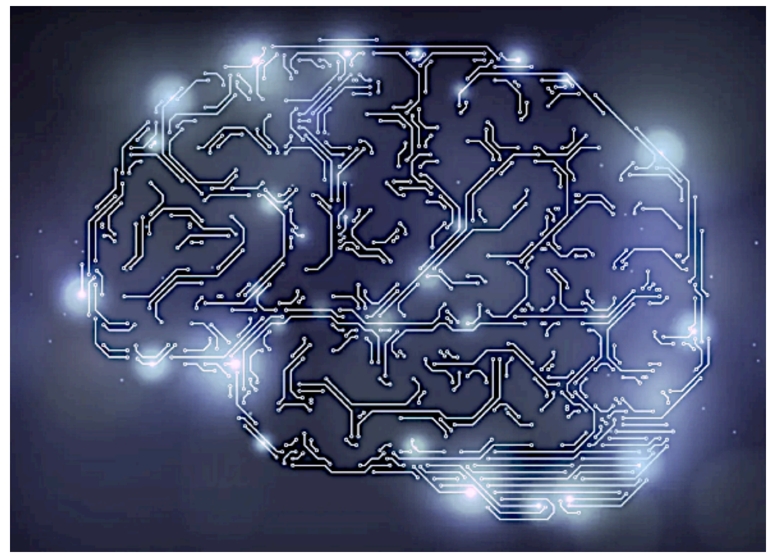
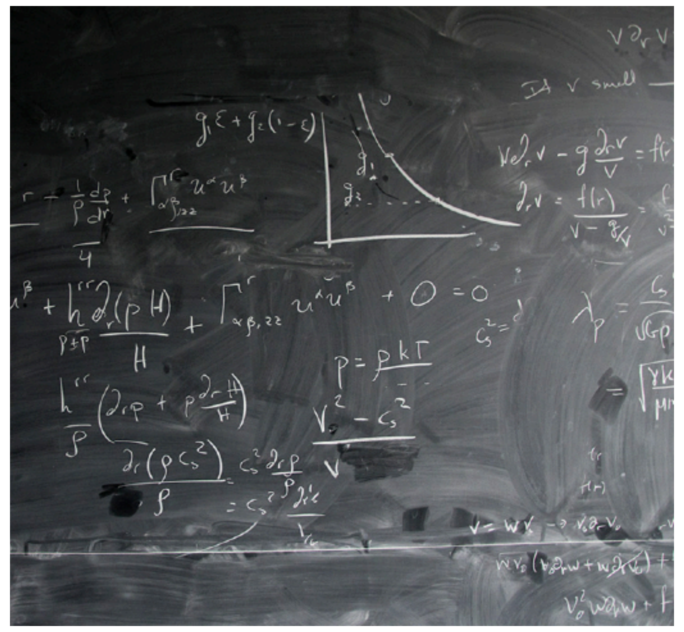
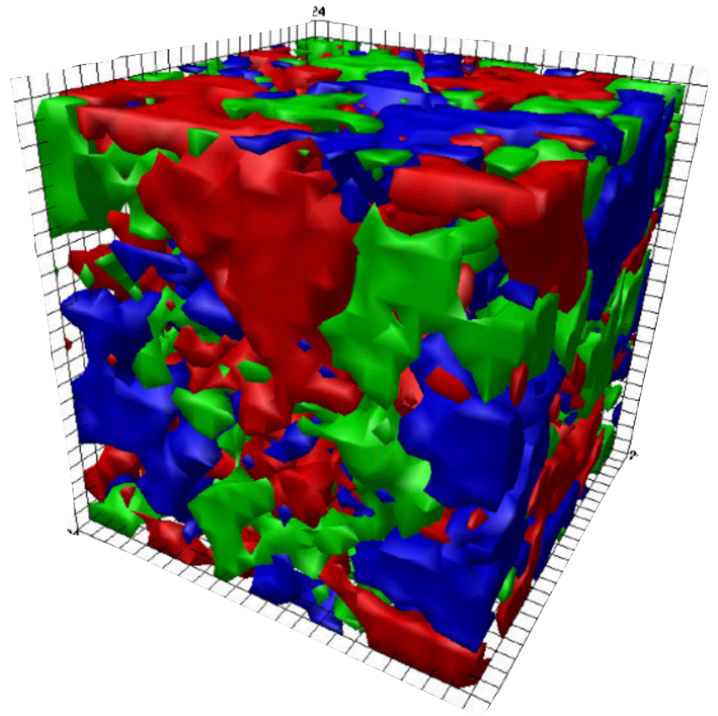
AI for HEP theory



{  ,  , ... }

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Chancellor’s Fellow in AI & Datascience
University of Edinburgh

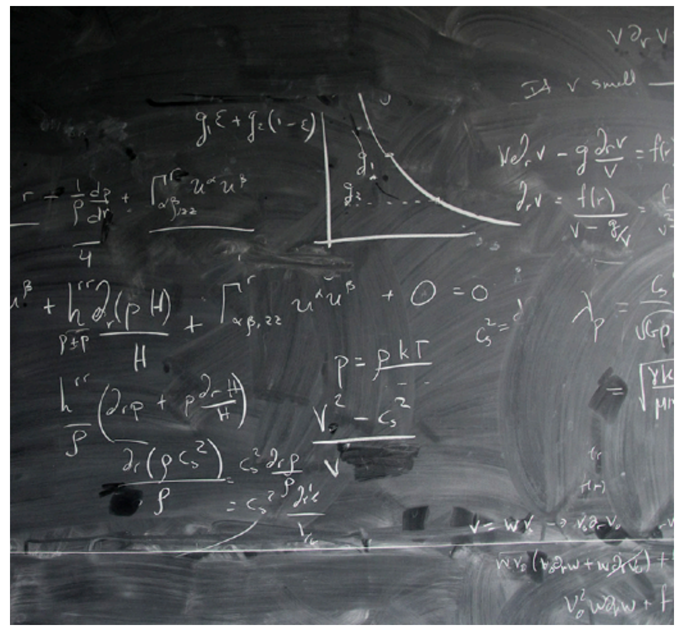
Sept 17th, 2025
Enabling AI in HEP

Survey of efforts

This is just a (hopefully representative) selection!

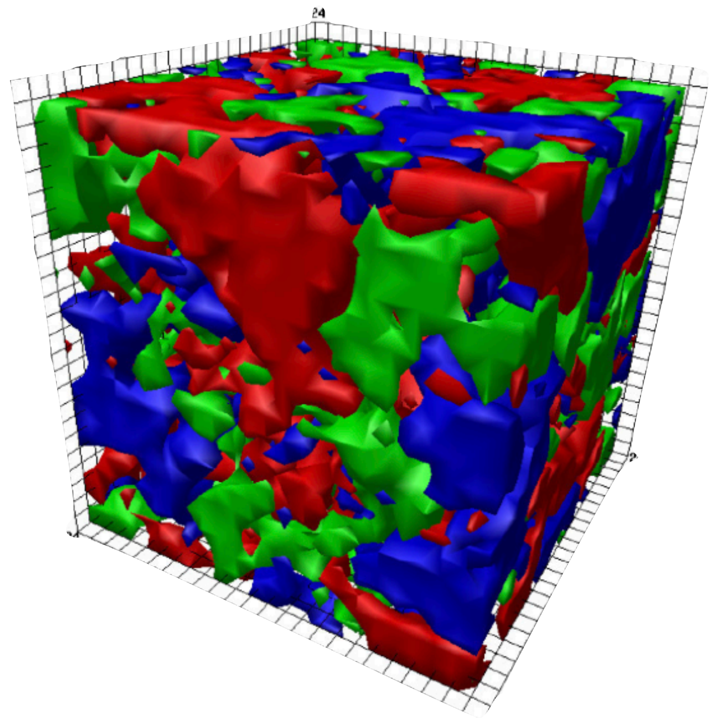
Perturbative calculations

- Loop and phase space integrals
- ML-assisted numerical integration



Lattice QCD

- Monte Carlo sampling
- NN fits (cf. NNPDF)
- “Perfect actions”

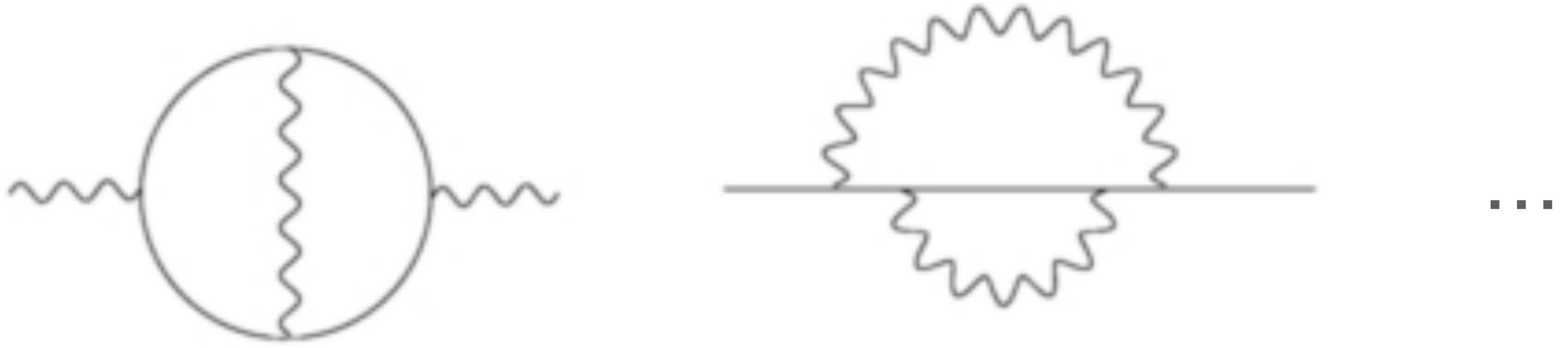


Speculative efforts

- Symbolic regression on Feynman integrals
- Field complexification for lattice sign problems

ML for loop integrals

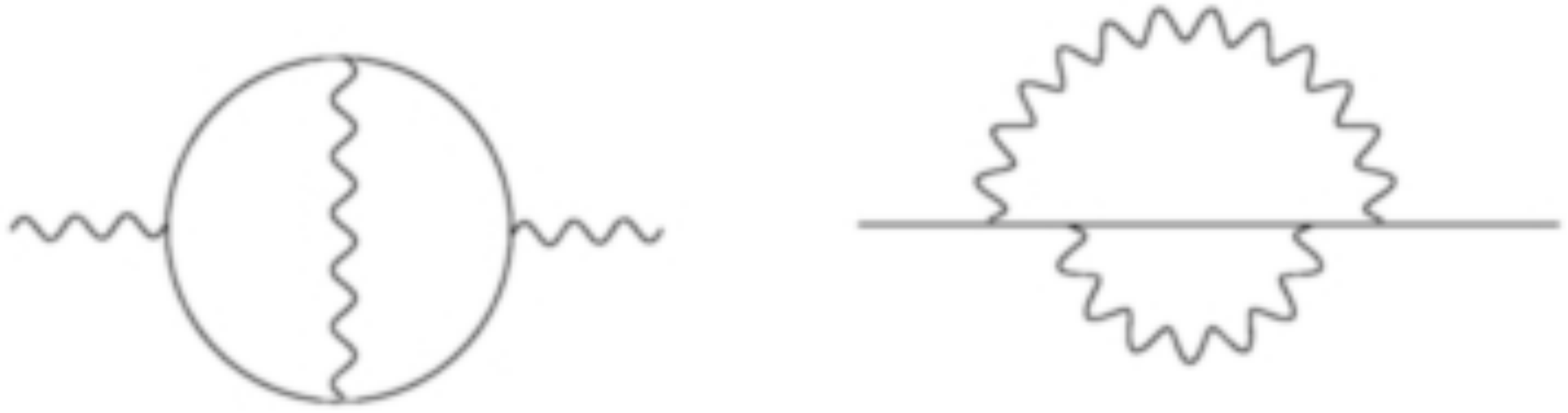
Numerical integration of multi-loop Feynman diagrams often useful



- Also needed for finite volume effects in lattice QCD calculations
- Standard approach via VEGAS, but struggles with certain integrand structures
- **ML approach based on normalizing flows**
- Related to phase space integrals for event generators

ML for loop integrals

Numerical integration of multi-loop Feynman diagrams often useful



- Also needed for finite volume effects in lattice QC
- Standard approach via VEGAS, but struggles with
- **ML approach based on normalizing flows**
- Related to phase space integrals for event generators

Efficient many-jet event generation with Flow Matching

E. Bothmann [a,c] T. Janßen [b,c] M. Knobbe [d] B. Schmitzer[b,e] and F. Sinz[b,e]

[a] *IT Department, CERN, 1211 Geneva 23, Switzerland*
[b] *Campus Institute Data Science, University of Göttingen, Germany*
[c] *Institute for Theoretical Physics, University of Göttingen, Germany*
[d] *Theoretical Physics Division, Fermi National Accelerator Laboratory, USA*
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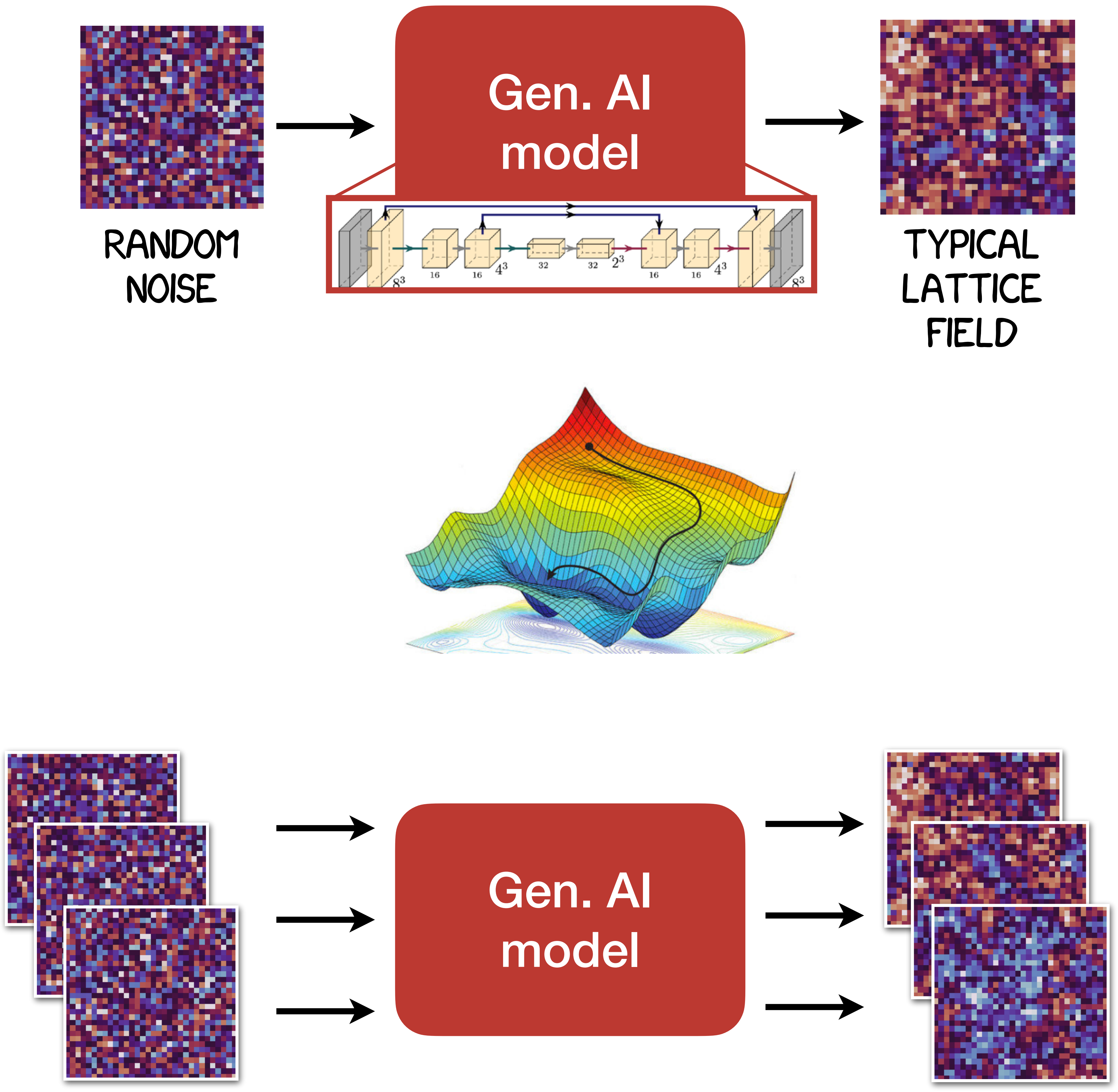
Gen. AI for Lattice QCD Monte Carlo



Parameterize transformation using neural networks

SPECIALIZED NNs FOR QCD

"Self-training" step

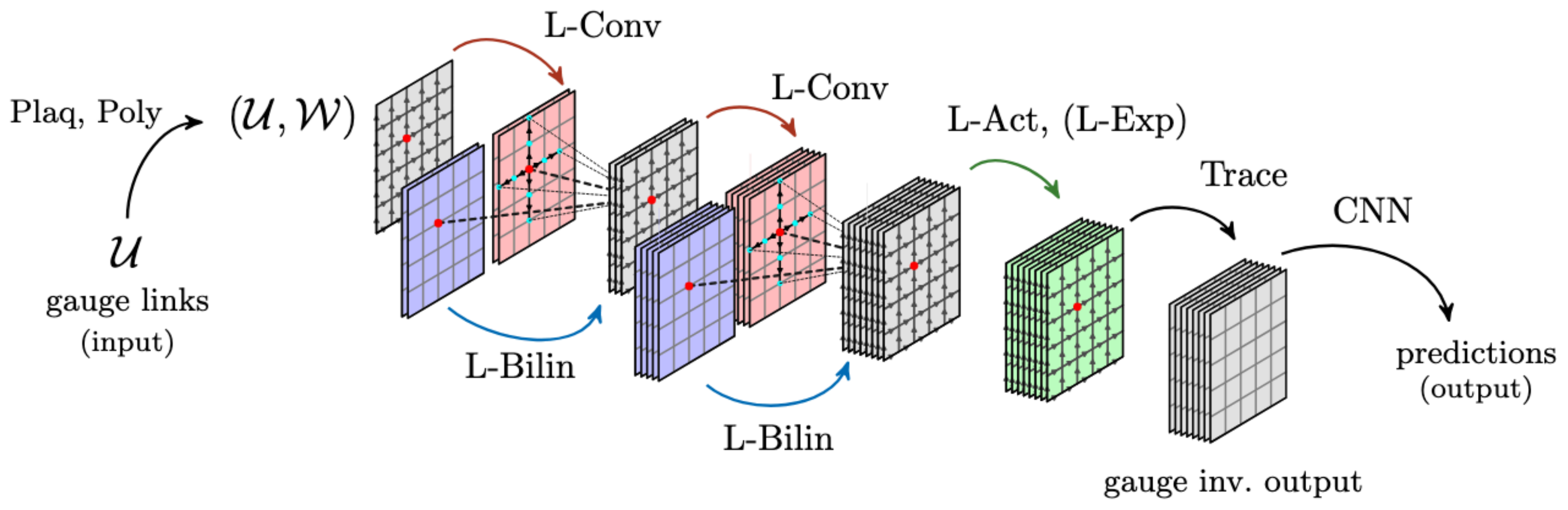
Save trained model

Draw samples and apply bias correction

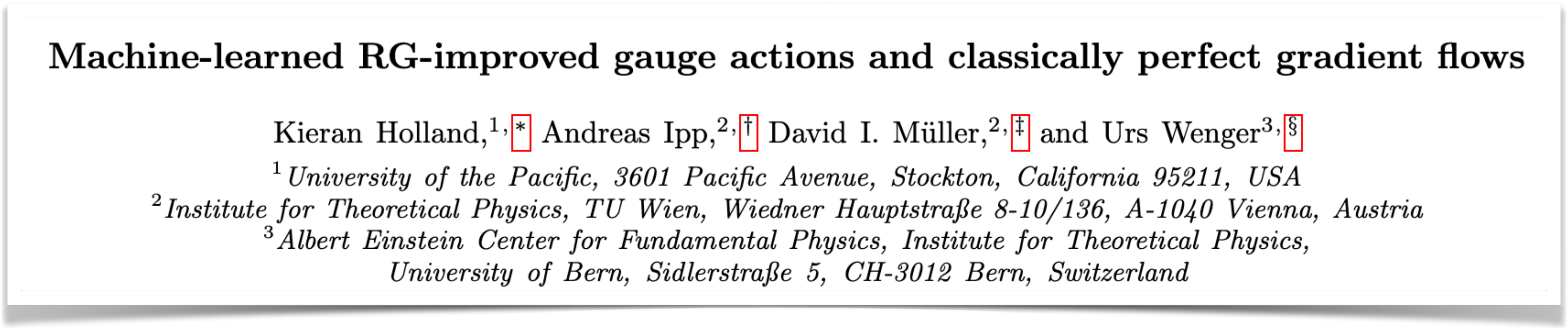
Lattice QCD perfect actions

Motivation: Minimize discretization artifacts, understand RG flow of QCD

- Specialized neural networks required (gauge symmetry) Favoni, et al. PRL128 (2022) 032003

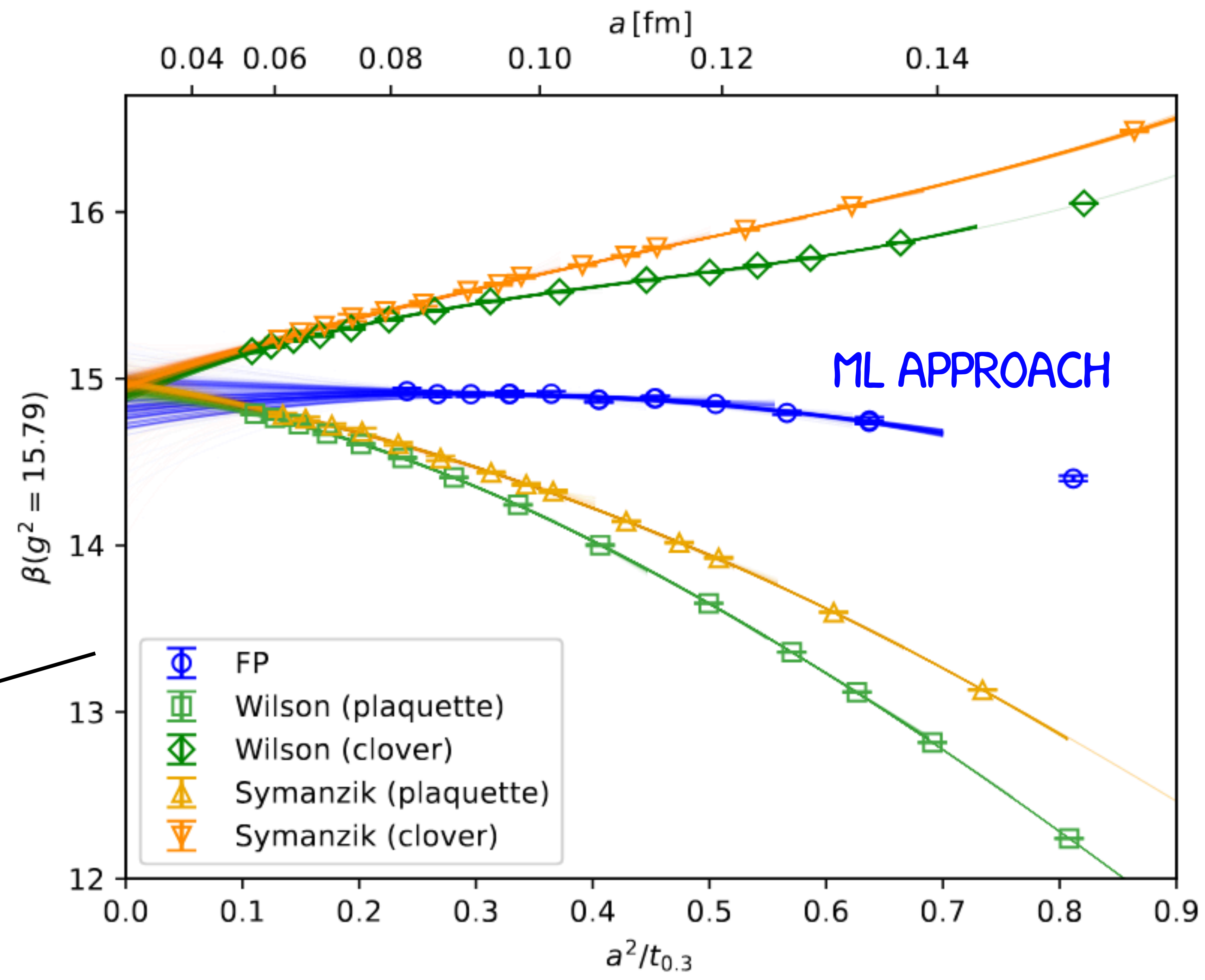


- Early learned actions look promising


Machine-learned RG-improved gauge actions and classically perfect gradient flows

Kieran Holland,[1,*] Andreas Ipp,[2,†] David I. Müller,[2,‡] and Urs Wenger[3,§]

[1] *University of the Pacific, 3601 Pacific Avenue, Stockton, California 95211, USA*
[2] *Institute for Theoretical Physics, TU Wien, Wiedner Hauptstraße 8-10/136, A-1040 Vienna, Austria*
[3] *Albert Einstein Center for Fundamental Physics, Institute for Theoretical Physics, University of Bern, Sidlerstraße 5, CH-3012 Bern, Switzerland*



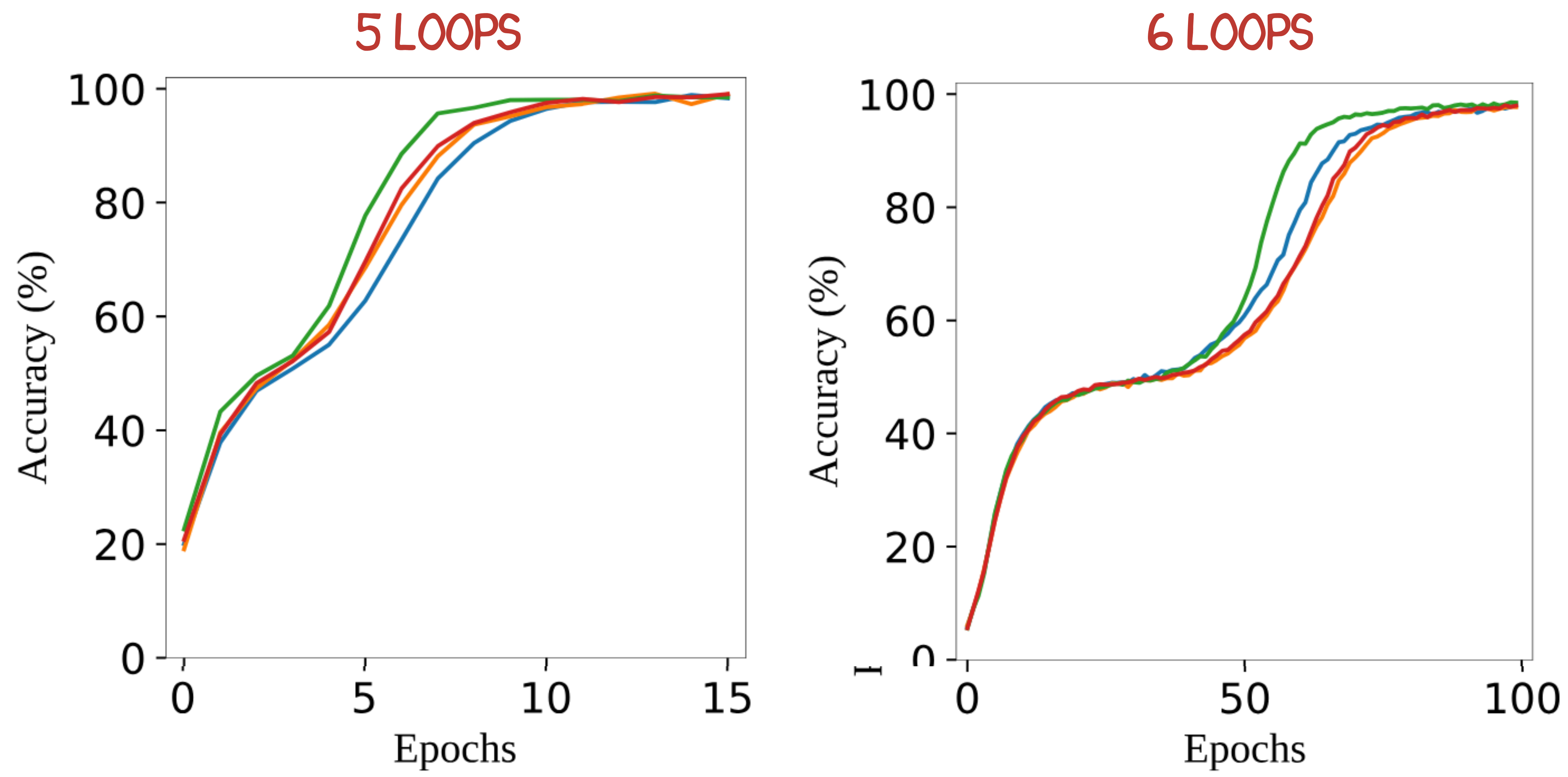
Symbolic regression for amplitudes?

HEP theory also looking at promising, but speculative possibilities

- Scattering amplitudes very constrained
- Full scope of constraints and structures unknown
- Can ML methods learn what humans have not (yet)?

Transforming the bootstrap: using transformers to compute scattering amplitudes in planar $\mathcal{N} = 4$ super Yang–Mills theory

Tianji Cai[1,5,*], Garrett W Merz[2,5,*], François Charton[3,5], Niklas Nolte[3], Matthias Wilhelm[4], Kyle Cranmer[2] and Lance J Dixon[1]



Needs: Exactness

Most applications demand control of systematic uncertainties

- Biases from models could lead to (uncontrolled) biases in outputs
- Numerical integration, Monte Carlo are fully controlled, **exact unbiasing is possible:**

For each U_i drawn from the model, we know $\underbrace{q(U_i)}_{\text{Our ML models provide this.}}$ and $\underbrace{p(U_i)}_{\text{Known in terms of the target integrand.}}$

Exact bias correction possible

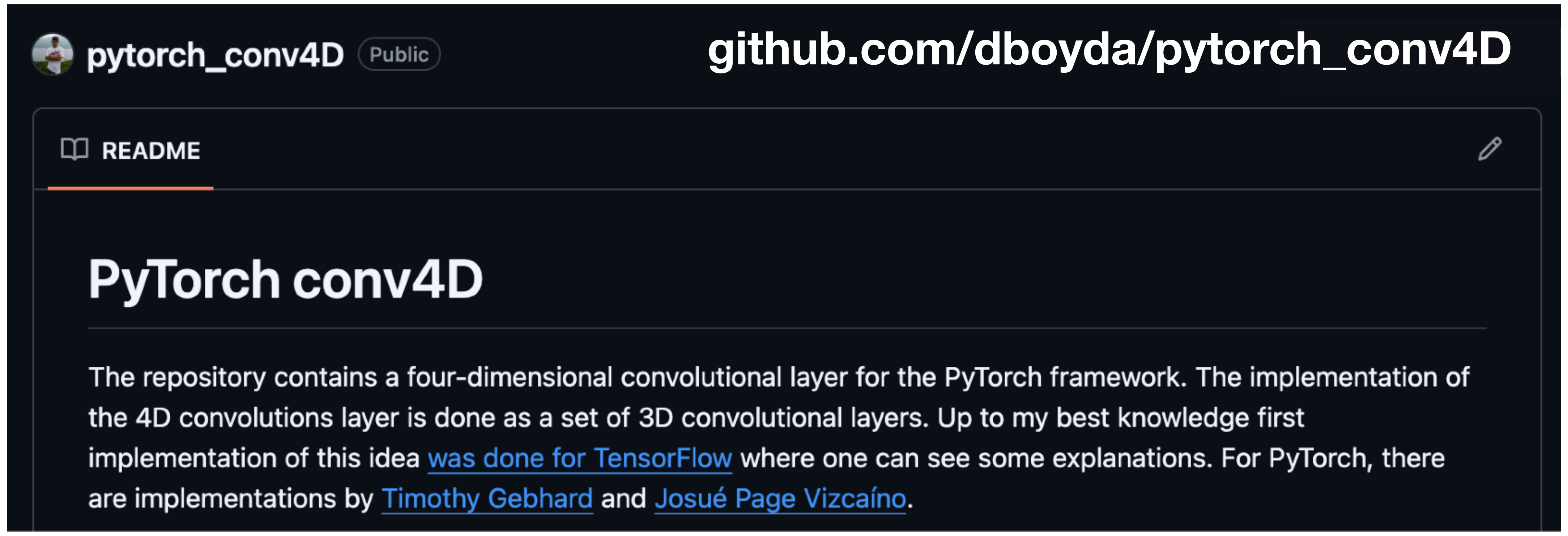
$$\langle \mathcal{O} \rangle_p = \frac{\langle \mathcal{O}(U)\, p(U)/q(U) \rangle_q}{\langle p(U)/q(U) \rangle_q}$$

- Other cases may need **bias correction strategies** from the broader ML field

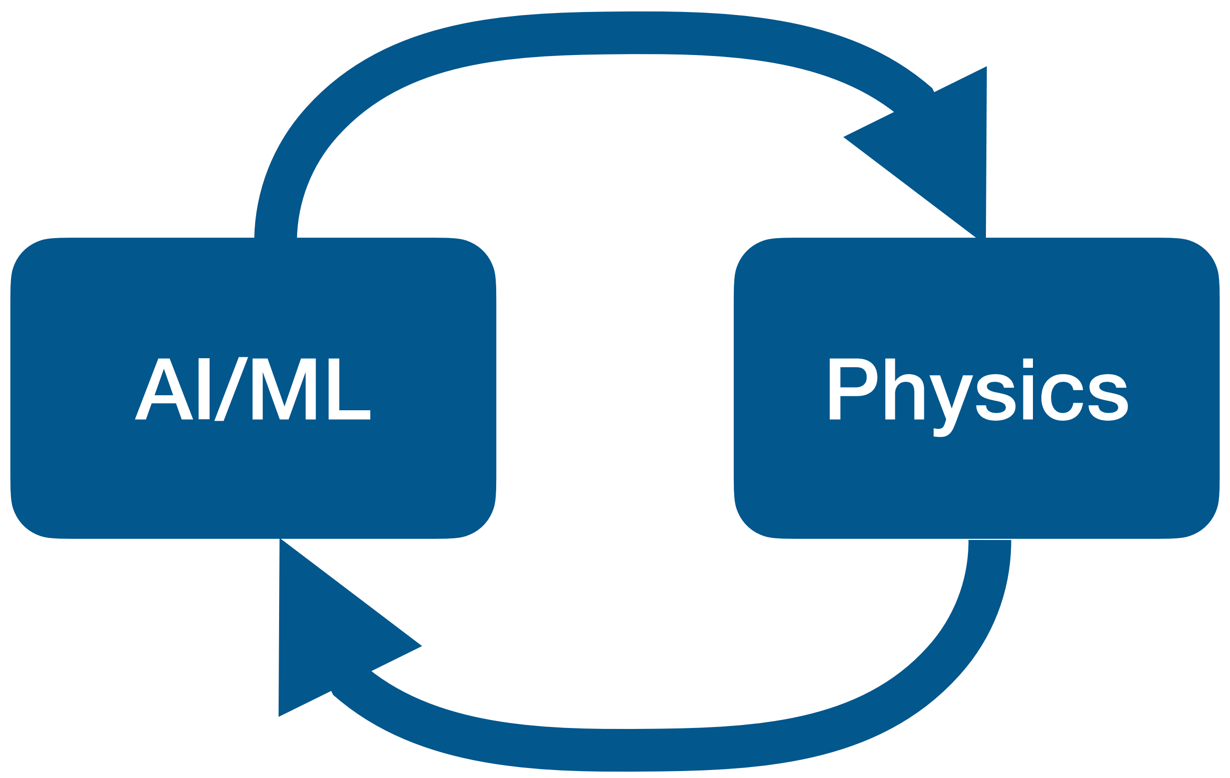
Needs: Computational methods / HW

- **Execution on GPUs**
  - Simple applications: $O(500)$ GPU-hours training
  - ML for LQCD targeting > 100k GPU-hours
  - FP64 important!
  - Memory intensive (computational graphs)

- **Model** and **data parallelism**
  - Pytorch FSDP
  - Custom code for 4D, distributed (LQCD)



Needs: Knowledge and skills



Going beyond users to **AI/ML researchers**

- Specialized neural networks being developed
- Contributing back to ML community (papers in ML conferences, journals)

HEP theory PhDs, postdocs, and PIs need to learn ML research practices

- **Intersectional specialization** is hard
- **Rapid progress in ML** makes it difficult to stay up-to-date
- Unique challenges of ML research: organizing and interpreting **many experiments**, sensitivity to **arbitrary choices**, significant **programming efforts**