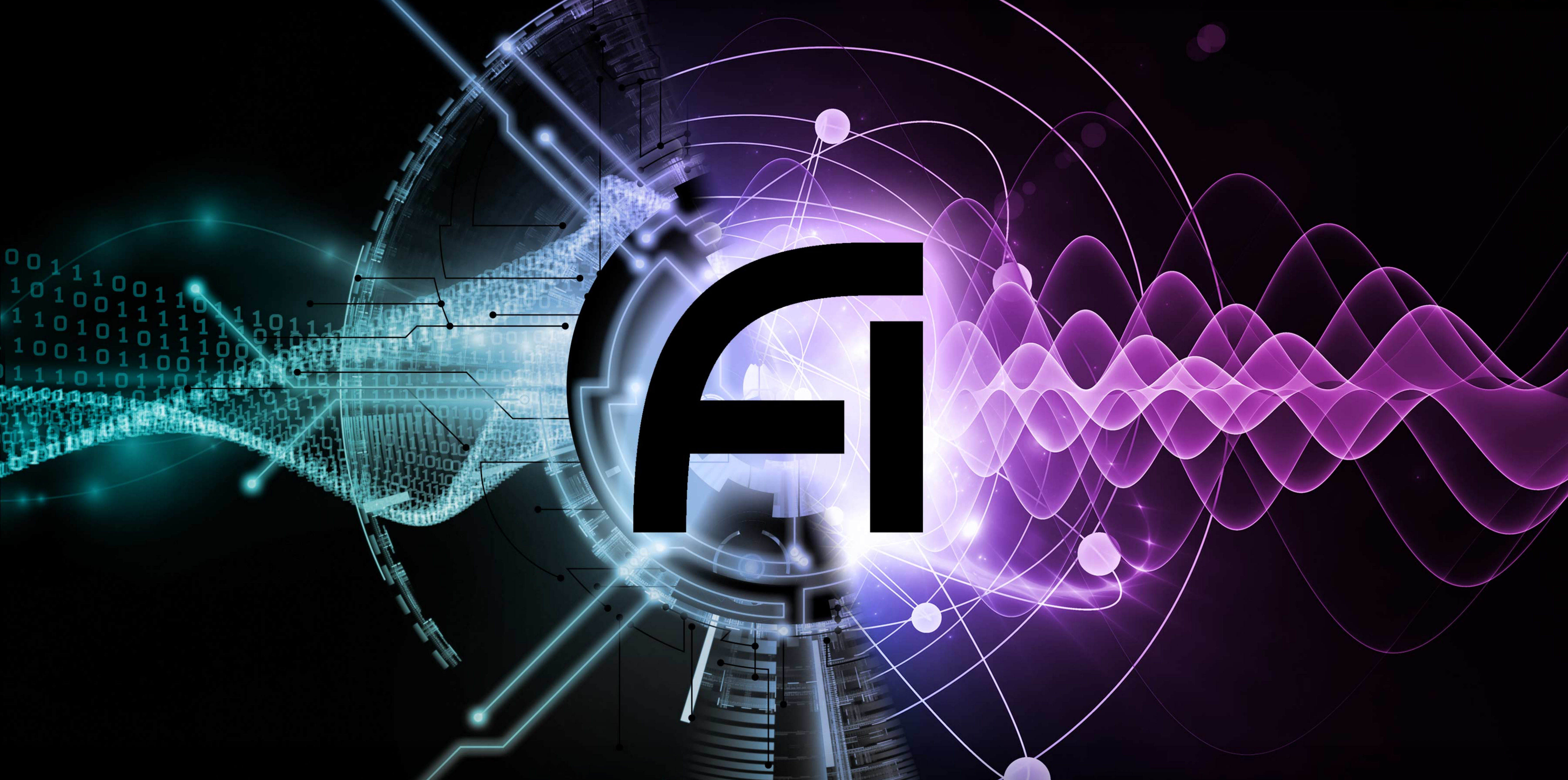
CIFAR benchmark image set for machine learning

- Each image has meaning
- 32 x 32 pixels x 3 cols ...000 numbers
- ...fram...

Need custom ML for physics from the ground up

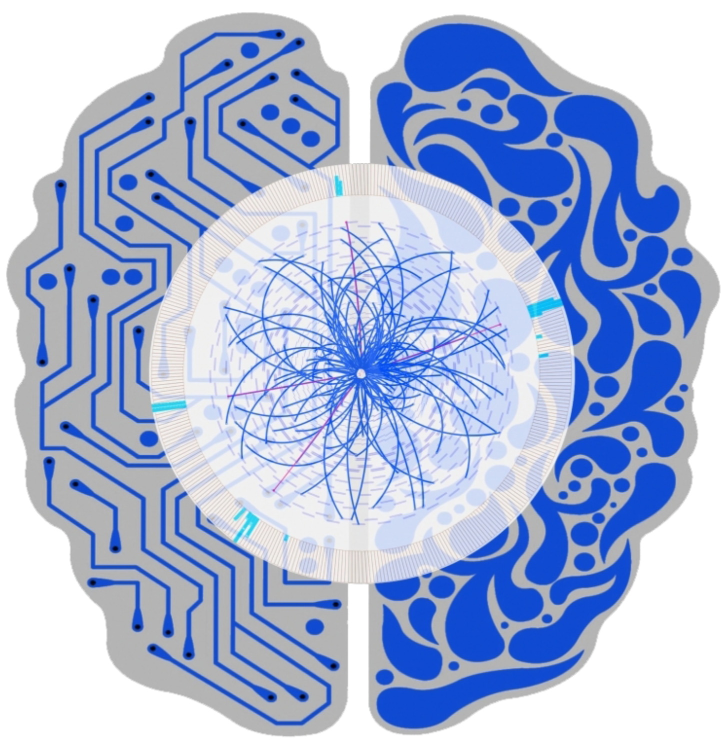
AB-INITIO AI

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



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

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"

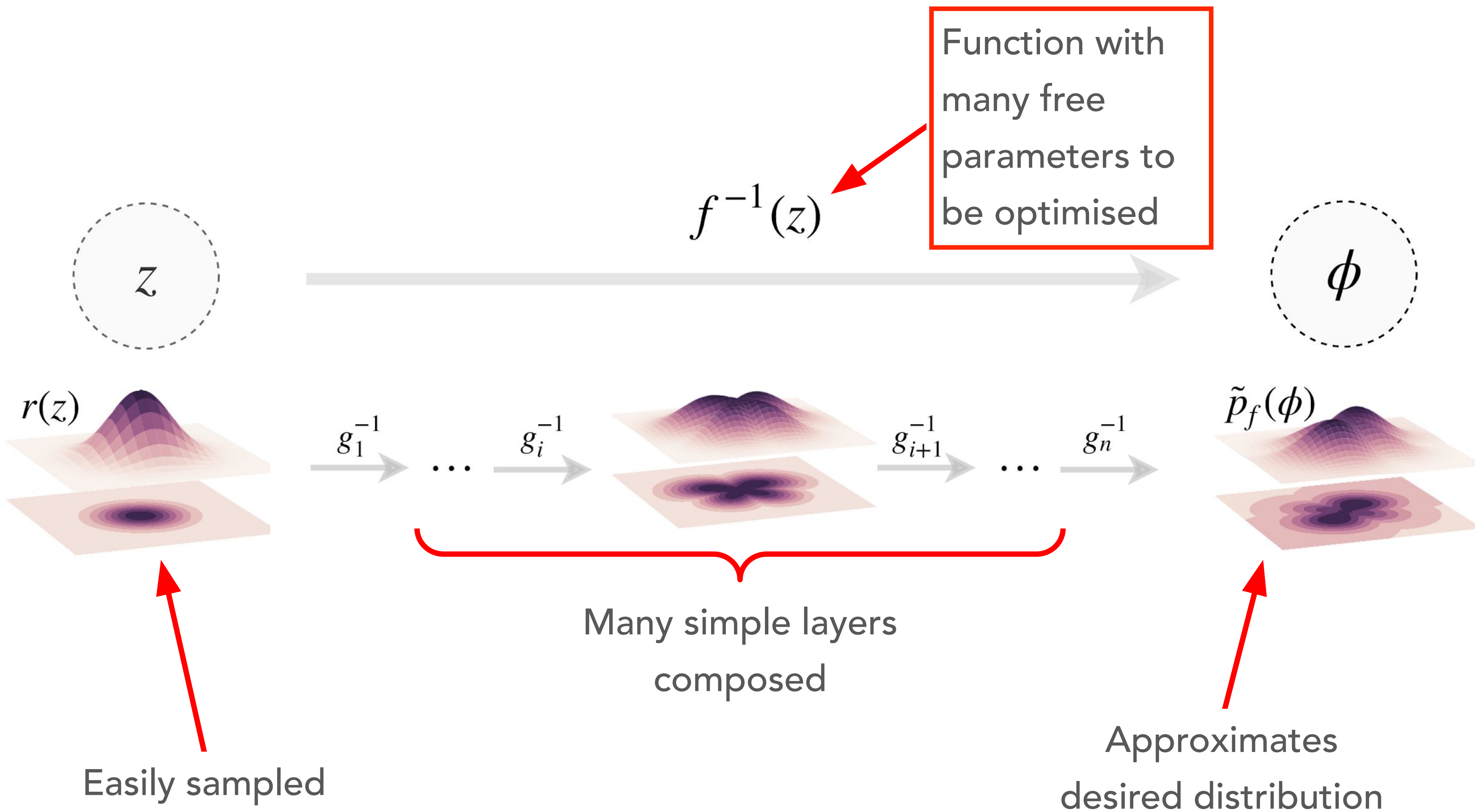
Symmetries, conservation laws, scaling relations, limiting behaviors, locality, causality, unitarity, gauge invariance, entropy, least action, factorization, unit tests, exactness, systematic uncertainties, reproducibility, verifiability, …

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

Generative flow models

Flow-based models learn a change-of-variables that transforms a known distribution to the desired distribution [Rezende & Mohamed 1505.05770]

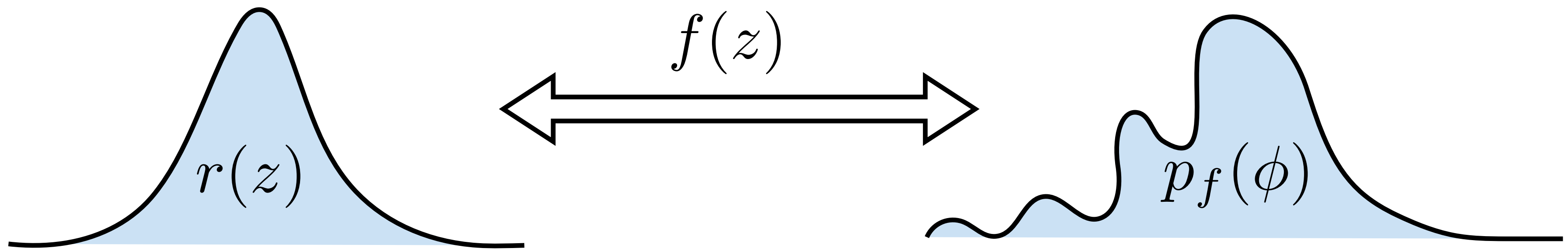
Can be made exact through accept/reject! [*Phys.Rev.D* 100 (2019), 034515]



Flow models for QCD

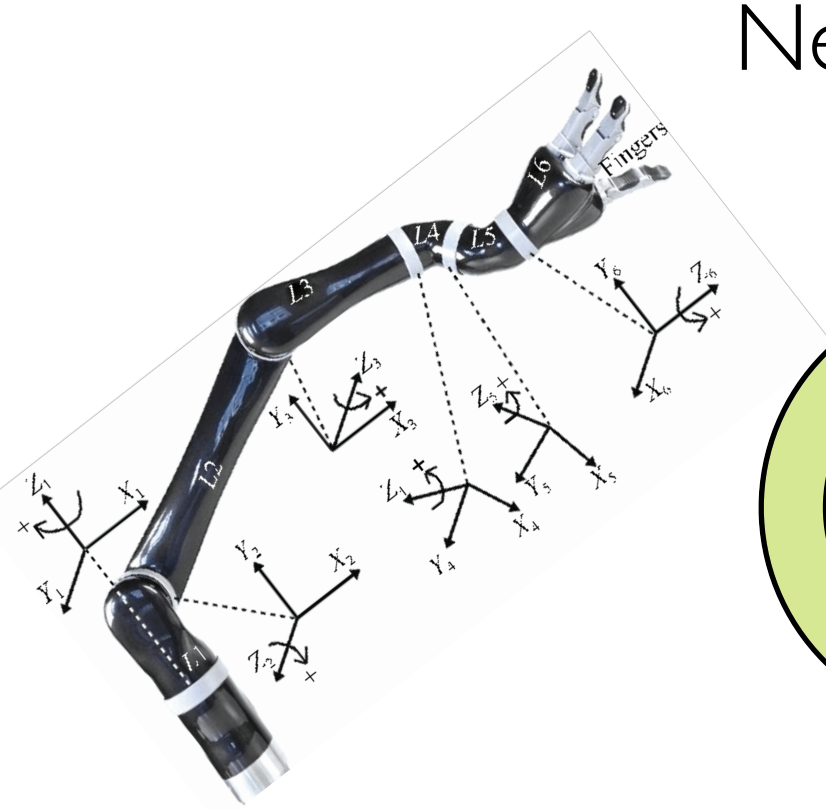
Flows on compact, connected manifolds

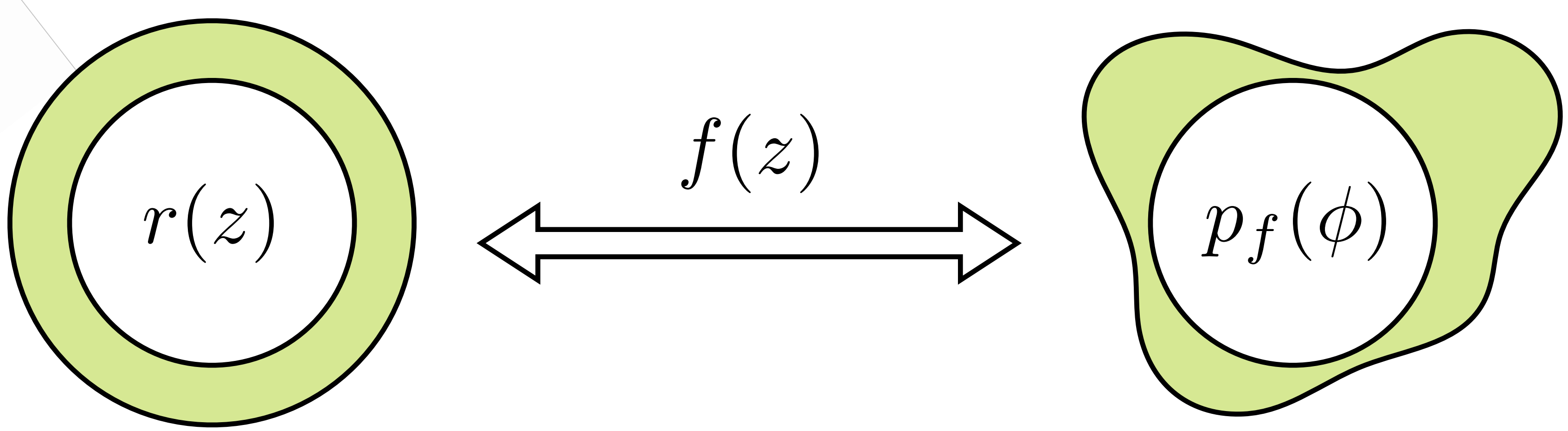
Previously: **Flows on real numbers**



Need: **Flows on compact, connected manifolds**

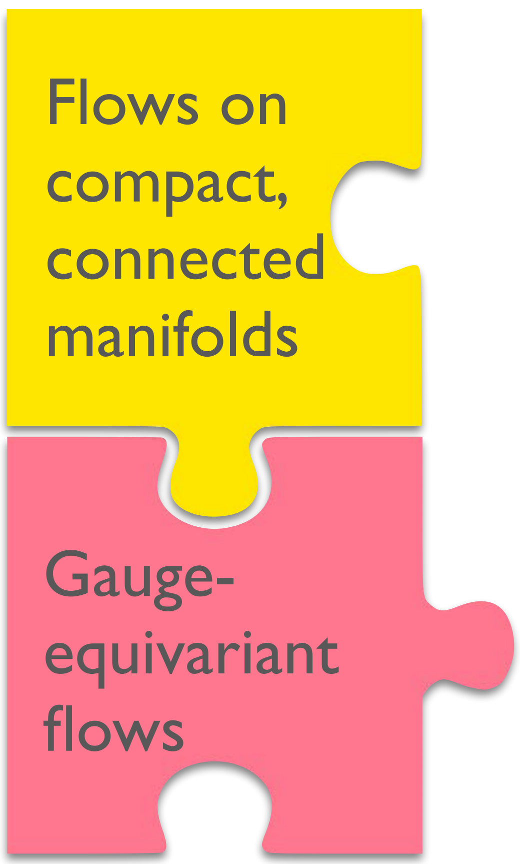
e.g., circles, tori, spheres





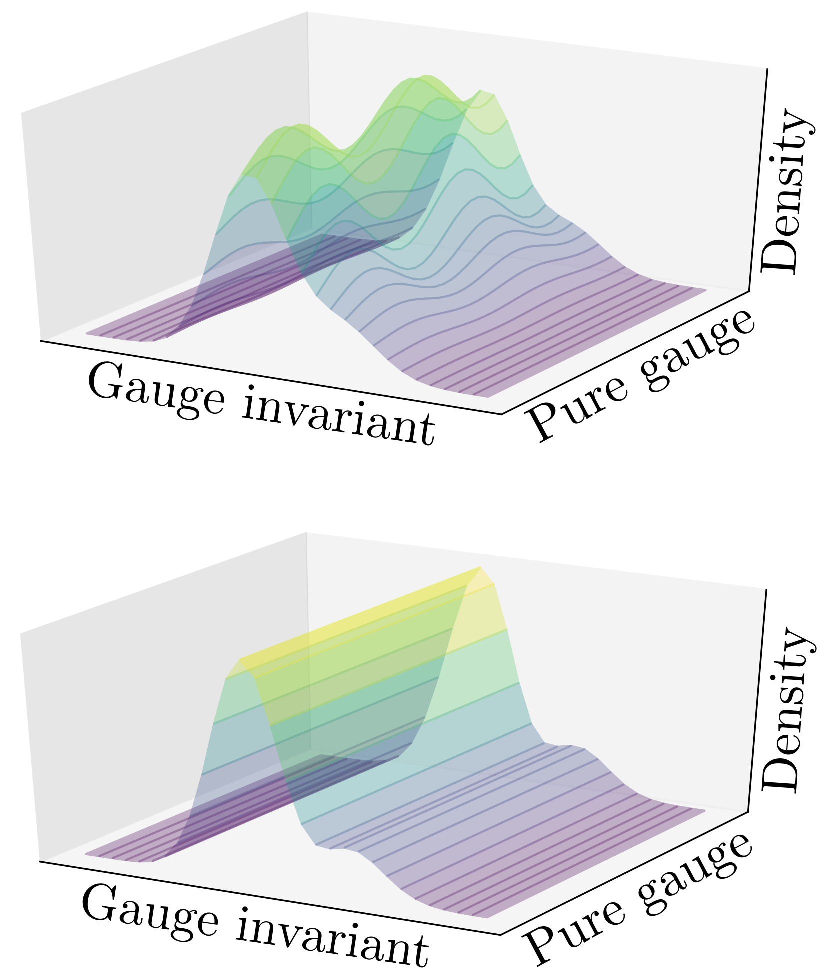
[PLMR 8083-8092 (2020)]

Flow models for QCD



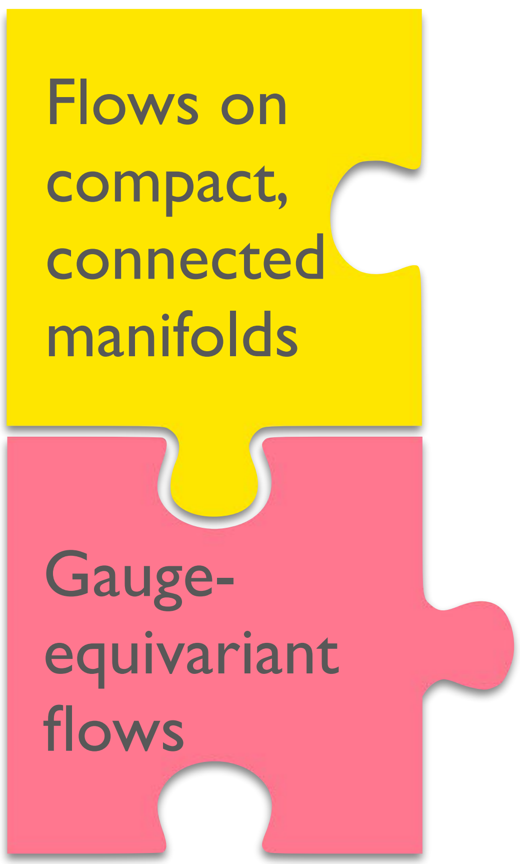
Incorporating symmetries

- Not essential for correctness of ML-generated ensembles
- BUT: Crucially important in training high-dimensional models
especially with high-dimensional symmetries



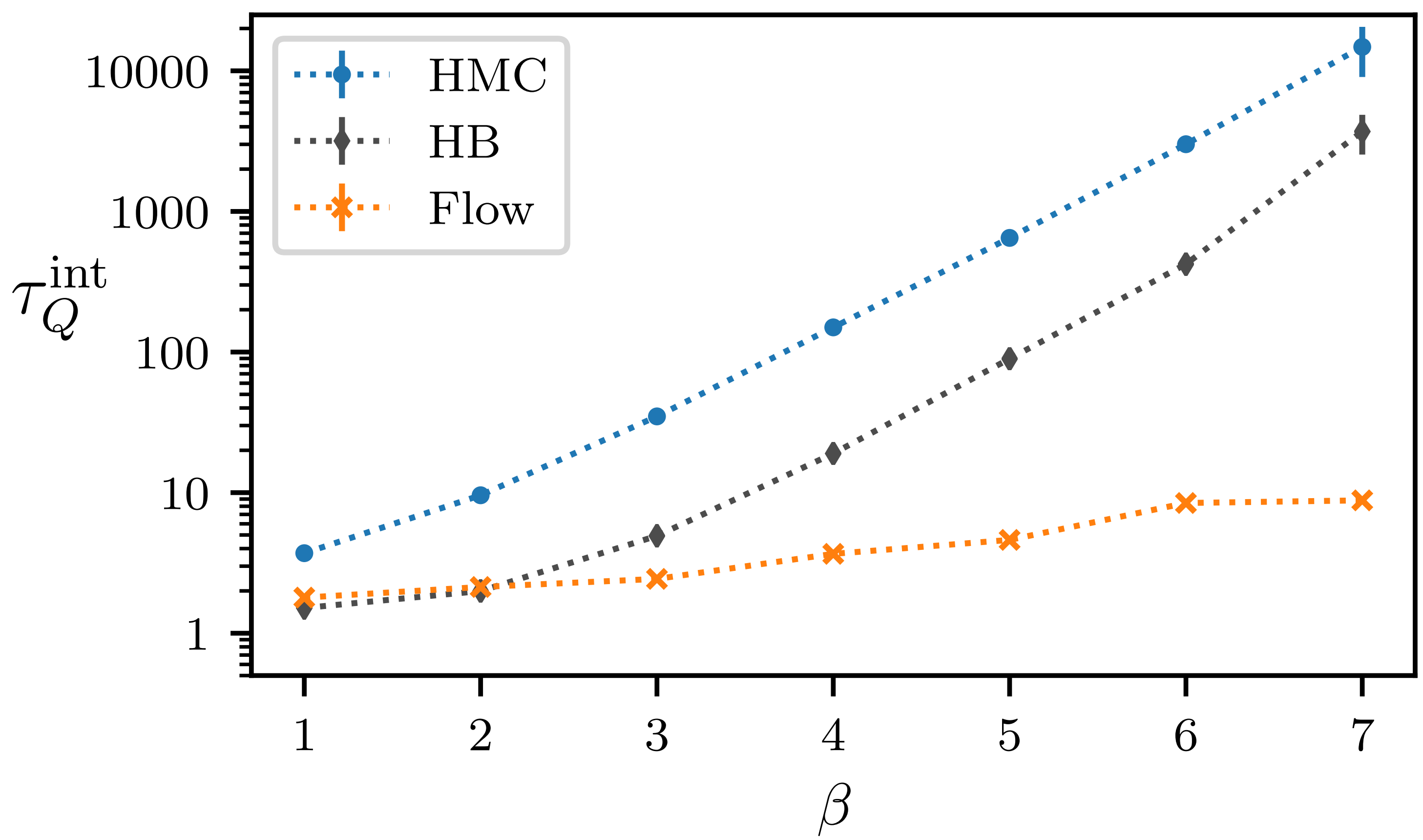
[Phys.Rev.Lett. 125, 121601 (2020), Phys.Rev.D 103, 074504 (2021)]

Flow models for QCD



First gauge theory application:
2D U(1) field theory

Cost per independent sample



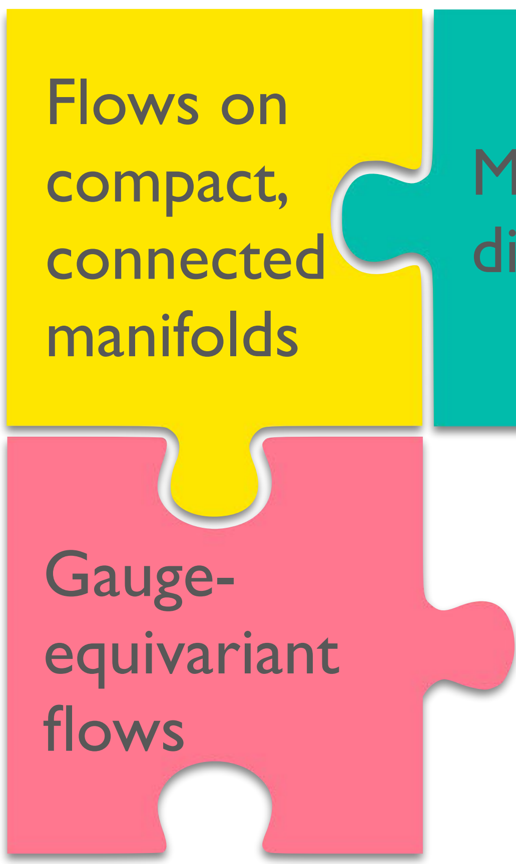
Conventional approaches

ML algorithm

Parameter of theory

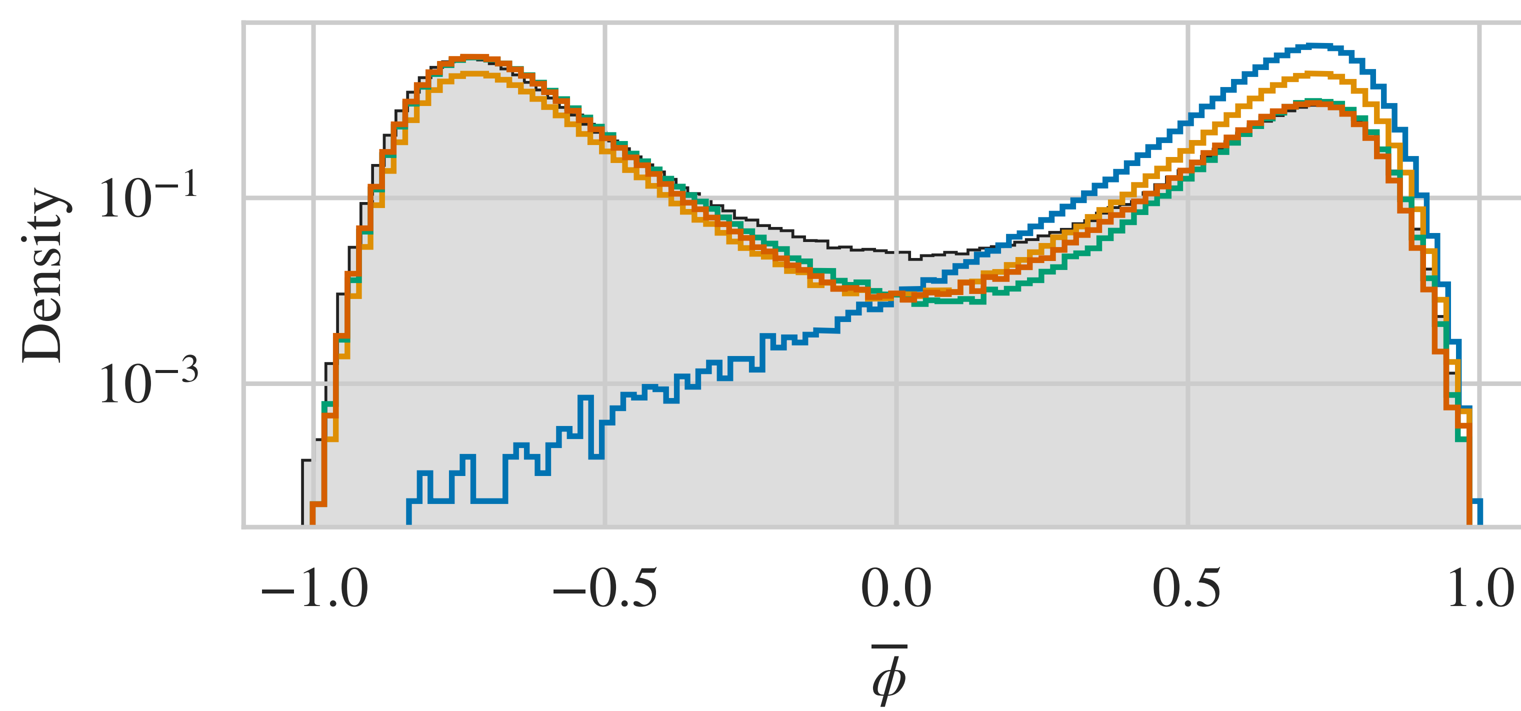
[*Phys.Rev.Lett.* 125, 121601 (2020)]

Flow models for QCD



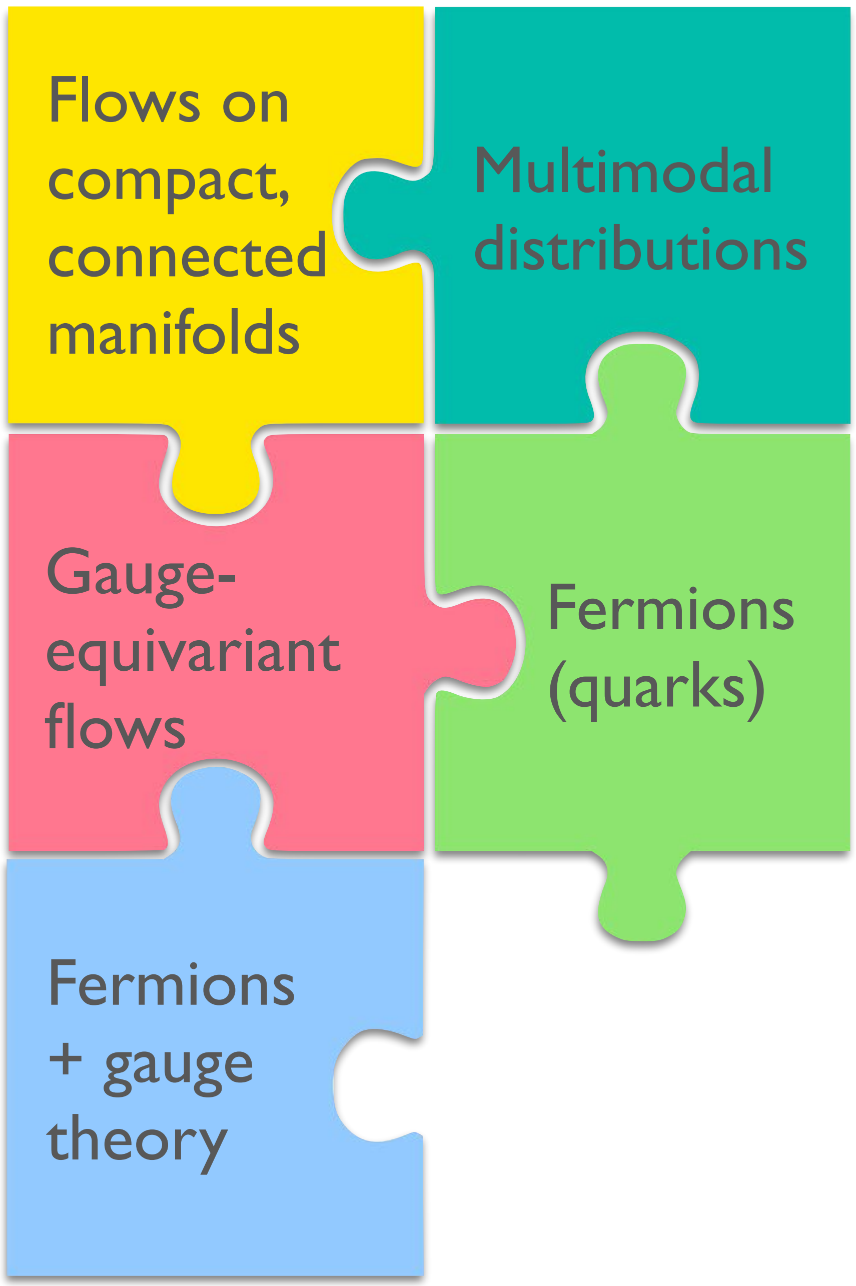
Systems with complex topologies

Need: **Unbiased sampling from multi-modal distributions**



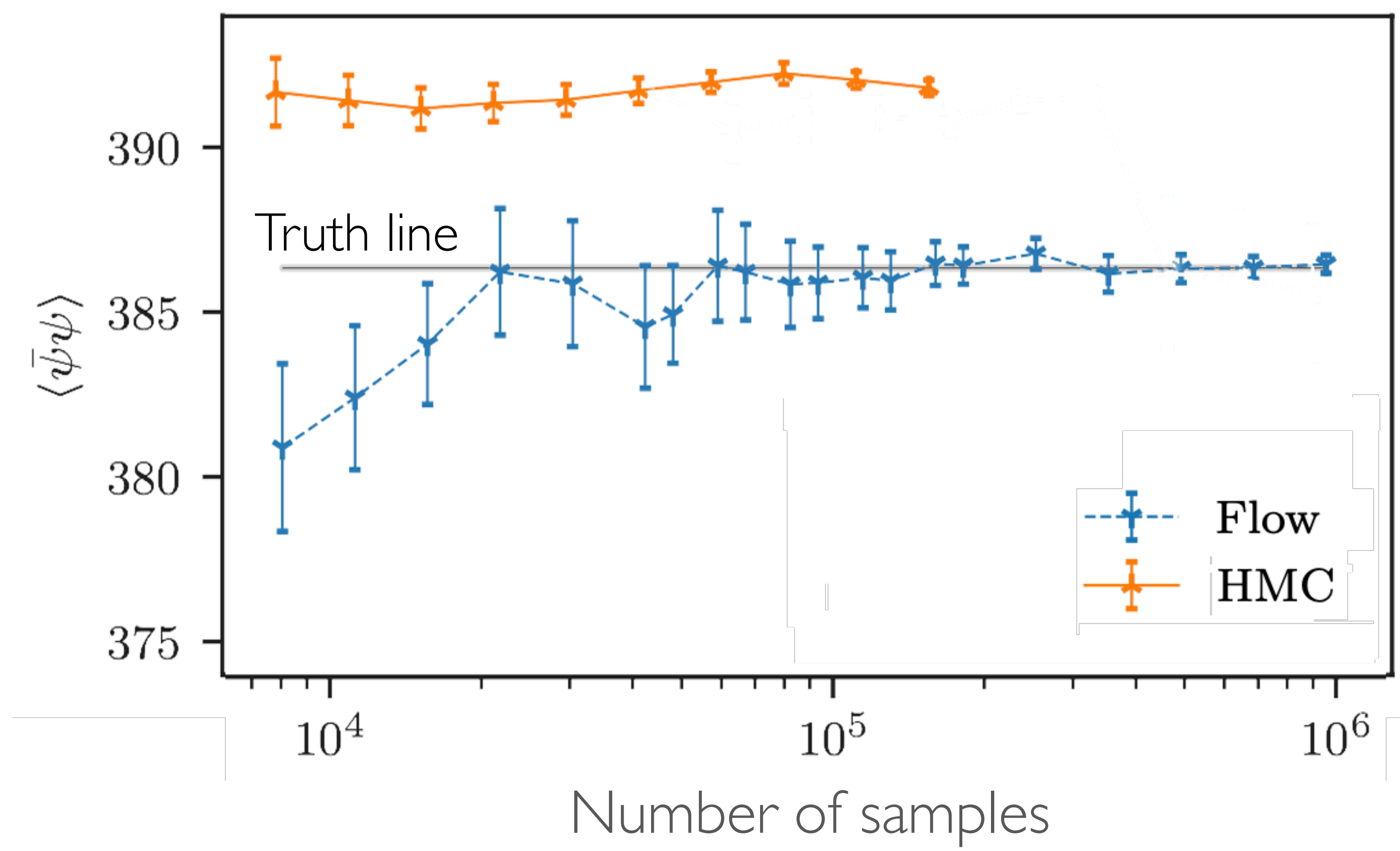
[2107.00734 (2021)]

Flow models for QCD



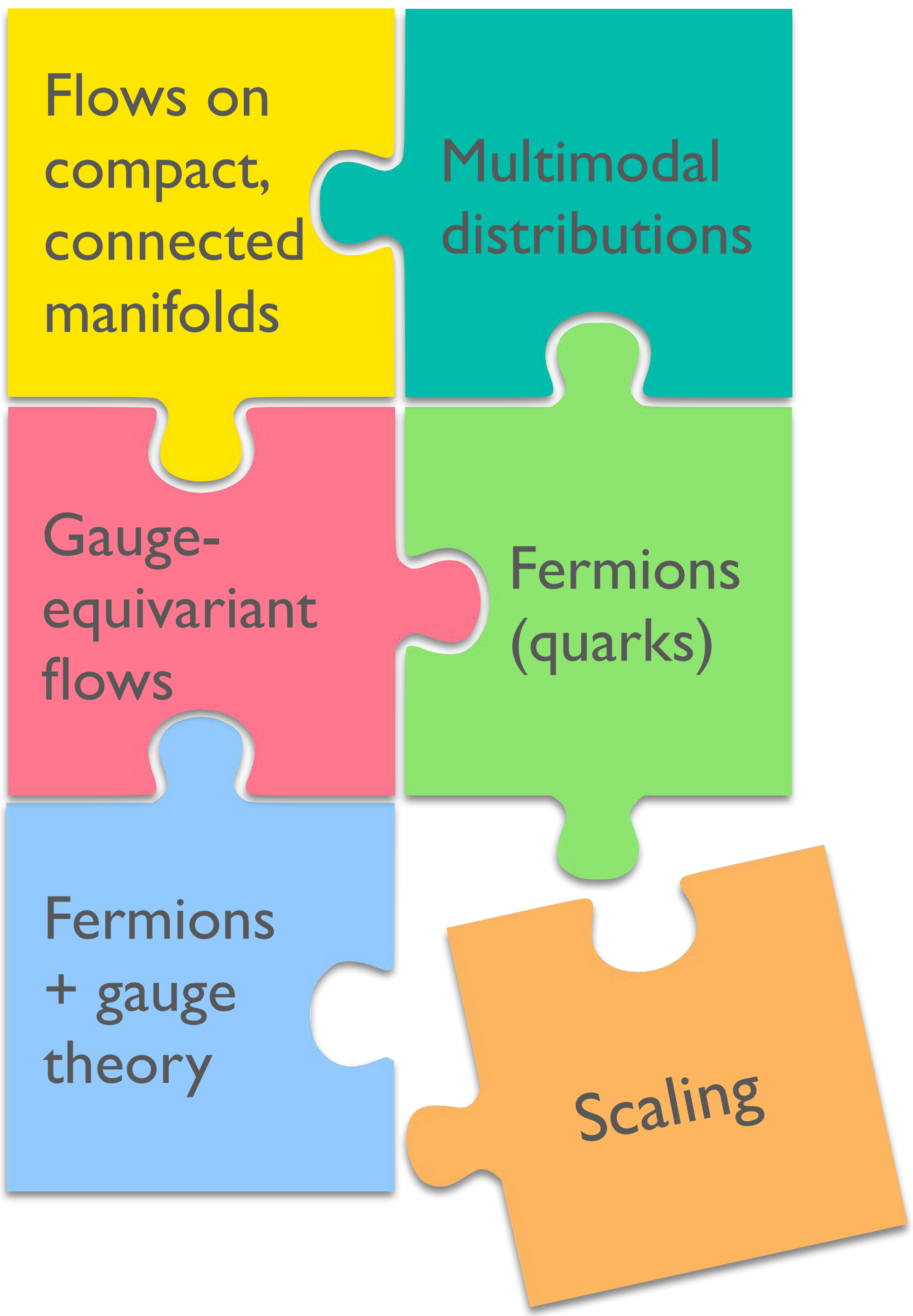
First gauge + fermion theory application:
2D Schwinger model

Measured value of observable

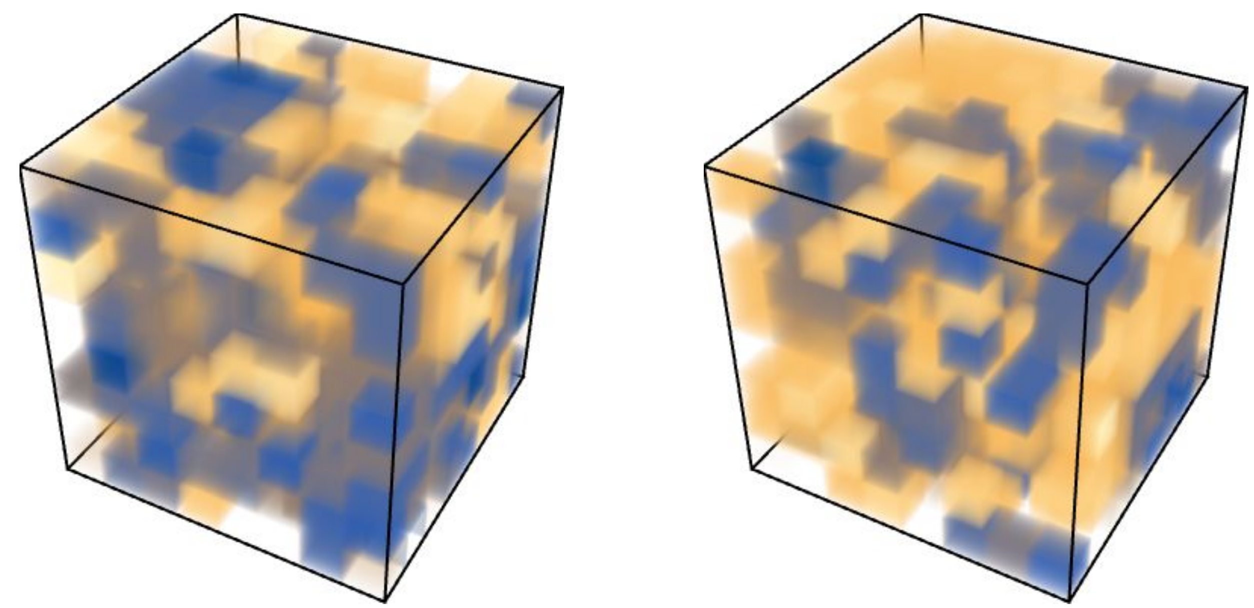


[*Phys.Rev.D* 104 (2021), 114507, arXiv:2202.11712 (2022)]

Flow models for QCD



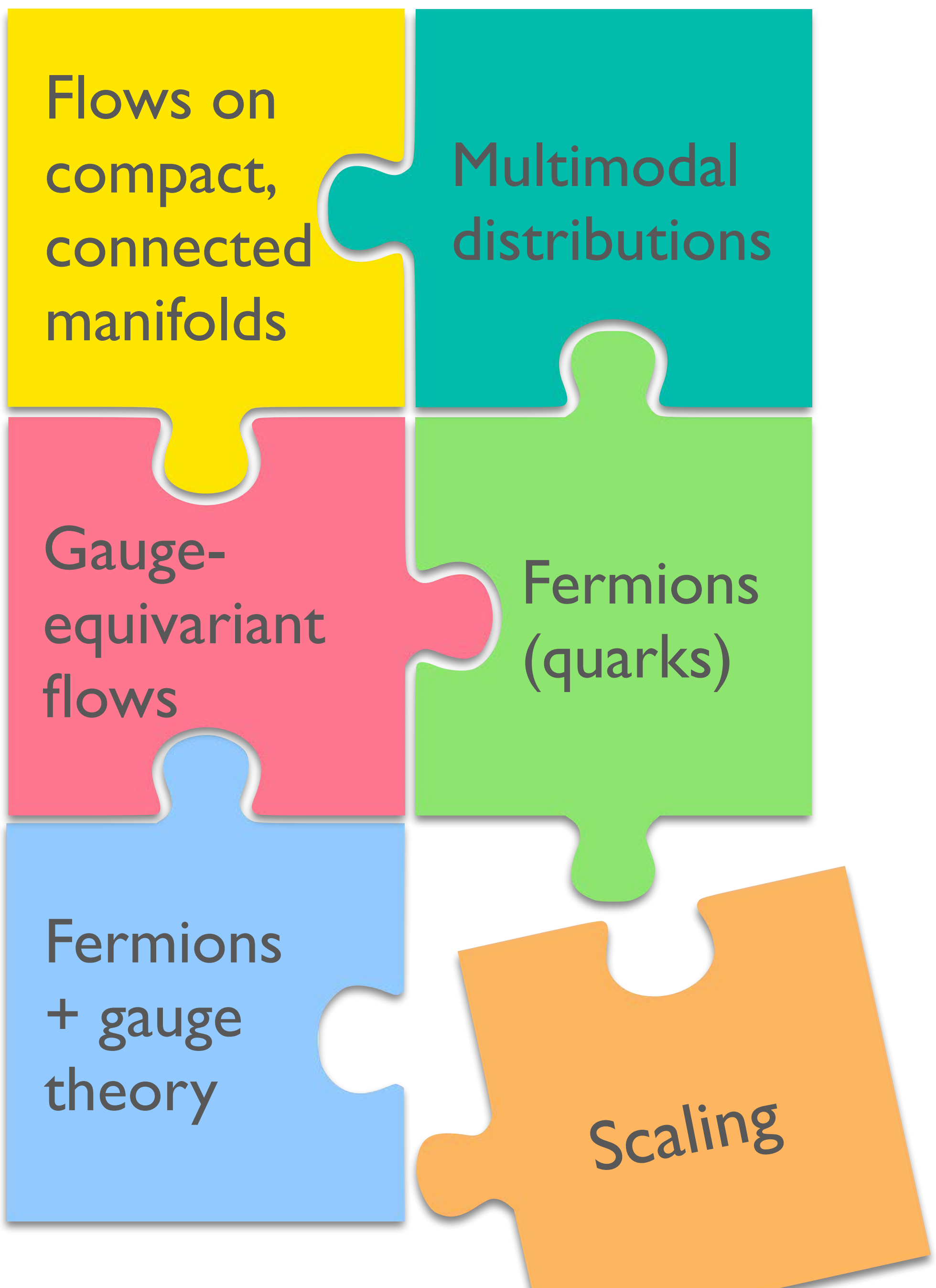
Scale to state-of-the-art volumes (4D)



Google DeepMind

AURORA | EARLY SCIENCE PROGRAM FOR DATA & LEARNIN

Flow models for QCD



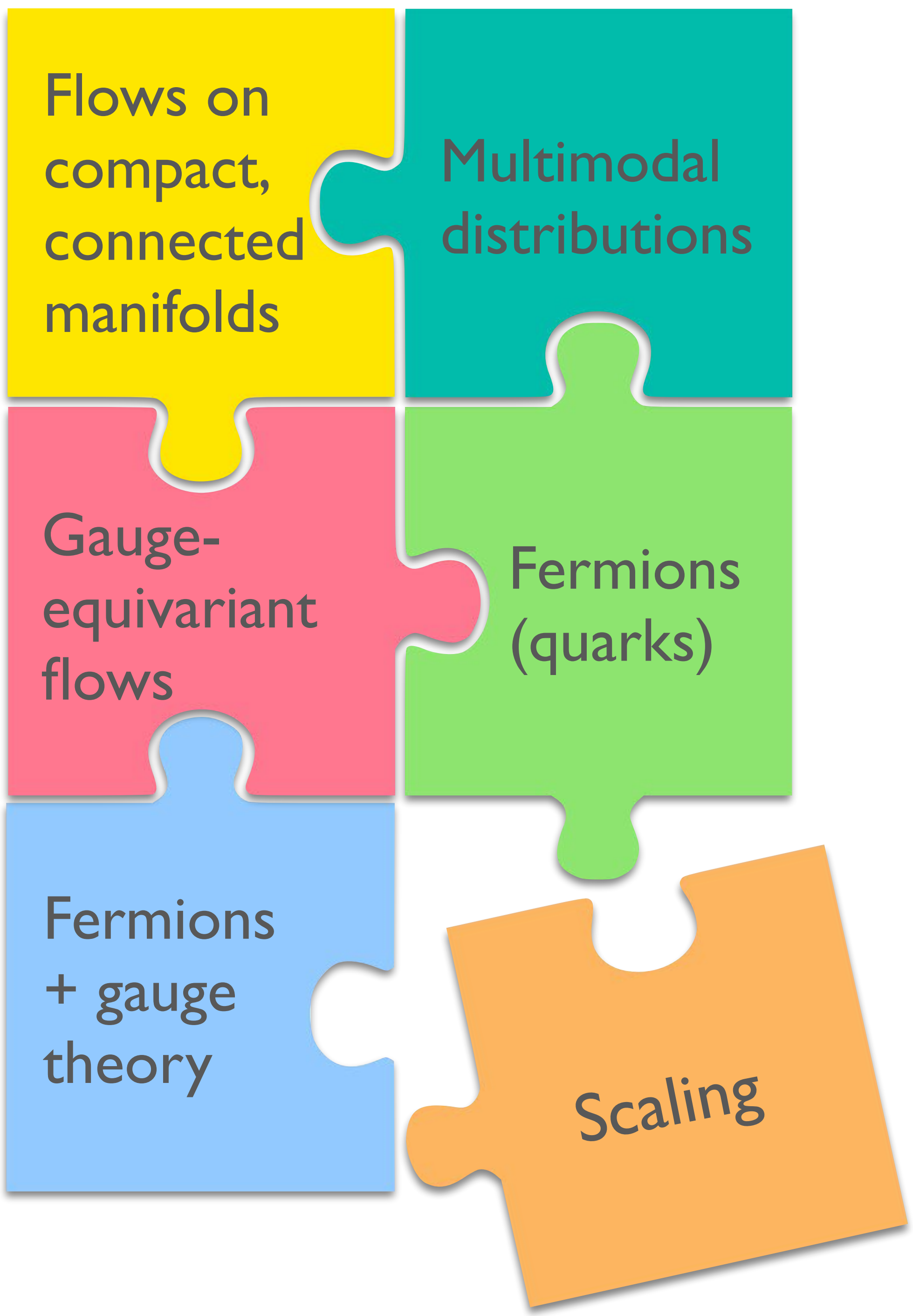
Machine learning for LQCD

- **Provably-exact** machine-learning-accelerated sampling algorithm
- Orders of magnitude more **efficient** than conventional algorithms overcoming critical slowing-down
- **Unbiased** results where traditional approaches fail

Deployment for state-of-the-art QCD scheduled for Aurora 2023 first science time

[2107.00734; 2101.08176, *Phys.Rev.D* 104, 114507; *Phys.Rev.D* 103, 074504 (2021); *Phys.Rev.Lett.* 125, 121601; PMLR 8083-8092 (2020); *Phys.Rev.D* 100, 034515 (2019); *Phys.Rev.D* 97, 094506 (2018)]

Flow models for QCD



- **Costs of fine lattice spacings contribute to systematic limitations** for high-precision QCD predictions of proton structure, e.g.,
  - first-principles PDFs, TMDs
  - muon g-2
- **Finer spacings needed for first controlled calculations of nuclei**
  - theory input for intensity-frontier experiments, e.g., dark matter direct detection, DUNE
  - nuclear reactions incl. big bang nucleosynthesis pathway

Machine learning for first-principles theory

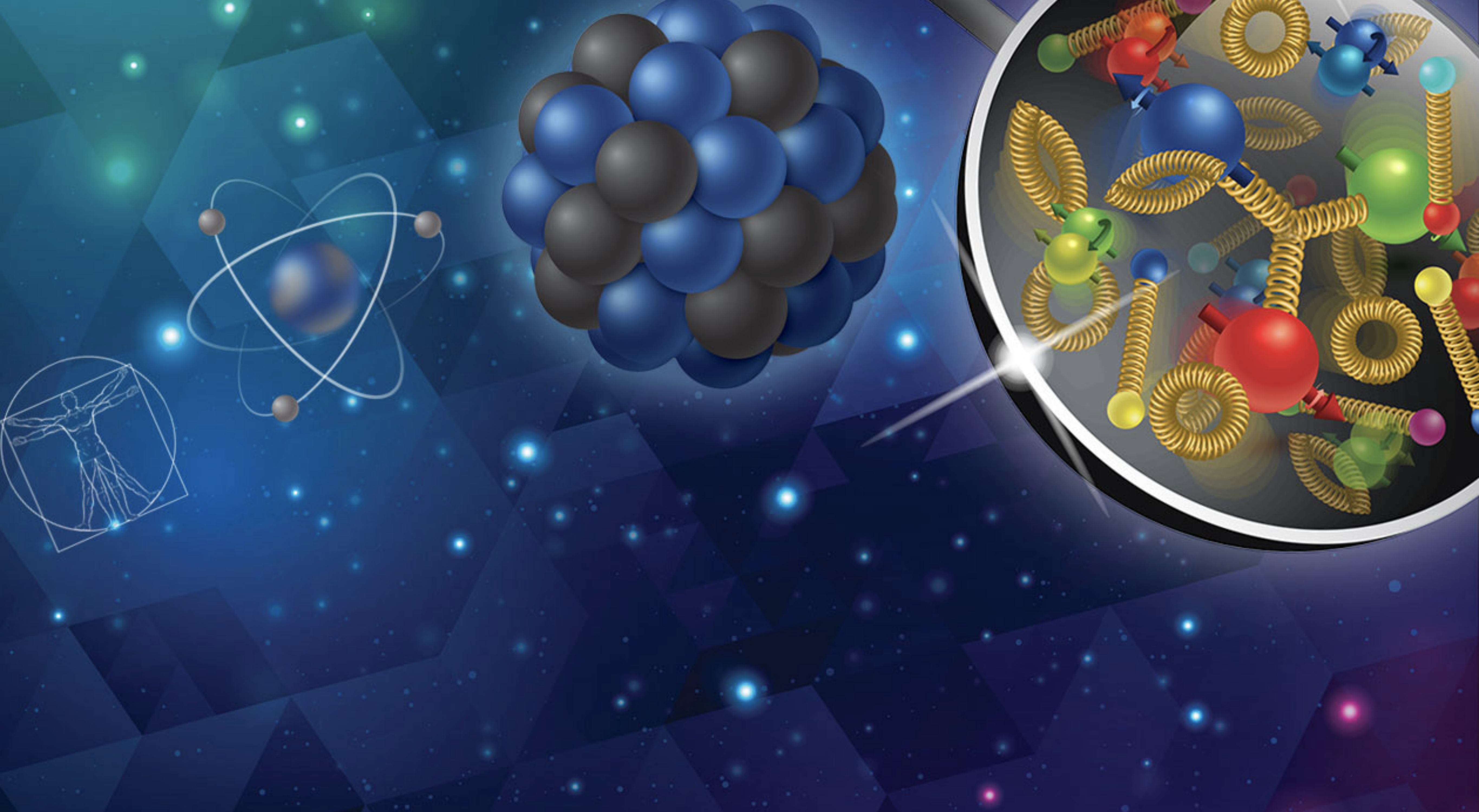
```
Compute exact results from known theory
Use AI/ML to do it faster
```

e.g., calculations of the Standard Model, BSM model, EFT, …

Require **mathematical guarantees of exactness** to preserve rigour of first-principles calculations

Potentially high-impact applications in development across theory areas, often require significant investment

- Developing new ML approaches from the ground up
- Engineering: scaling up to state-of-the-art HPC facilities



C²QA
Co-design Center for
Quantum Advantage

Massachusetts
Institute of
Technology

NSF

USQCD

NERSC

AURORA | EARLY SCIENCE PROGRAM FOR DATA & LEARNING

TACC

OLCF
OAK RIDGE LEADERSHIP COMPUTING FACILITY