


KISS

KI zur schnellen Simulation von wissenschaftlichen Daten

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BDA Annual Meeting — 13.03.2025

CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE



Universität Hamburg

DER FORSCHUNG | DER LEHRE | DER BILDUNG



DASHH



Partnership of
Universität Hamburg and DESY

GEFÖRDERT VOM



Bundesministerium
für Bildung
und Forschung

Emmy
Noether-
Programm

Deutsche
Forschungsgemeinschaft
DFG



Motivation

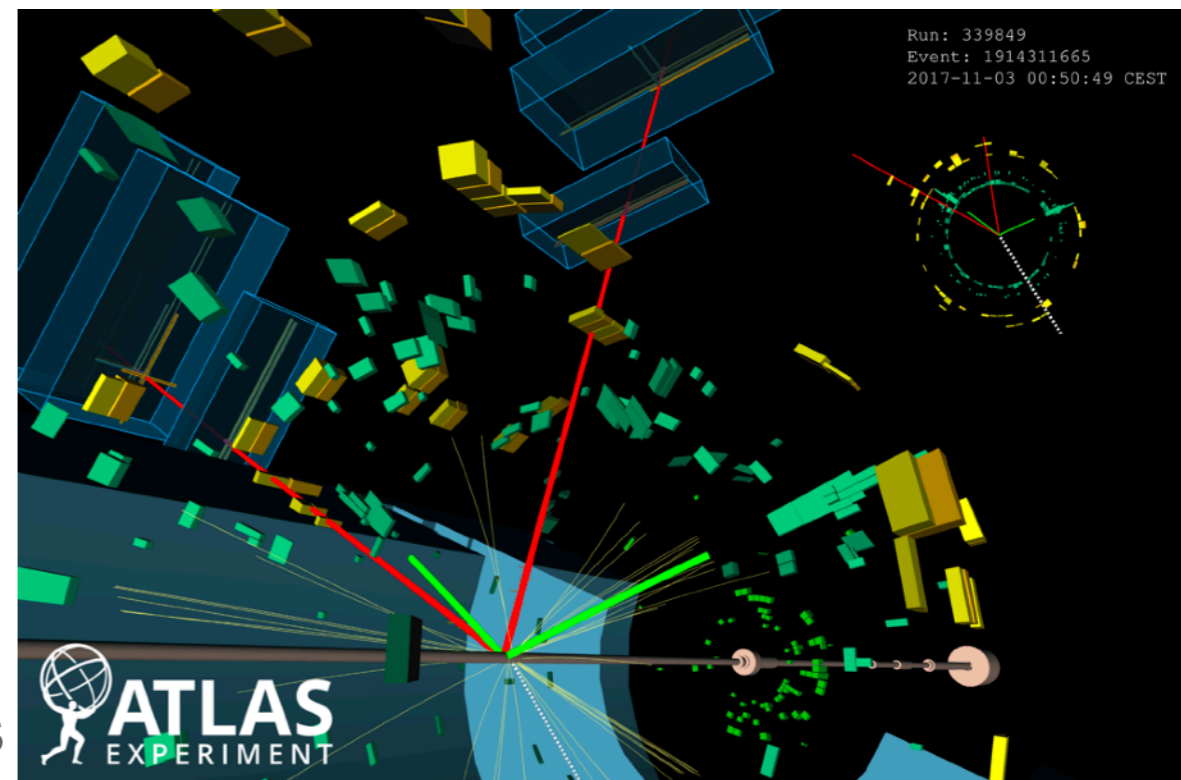
Simulations relate fundamental physical structures to observable quantities.

$$\begin{aligned}\mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + h.c. \\ & + \chi_i Y_{ij} \chi_j \phi + h.c. \\ & + |D_\mu \phi|^2 - V(\phi)\end{aligned}$$

Complex chain
of simulations

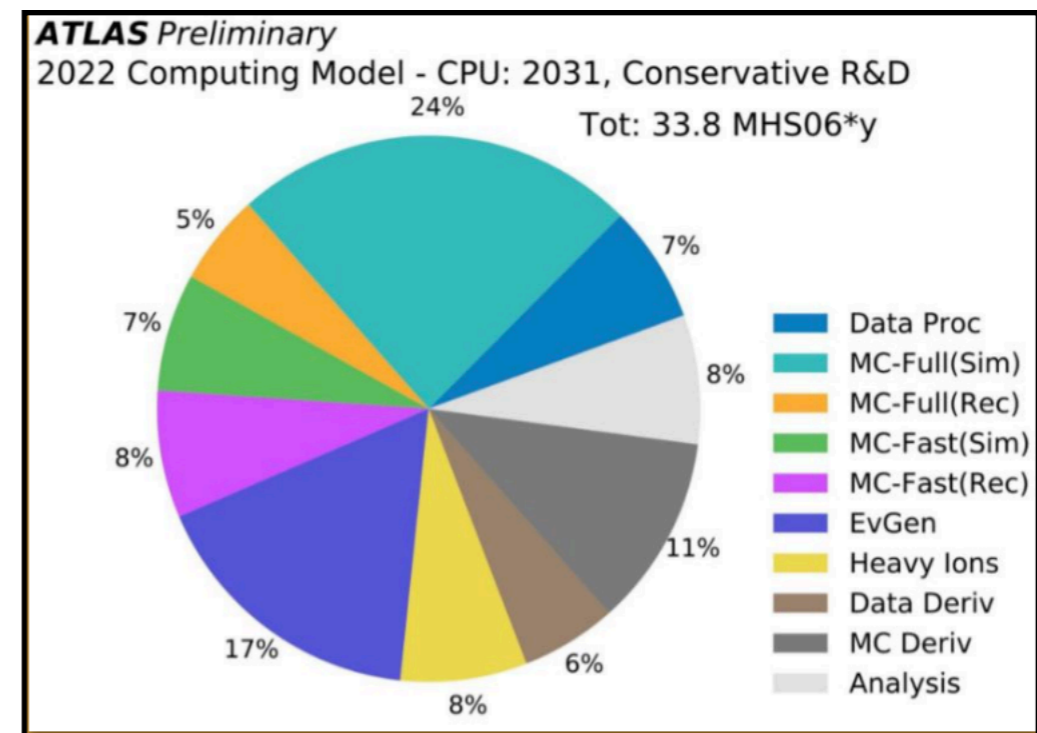
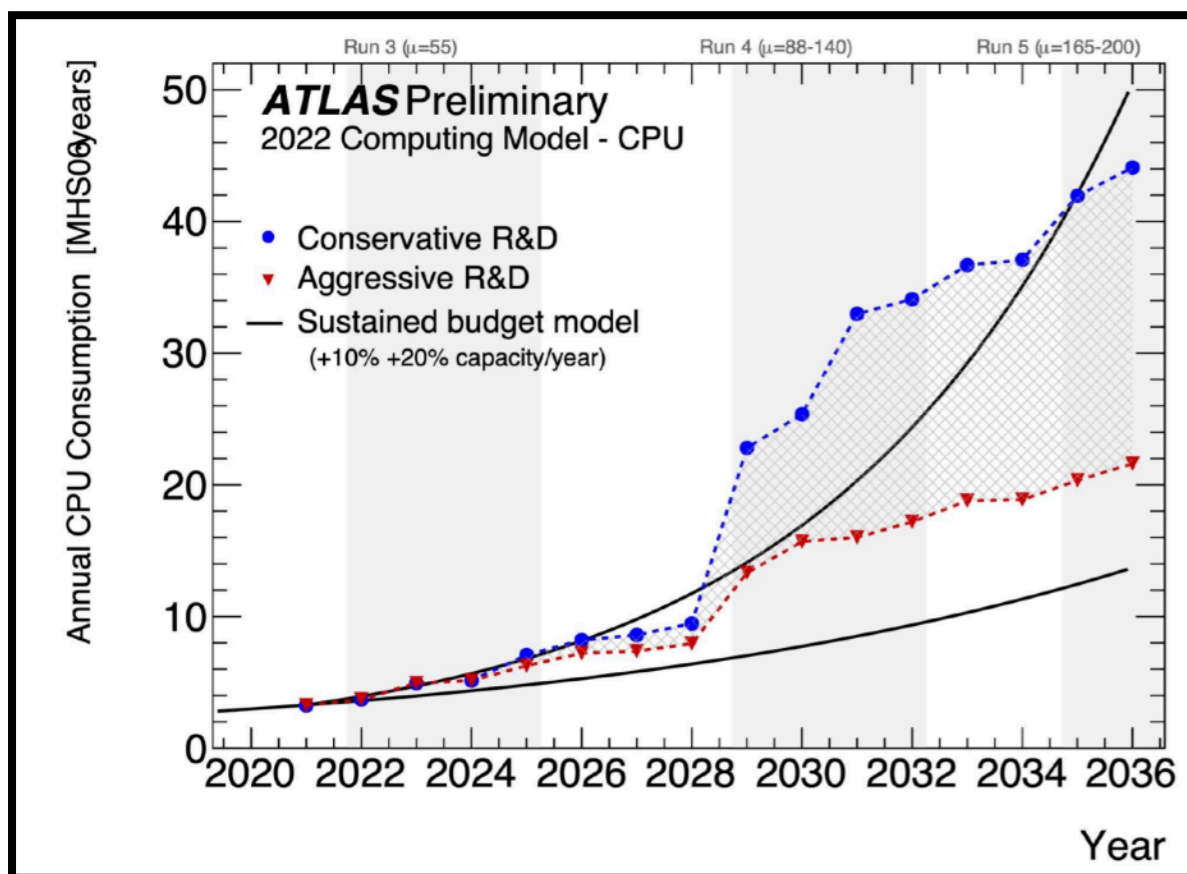


Simulation-aided
inverse problems



Motivation

Simulations relate fundamental physical structures to observable quantities, but are computationally very expensive.

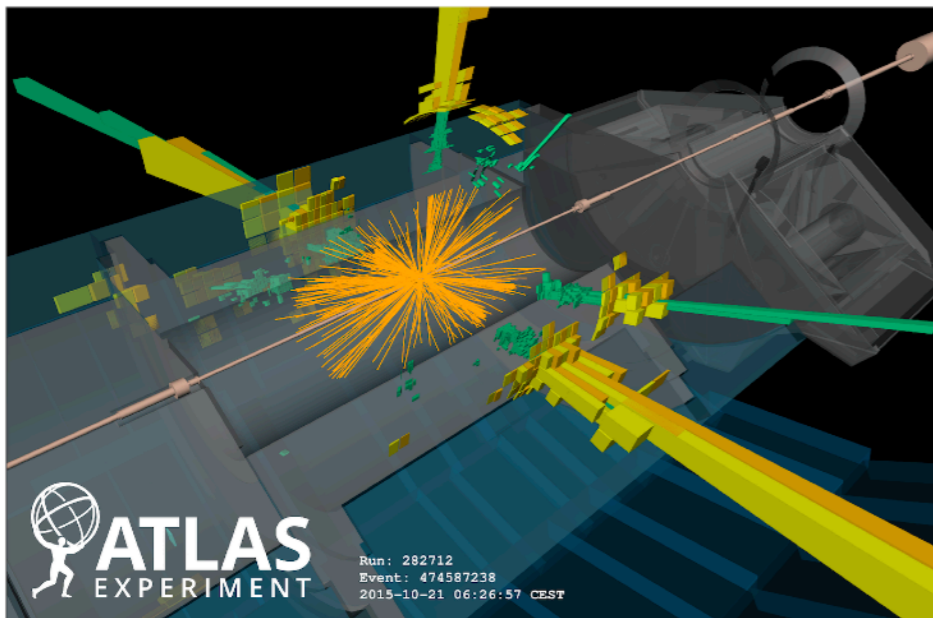


Example for collider physics, similar issues in all domains

Motivation

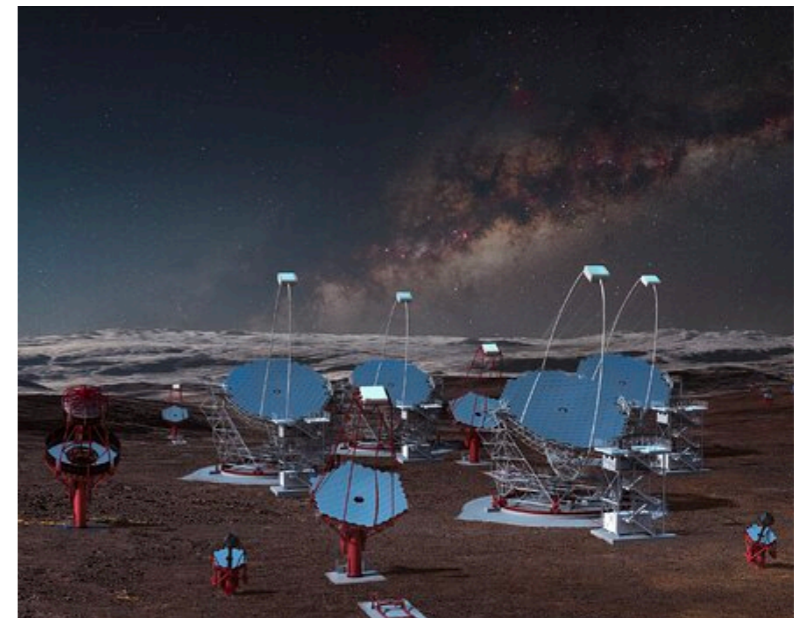
Simulations relate fundamental physical structures to observable quantities, but are computationally very expensive.

They are crucially required for research in particle physics, hadron- and nuclear physics, astro-particle physics, and astronomy.



Between particle physics and astronomy, KISS covers 45 orders of magnitudes.

Experimental particle physics probes nature at length scales of 10^{-18} meters.

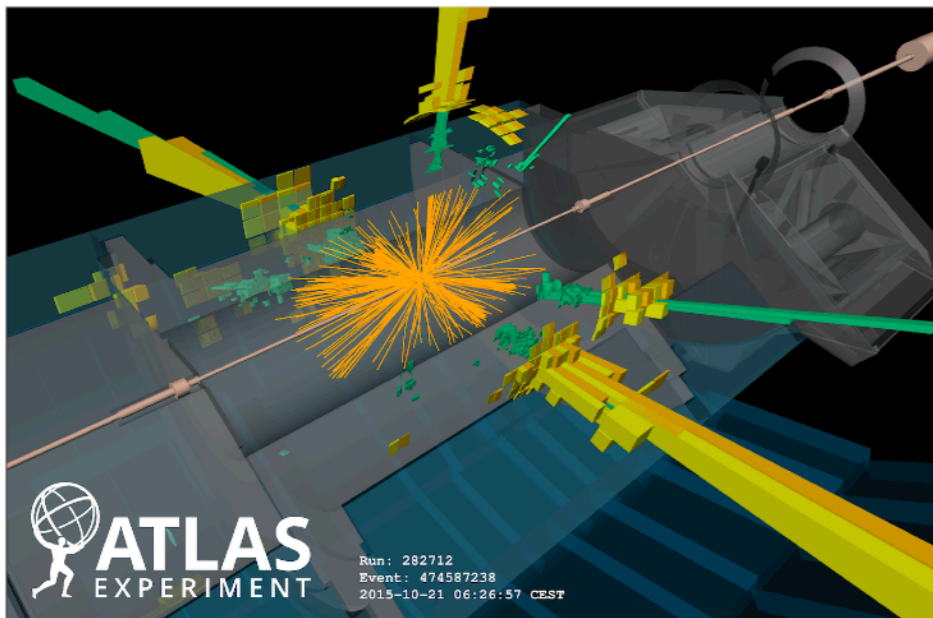


The observable universe has a diameter of 10^{27} meters.

Motivation

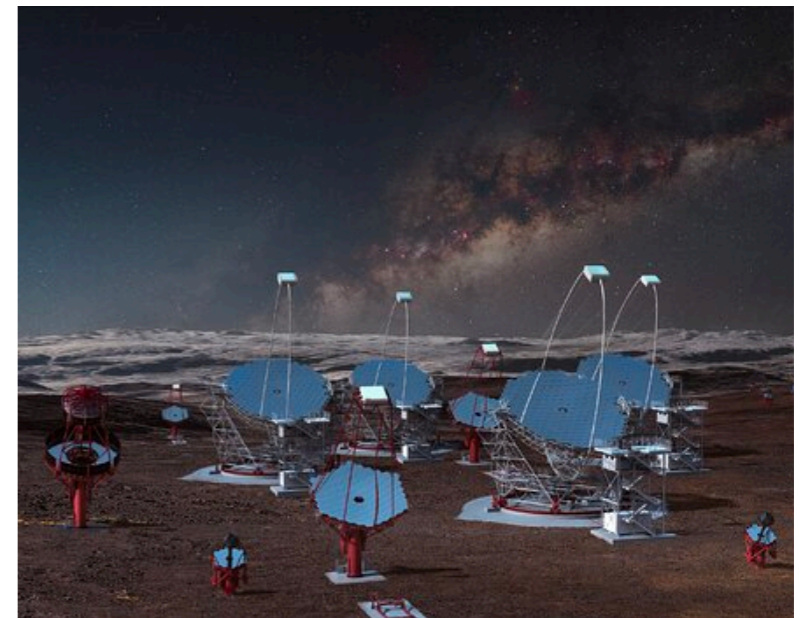
Simulations relate fundamental physical structures to observable quantities, but are computationally very expensive.

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United by scientific questions and key methods

Experimental particle physics probes nature at length scales of 10^{-18} meters.



The observable universe has a diameter of 10^{27} meters.

Motivation

Simulations relate fundamental physical structures to observable quantities.

They are crucially required for research in particle physics, hadron- and nuclear physics, astro-particle physics, and astronomy.

KISS develops and researches generative AI tools to increase the efficiency of scientific simulations



Composition



DESY (KET, KAT)



München (KET, RdS)



Dresden (KET)



Dortmund (KET, KAT, RdS)



Göttingen (KET)



UNIVERSITÄT HEIDELBERG
ZUKUNFT SEIT 1386

Heidelberg (KET)



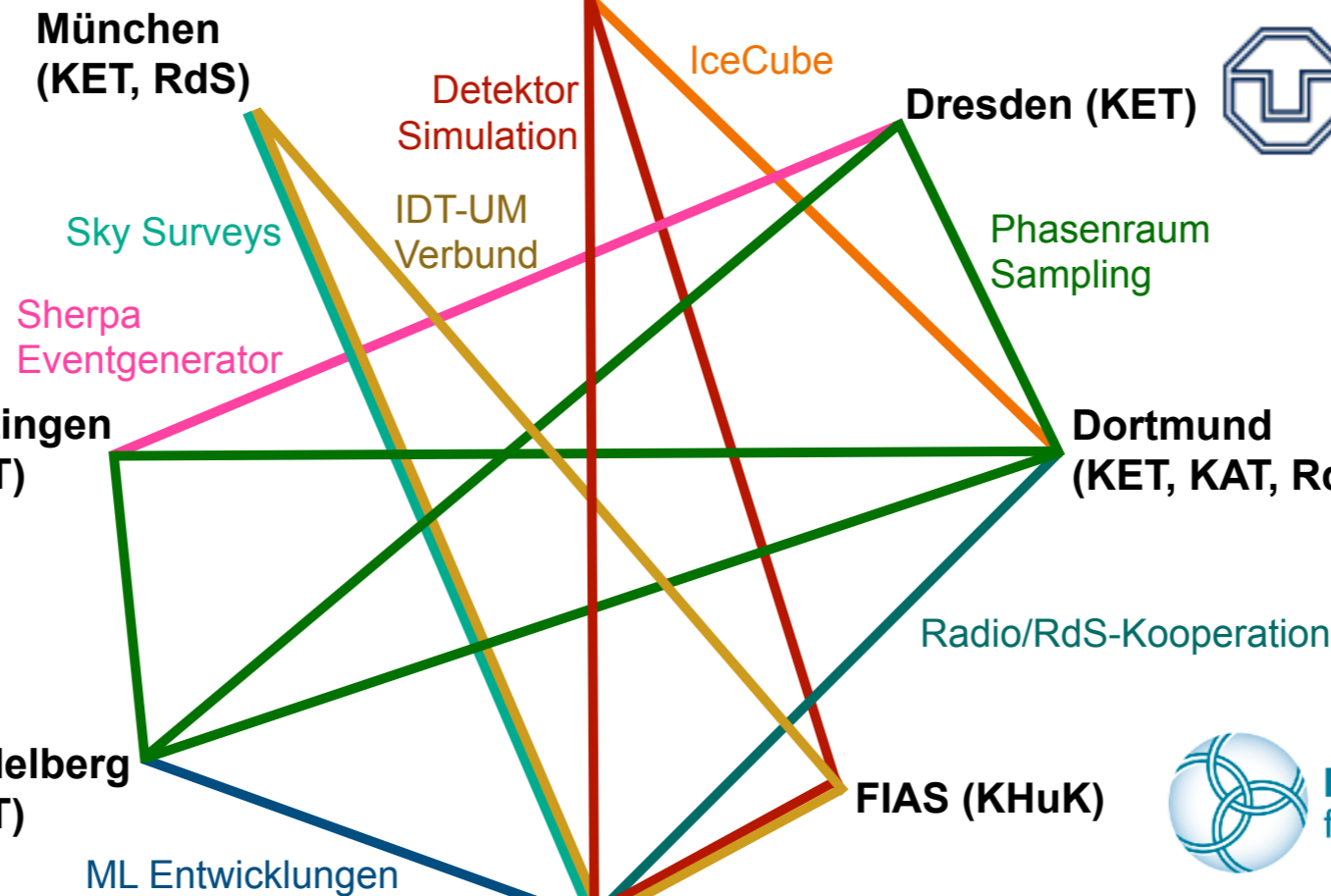
FIAS (KHuK)



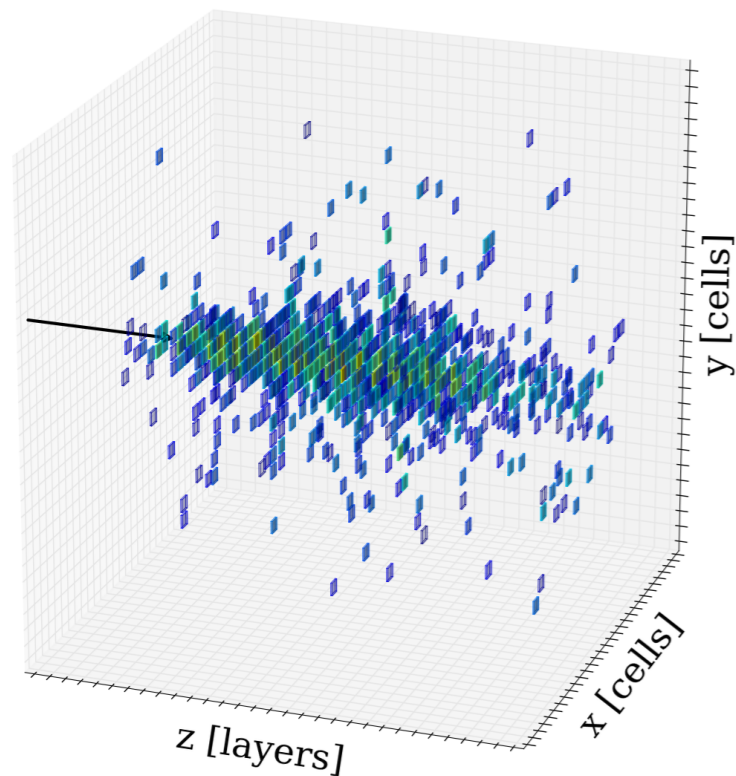
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Hamburg (KET, RdS)

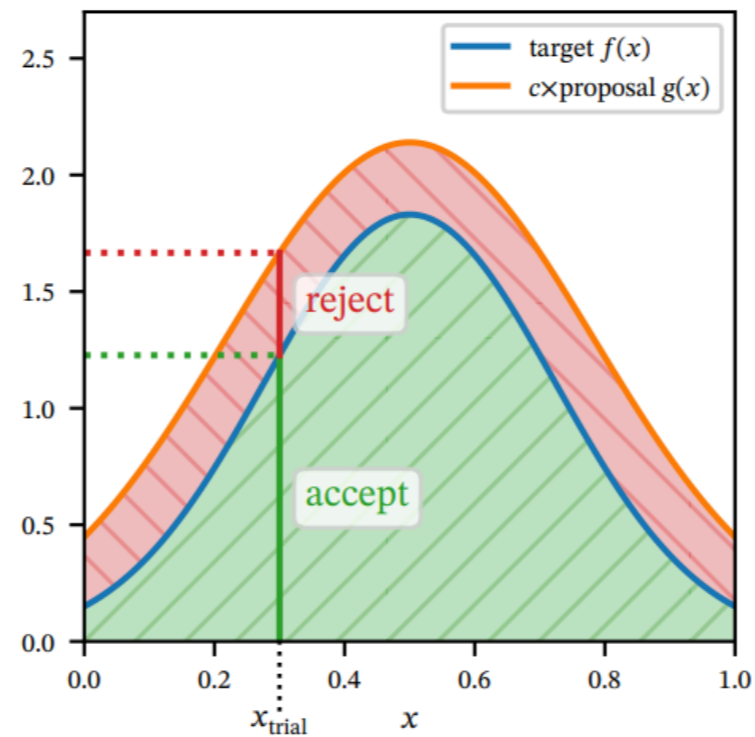
Associated:



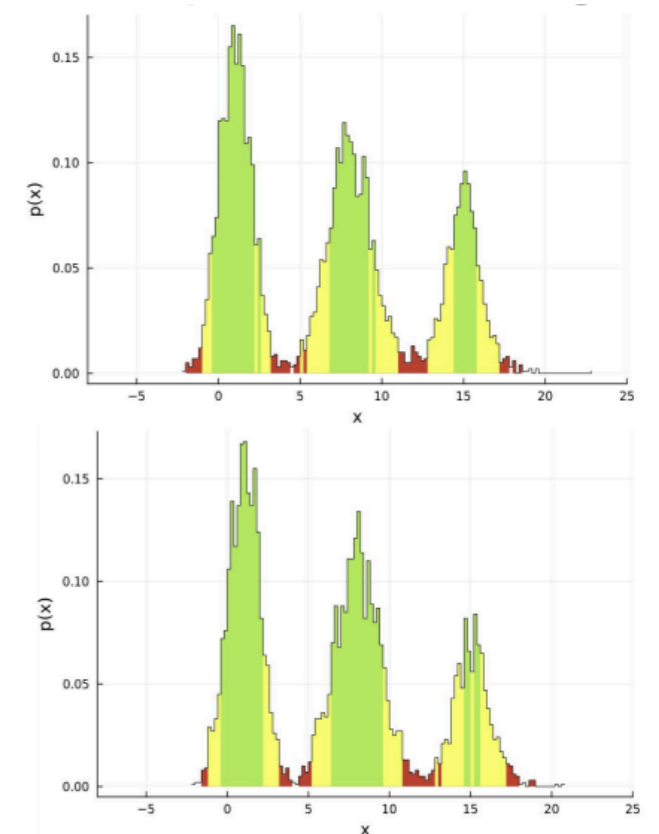
Overview



Surrogates



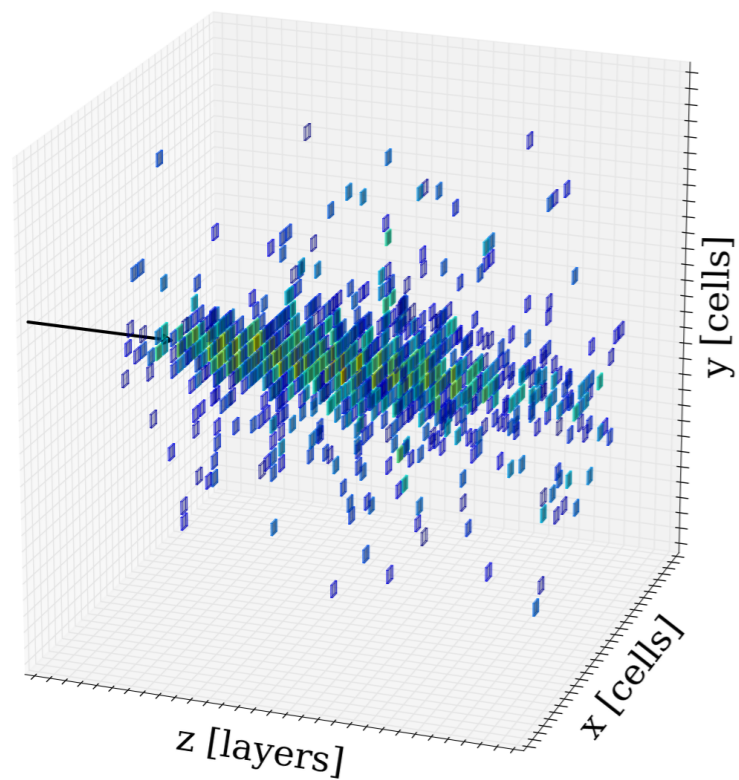
Sampling



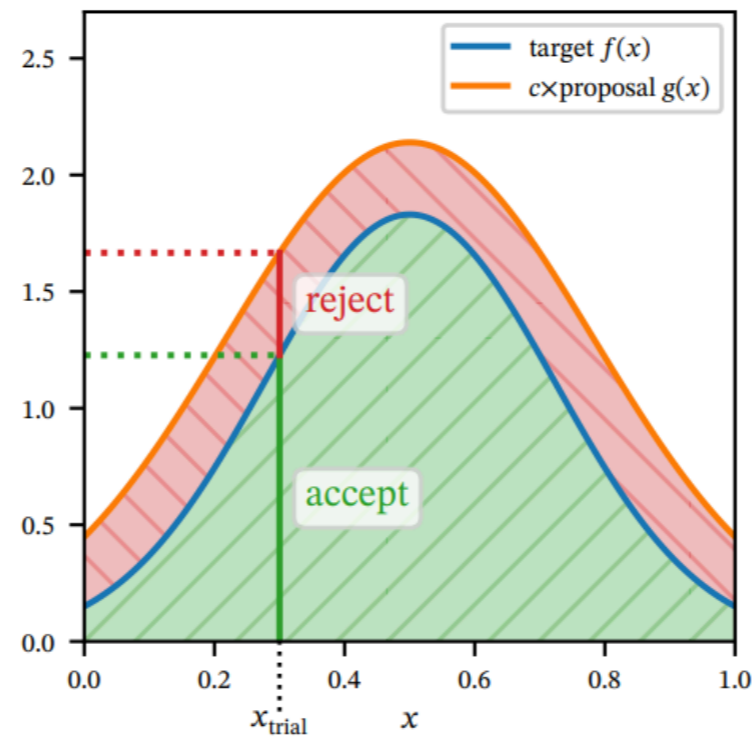
Quality

*apologies for
selection bias!

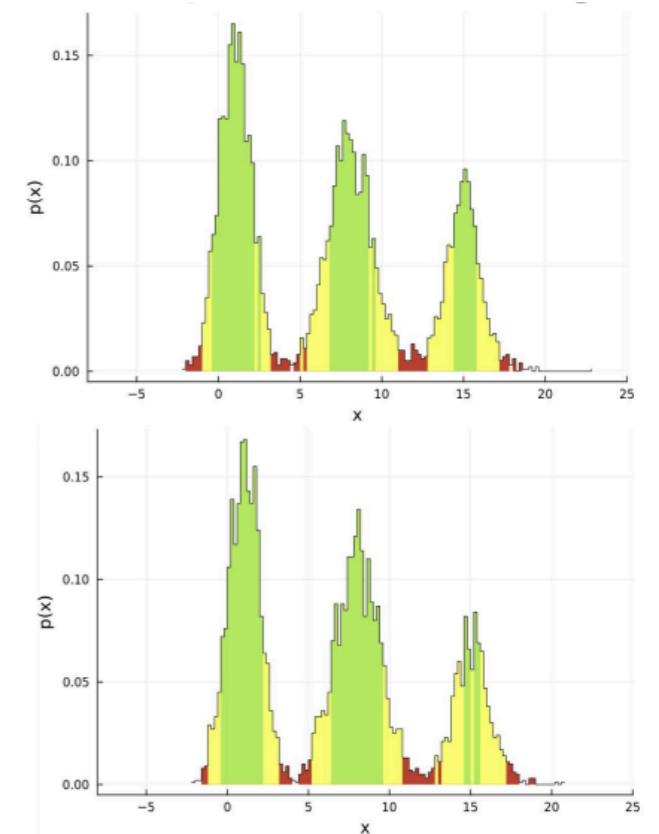
Overview



Surrogates



Sampling

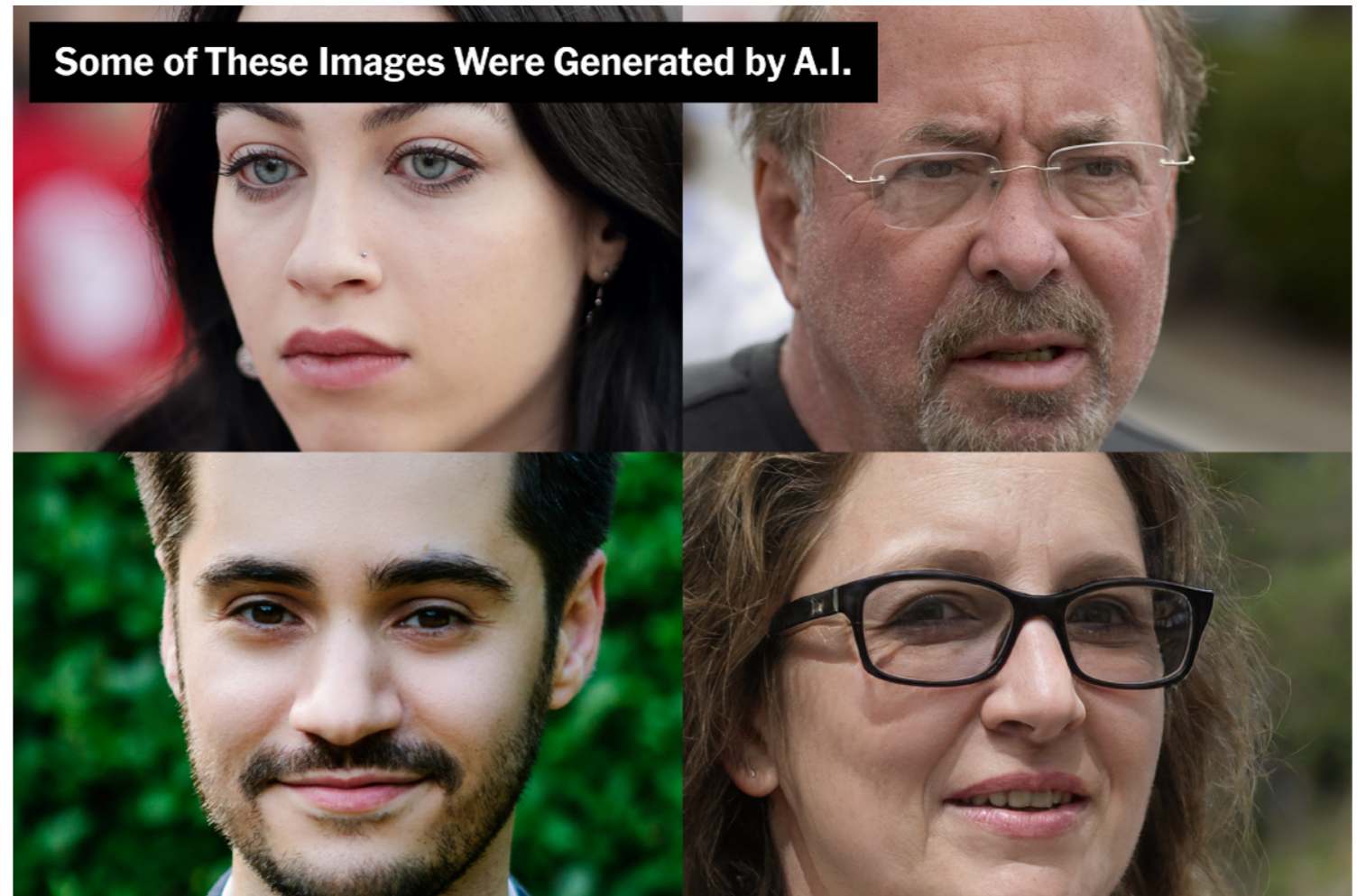


Quality

Generative Image Models



Massive progress in the generation of artificial images

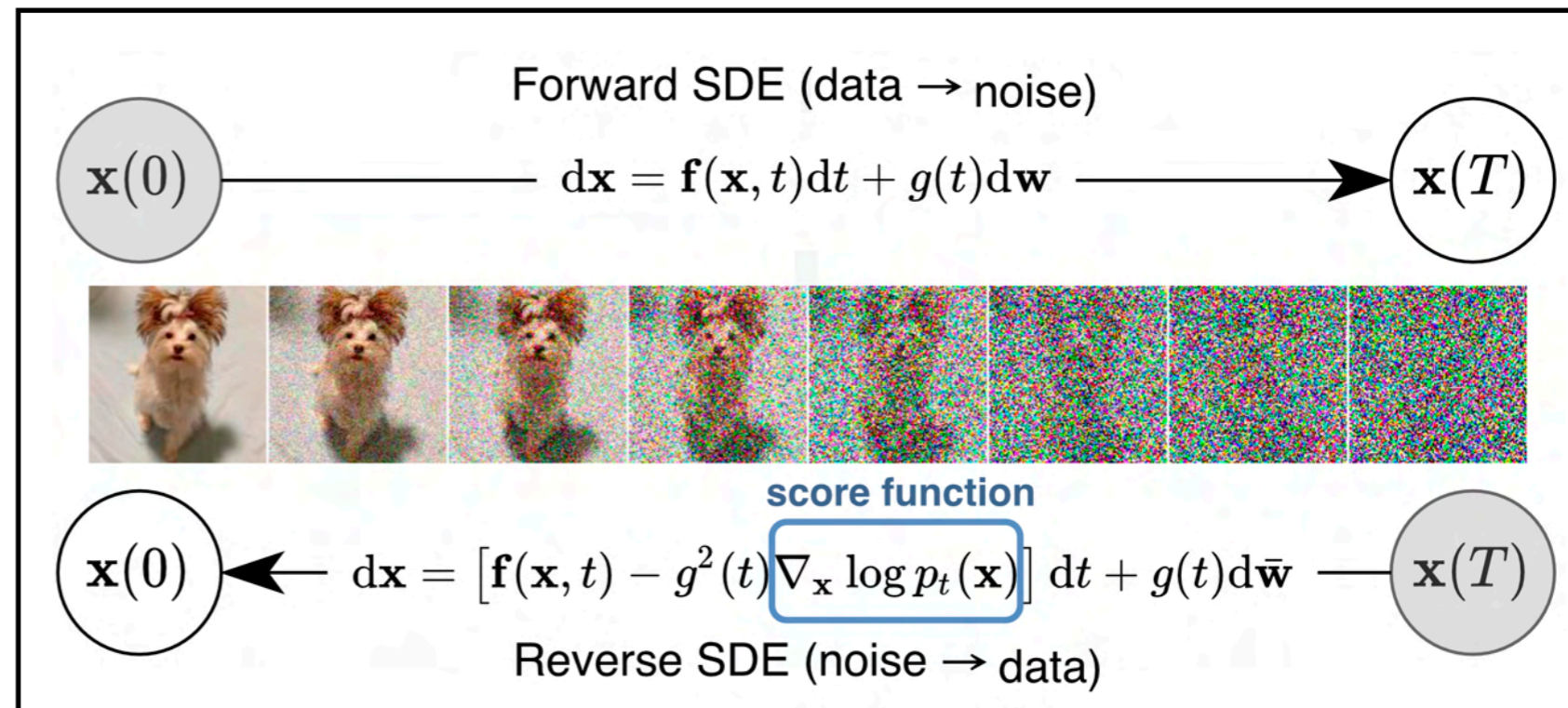


2024

Generative Image Models

Massive progress in the generation of artificial images

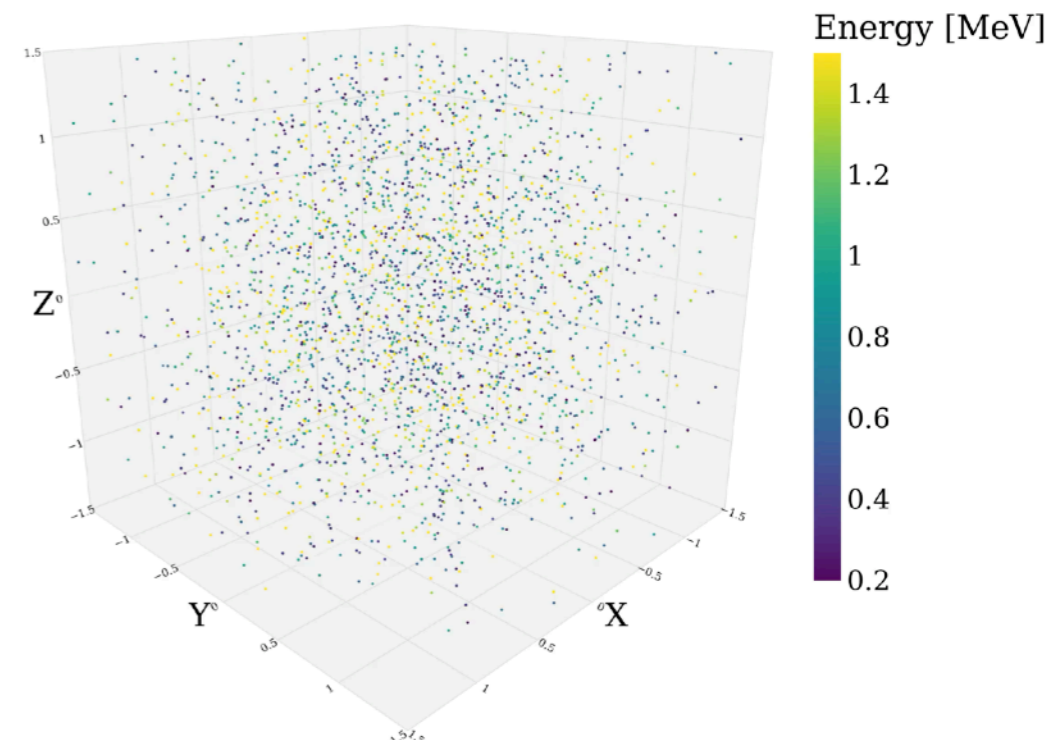
Main driver: Normalising flows and **diffusion**



Idea:
Use **classical simulation** to
produce initial training data for
generative model

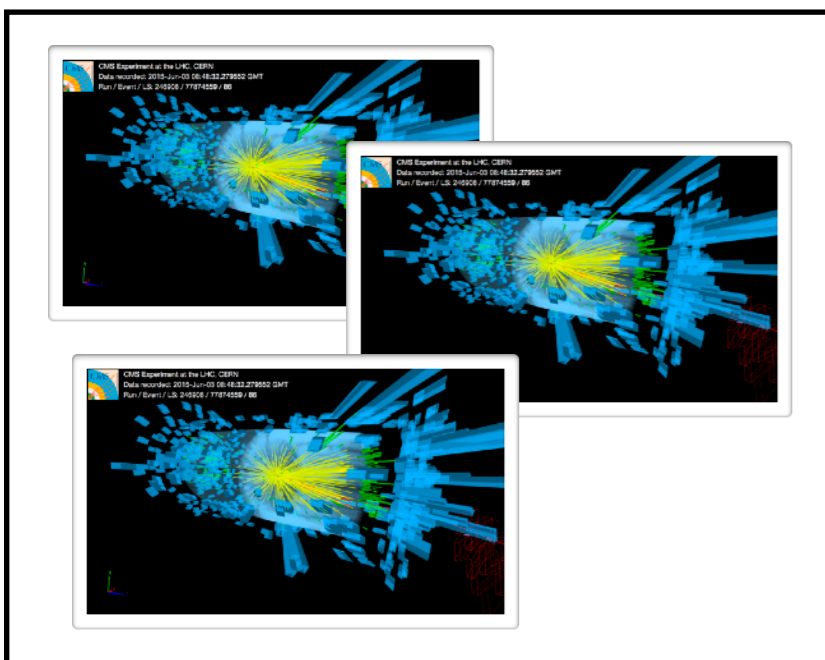
Example: **surrogate
model** for particle interaction
in high granularity detector.

CaloCloud, time stamp: t_{99}



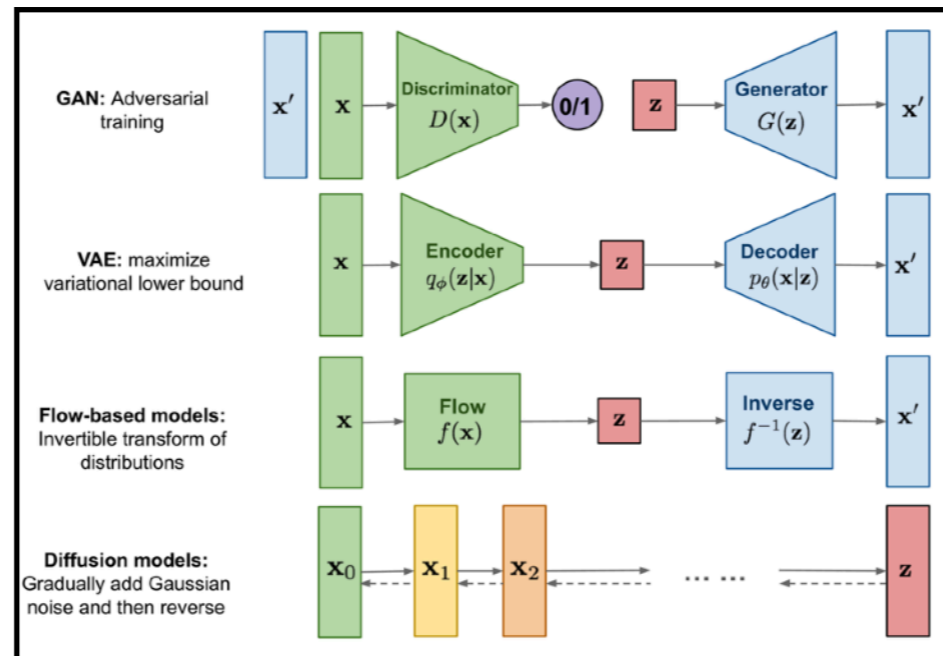
Strategy

1. Use classical simulation or data as input

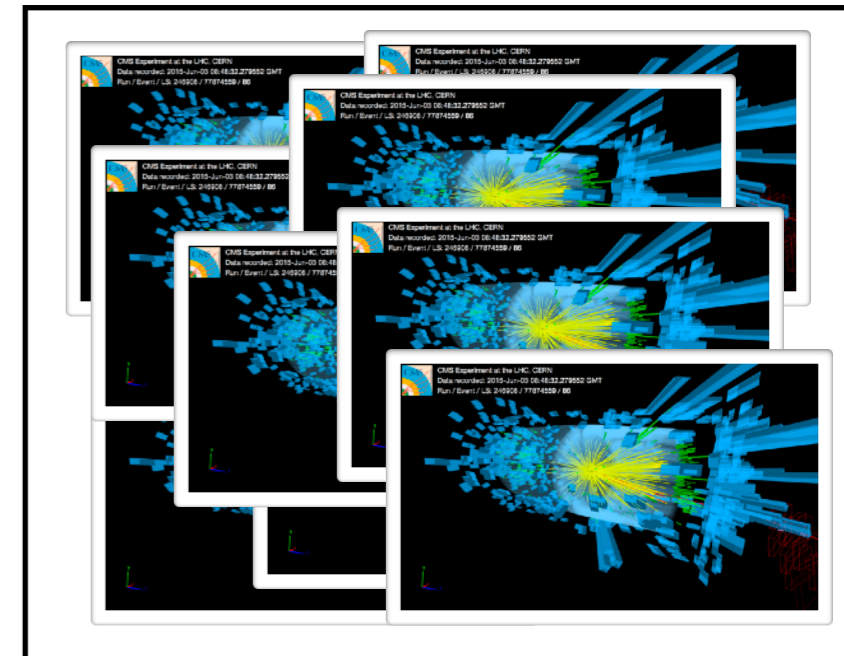


(slow)

2. Train generative surrogate



3. Oversample

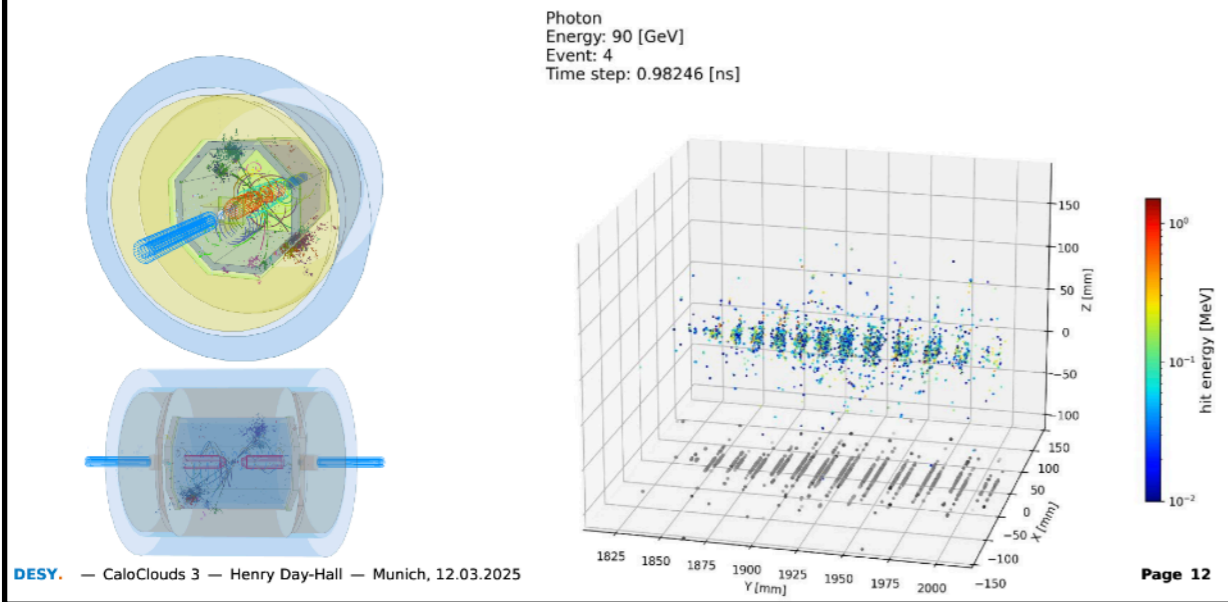


(fast)

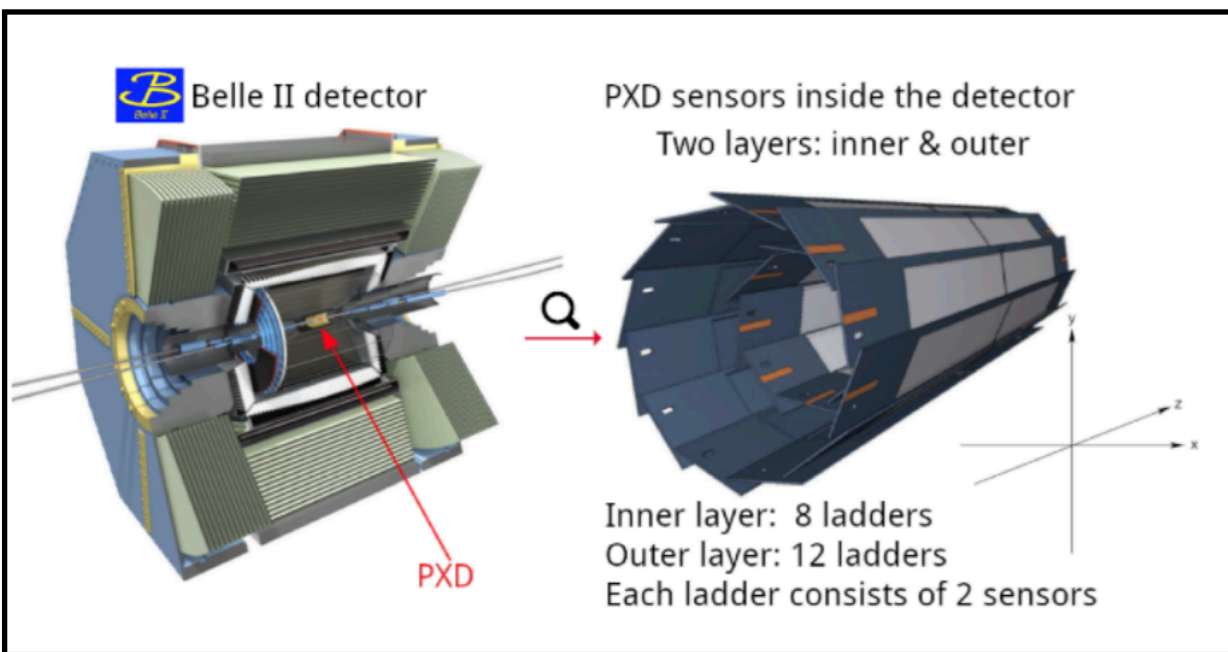
Targets

Our training data

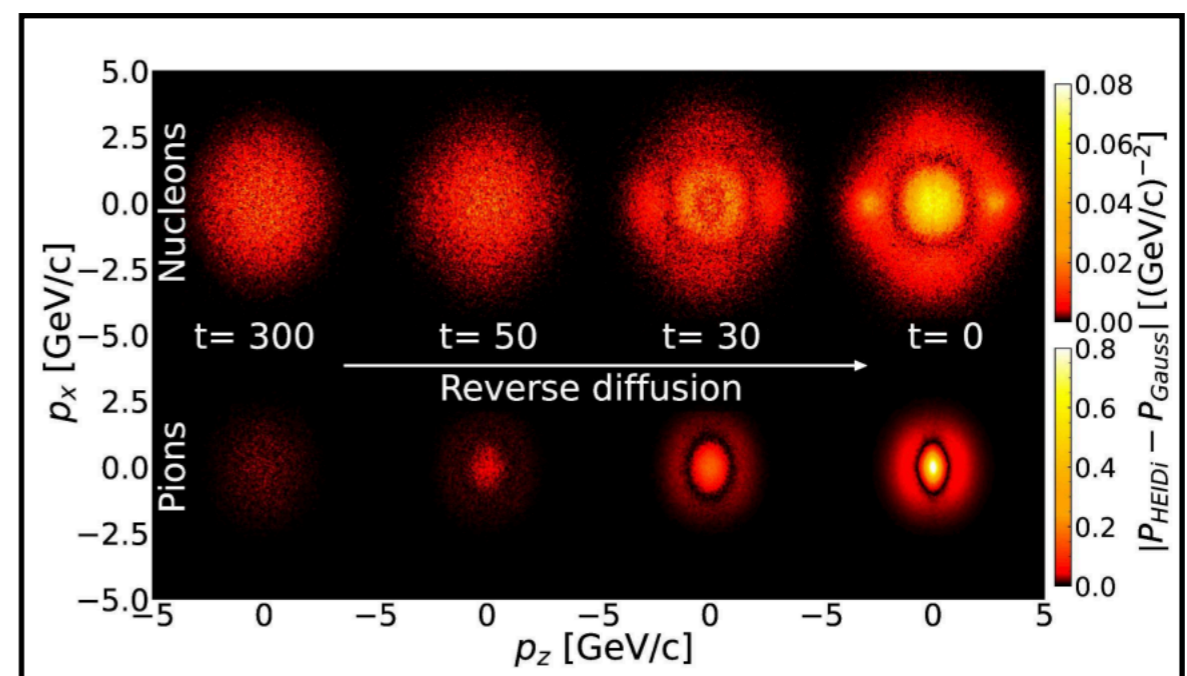
Photon showers in the ILC EM calorimeter



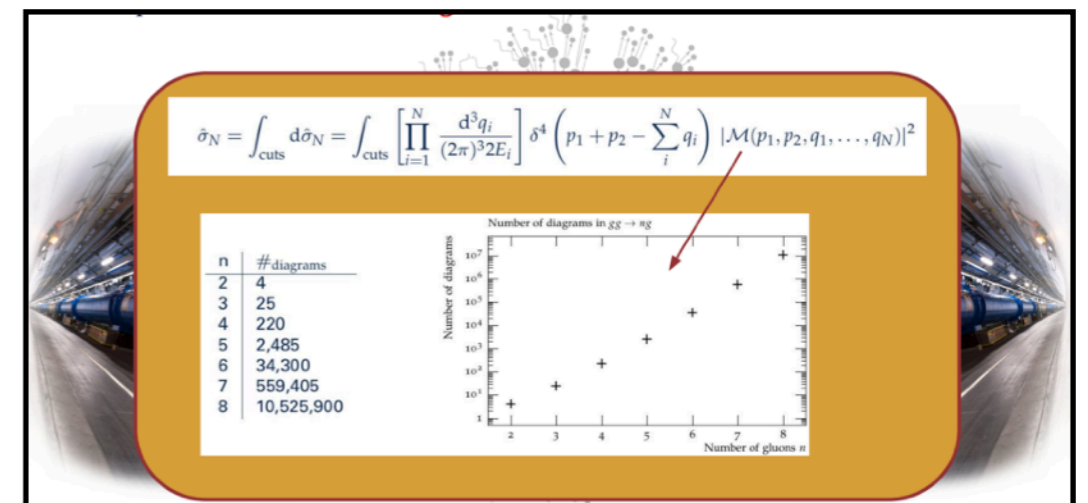
Particle showers in calorimeters



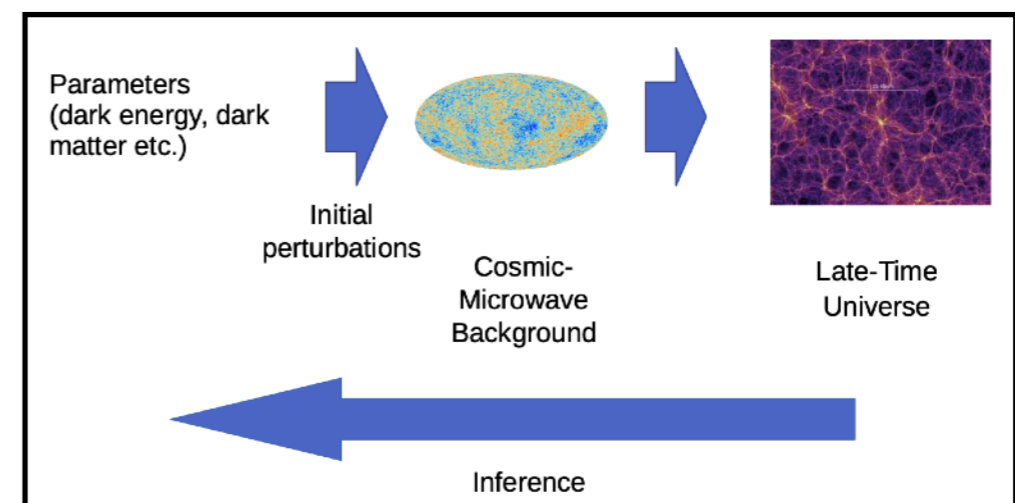
Background hits in pixel sensors



Heavy ion collisions



Hard-scattering matrix elements



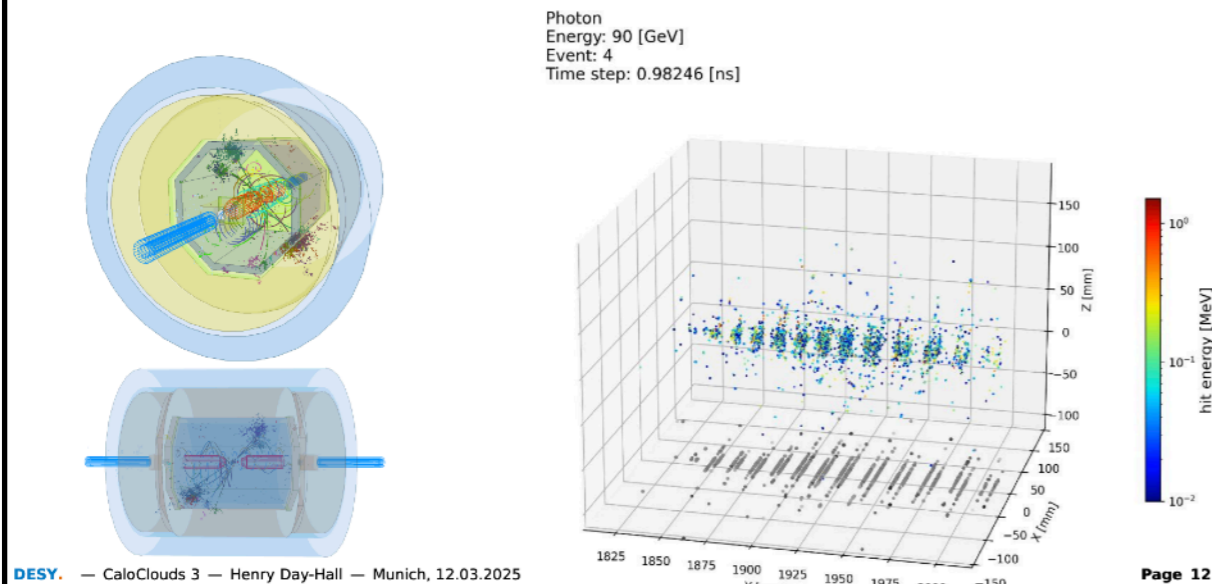
Distributions of galaxies

Targets

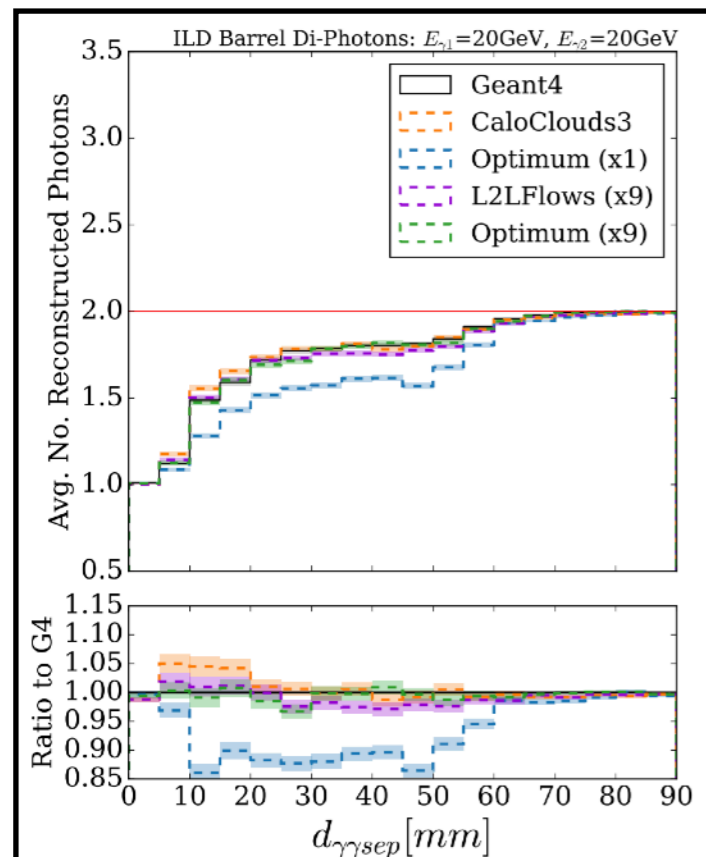
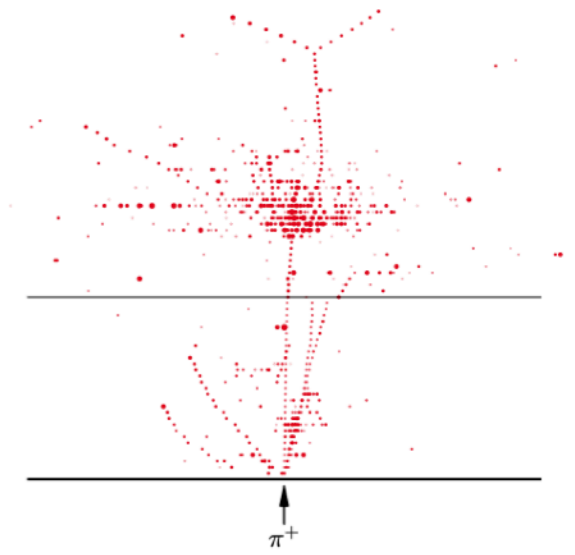
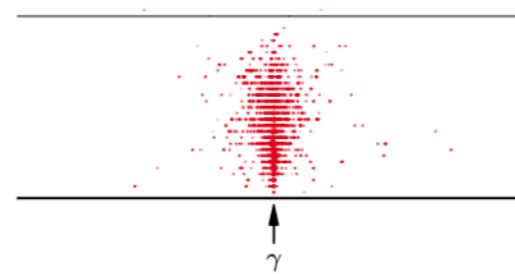
Addressing more **complex pion showers**

Our training data

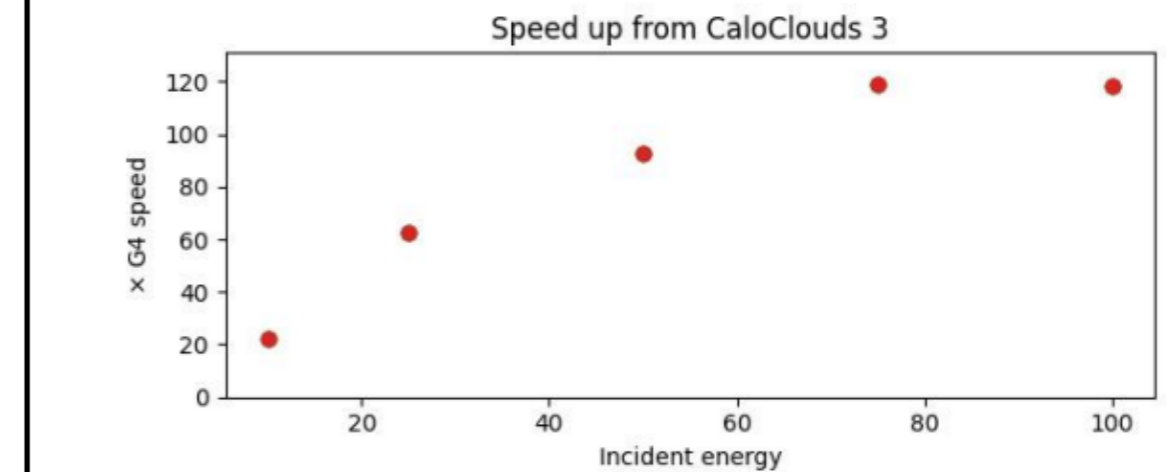
Photon showers in the ILC EM calorimeter



- ▶ hadronic showers are complex
- ▶ difficult to model
- ▶ naive binning with 3×3 bins per ECAL cell results in more than 10^7 bins
- ▶ represent as a point cloud
- ▶ binning points to clusters

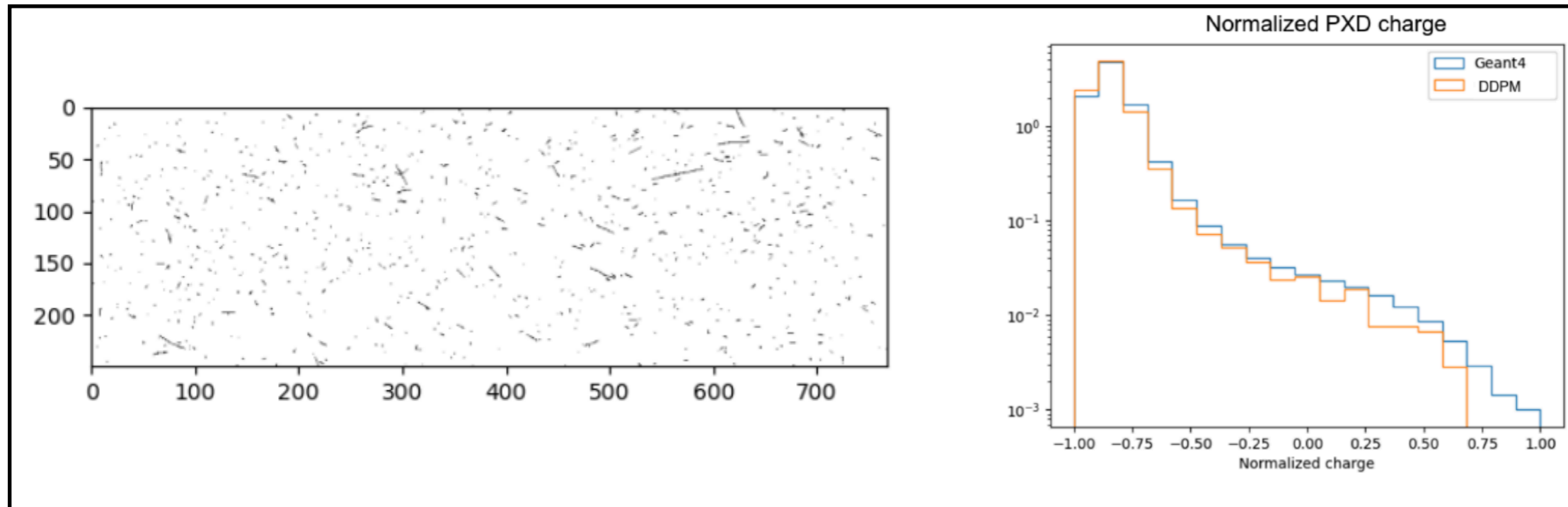


Point-cloud diffusion model (CaloClouds) with very **good generative fidelity**

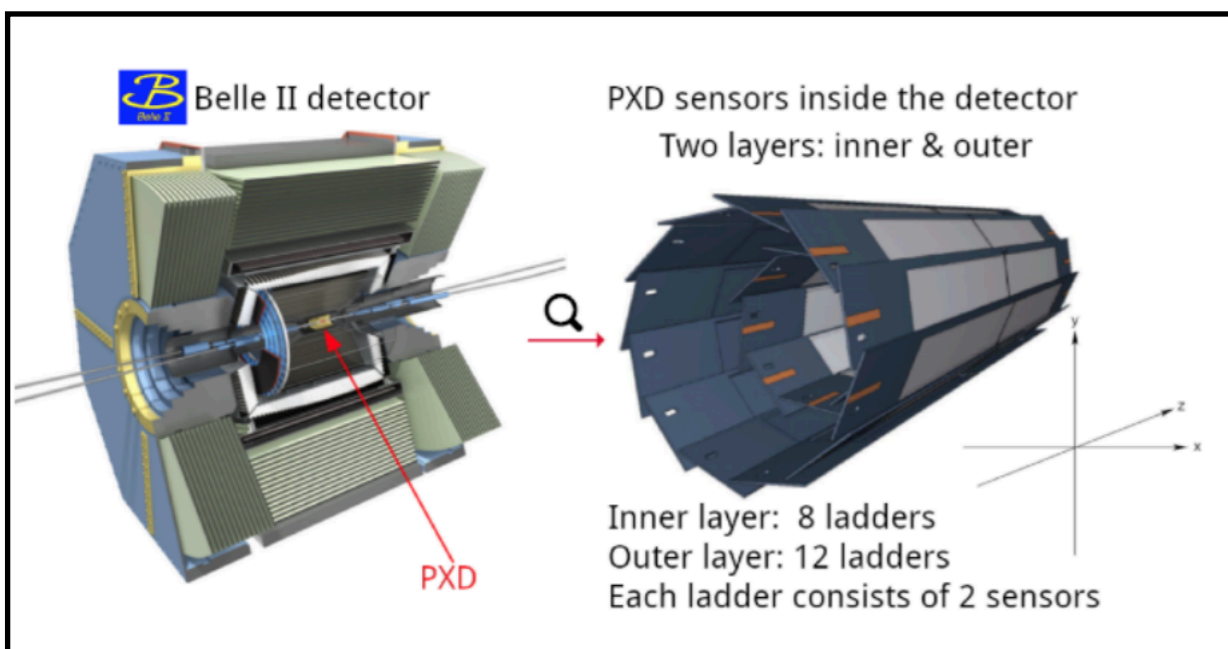


2 orders of magnitude speed-up on same hardware

Targets

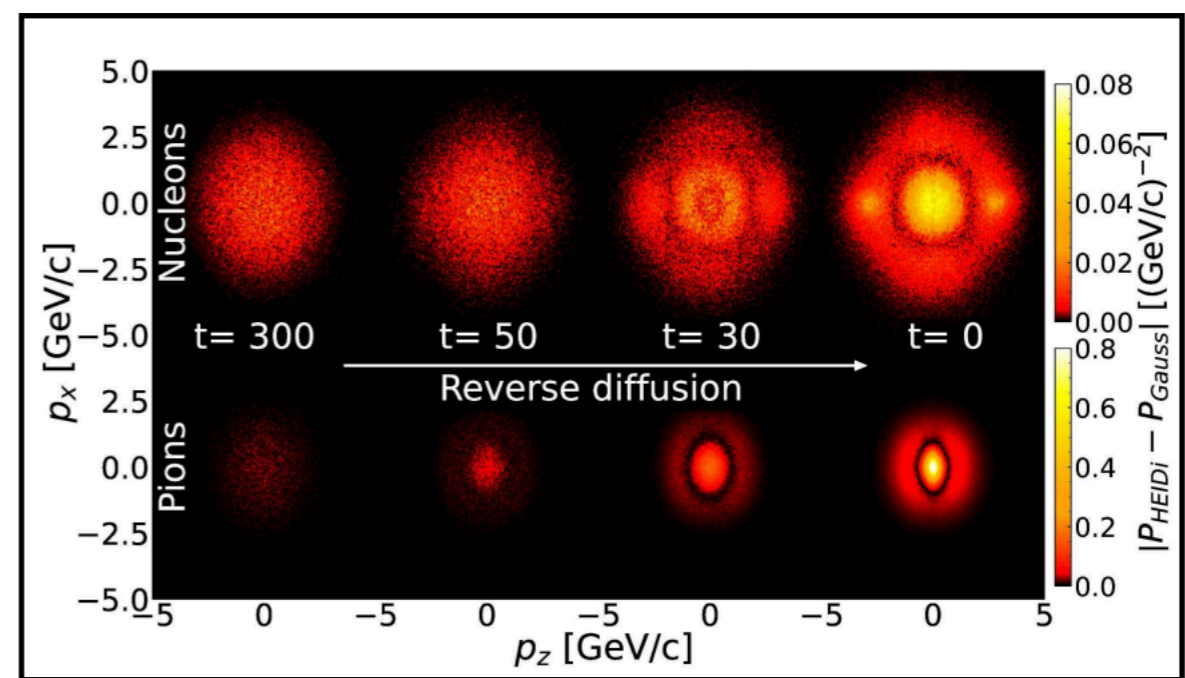


Diffusion model simulates difficult background hits
Good agreement on charge, more tuning needed on correlations



Background hits in pixel sensors

Targets



Heavy ion collisions

HEIDI: Heavy-ion Events through Intelligent Diffusion

Manjunath Omana Kuttan, Kai Zhou, Jan Steinheimer, Horst Stöcker

[arXiv:2412.10352](https://arxiv.org/abs/2412.10352), [arXiv:2502.16330](https://arxiv.org/abs/2502.16330)



Dedicated talk
(Spoiler: substantial speed-up)

Targets

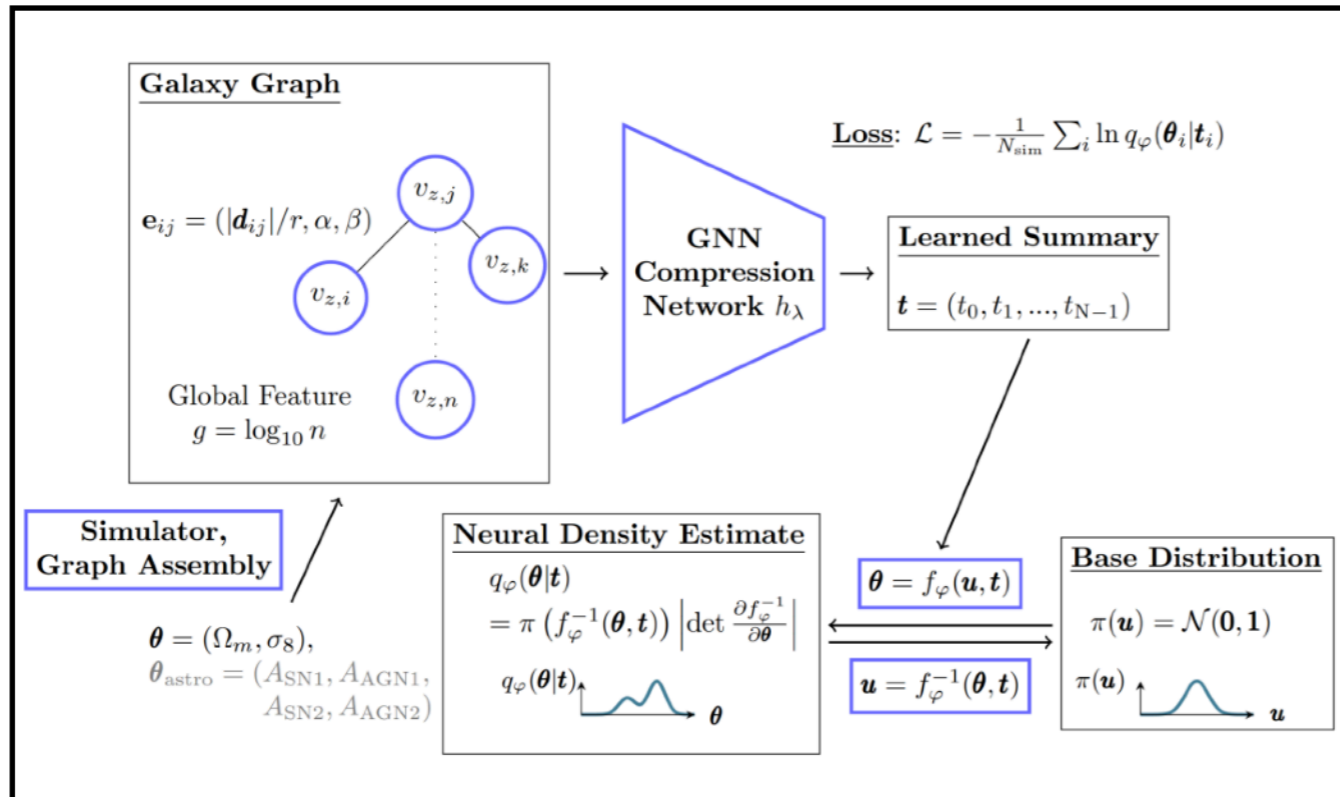
 Ω_m
 σ_8
 A_{AGN1}
 A_{AGN2}
 A_{SN1}
 A_{SN2}

Matter
content

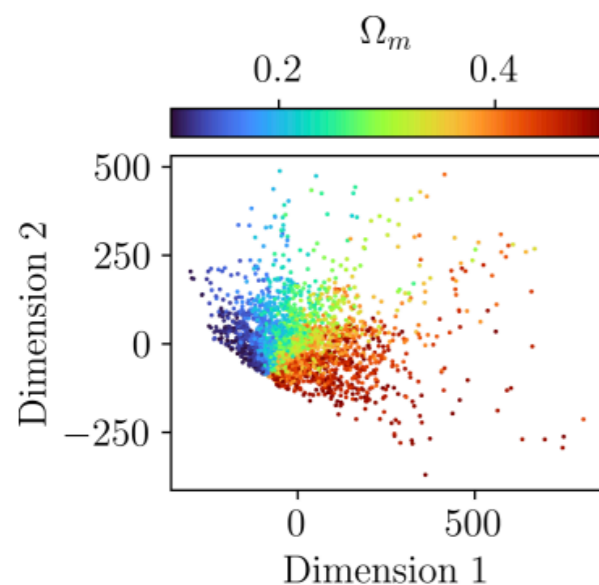
Density
fluctuations

BH feedback

Stellar feedback

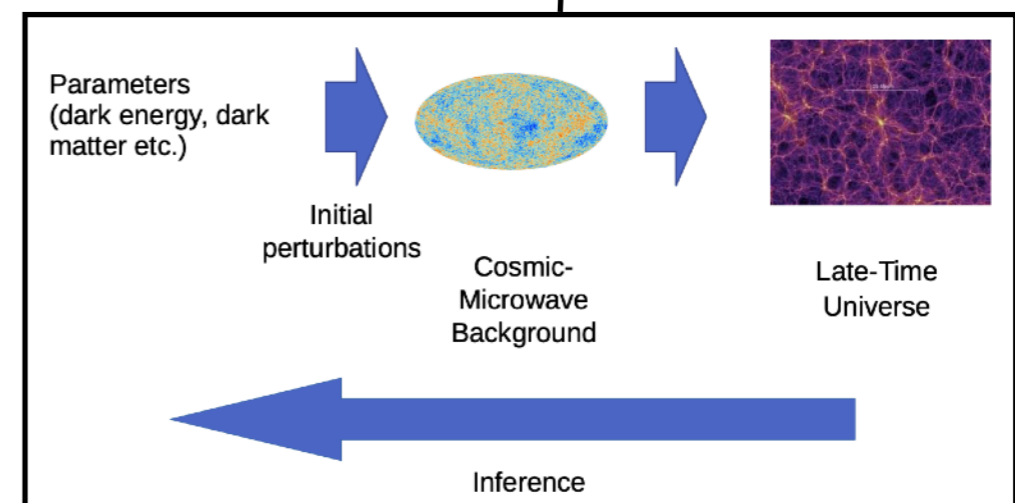


Learn parametrised surrogate of 3000 baryonic simulations, parametrised by 6 physics quantities



GNN summaries

Identify physics obs. in latent space



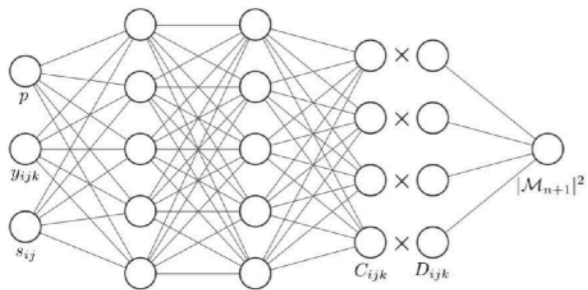
Distributions of galaxies

Targets

KISS AI: Can we replace MEs with ML-based surrogates?

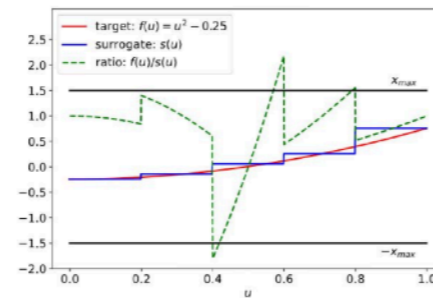
Machine Learning:

Design and train **suitable surrogate models**.



Monte Carlo:

Develop **unbiased algorithm** to use surrogates.

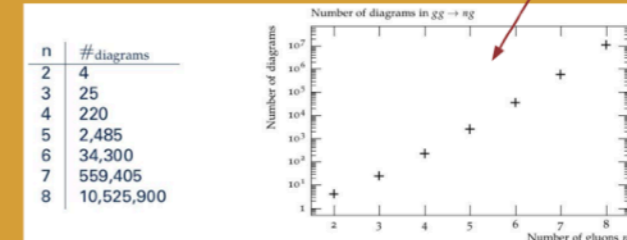


→ Monte Carlo unweighting in 2 stages: surrogate, real ME

Surrogate + Sampling
to remove bias

Expect **savings of O(50)**
Million CPU years!

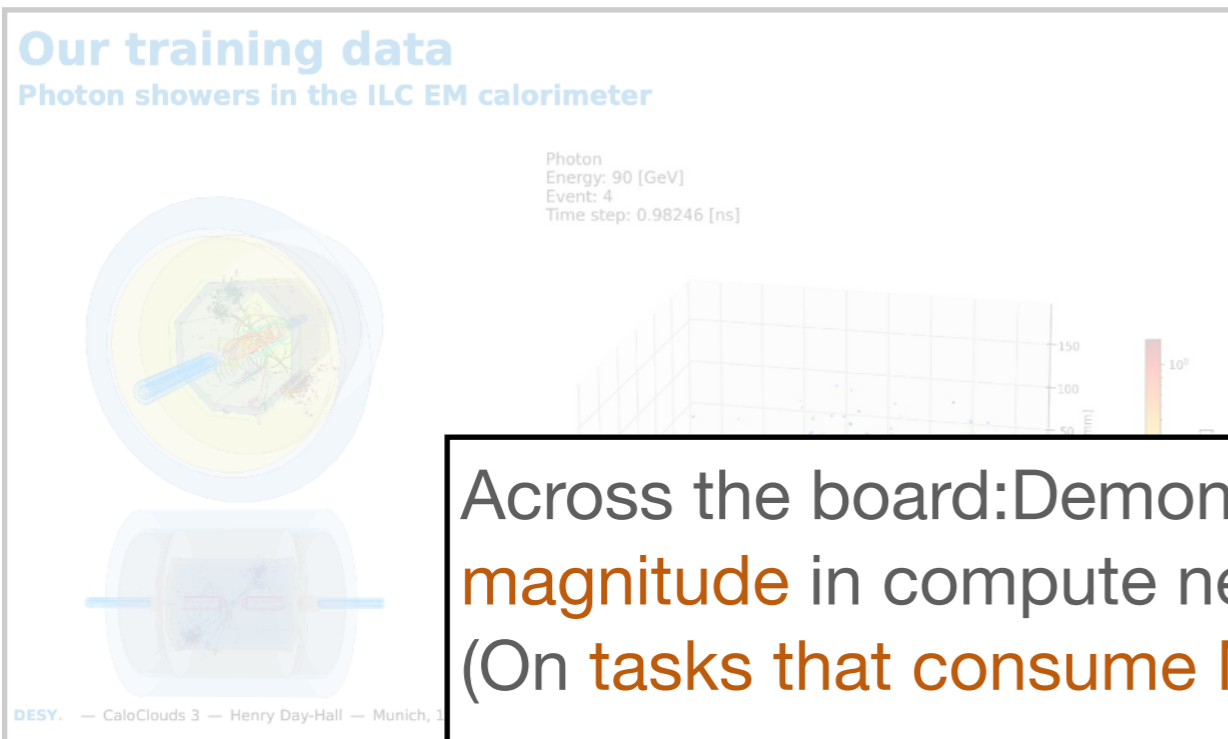
$$\hat{\sigma}_N = \int_{\text{cuts}} d\hat{\sigma}_N = \int_{\text{cuts}} \left[\prod_{i=1}^N \frac{d^3 q_i}{(2\pi)^3 2E_i} \right] \delta^4 \left(p_1 + p_2 - \sum_i q_i \right) |\mathcal{M}(p_1, p_2, q_1, \dots, q_N)|^2$$



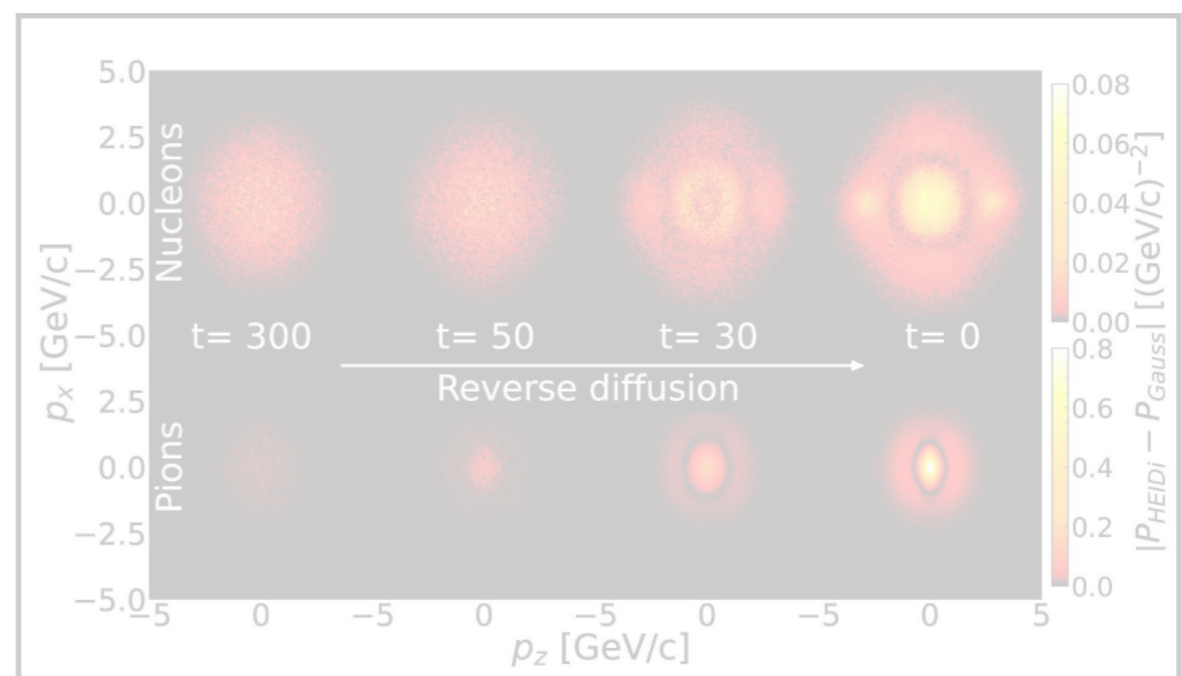
Hard-scattering matrix elements

Process	Events [M]	Summed [MHS23*y]	Sampled [MHS23*y]	Surrogates [MHS23*y]	Ratio
Z + ≤0 jets	53 797	0.03	0.03	-	
Z + ≤1 jets	164 479	0.10	0.10	-	
Z + ≤2 jets	456 960	0.29	0.30	-	
Z + ≤3 jets	835 797	0.58	0.74	-	
Z + ≤4 jets	1 164 974	1.16	2.25	-	
Z + ≤5 jets	1 381 719	8.93	18.08	3.10	2.8
Z + ≤6 jets	1 505 067	161.32	51.68	7.57	6.7

Targets



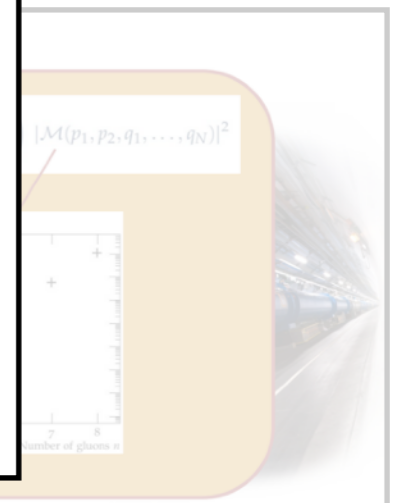
Particle shower



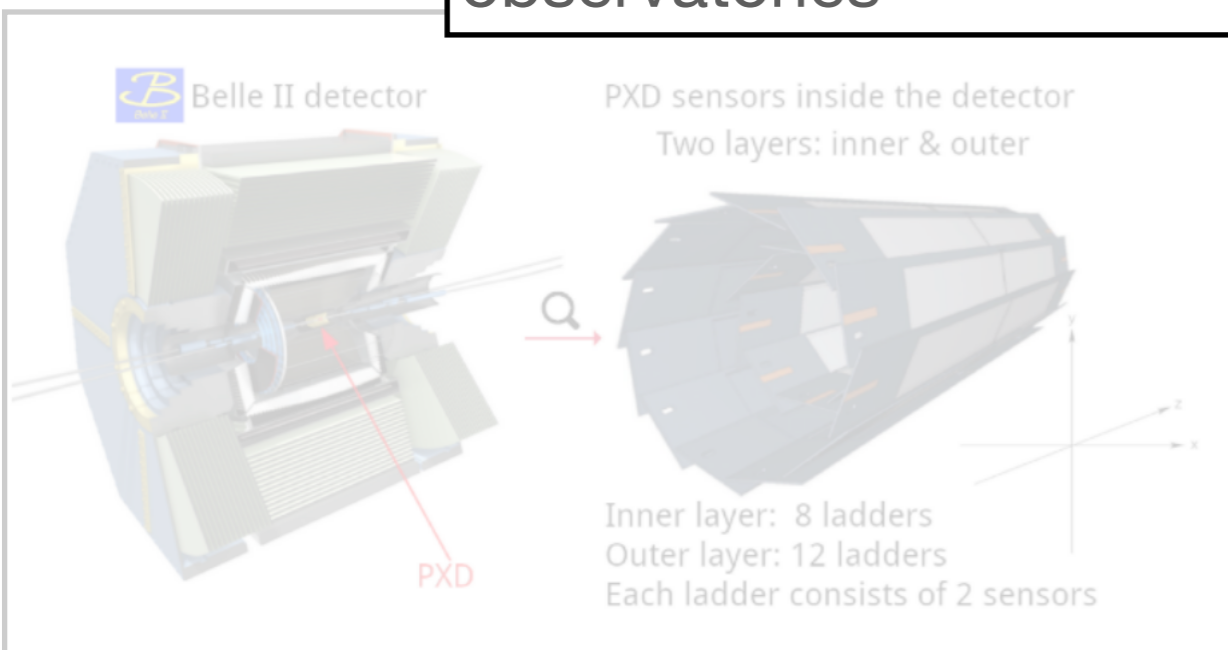
Heavy ion collisions

Across the board: Demonstrate **saving 1-3 orders of magnitude** in compute needs for simulation
(On **tasks that consume Millions of CPU years/year**)

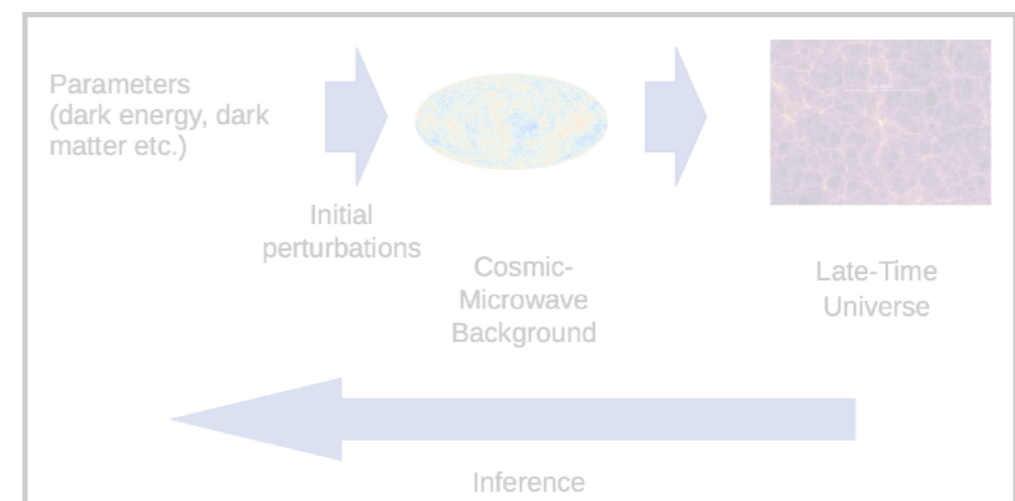
Required for next generation experiments and observatories



Hard-scattering matrix elements

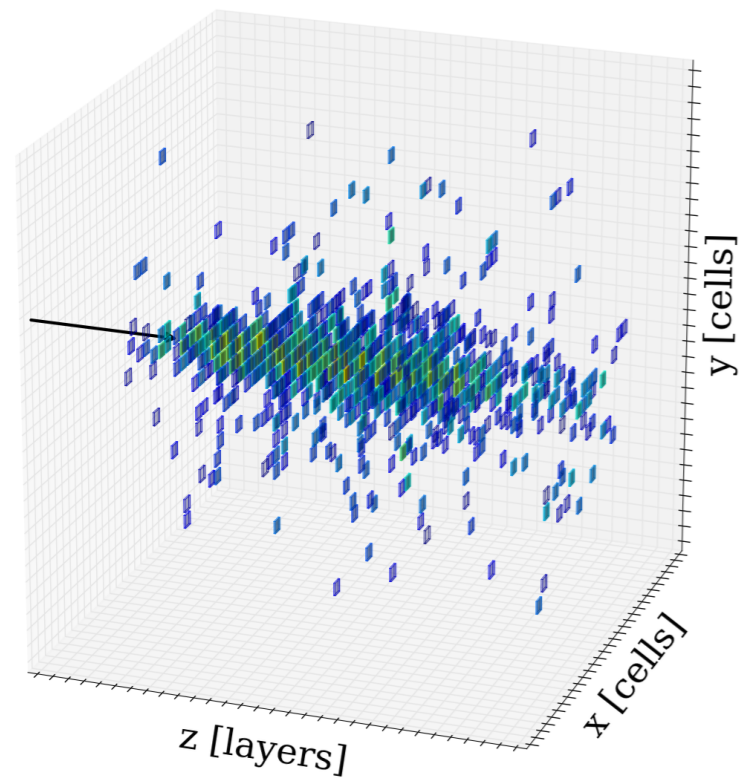


Background hits in pixel sensors

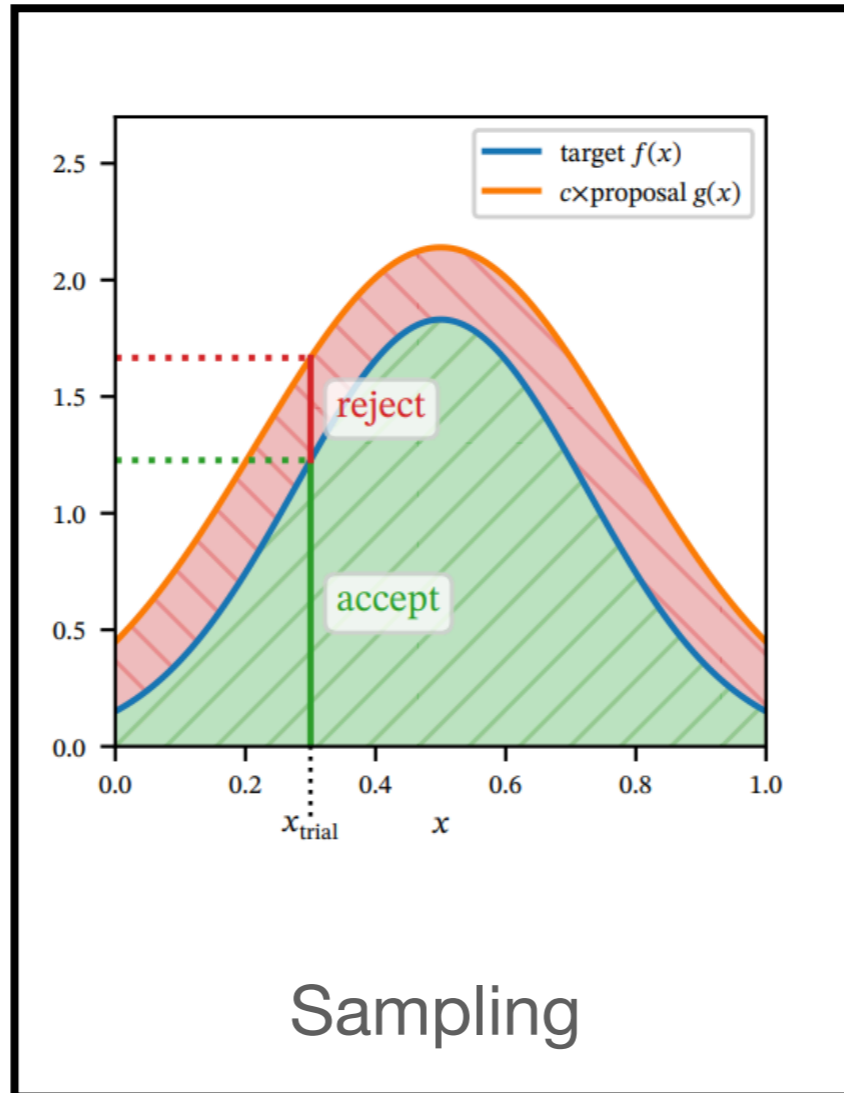


Distributions of galaxies

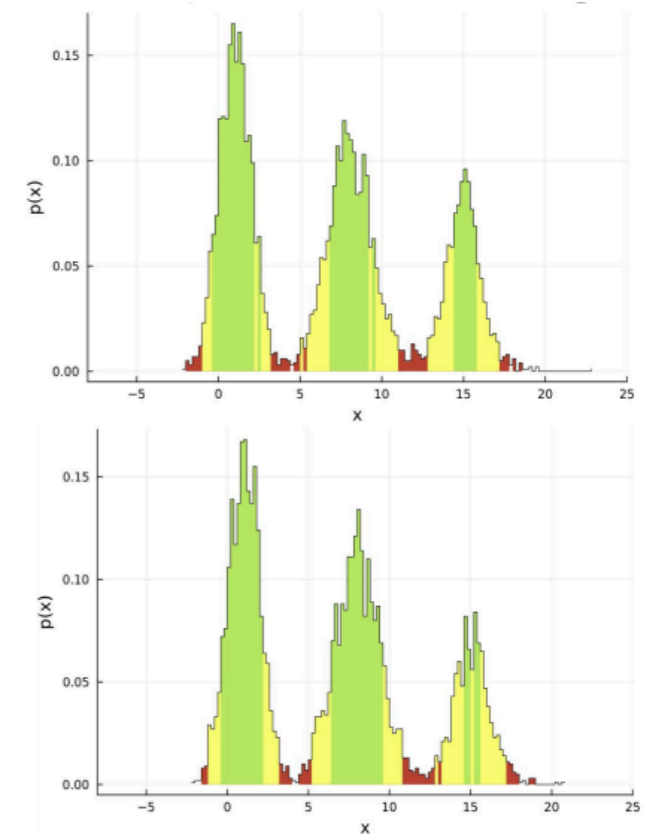
Overview



Surrogates

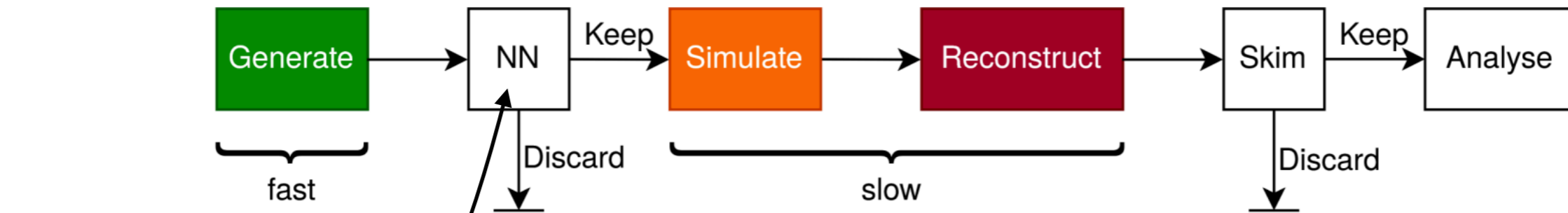


Sampling

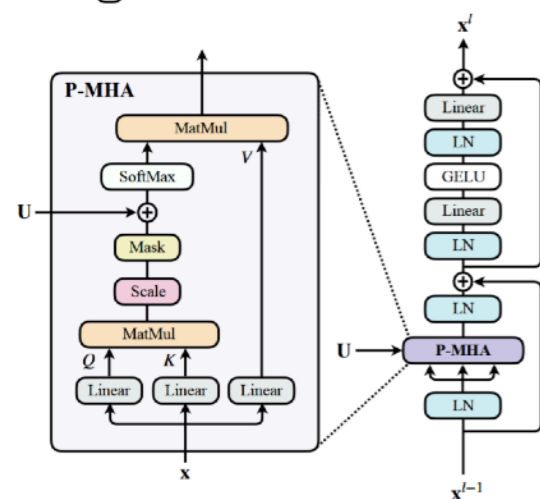
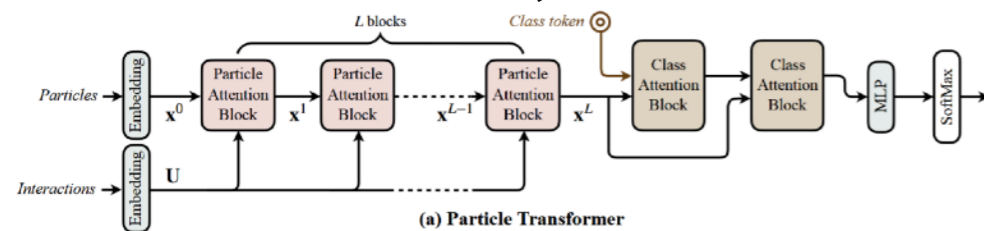


Quality

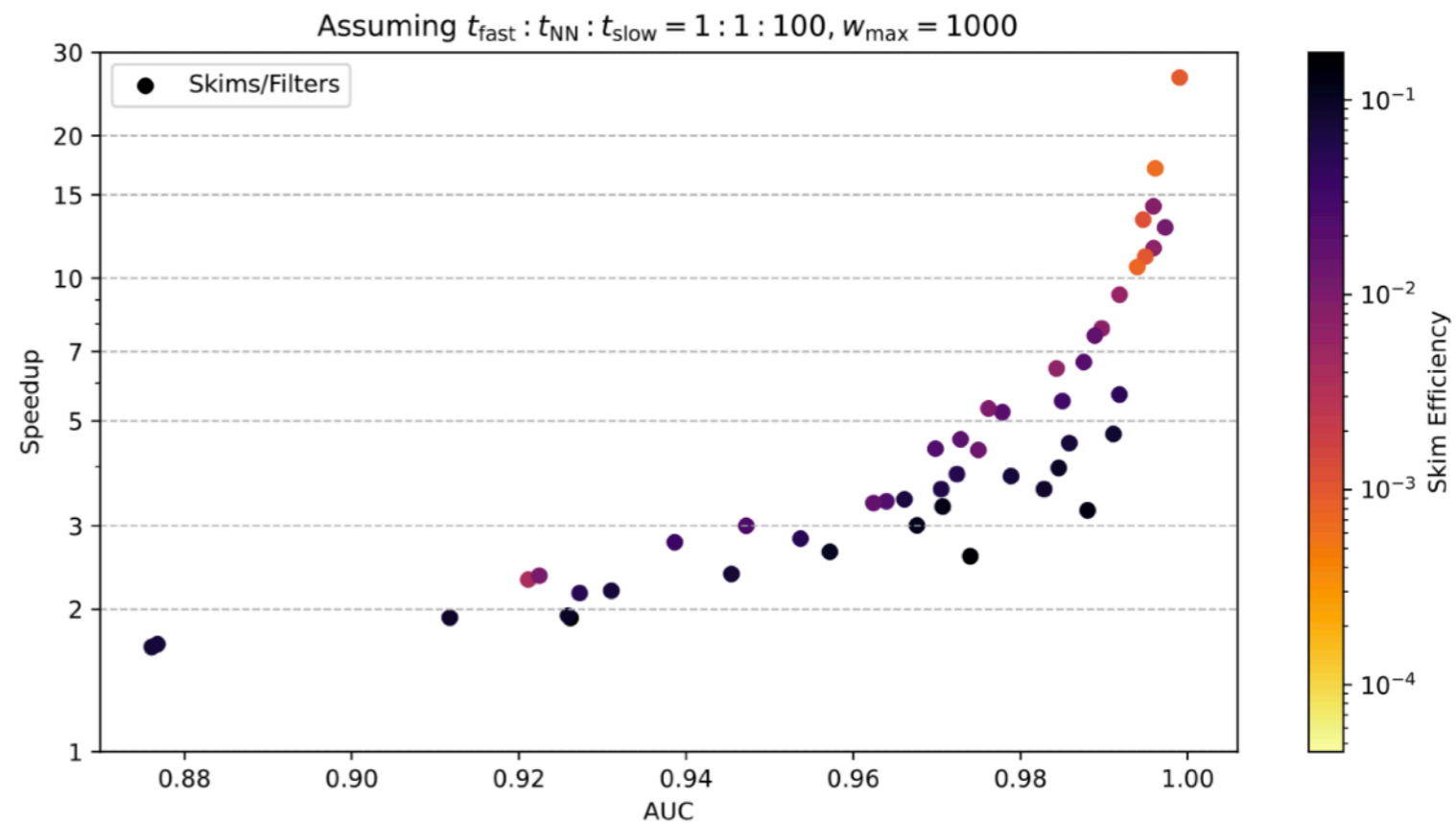
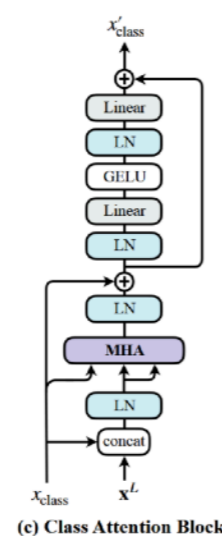
Smart background simulation



Transformer

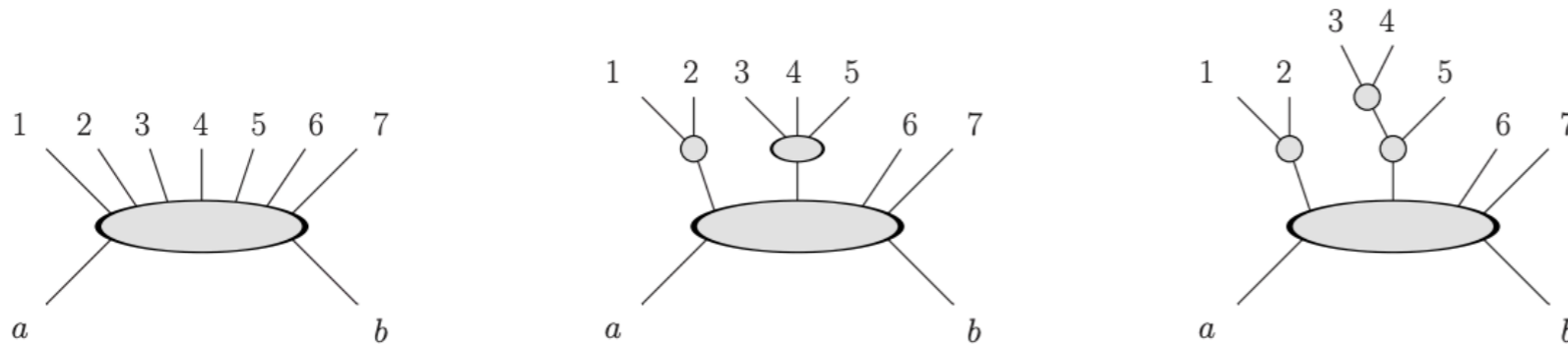


(b) Particle Attention Block
KISS annual meeting - 12.03.2025

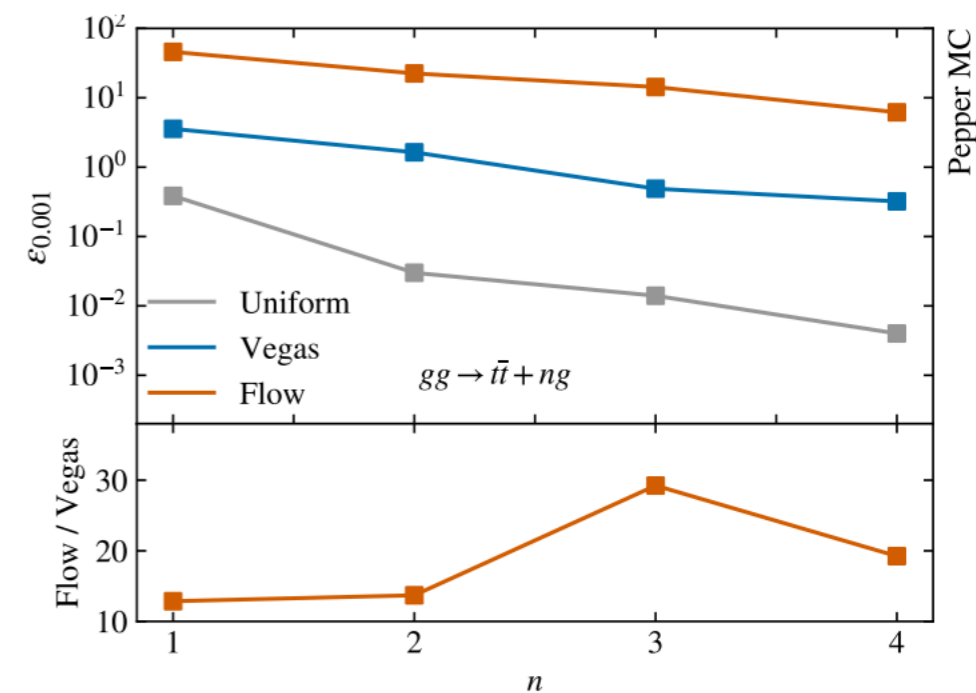
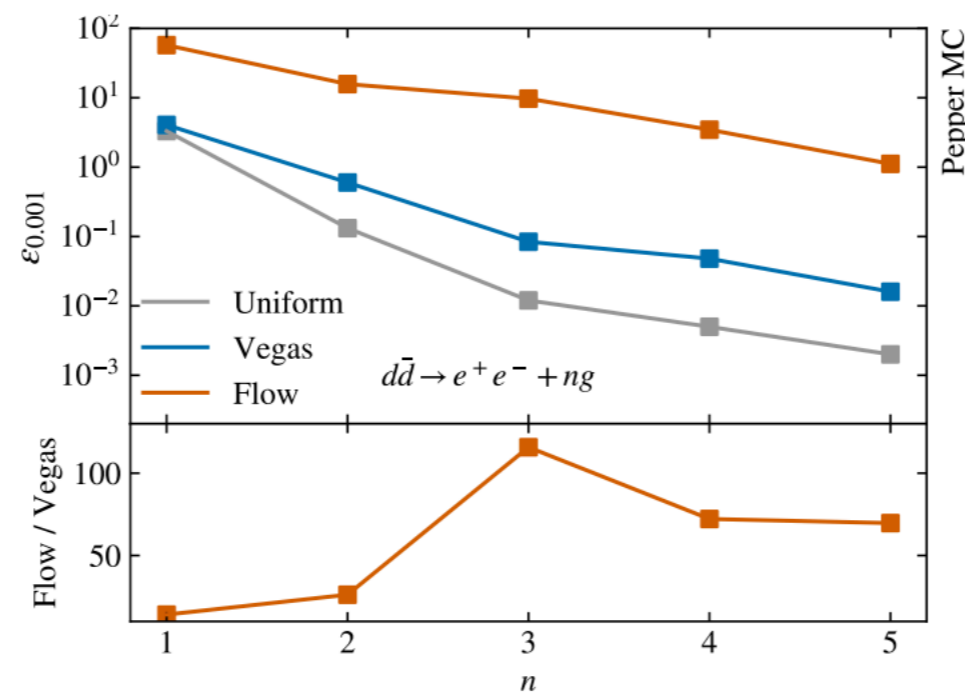


Speed-up depends on
physics selection: **~1 order
of magnitude**

Smart background simulation



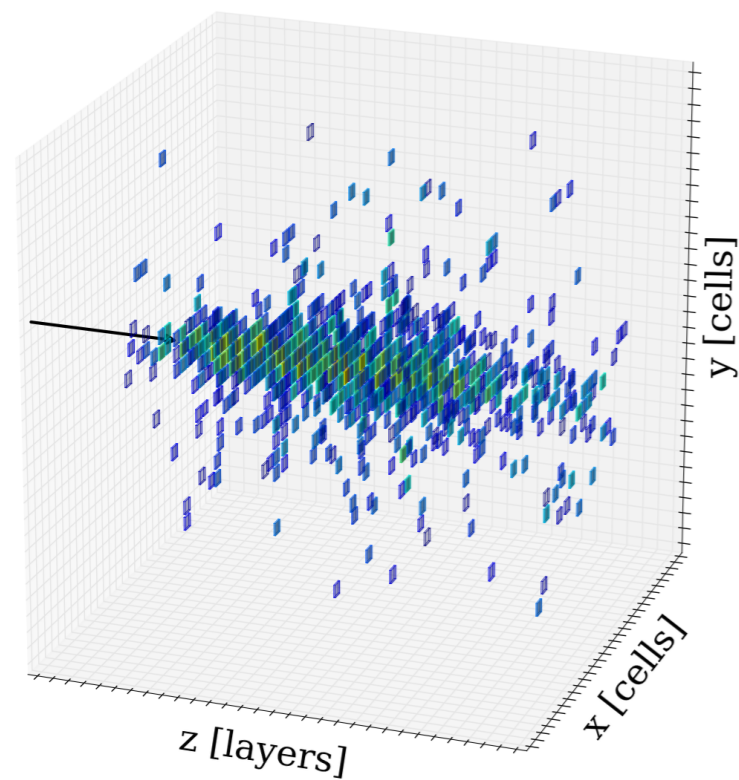
Use normalising
flows to predict
sampling
distributions at LO/
NLO



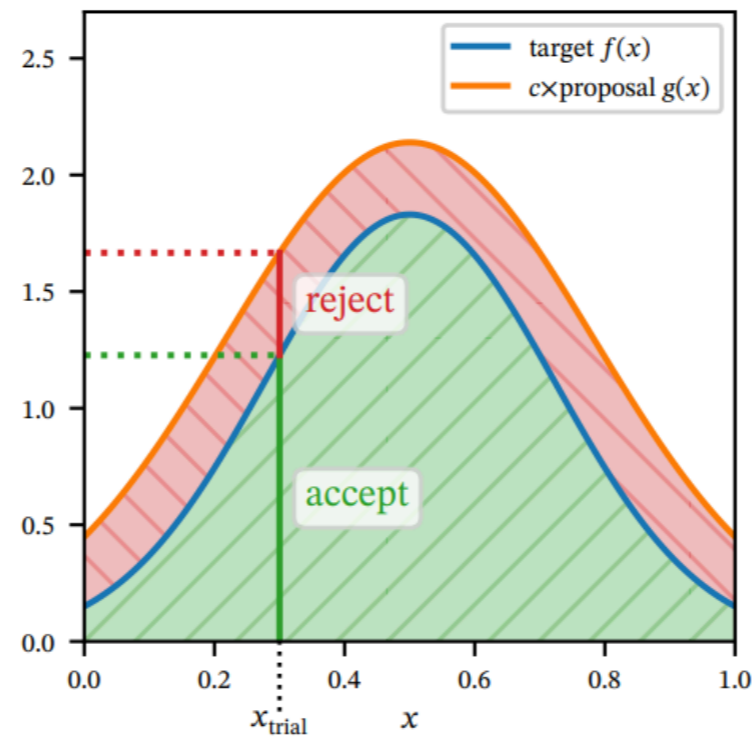
- ▶ significantly increased unw. eff. for all multiplicities
- ▶ factors up to 115
- ▶ seems to scale well

Again, 1-2 order of
magnitude

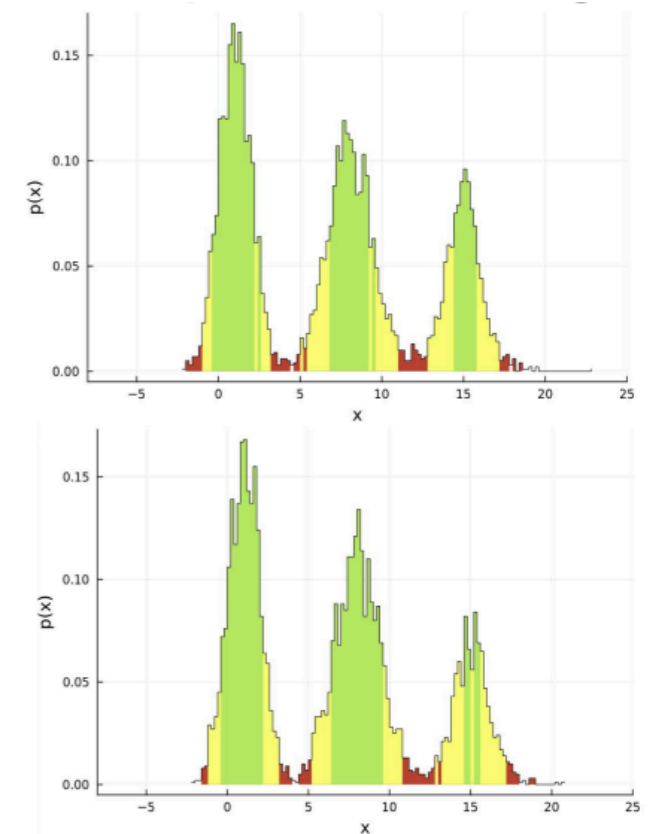
Overview



Surrogates

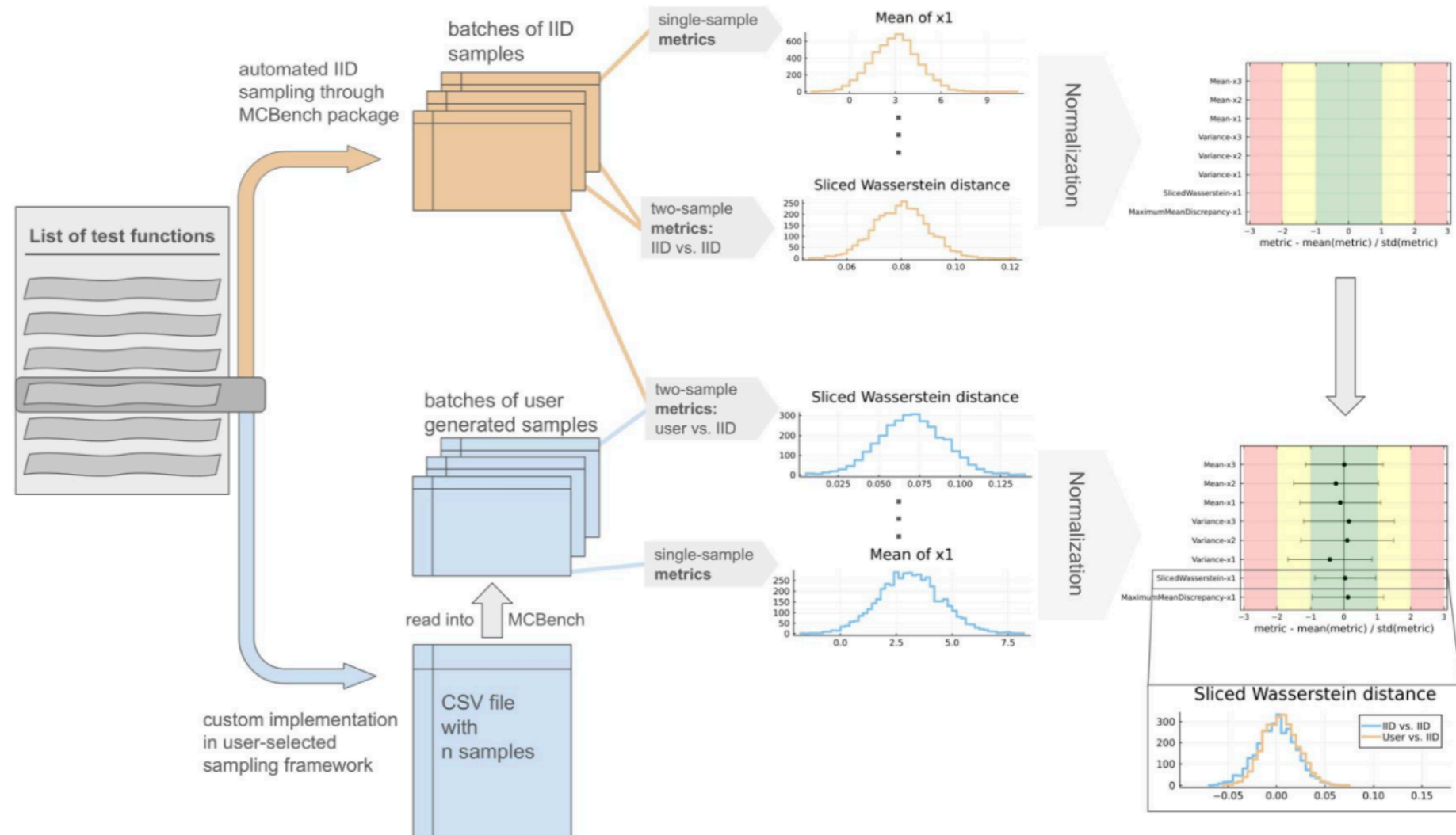
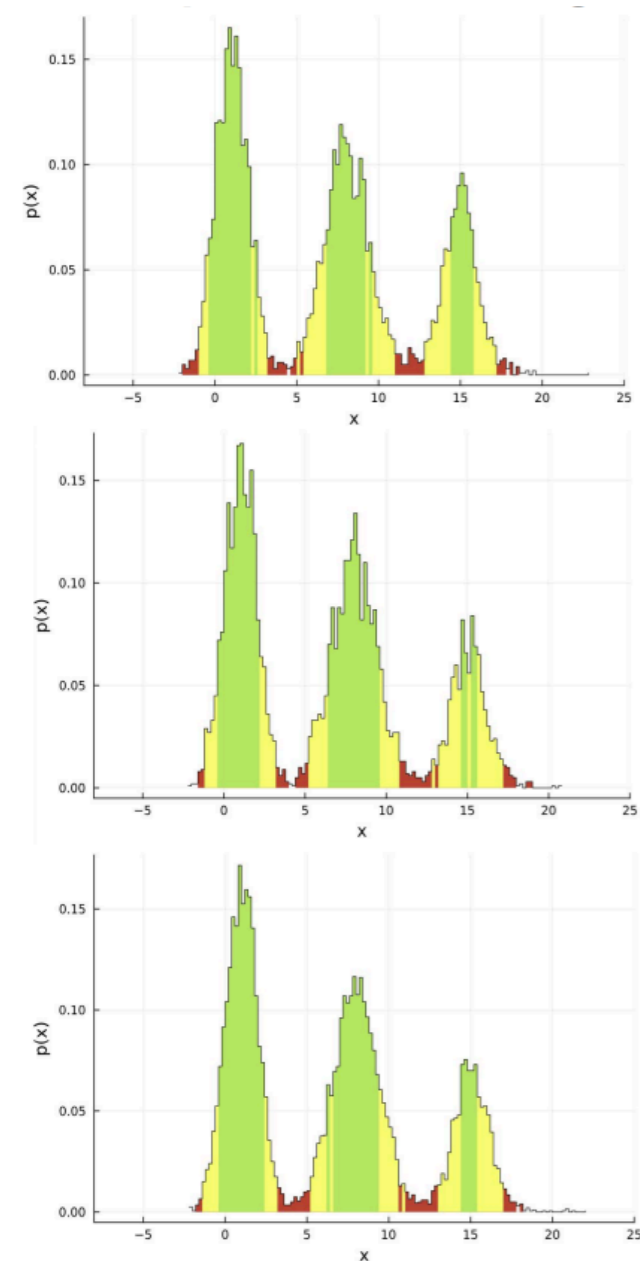


Sampling



Quality

Foundational Topics



Which samples are drawn from the same underlying distribution?

Build automated tools for comparing and benchmarking distributions

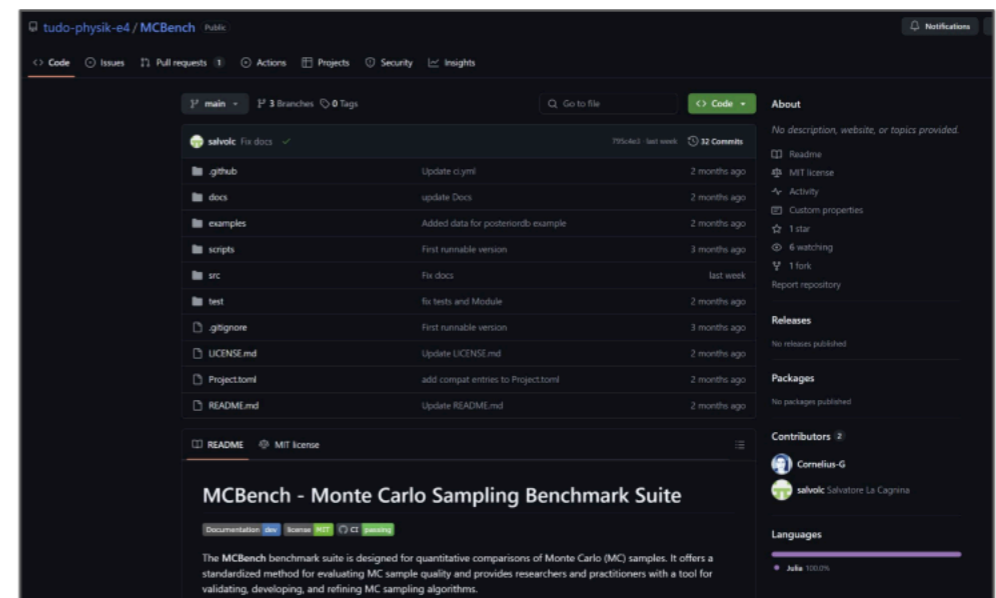
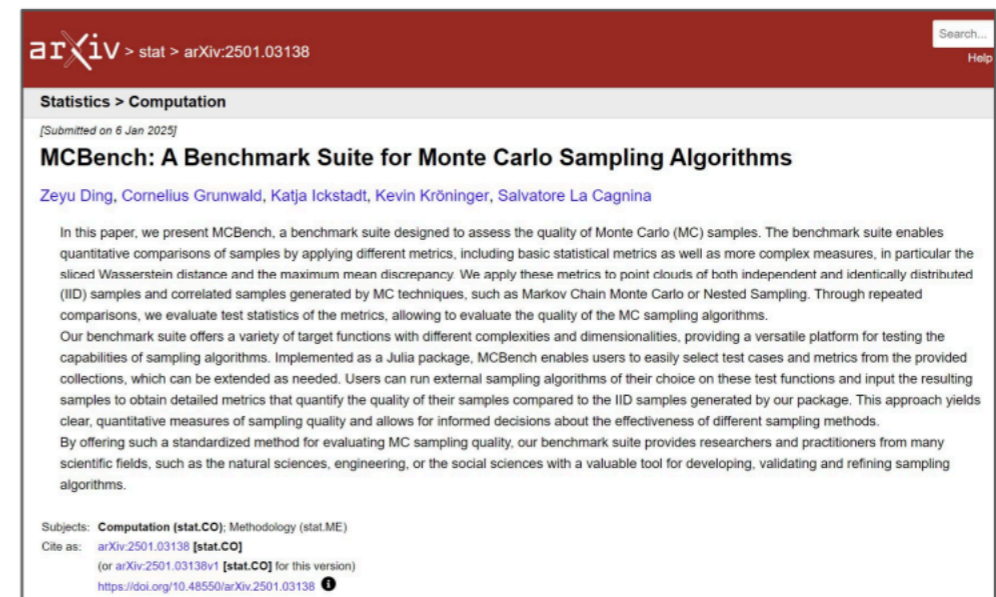
Foundational Topics

Summary and Conclusions

- Developed a test suite (in the julia programming language)
- Compare samplers to IID samples using metrics
- Provide a selection of (IID sampleable) test functions and (one and two-sample) metrics
- Visit our suite on github and paper on arxiv
 - <https://github.com/tudo-physik-e4/MCBench>
 - <https://arxiv.org/abs/2501.03138>

Next Steps:

- Add full test case support for different platforms (R, stan, pymc) including testpoints
- Lookout to include more complex test cases and applications

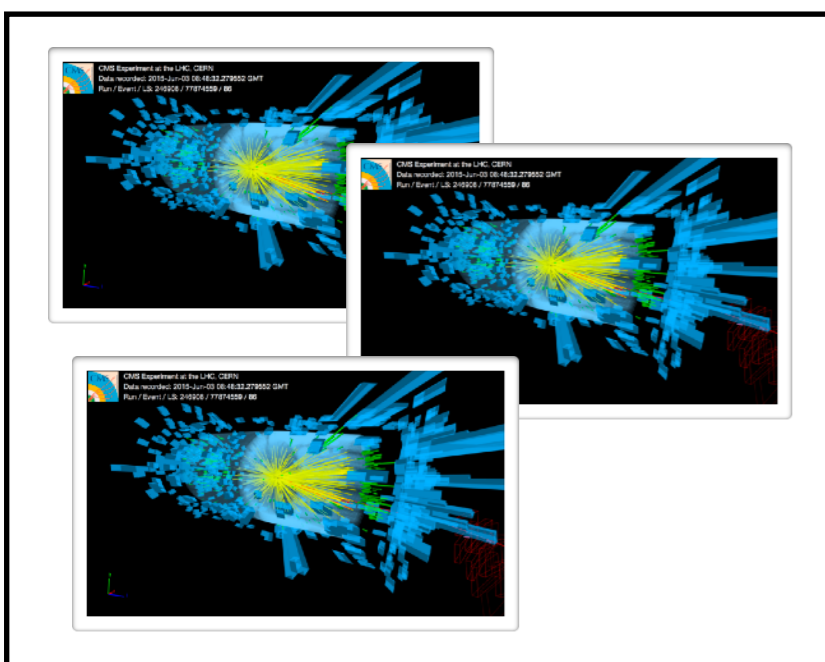


Paper & code now
publically available!

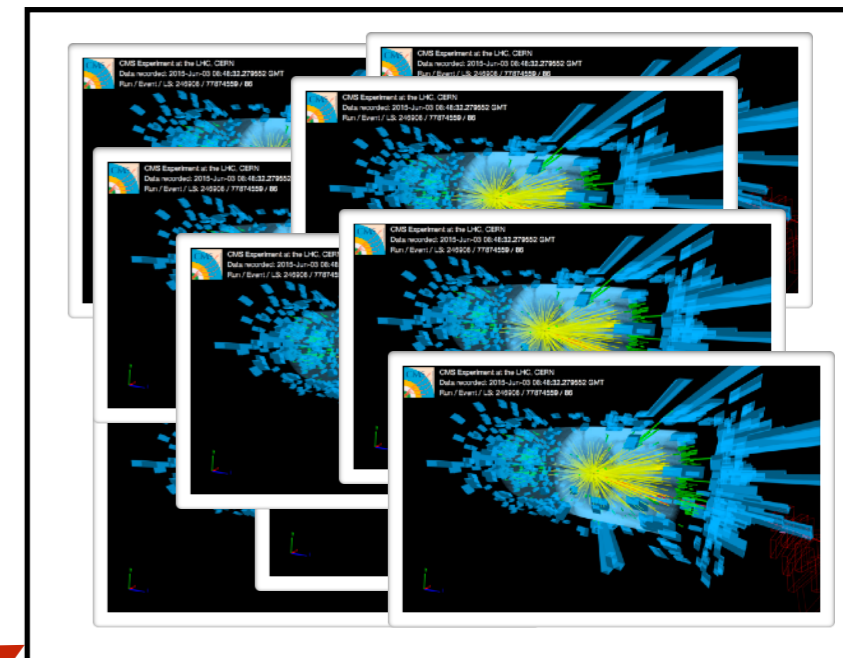
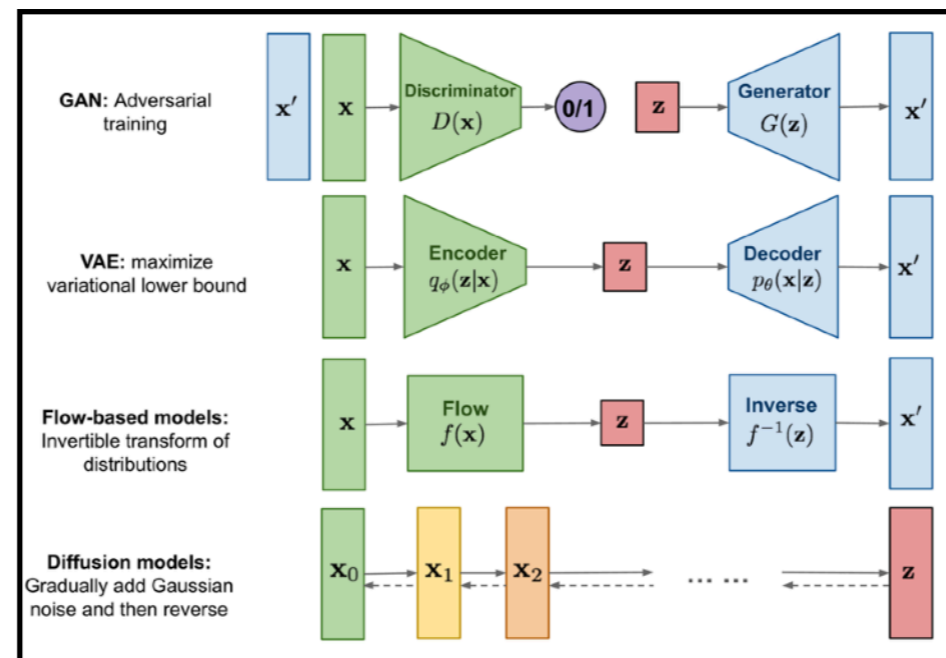
1. Use classical simulation or data as input

2. Train generative surrogate

3. Oversample

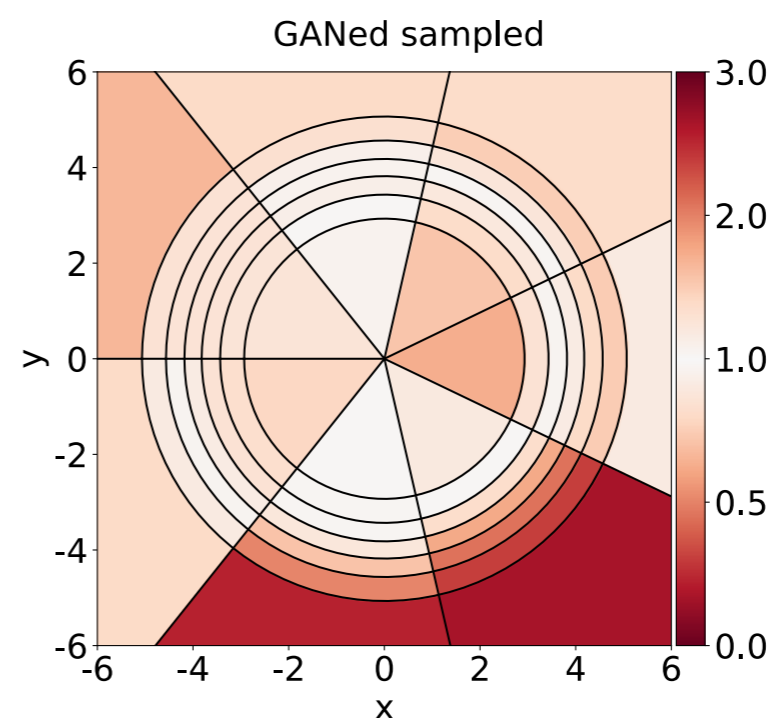
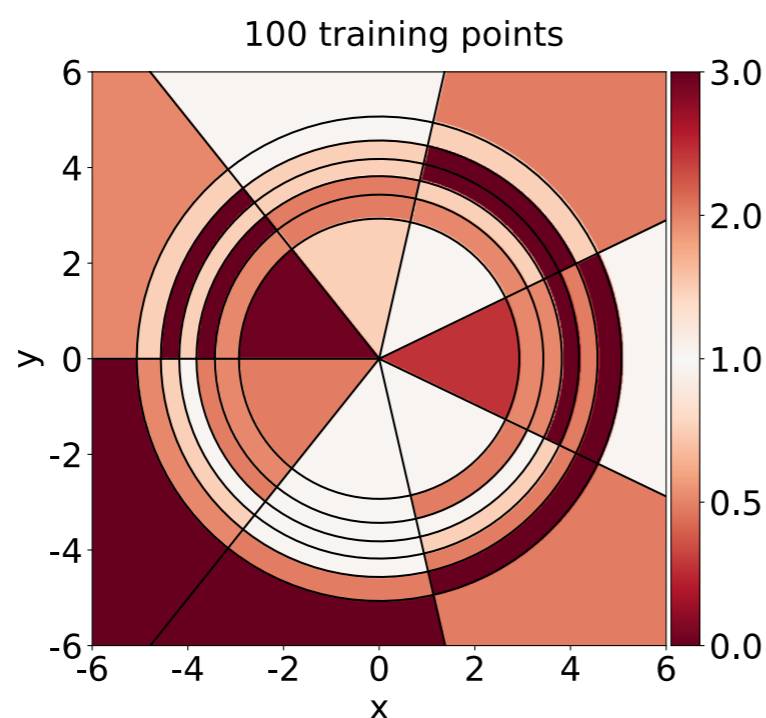


(slow)

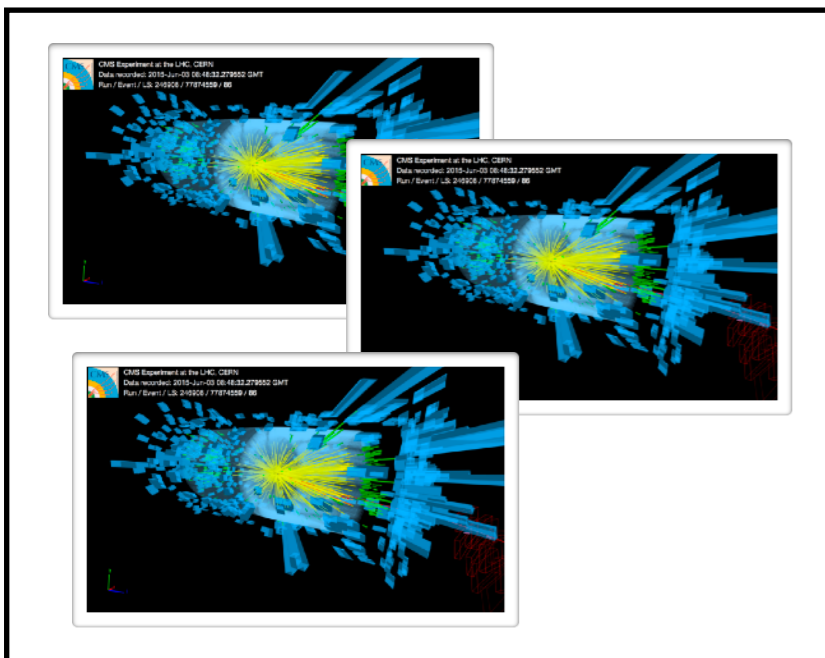


(fast)

Does this even make sense?

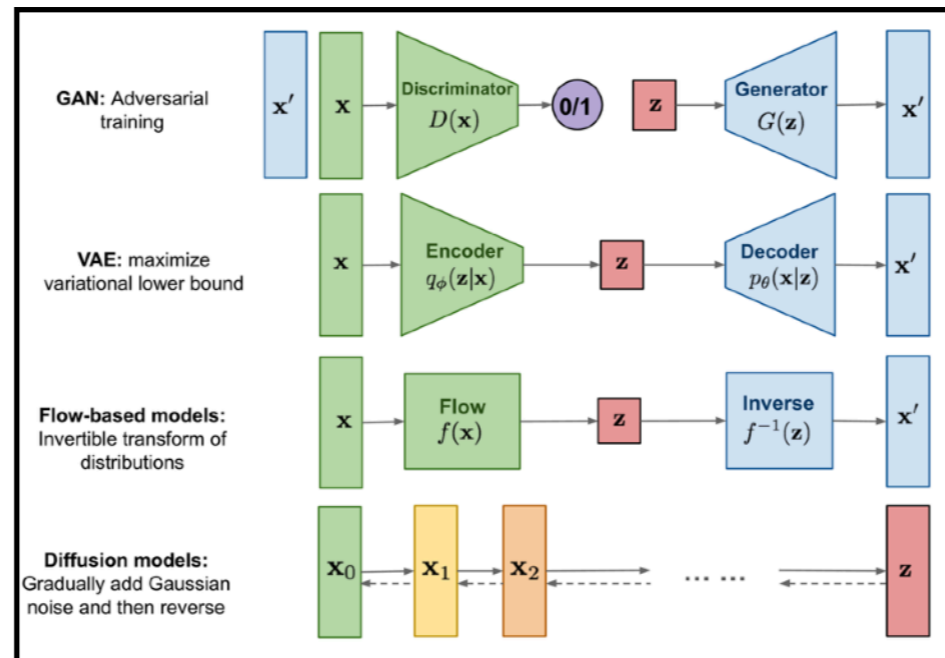


1. Use classical simulation or data as input

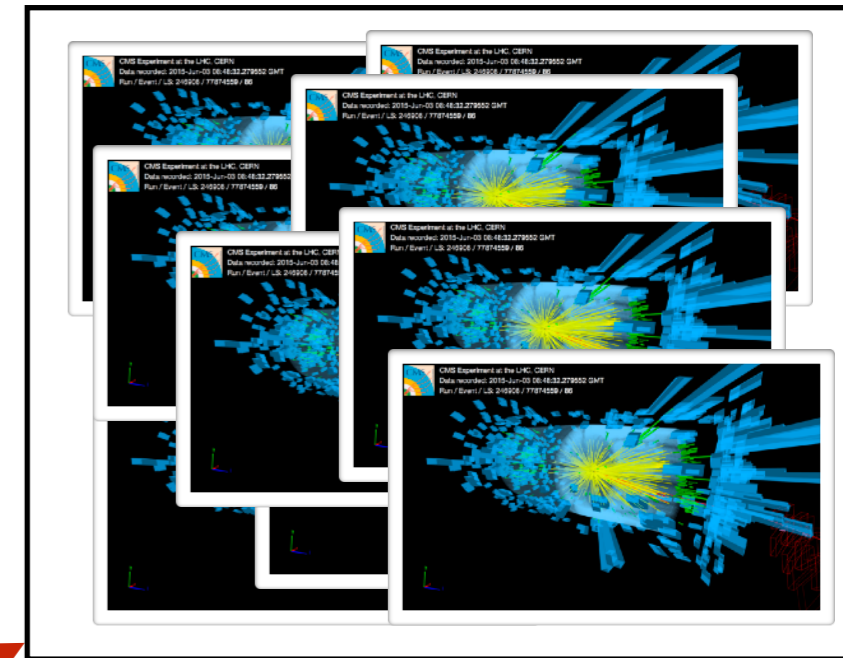


(slow)

2. Train generative surrogate

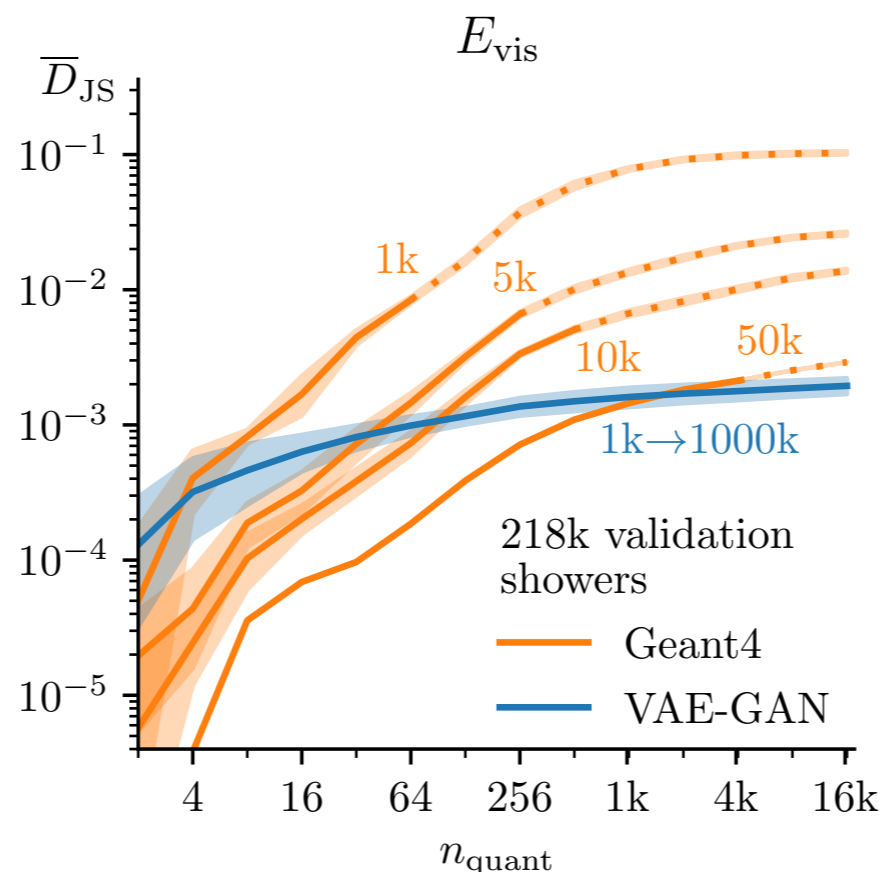
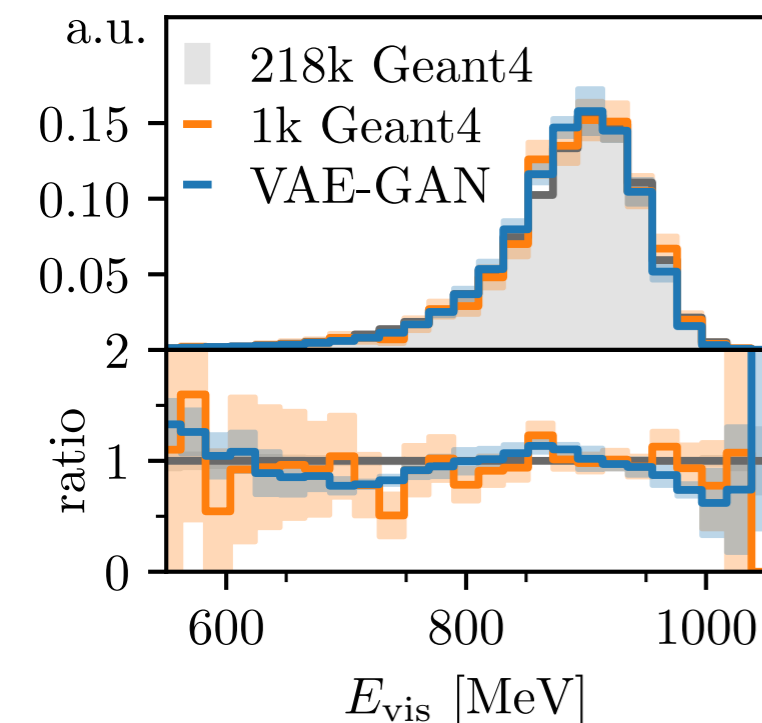


3. Oversample



(fast)

Does this even make sense?: Yes!



Scaling of difference to ground truth with resolution again better for the generative model.

Follow-up work with statisticians

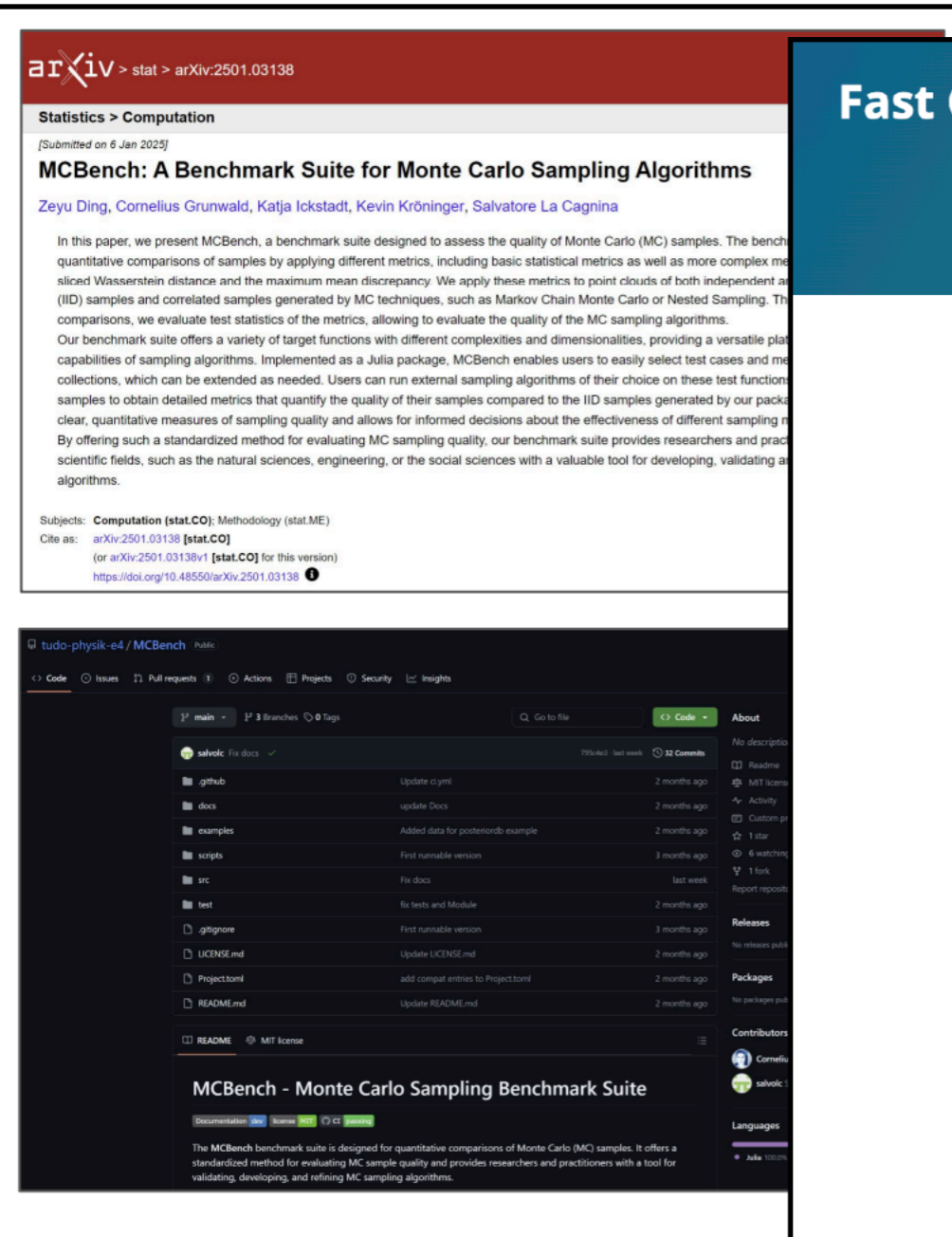
Closing

New angles on fast calorimeter shower simulation	https://inspirehep.net/literature/2647716
CaloClouds: fast geometry-independent highly-granular calorimeter	https://inspirehep.net/literature/2657637
CaloClouds II: ultra-fast geometry-independent highly-granular calorimeter	https://inspirehep.net/literature/2696622
EPiC-ly Fast Particle Cloud Generation with Flow-Matching and Diffusion	https://inspirehep.net/literature/2705220
Flow Matching Beyond Kinematics: Generating Jets with Particle-ID and	https://inspirehep.net/literature/2729197
Simulating images of radio galaxies with diffusion models	https://ui.adsabs.harvard.edu/abs/2024arXiv241007794V/abstract
Deep-learning-based radiointerferometric imaging with GAN-aided training	https://ui.adsabs.harvard.edu/abs/2023A%26A...677A.167G/abstract
Convolutional L2LFlows: generating accurate showers in highly granular	https://inspirehep.net/literature/2793021
Calibrating Bayesian Generative Machine Learning for Bayesiamplication	https://inspirehep.net/literature/2814095
How to understand limitations of generative networks	https://inspirehep.net/literature/2663017
Precision-Machine Learning for the Matrix Element Method	https://inspirehep.net/literature/2709868
The MadNIS reloaded	https://inspirehep.net/literature/2718812
Kicking it Off(-shell) with Direct Diffusion	https://inspirehep.net/literature/2727894
Normalizing Flows for High-Dimensional Detector Simulations	https://inspirehep.net/literature/2737698
The Landscape of Unfolding with Machine Learning	https://inspirehep.net/literature/2781602
CaloDREAM -- Detector Response Emulation via Attentive flow Matching	https://inspirehep.net/literature/2787493
Lorentz-Equivariant Geometric Algebra Transformers for High-Energy	https://inspirehep.net/literature/2789600
Differentiable MadNIS-Lite	https://inspirehep.net/literature/2814426
Machine learning study to identify collective flow in small and large colliding	https://inspirehep.net/literature/2660500
Building imaginary-time thermal field theory with artificial neural networks	https://inspirehep.net/literature/2787839
Phase Transition Study Meets Machine Learning	https://inspirehep.net/literature/2721834
Diffusion models as stochastic quantization in lattice field theory	https://inspirehep.net/literature/2704849
Mass and tidal parameter extraction from gravitational waves of binary	https://inspirehep.net/literature/2673529
Exploring QCD matter in extreme conditions with Machine Learning	https://inspirehep.net/literature/2646083
Improved selective background Monte Carlo simulation at Belle II with graph	https://inspirehep.net/literature/2676588
Ultra-high-granularity detector simulation with intra-event aware generative	https://inspirehep.net/literature/2642136
Improved selective background Monte Carlo simulation at Belle II with graph	https://indico.cern.ch/event/1253794/contributions/5588582/
QCD Equation of State of Dense Nuclear Matter from a Bayesian Analysis of	https://inspirehep.net/literature/2512939
Efficient phase-space generation for hadron collider event simulation	https://inspirehep.net/literature/2630465
A Portable Parton-Level Event Generator for the High-Luminosity LHC	https://inspirehep.net/literature/2721108
Unweighting multijet event generation using factorisation-aware neural	https://inspirehep.net/literature/2628385
Development of the time-of-flight particle identification for future Higgs	https://inspirehep.net/literature/2720464
Improving Monte Carlo simulations in high energy physics using machine	https://inspirehep.net/literature/2698487
Event generation with Sherpa 3	https://inspirehep.net/literature/2843469
Learning Optimal and Interpretable Summary Statistics of Galaxy Catalogs	https://inspirehep.net/literature/2848384
MCBench: A Benchmark Suite for Monte Carlo Sampling Algorithms	https://arxiv.org/abs/2501.03138
Full phase space resonant anomaly detection	https://arxiv.org/abs/2310.06897
Generative Diffusion Models for Lattice Field Theory	https://arxiv.org/abs/2311.03578
Accurate Surrogate Amplitudes with Calibrated Uncertainties	https://inspirehep.net/literature/2860406
Phase space sampling with Markov Chain Monte Carlo methods	https://inspirehep.net/literature/2860425
Advancing Tools for Simulation-Based Inference	https://inspirehep.net/literature/2838939

40+ KISS papers
since 1.3.2023

<https://kiss.pages.desy.de/website/page/activities/>

Code & data for KISS projects



Fast Calorimeter Simulation Challenge 2022

[View on GitHub](#)

Welcome to the home of the first-ever Fast Calorimeter Simulation Challenge!

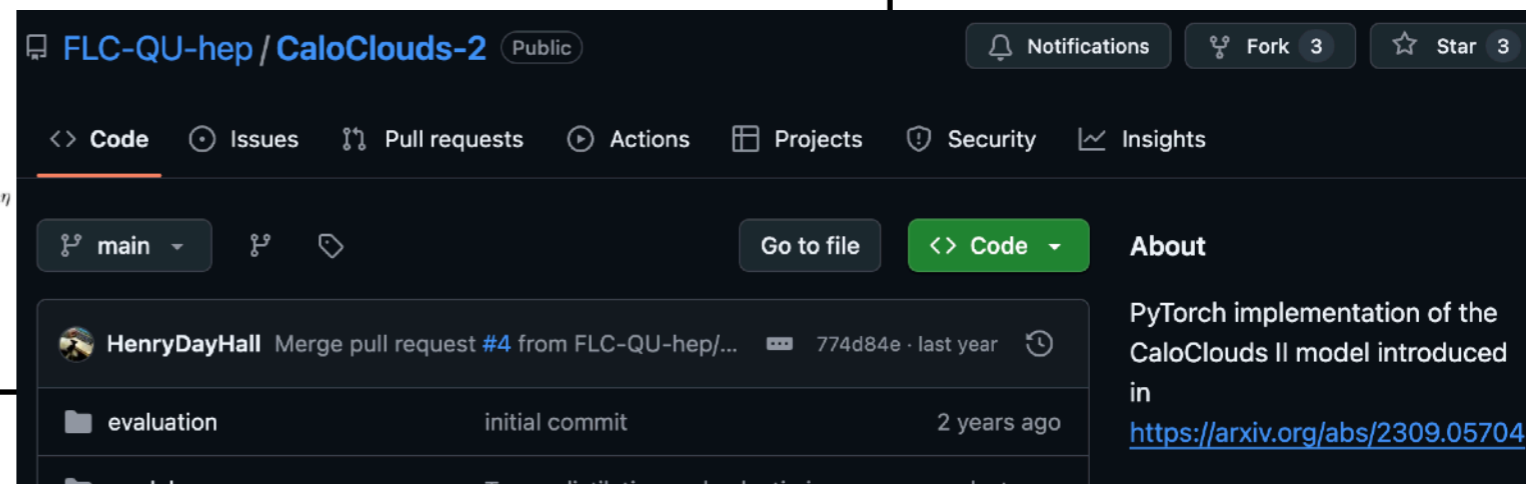
The purpose of this challenge is to spur the development and benchmarking of fast and high-fidelity calorimeter shower generation using deep learning methods. Currently, generating calorimeter showers of interacting particles (electrons, photons, pions, ...) using GEANT4 is a major computational bottleneck at the LHC, and it is forecast to overwhelm the computing budget of the LHC experiments in the near future. Therefore there is an urgent need to develop GEANT4 emulators that are both fast (computationally lightweight) and accurate. The LHC collaborations have been developing fast simulation methods for some time, and the hope of this challenge is to directly compare new deep learning approaches on common benchmarks. It is expected that participants will make use of cutting-edge techniques in generative modeling with deep learning, e.g. GANs, VAEs and normalizing flows.

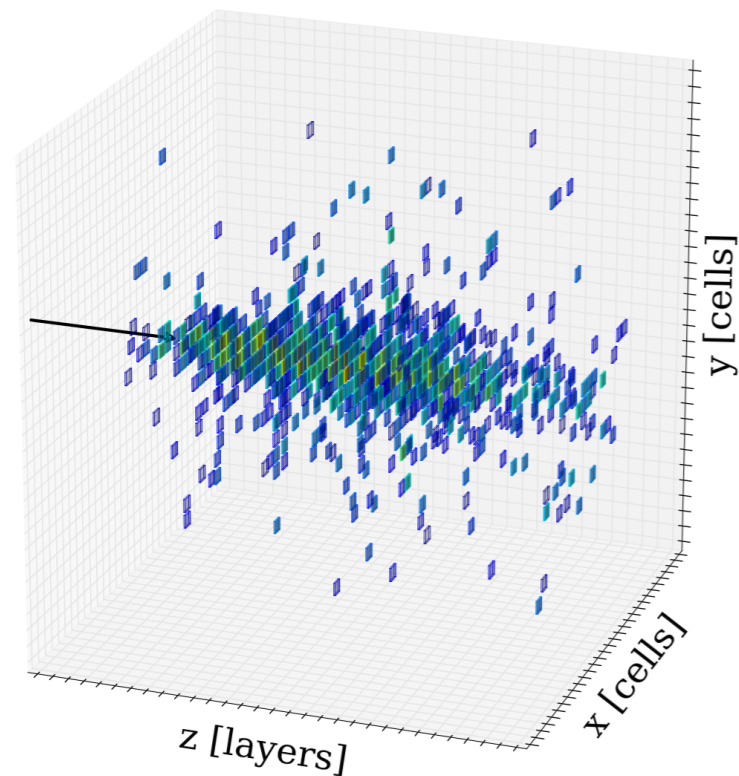
This challenge is modeled after two previous, highly successful data challenges in HEP – the [top tagging community challenge](#) and the [LHC Olympics 2020 anomaly detection challenge](#).

Datasets

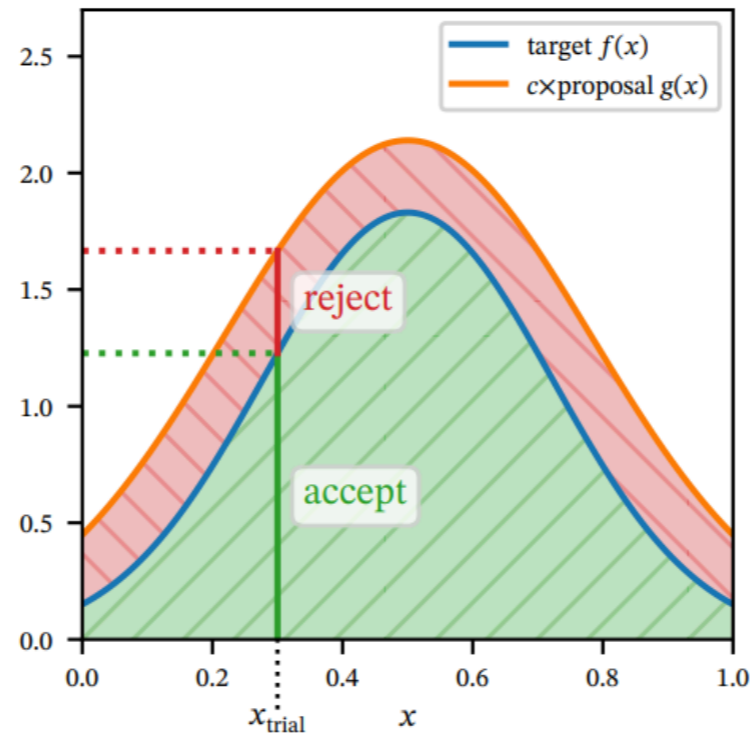
The challenge offers three datasets, ranging in difficulty from “easy” to “medium” to “hard”. The difficulty is set by the dimensionality of the calorimeter showers (the number layers and the number of voxels in each layer).

Each dataset has the same general format. The detector geometry consists of concentric cylinders with particles propagating along the z-axis. The detector is segmented along the z-axis into discrete layers. Each layer has bins along the radial direction and some of them have bins in the angle α . The number of layers and the number of bins in r and α is stored in the binning .xml files and will be read out by the HighLevelFeatures class of helper functions. The coordinates $\Delta\phi$ and $\Delta\eta$ correspond to the x- and y axis of the cylindrical coordinates. The image below shows a 3d view of a geometry with 3 layers, with each layer having 3 bins in radial and 6 bins in angular direction. The right image shows the front view of the geometry, as seen along the z axis.

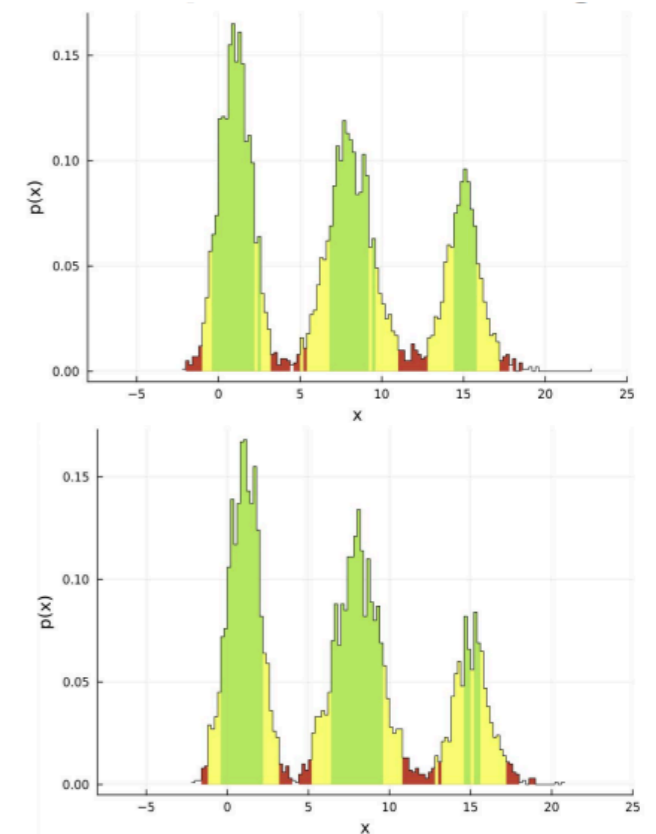




Surrogates



Sampling



Quality

Major improvements
(x10-x100) of
efficiency for key
simulation needs

Substantial
publications and
public data & code

Generally usable
tools and
foundational work
with statistics

