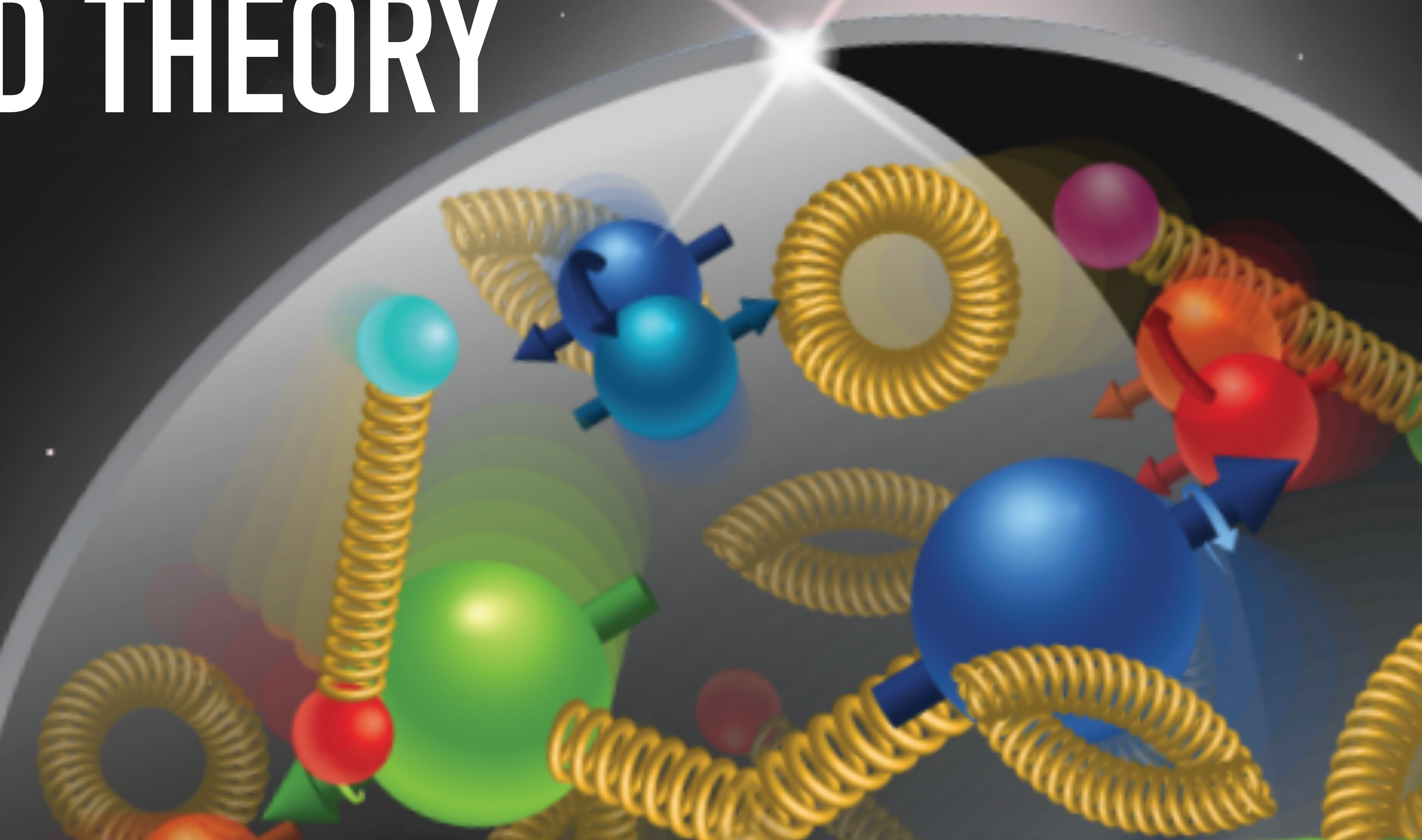
PHIALA SHANAHAN

MACHINE LEARNING AND ARTIFICIAL INTELLIGENCE FOR QCD THEORY



NSF | AI
Massachusetts Institute of Technology

AI/ML in the context of QCD theory

Machine learning is a class of tools for optimising the parameters of complex models

- **Given data:** describe/model/approximate data, identify correlations/features, …
- **Without data:** approximate known or unknown functions, reinforcement-based optimisation…

Applications of AI/ML target almost **all facets of QCD theory**

1. Data analysis
   i.e., global fits, classification, interpretation, …
2. First-principles theory
   i.e., Lattice QCD, perturbative QCD, EFT, nuclear many-body, …

AI/ML in the context of QCD theory

Applications of AI/ML target almost **all facets of QCD theory**

- No time for a review (or even summary) of the state-of-the-art: examples only. See many focused workshops on this issue

INT Program 22-1

Machine Learning for Nuclear Theory

March 28 - April 22, 2022

Workshop: Theory for EIC in the next decade

20–22 Sep 2022
MIT, Maclaurin Buildings, Building 4
US/Eastern timezone

Computational Nuclear Physics and AI/ML Workshop

6-7 September, 2022 / SURA headquarters

arXiv:2112.02309v2 [nucl-th] 2 May 2022

Machine Learning in Nuclear Physics

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The NSF AI Institute for Artificial Intelligence and Fundamental Interactions

et al.

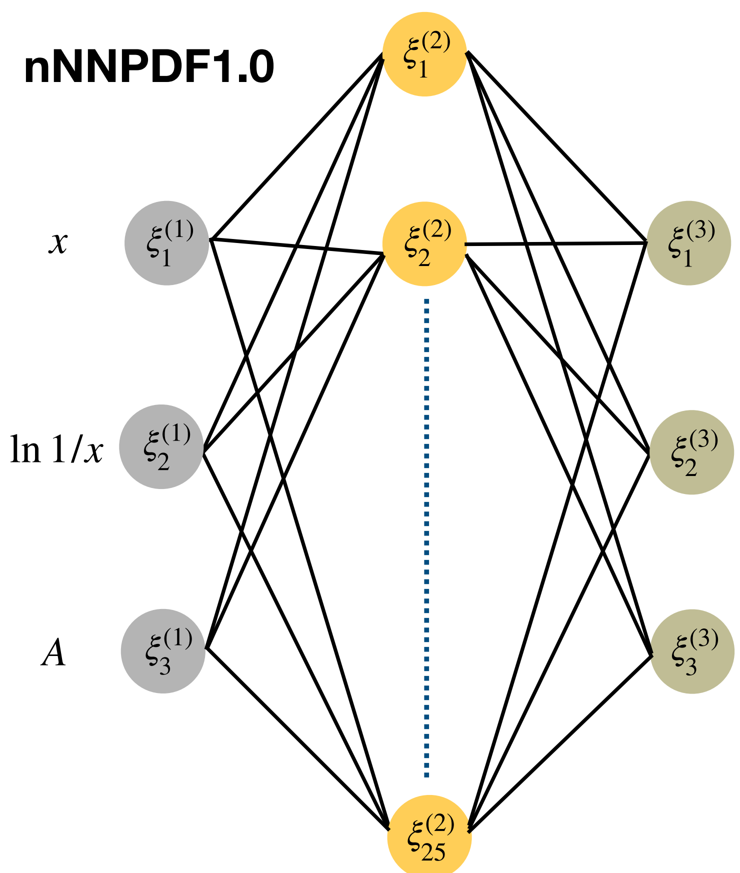
1. AI/ML for data analysis (theory)

Data analysis example #1:

Global fits to parton distribution functions

Global fits

- Neural network parameterisations of nucleon and nuclear PDFs
- ML approach allows efficient exploration of a large class of functional parameterisations
- EIC will significantly reduce uncertainties in nuclear PDFs at low x



$$g(x, Q_0, A) = B_g x^{-\alpha_g}(1-x)^{\beta_g}\,\xi_1^{(3)}$$

$$\Sigma(x, Q_0, A) = x^{-\alpha_\Sigma}(1-x)^{\beta_\Sigma}\,\xi_2^{(3)}$$

$$T_8(x, Q_0, A) = x^{-\alpha_{T_8}}(1-x)^{\beta_{T_8}}\,\xi_3^{(3)}$$

N3PDF Machine Learning • PDFs • QCD

NNPDF

[Eur.Phys.J.C 82 (2022), 2109.02653; Eur. Phys. J. C 79 (2019), 1904.00018]

1.

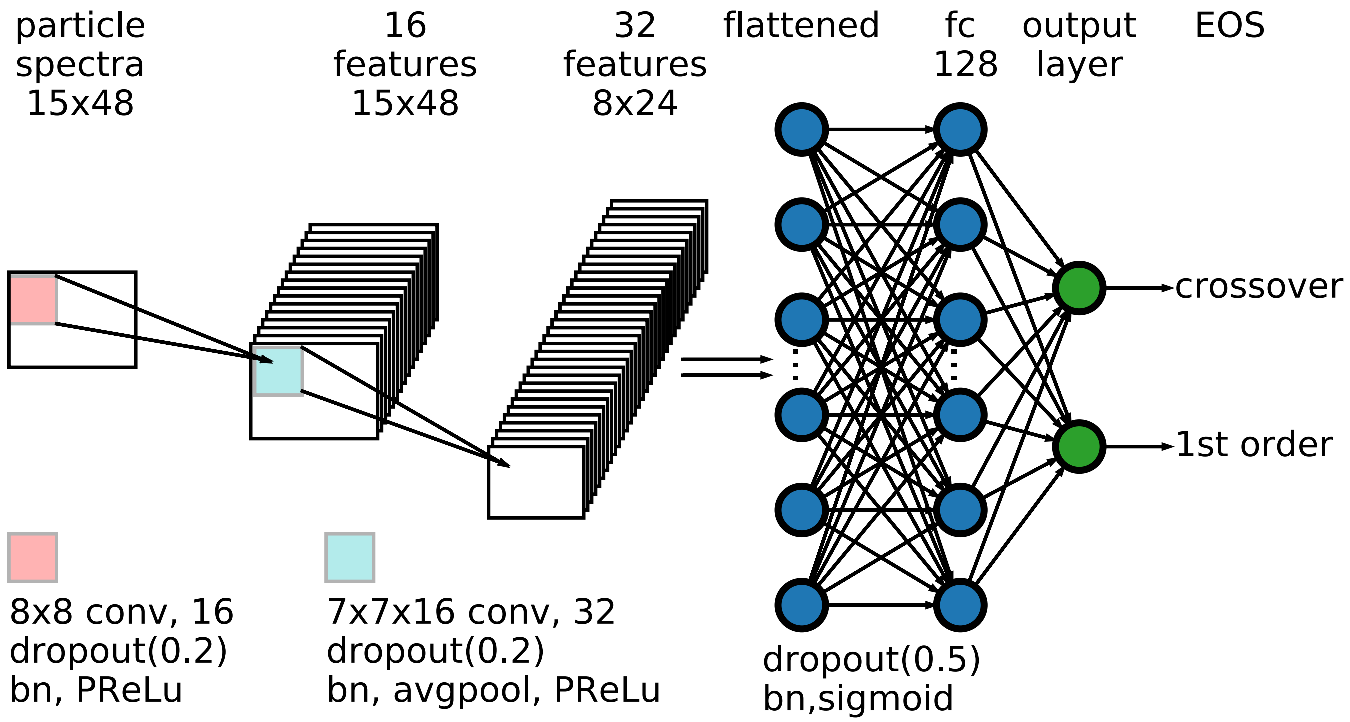
AI/ML for data analysis (theory)

Data analysis example #2:

Detect nature of QCD transition in heavy-ion collisions

Classification

- Neural network trained to identify nature of equation-of-state from heavy-ion collision data
- Successful proof-of-principle using hydrodynamics simulation data
- Based on identifying complex correlations in input data



In: Final-state particle distributions in longitudinal momentum (rapidity), transverse momentum and azimuthal angle

Out: Identification of class of equation-of-state

[Nature Commun. 9 (2018) 1, 210, 1612.04262]

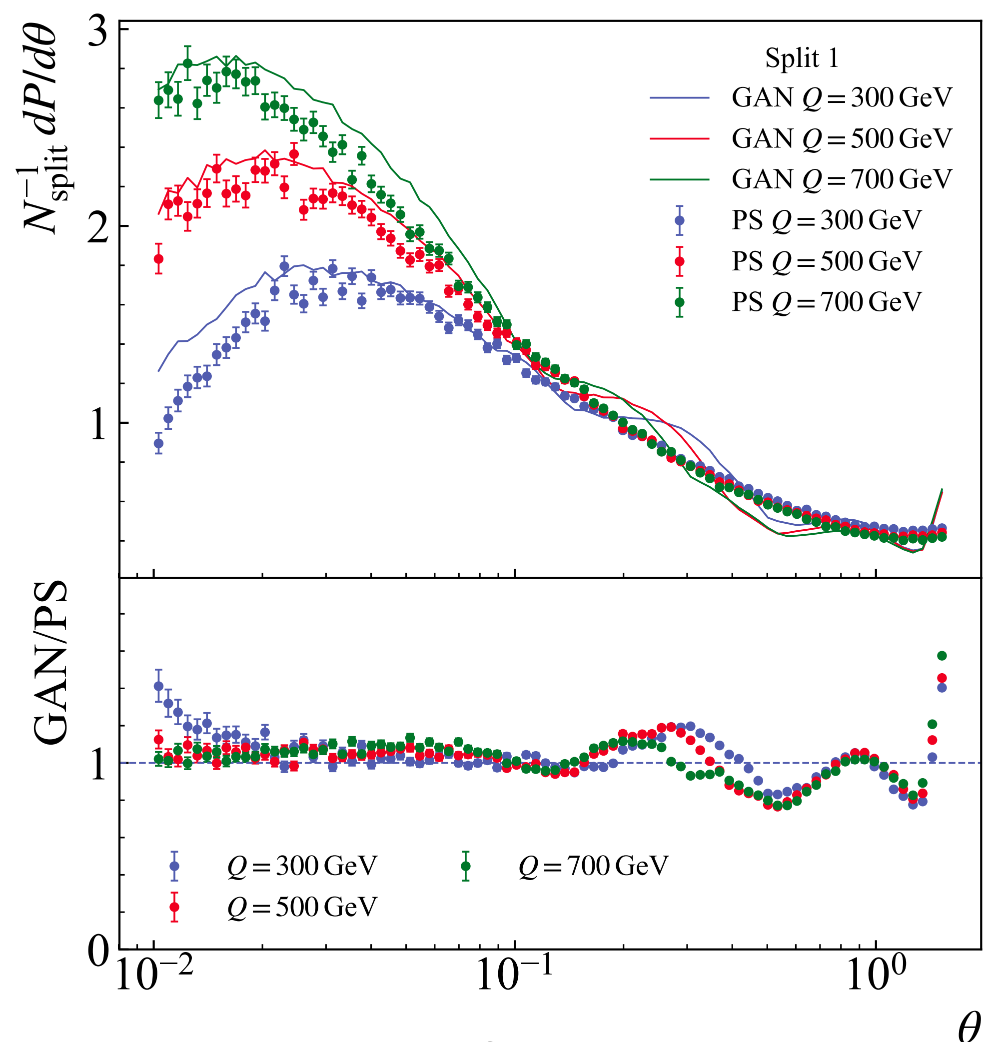
1.

AI/ML for data analysis (theory)

Data analysis example #3:
Learn parton branching mechanism from simulated data

Interpretation

- Generative network trained using DGLAP-based parton shower Monte Carlo event generator
- Explainable/"white-box" architecture identifies physics of individual splitting processes
- Future applications incl. modification of the vacuum parton shower in heavy-ion collision or electron-nucleus collisions at EIC



Splitting angle of daughter partons

[Phys.Lett.B 829 (2022), 2012.06582]

2.

AI/ML for first-principles theory

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

e.g., Lattice QCD, perturbative QCD, EFT, nuclear many-body, …

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

Potential for transformative impact by enabling calculations that would otherwise be computationally intractable

AI/ML for first-principles theory

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

a. 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]

AI/ML for first-principles theory

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

b. Transform to a computationally easier problem with the 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 complex integration contour leaves observables unaltered but modifies variance]

Phiala Shanahan, MIT

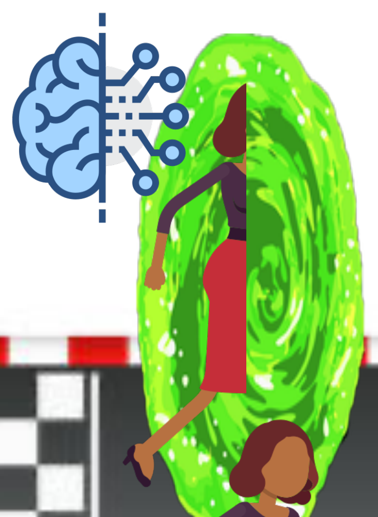
AI/ML for first-principles theory

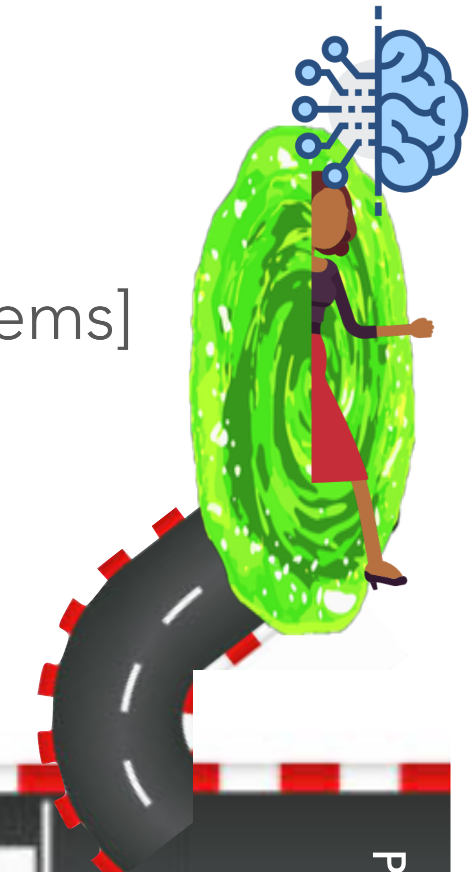
Compute **exact** results from known theory
Use AI/ML to do it **faster**

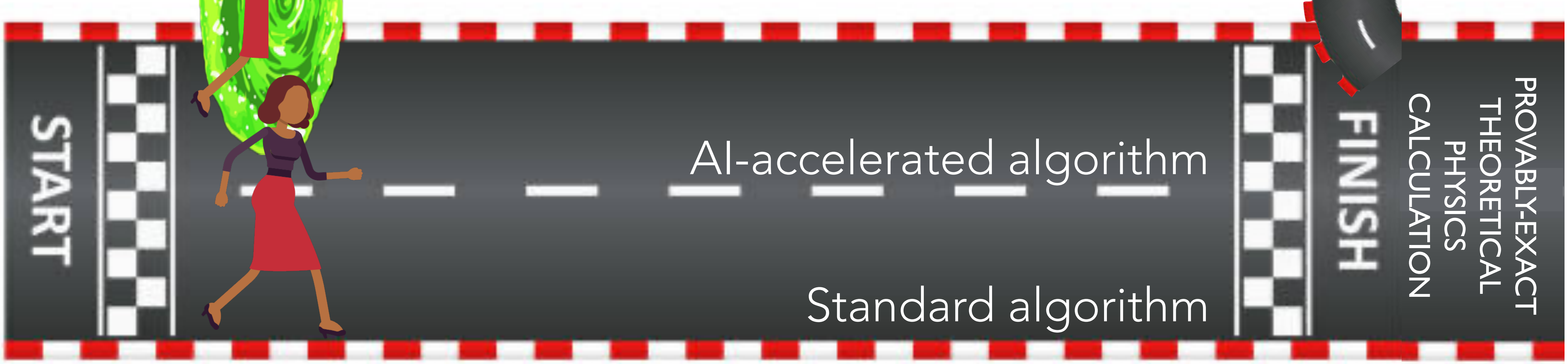
c. Solve a different problem, apply a known correction

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

2.

AI/ML for first-principles theory

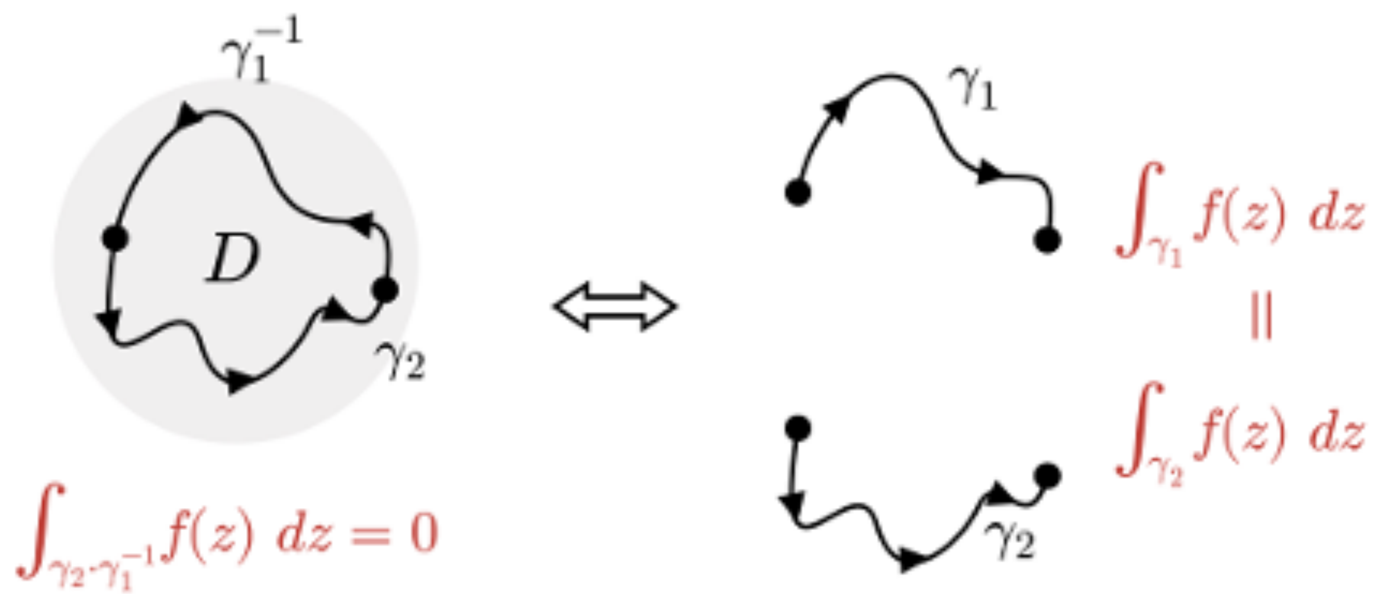
First-principles theory example #1:
Contour deformation of complex integrals

Problem transformation

- ML-based deformation of integration contours: different integral with same solution but better signal-to-noise properties/ faster evaluation

- Lattice field theory:
  Exponentially improved signal-to-noise in proof-of-principle applications

- Perturbative QCD:
  Acceleration of multi-loop Feynman integrals



[Phys. Rev. D 103, 094517 (2021), 2101.12668; SciPost Phys. 12, 129 (2022), 2112.09145]

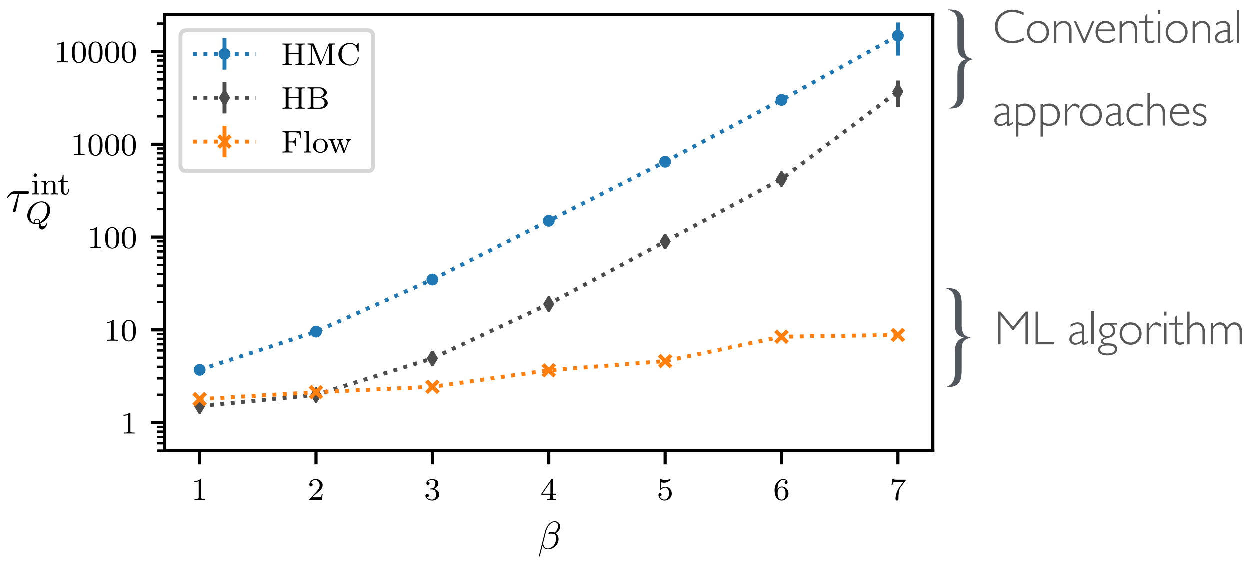
2. AI/ML for first-principles theory

First-principles theory example #2:
Accelerate gauge field generation (sampling) in lattice QCD

Generative modeling

- Generative models used to accelerate provably-exact sampling of lattice QCD gauge fields
- Success in proof-of-principle examples
- Requires custom model architectures with physics built in
- Example of successful partnership with industry

Cost per independent sample



Parameter of theory

Google DeepMind

AURORA | EARLY SCIENCE PROGRAM FOR DATA & LEARNING

IAIFI

[Phys.Rev.Lett. 125 (2020) 12, 121601, 2003.06413]

Exploiting AI/ML for QCD theory: needs

Capitalising on **great potential** for transformative impact on QCD theory **requires targeted action**

BUT Planning is difficult given rapidly changing and diverse requirements!

- **Advances to be made at every level of complexity and scale**
  Complexity: Existing tools → Custom approaches
  Scale: Laptop → Exascale hardware
- Many applications are in an early phase of development
- We have not yet explored the full space of possibilities: **new paradigms certainly still to come in next decade**

Strong overlap with approaches and challenges on experimental side, but also **unique demands and opportunities**

Exploiting AI/ML for QCD theory: needs

Capitalising on **great potential** for transformative impact on QCD theory **requires targeted action**

- Full exploitation requires true "ground-up" ML/AI for physics problems
    - **Requires support (people+hardware) for exploratory and developmental research at *both* universities and labs**
    - **Must train and retain talent at physics/AI intersection**
      Collaborations with AI/ML "experts" external to physics community are necessary but not sufficient
- Computational workflow of AI/ML problems can be different to other algorithmic problems
    - **Demands supporting AI/ML workflows in hardware purchasing and computing allocation policies**

Computational nuclear physics: needs

Computational Nuclear Physics and AI/ML Workshop

- Organized by:
  - Alessandro Lovato (ANL)
  - Joe Carlson (LANL)
  - Phiala Shanahan (MIT)
  - Bronson Messer (ORNL)
  - Witold Nazarewicz (FRIB/MSU)
  - Amber Boehnlein (JLab)
  - Peter Petreczky (BNL)
  - Robert Edwards (JLab)
  - David Dean (JLab)
- 6-7 September 2022 at SURA in Washington, DC
- 60 registered participants (40 in person, 20 on line), including DOE
- https://indico.jlab.org/event/581/
  - All talks archived
  - Short white paper being prepared for the LRP

Computational Nuclear Physics and AI/ML Workshop

6-7 September, 2022 / SURA headquarters

Organized by:
Alessandro Lovato – Joe Carlson (LANL), Phiala Shanahan (MIT), Bronson Messer (ORNL)
Witold Nazarewicz (FRIB/MSU), Amber Boehnlein (JLab), Peter Petreczky (BNL)
Robert Edwards (JLab), David Dean (JLab)

Admin support: Jae Cho jcho@jlab.org Tea Jojua tjojua@sura.org Sherry Thomas sthomas@jlab.org

Schedule
Registration, schedule, and other information can be found at: https://indico.jlab.org/event/581/

Tuesday, 6 September
1:00 – 1:05 Welcome, David Dean and Sean Hearne
1:05 – 1:20 DOE remarks, Tim Hallman
1:20 – 2:00 QCD, William Detmold (JLab) and Swagato Mukherjee (BNL)
2:00 – 2:40 Quantum many-body problems, Thomas Papenbrock (UT/ORNL)
2:40 – 3:00 BREAK
3:00 – 3:40 Fundamental Symmetries,Emanuele Mereghetti (LANL)
3:40 – 4:20 Astrophysics, George Fuller (UCSD)
4:20 – 5:00 AI/ML, Amber Boehnlein (JLab)
5:00 – 5:40 Preliminary list of recommendations discussion (Peter Petreczky, lead)
5:40 – 7:30 Reception

Wednesday, 7 September
7:45 – 8:30 Continental Breakfast
8:30 – 10:00 Breakout Sessions
1. QCD (Phiala Shanahan, lead)
2. Nuclear Structure and fundamental symmetries (Alessandro Lovato, lead)
3. Astrophysics (Bronson Messer, lead)

10:00 – 10:30 Break
10:30 – 12:00 Breakout reports
12:00 – 1:00 Lunch
1:00 – 2:30 Recommendations discussion and next steps

Jefferson Lab
Thomas Jefferson National Accelerator Facility
SURA

Computational nuclear physics: needs

Workshop Resolution

High-performance computing is essential to advance nuclear physics on the experimental and theory frontiers. Increased investments in computational nuclear physics will facilitate discoveries and capitalize on previous progress. Thus, we recommend a targeted program to ensure the utilization of ever-evolving HPC hardware via software and algorithmic development, which includes taking advantage of novel capabilities offered by AI/ML.

The key elements of this program are to:

1) Strengthen and expand programs and partnerships to support immediate needs in HPC and AI/ML, and also to target development of emerging technologies, such as quantum computing, and other opportunities.
   i.e., it is critical to support software and algorithm development, as well as maintenance, sustainability e.g., DOE SciDAC, ECP, NSF AI institutes, CSSI programs
2) Take full advantage of exciting possibilities offered by new hardware and software and AI/ML within the nuclear physics community through educational and training activities.
3) Establish programs to support cutting-edge developments of a multi-disciplinary workforce and cross-disciplinary collaborations in high-performance computing and AI/ML.
4) Expand access to computational hardware through dedicated and high-performance computing resources. i.e., dedicated resources are needed to catalyse use of leadership-class e.g., expansion of successful USQCD program across nuclear theory