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Conditioned Calo4pQVAE: High-energy calorimeter-particle interactions using deep learning and quantum annealers

★arXiv:2410.22870

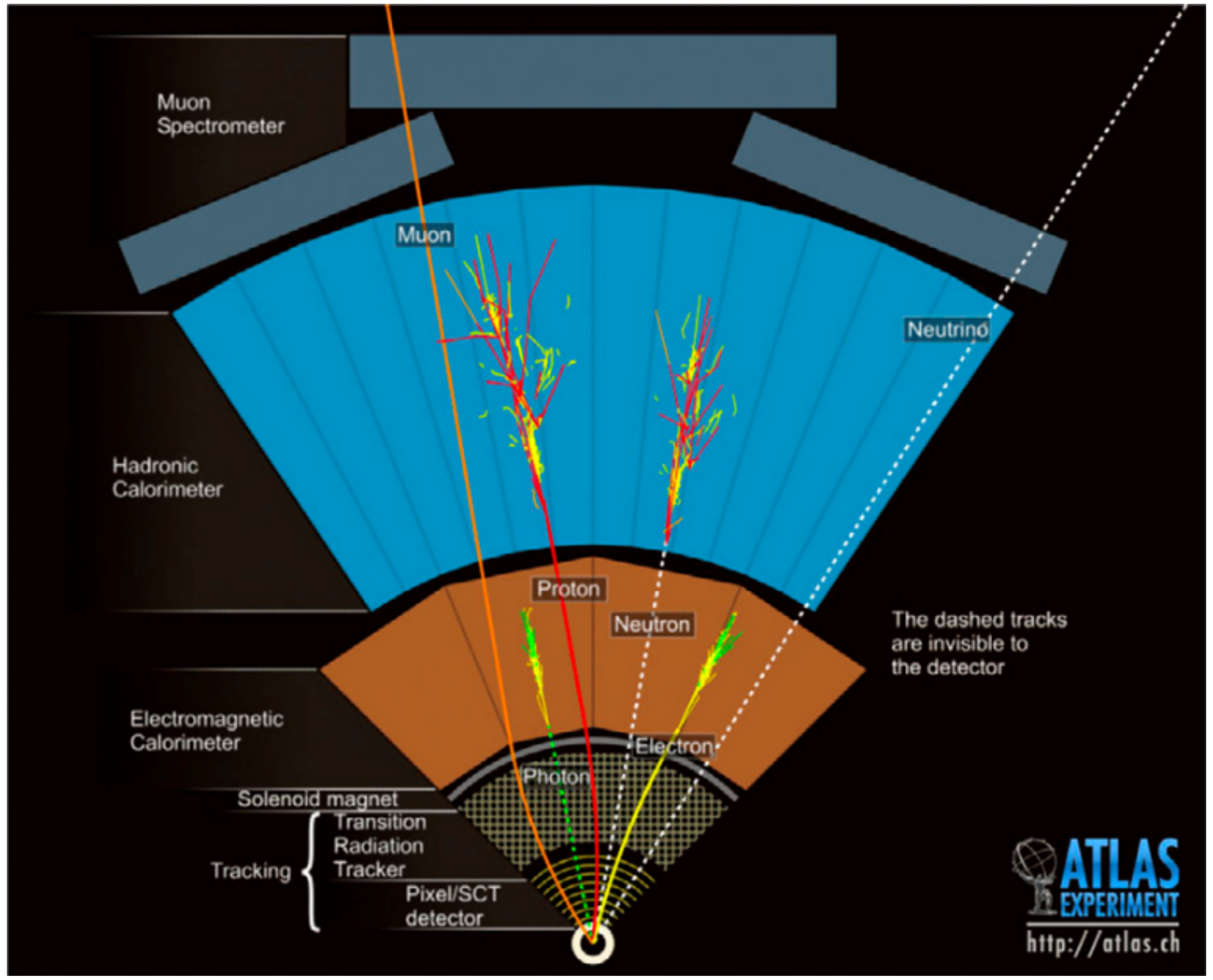
11/11/24 :: IFAE UAB

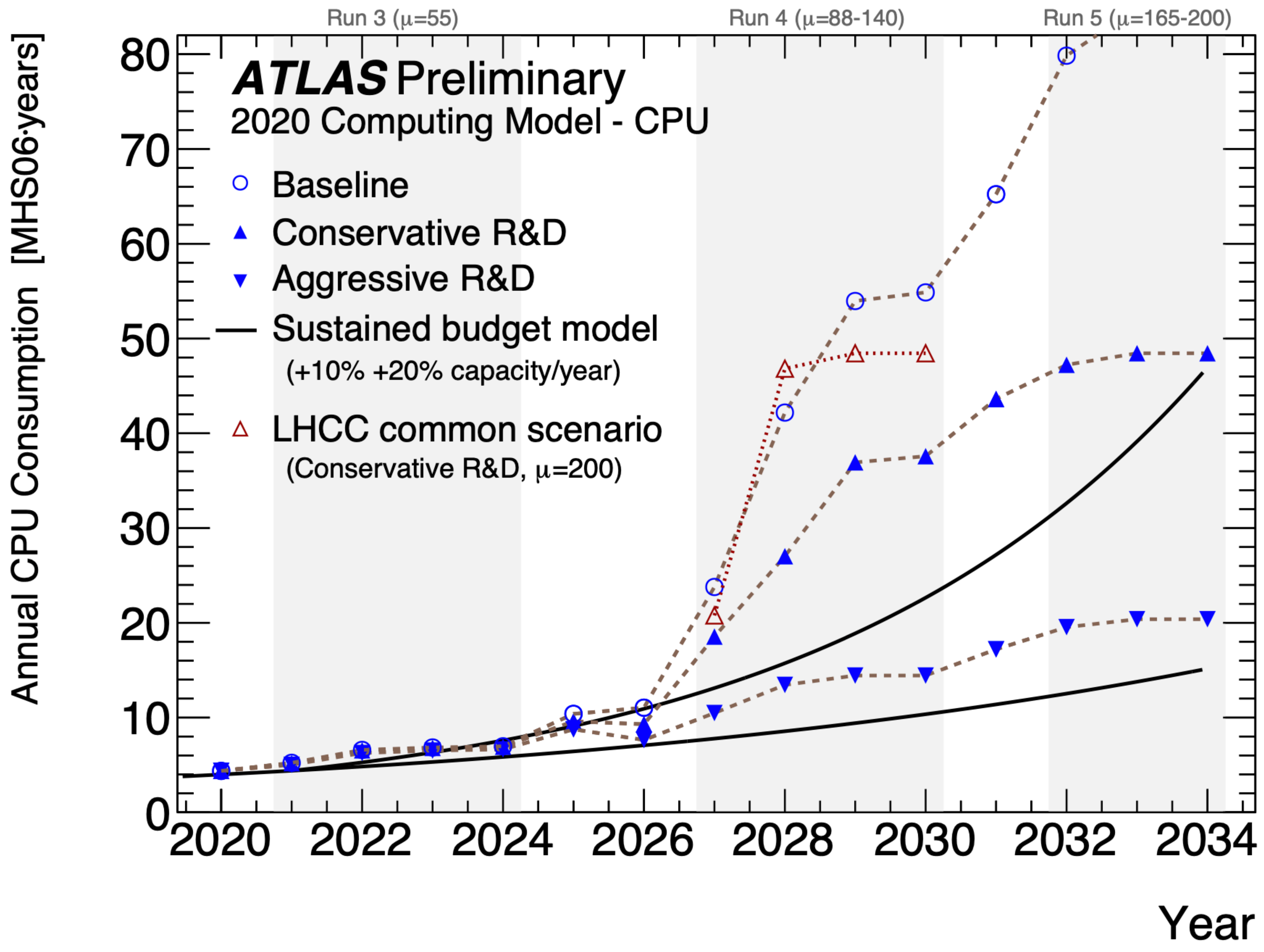
J. Quetzalcoatl Toledo-Marin
Quantum Machine Learning Research Associate

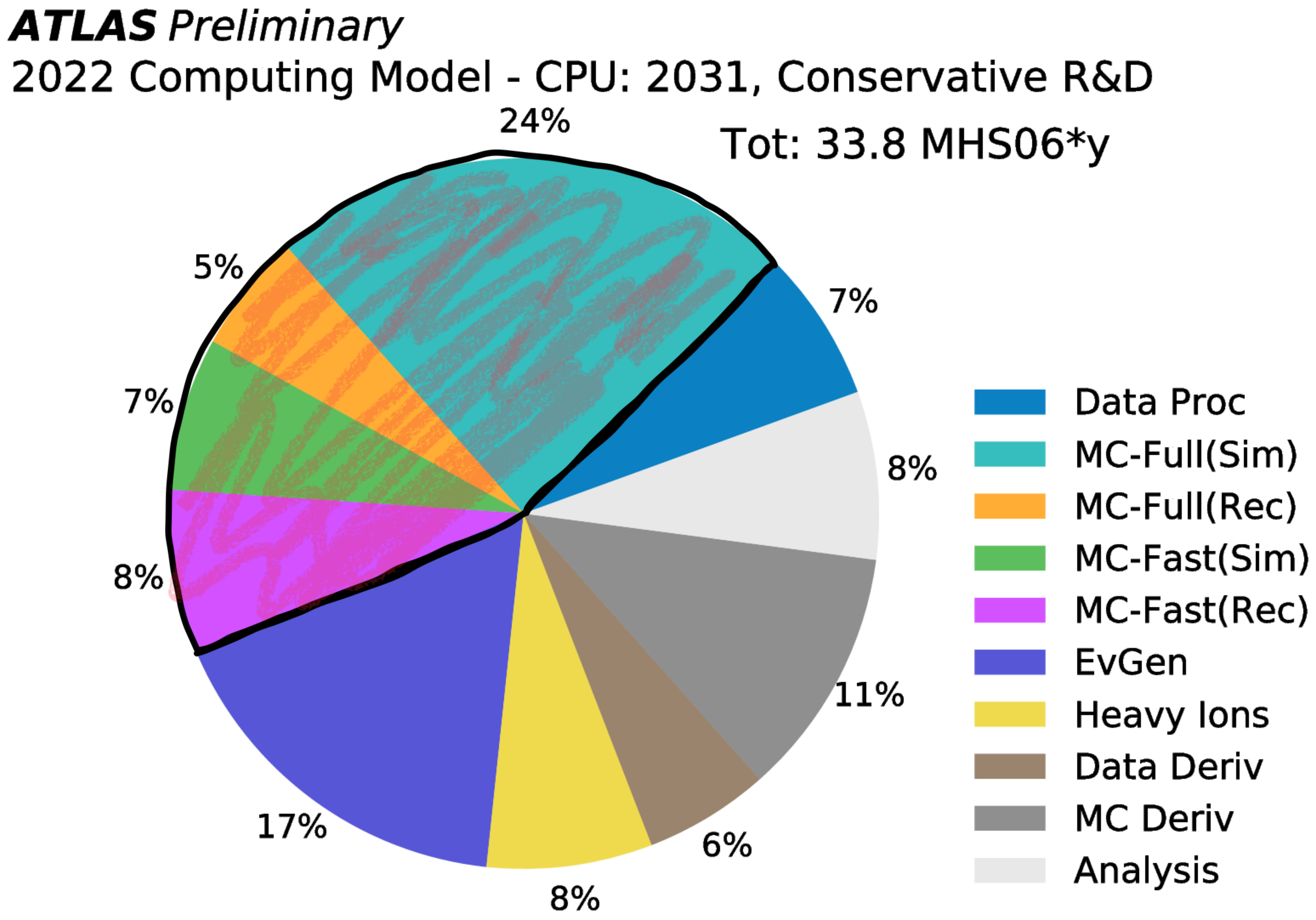
TRIUMF Canada's particle accelerator centre
Centre canadien d'accélération des particules

Motivation

- As we approach the launch of the High Luminosity Large Hadron Collider (HL-LHC) by the decade's end, the computational demands of traditional collision simulations have become untenably high.
- Current methods, relying heavily on Monte Carlo simulations for event showers in calorimeters, are projected to require millions of CPU-years annually, a demand far beyond current capabilities.
- This bottleneck presents a unique opportunity for breakthroughs in computational physics through the integration of generative AI with quantum computing technologies.

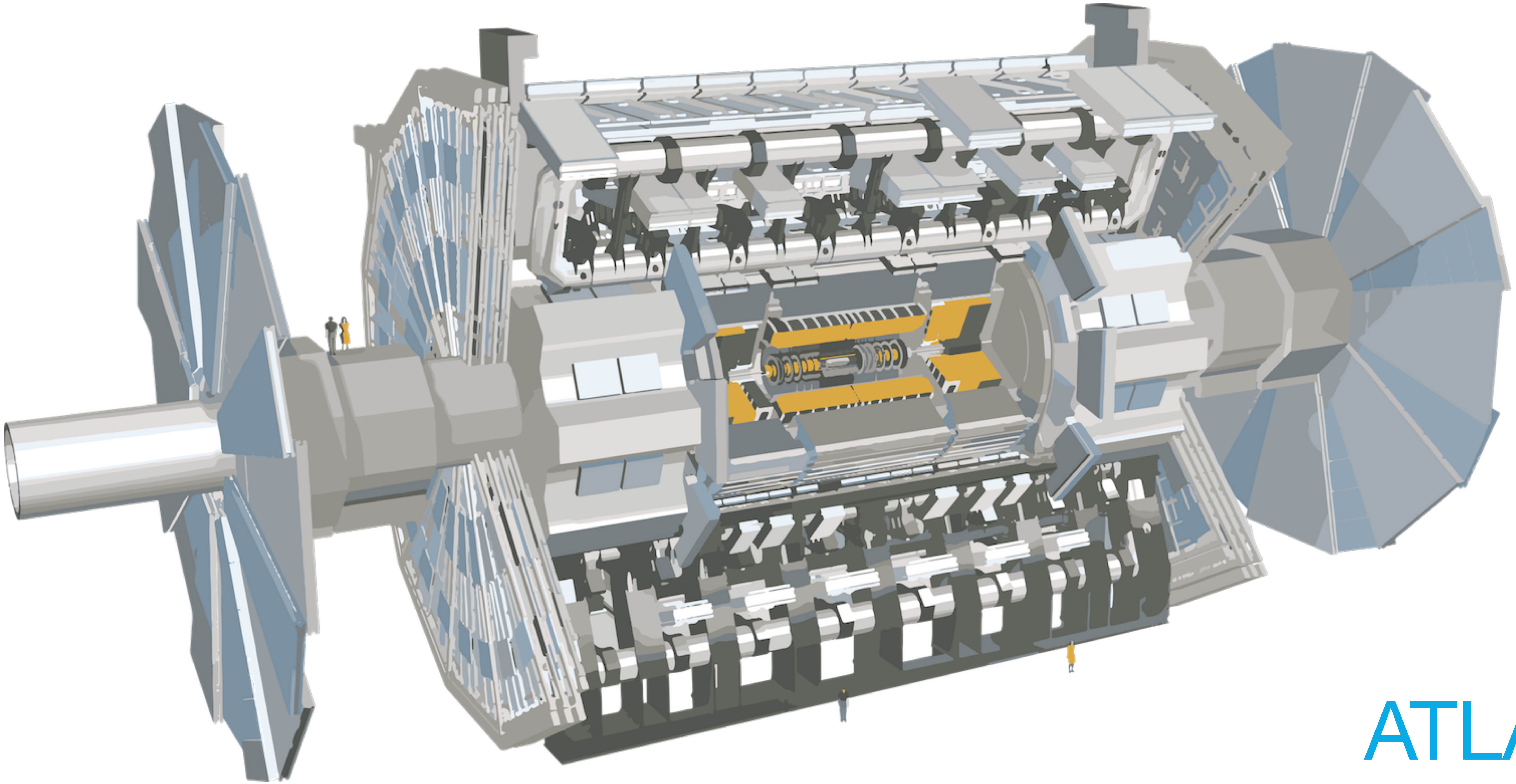






Scientific Data Lake for High Luminosity LHC project and other data-intensive particle and astro-particle physics experiments. InJournal of Physics: Conference Series 2020 Dec 1 (Vol. 1690, No. 1, p. 012166). IOP Publishing.

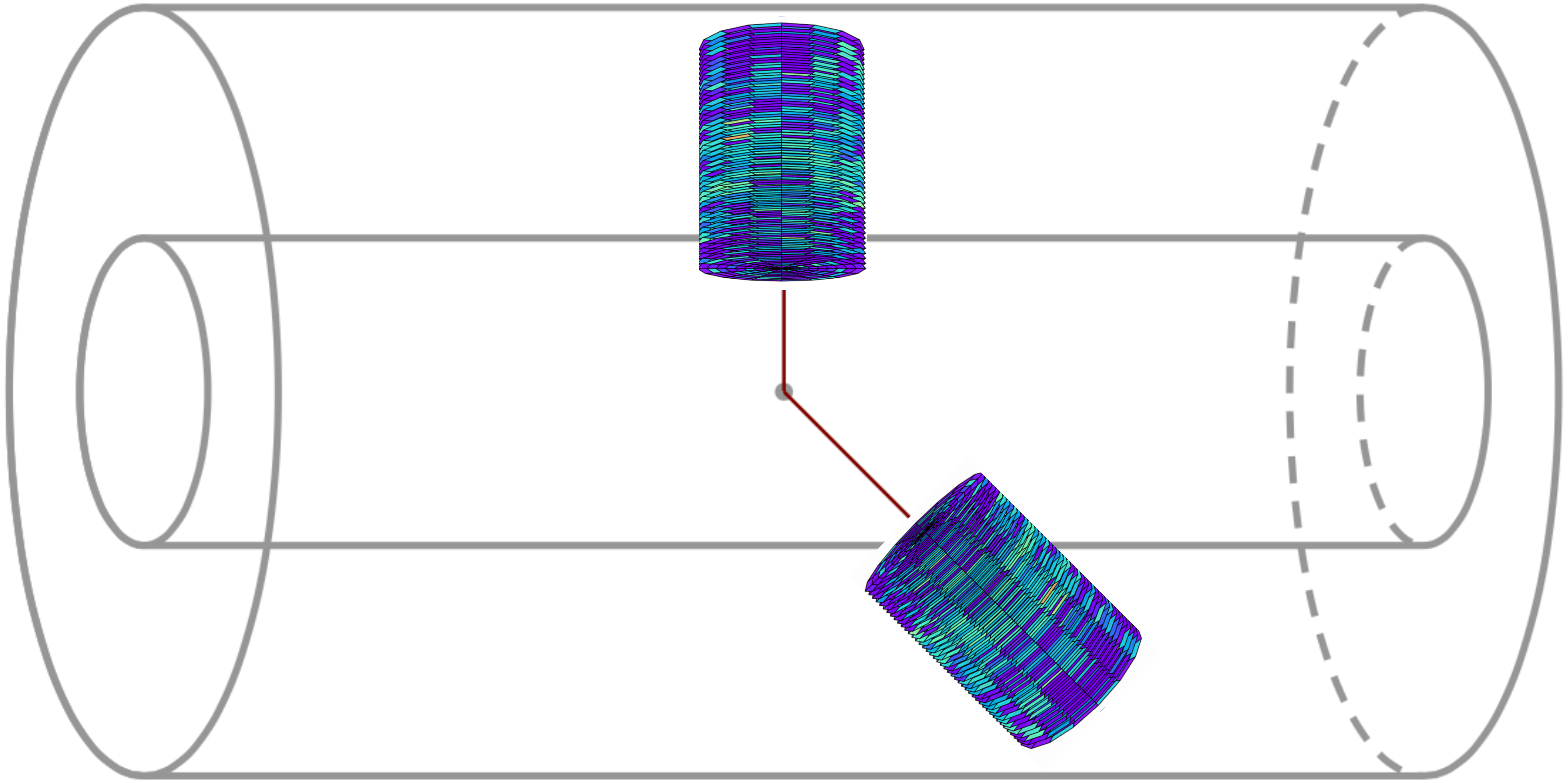
CaloChallenge



ATLAS Detector

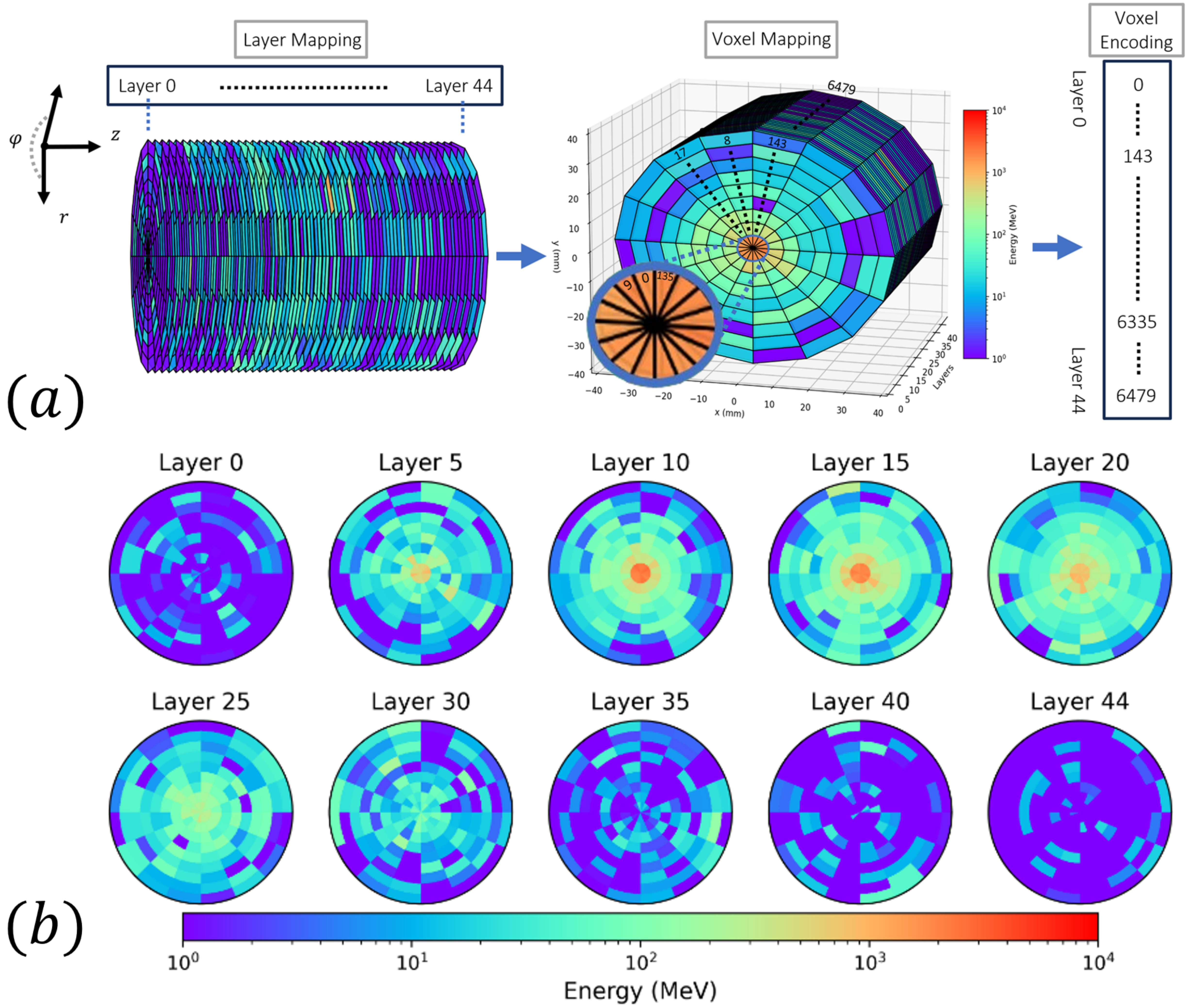
https://atlas.cern/Discover/Detector

CaloChallenge



ATLAS Detector
(Simplified)

CaloChallenge

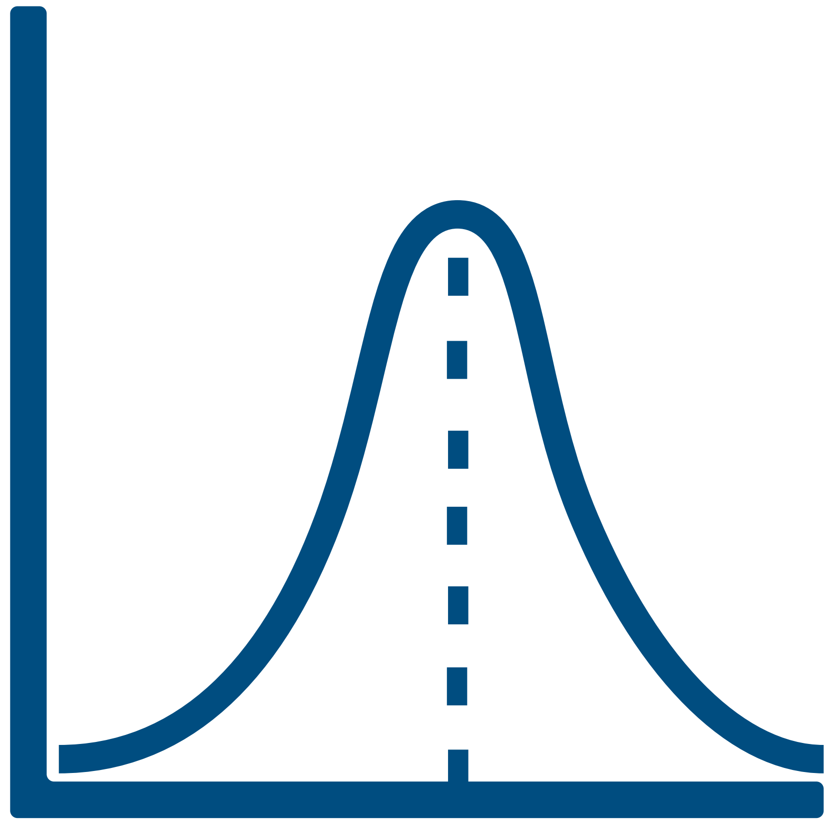


	Dataset
Particle type	Electron showers
Layers	45
Voxels per layer	9 radial * 16 angular
Incident energies	Log-uniform distribution (1GeV-1TeV)
N. of events	100,000

Generative Models

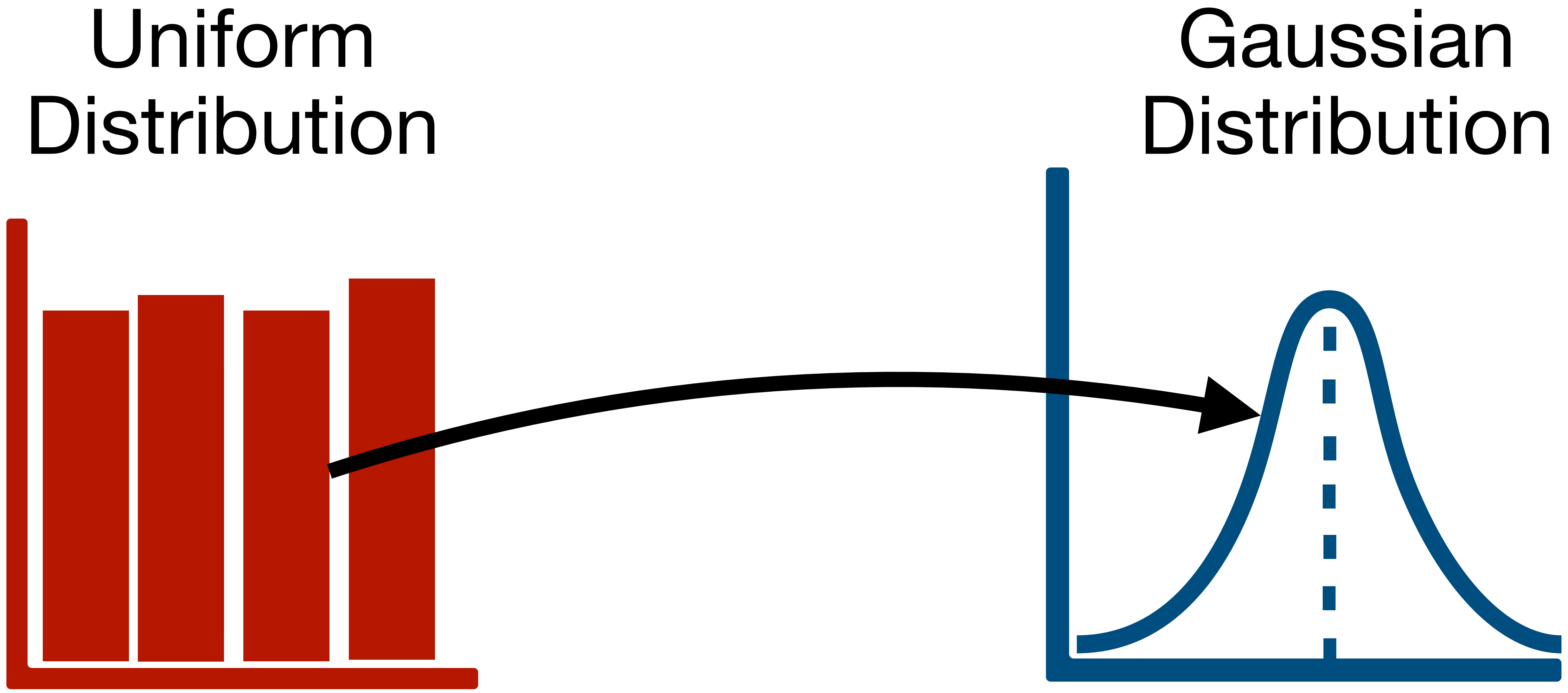
Simplest Example: Box-Muller Method

Gaussian
Distribution



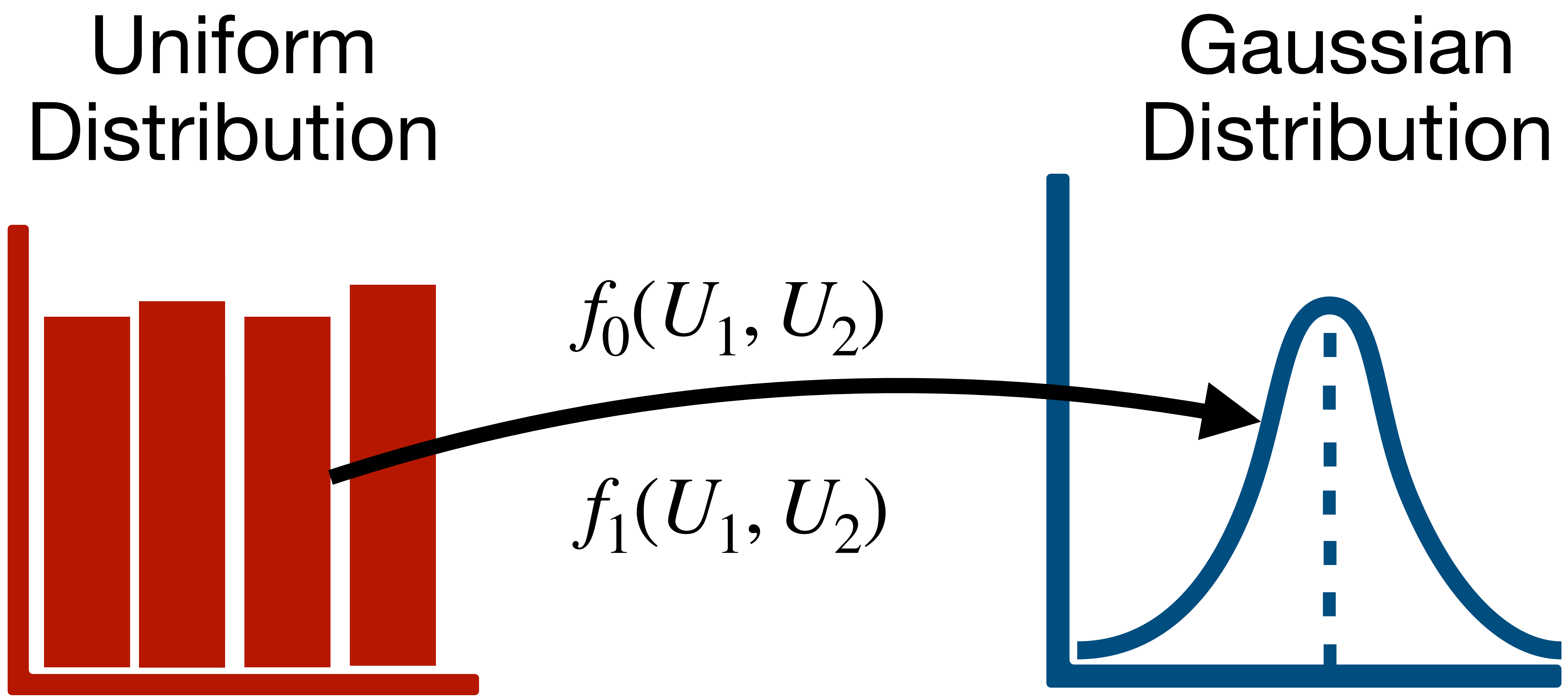
Generative Models

Simplest Example: Box-Muller Method



Generative Models

Simplest Example: Box-Muller Method



Recipe:

1. Generate two **uniformly** independent, identically distributed random numbers U_1 and U_2.

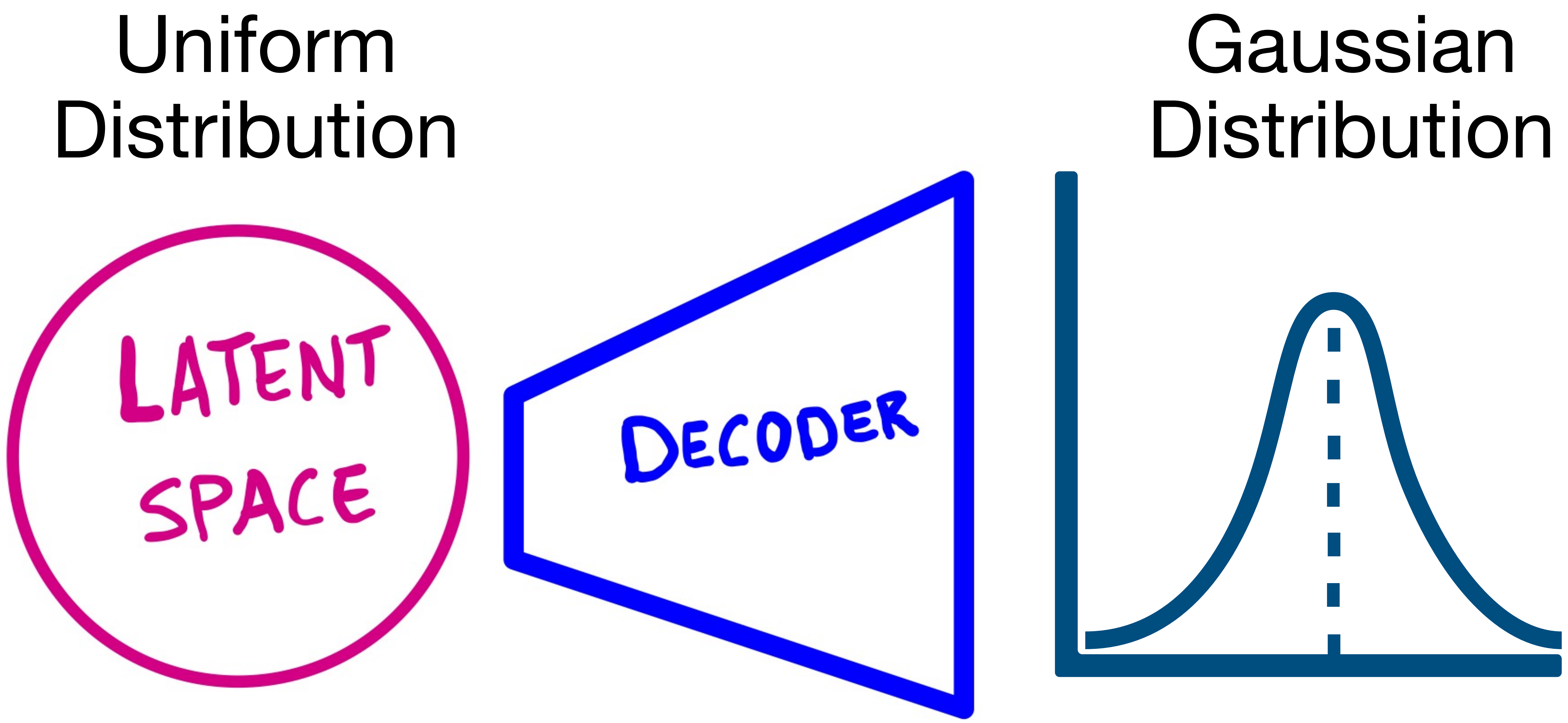
2. Substitute in:

$$Z_0 = f_0(U_1, U_2) = \sqrt{-2 \ln U_1} \cos(2\pi U_2)$$

$$Z_1 = f_1(U_1, U_2) = \sqrt{-2 \ln U_1} \sin(2\pi U_2)$$

Generative Models

Simplest Example: Box-Muller Method



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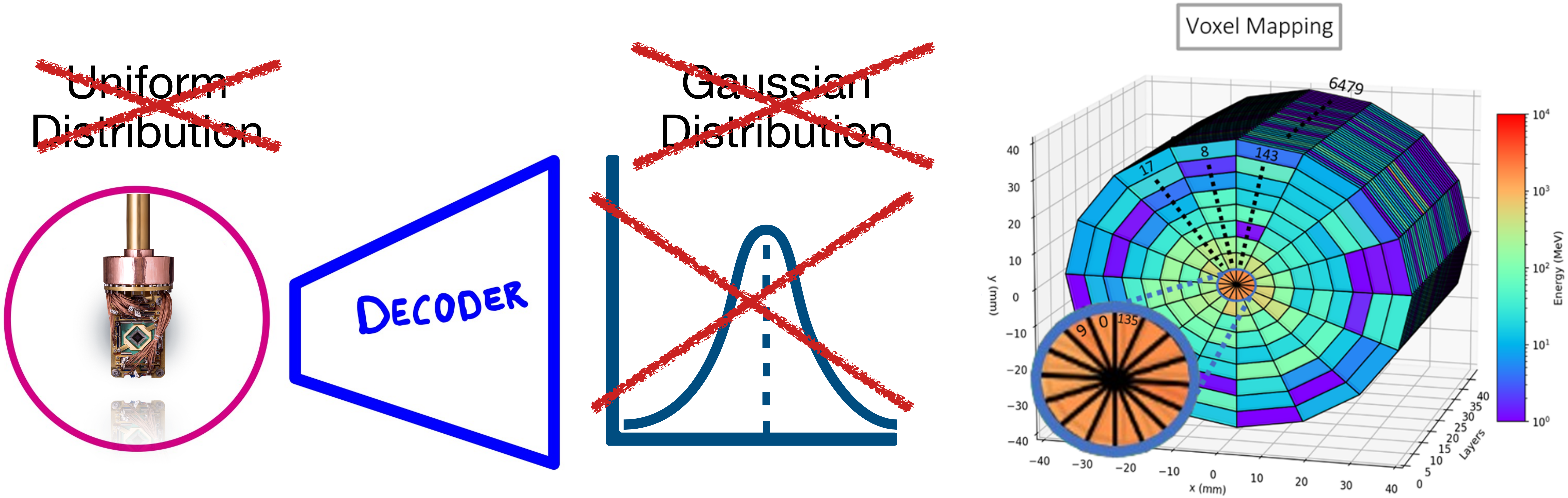
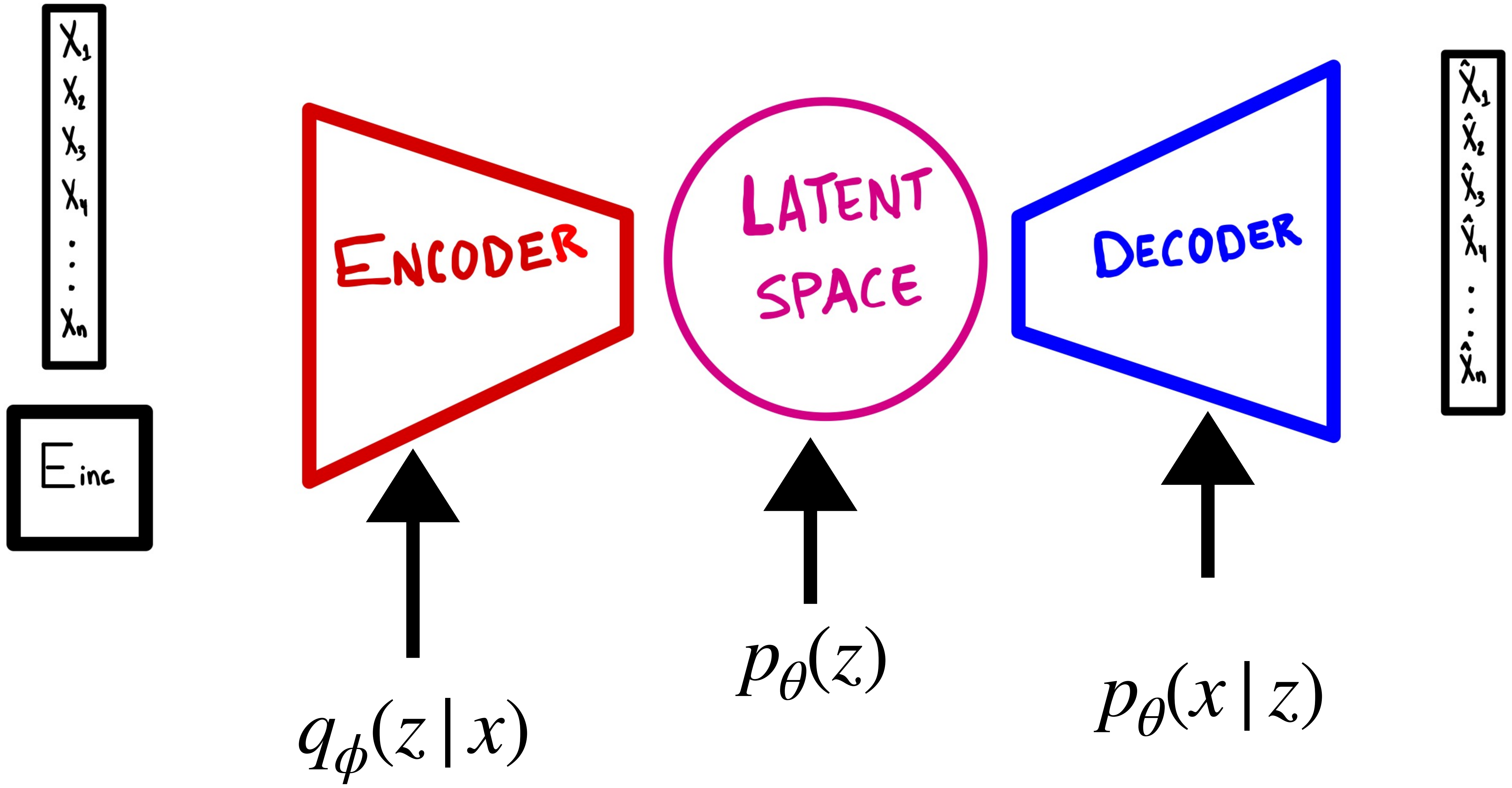
Generative Models

For particle-calorimeter interactions + quantum-assisted



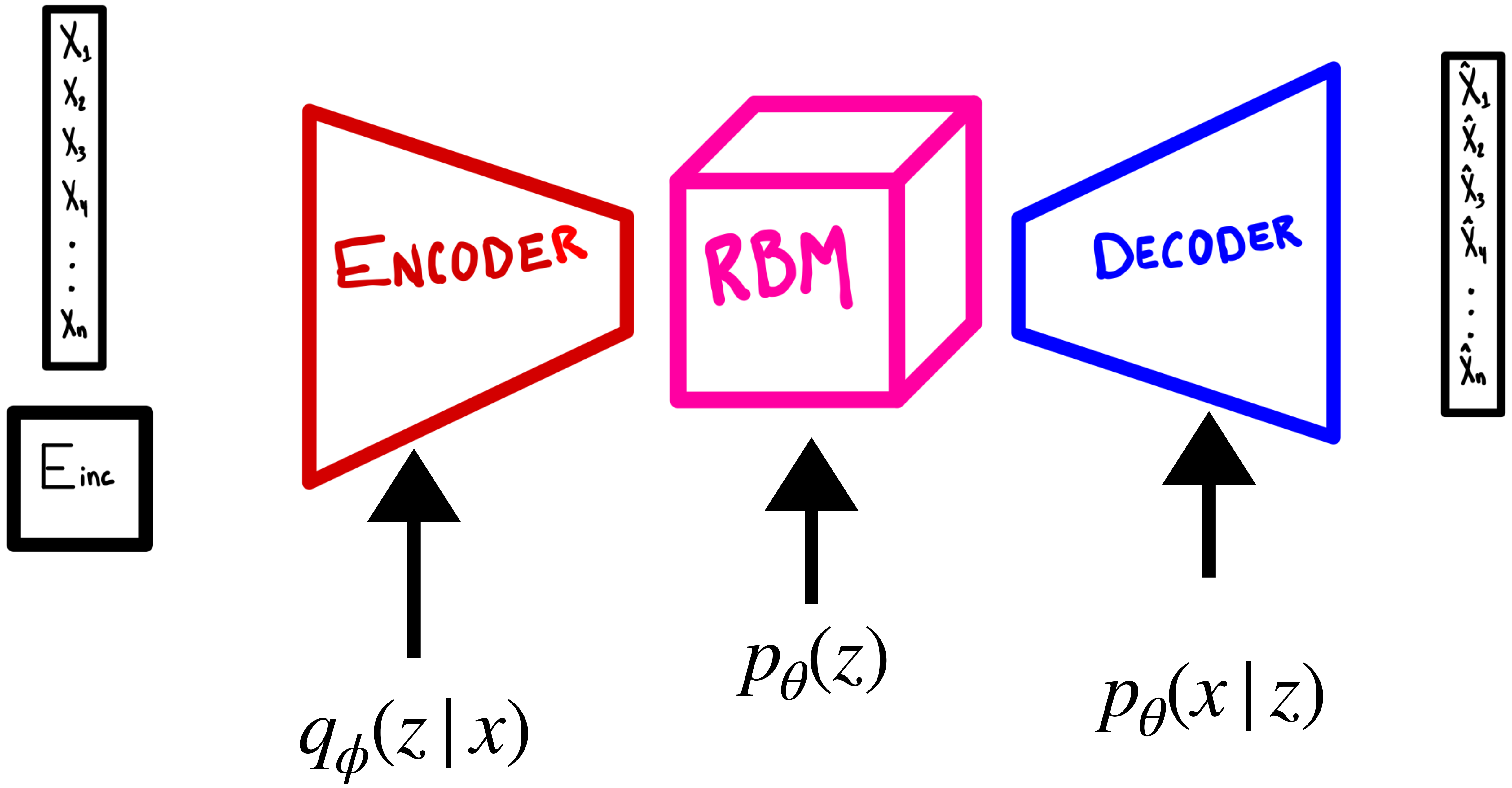
Variational Autoencoders (VAE)



$$\mathscr{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x\,|\,z)\rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\left\langle \ln \frac{q_\phi(z\,|\,x)}{p_\theta(z)} \right\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

- ✦Easy to train.
- ✦Average performance.
- ✦*Legacy* VAE assumes a Gaussian prior.

VAE + Restricted Boltzmann Machine



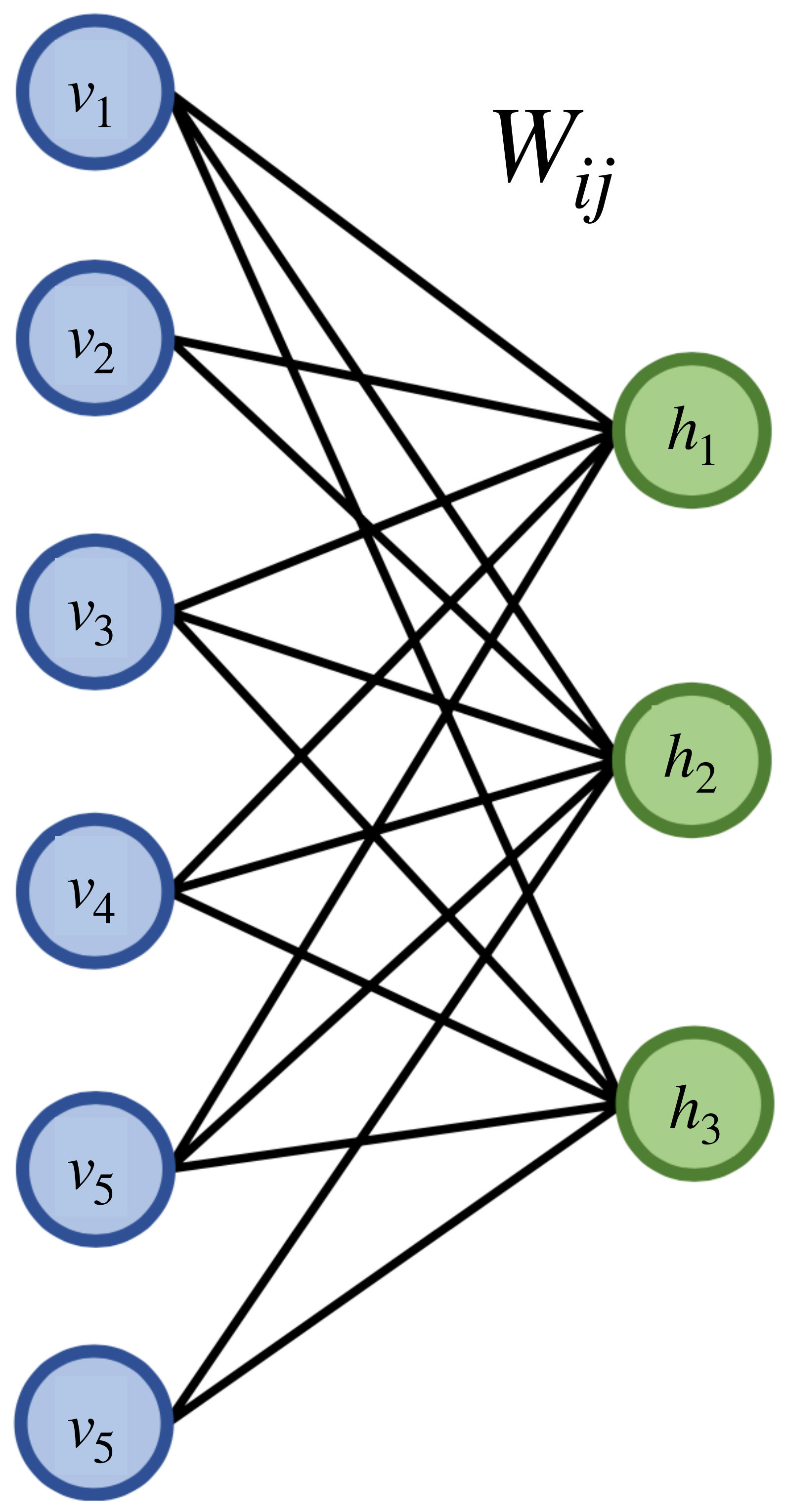
$$\mathscr{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x \mid z) \rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\left\langle \ln \frac{q_\phi(z \mid x)}{p_\theta(z)} \right\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

- Replace Gaussian prior with Boltzmann prior.
- More expressiveness.
- However, this comes at a cost.

Restricted Boltzmann Machine

Basics

$\langle v |$ $| h \rangle$



Suppose a data set $\{v^\alpha\}_{\alpha=1}^n$, such that $v_i \in \{0,1\}$.

I) An RBM will fit a Boltzmann distribution, $p(v)$, to the data set.

II) The fitting is done by maximizing the log-likelihood, $\ln p(v)$.

III) RBMs are composed by a two-partite graph, where **v** denotes the visible layer and **h** the hidden layer.

$$p(v,h) = \frac{\exp(-E(v,h))}{Z}$$

Boltzmann Dist

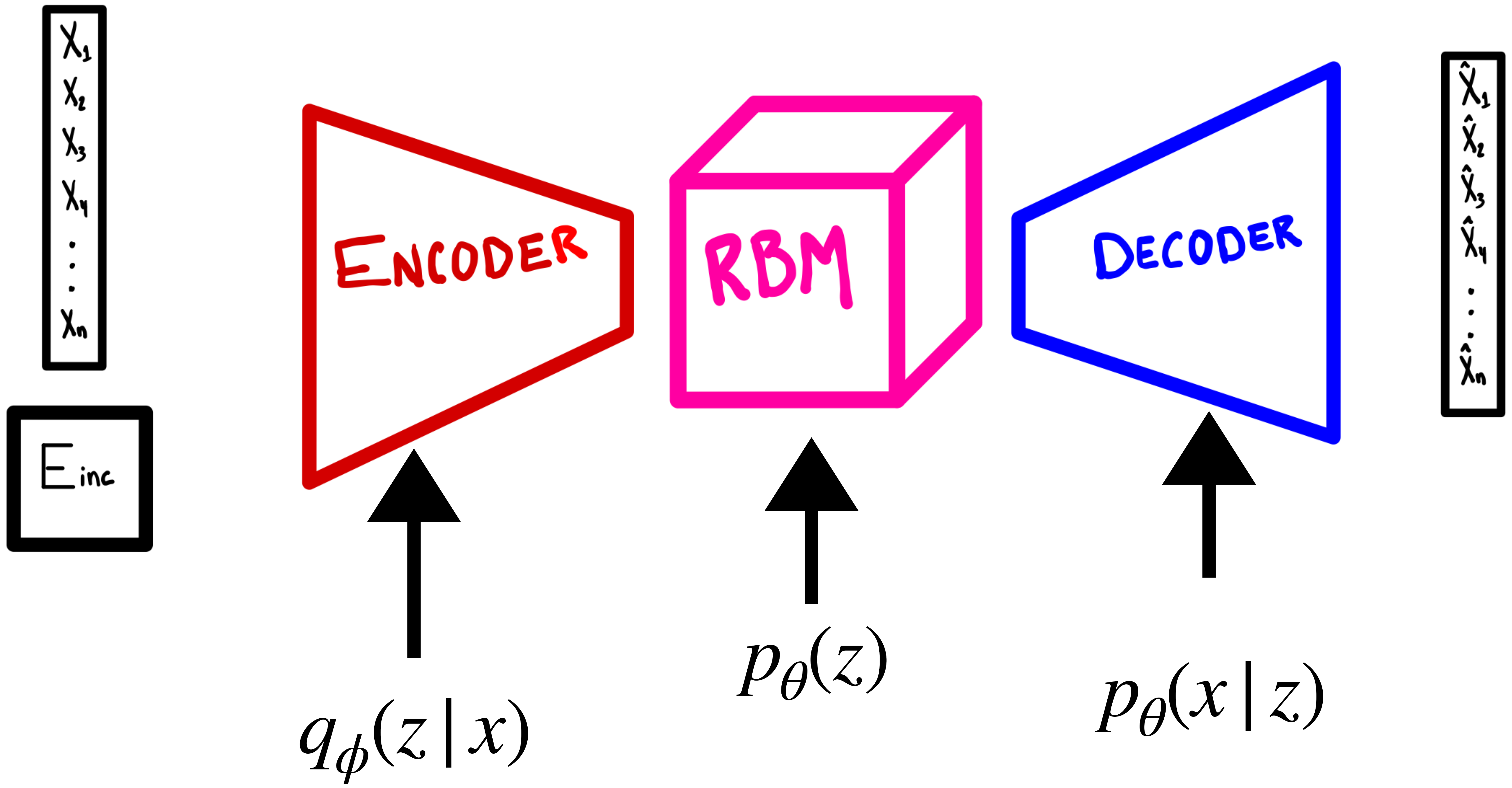
$$E(v,h) = -\sum_{i=1}^{n_v} v_i a_i - \sum_{j=1}^{n_h} b_j h_j - \sum_{i,j} v_i W_{ij} h_j$$

Energy

$$Z(W,a,b,\beta=1) = \sum_{v',h'} \exp(-E(v',h'))$$

Partition Function

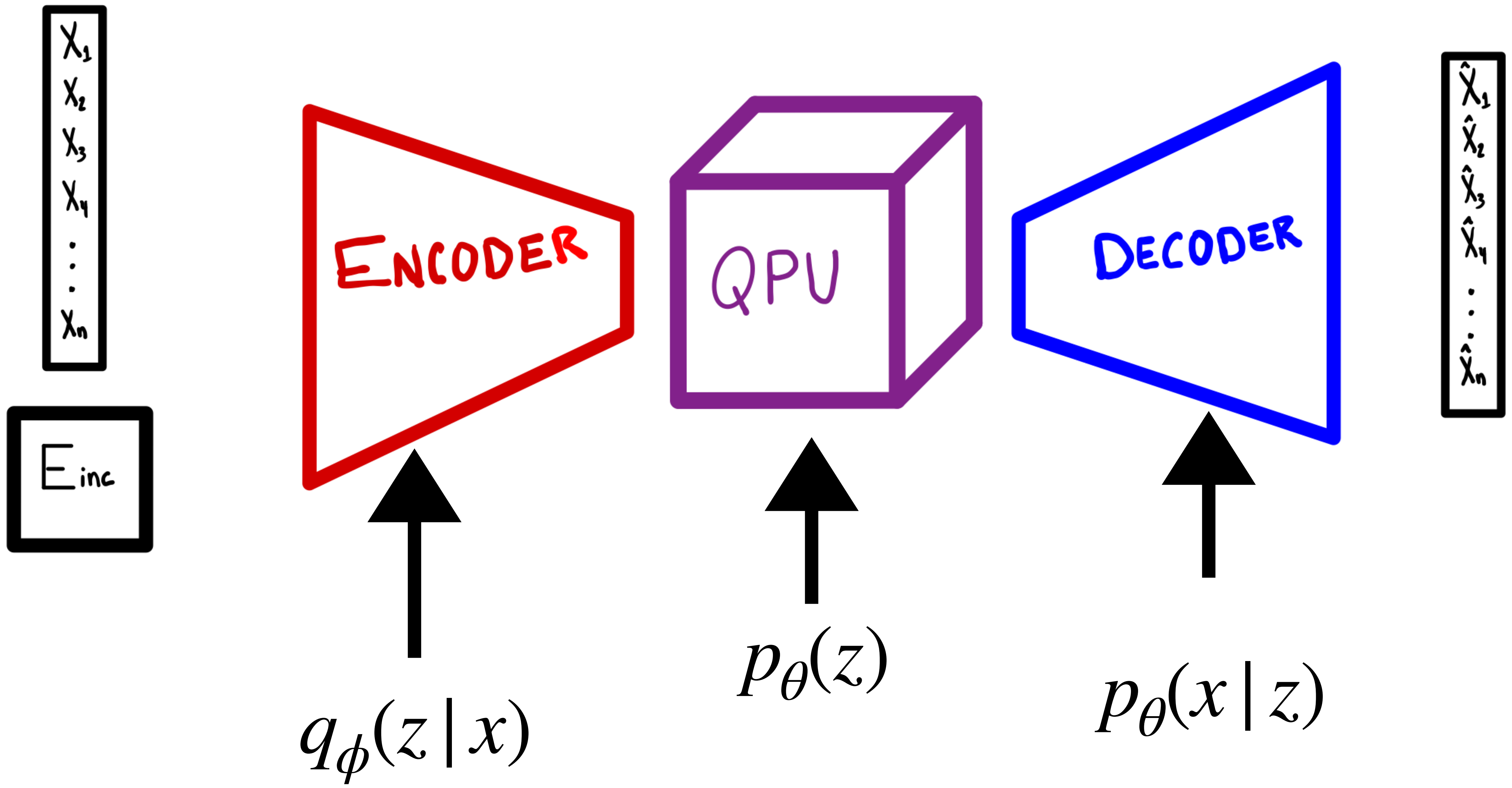
VAE + Restricted Boltzmann Machine



$$\mathcal{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x|z) \rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\left\langle \ln \frac{q_\phi(z|x)}{p_\theta(z)} \right\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

- Replace Gaussian prior with Boltzmann prior.
- More expressiveness.
- However, this comes at a cost.

Quantum-Assisted Discrete VAE



$$\mathcal{L}_{\phi,\theta}(x) = \underbrace{\langle \ln p_\theta(x|z) \rangle_{q_\phi(z|x)}}_{\text{Reconstruction}} - \underbrace{\left\langle \ln \frac{q_\phi(z|x)}{p_\theta(z)} \right\rangle_{q_\phi(z|x)}}_{\text{Regularizer}}$$

- Replace Gaussian prior with Boltzmann prior.
- More expressiveness.
- However, this comes at a cost.
- But we might be able to avoid Gibbs sampling…

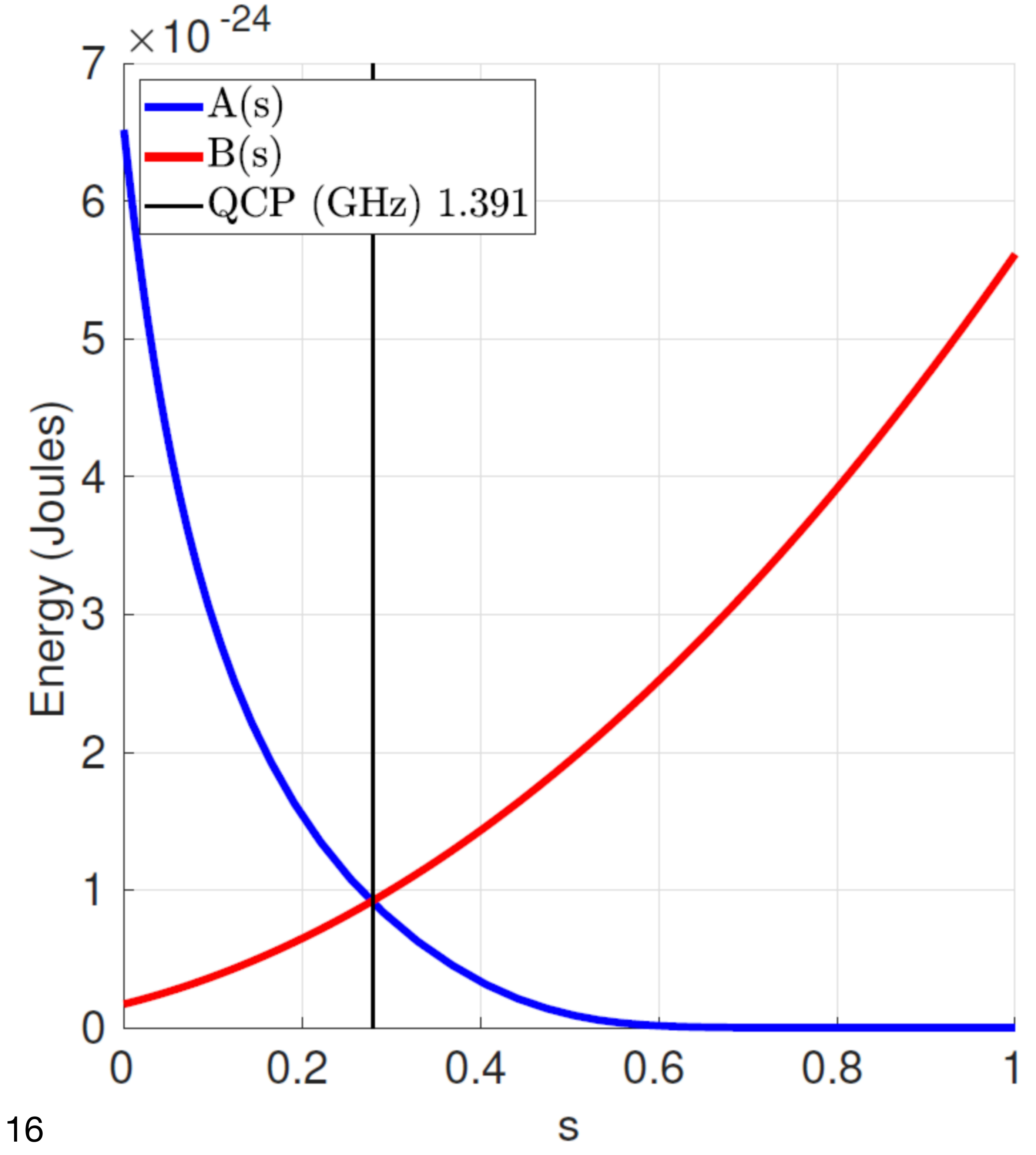
Quantum Annealer

Basics

$$\mathcal{H}_{ising} = \underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\text{Initial Hamiltonian}} + \underbrace{\frac{B(s)}{2}\left(\sum_i c_i \hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\text{Final Hamiltonian}}$$

H_1 $\qquad$ H_0

- An array of **superconducting flux quantum bits** with **programmable spin–spin couplings** and **self-fields**.
- Relies on the Adiabatic Approximation.
- The goal is to find the ground state of a Hamiltonian H_0.
- In practice, quantum annealers have a strong interaction with the environment which lead to **thermalization** and **decoherence**. It can also reach a ***dynamical arrest***.



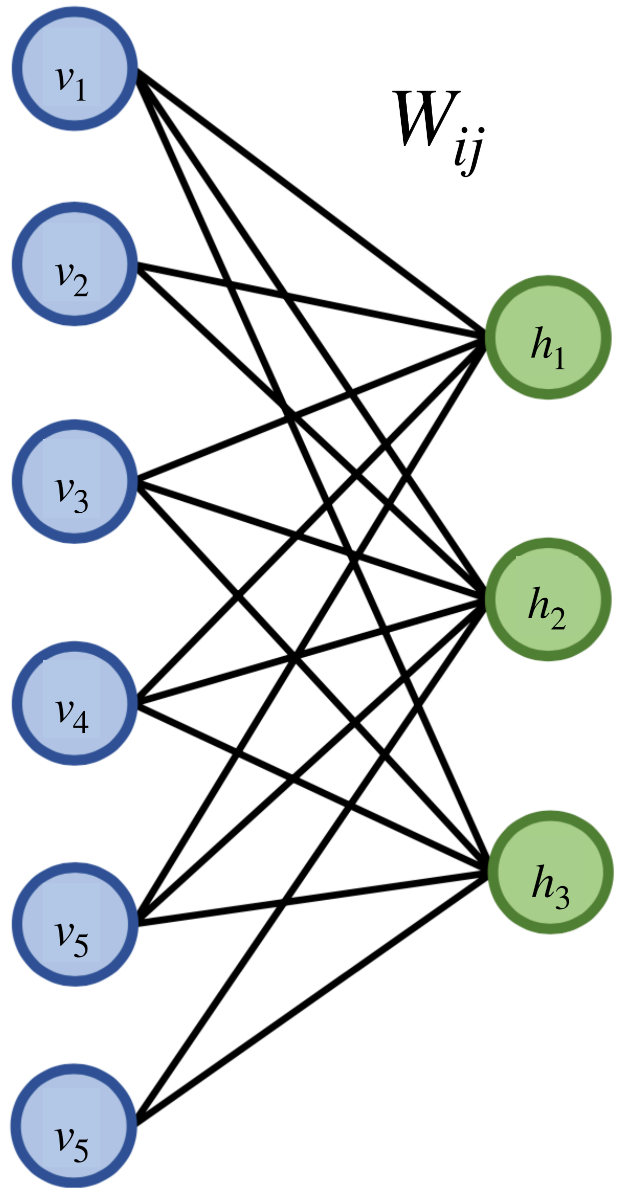
Amin MH. Searching for quantum speedup in quasistatic quantum annealers. Physical Review A. 2015 Nov 19;92(5):052323.

Quantum Annealer

Topologies

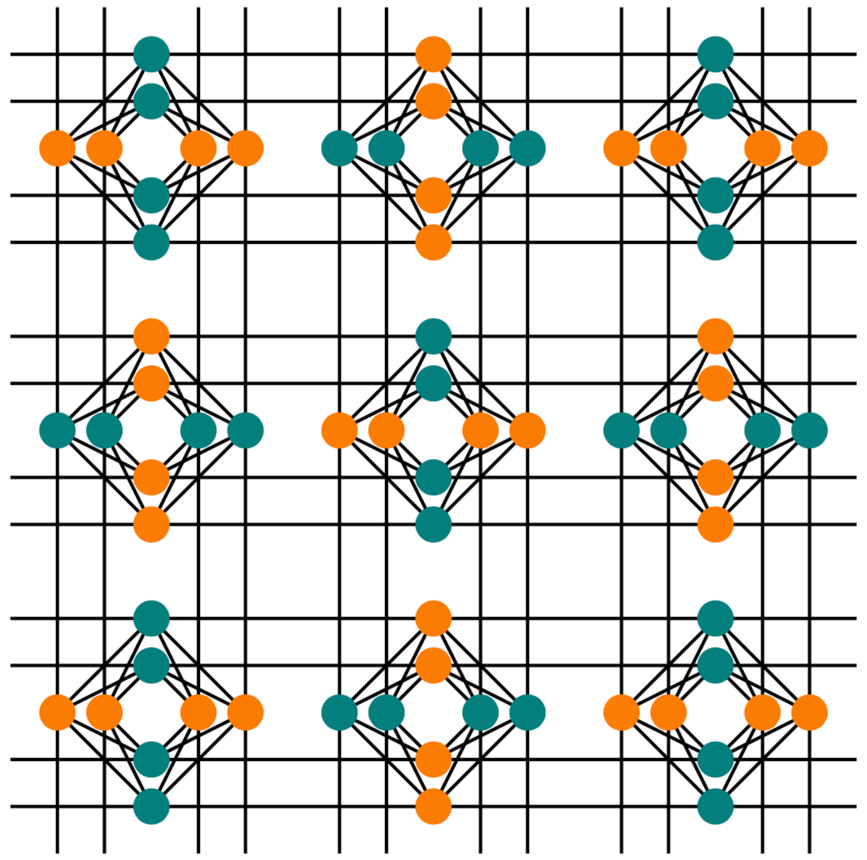
Fully Connected RBM

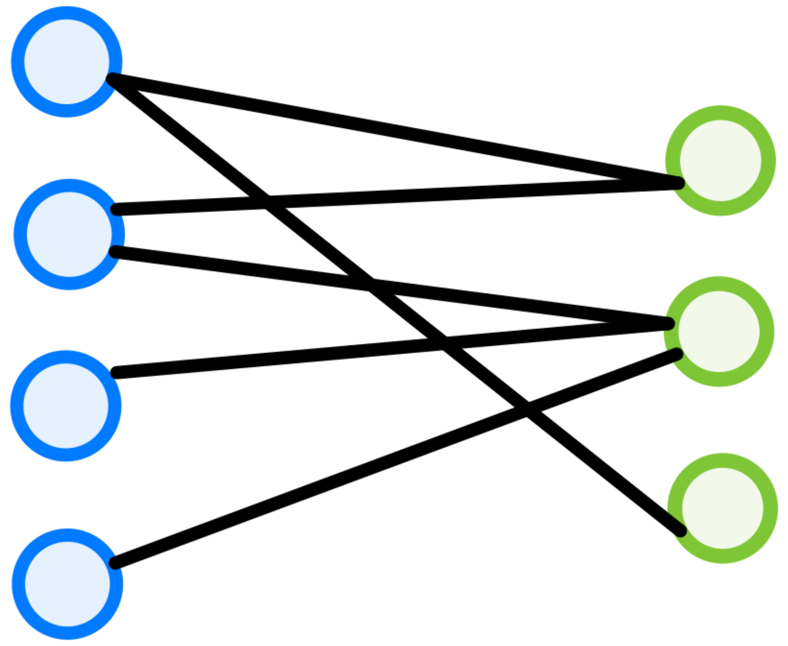
2-partite Graph



Chimera QA

2-partite Graph

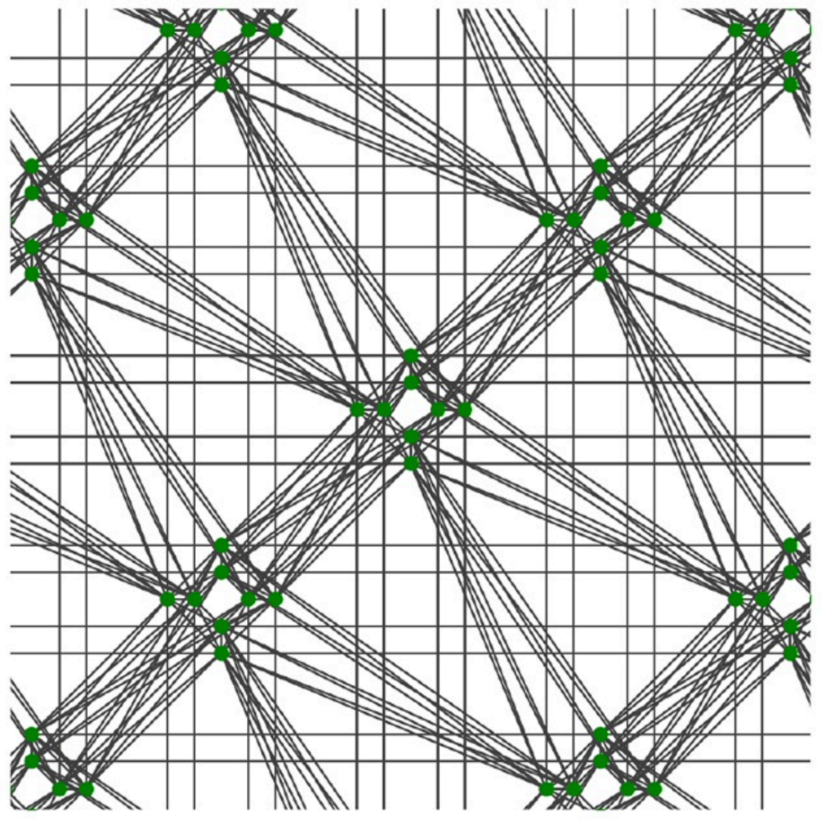


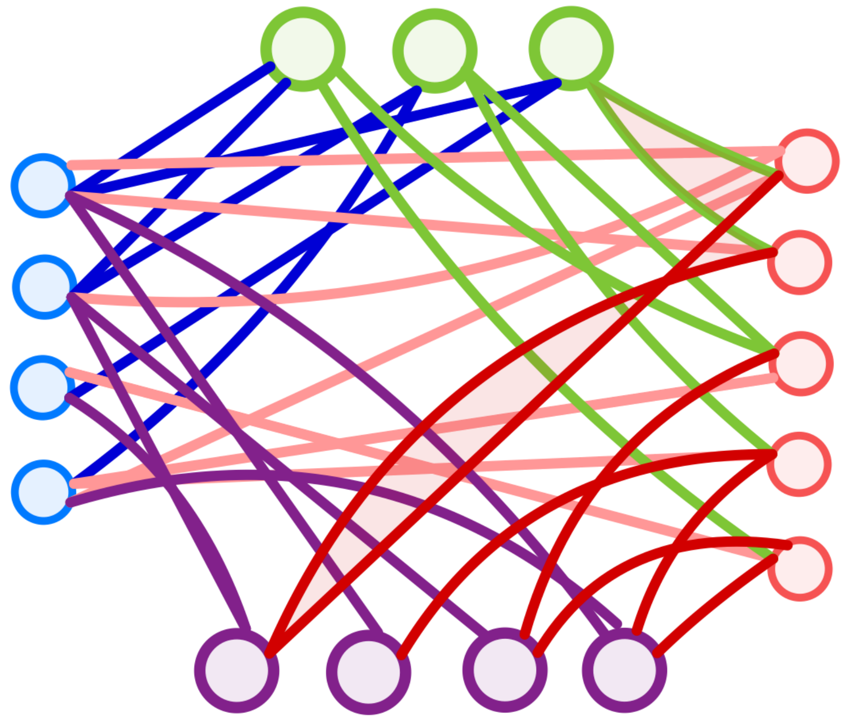


Pegasus QA

4-partite Graph

Max coord num=15

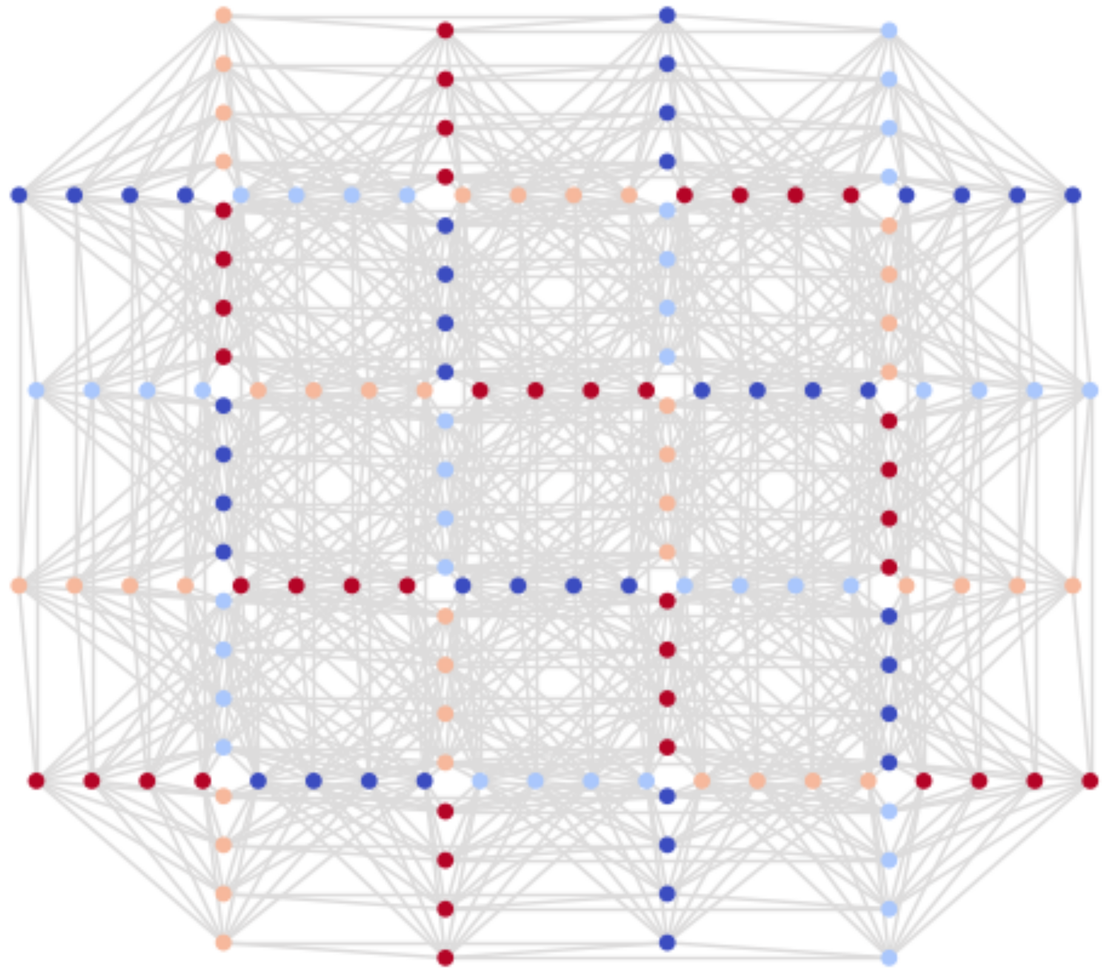




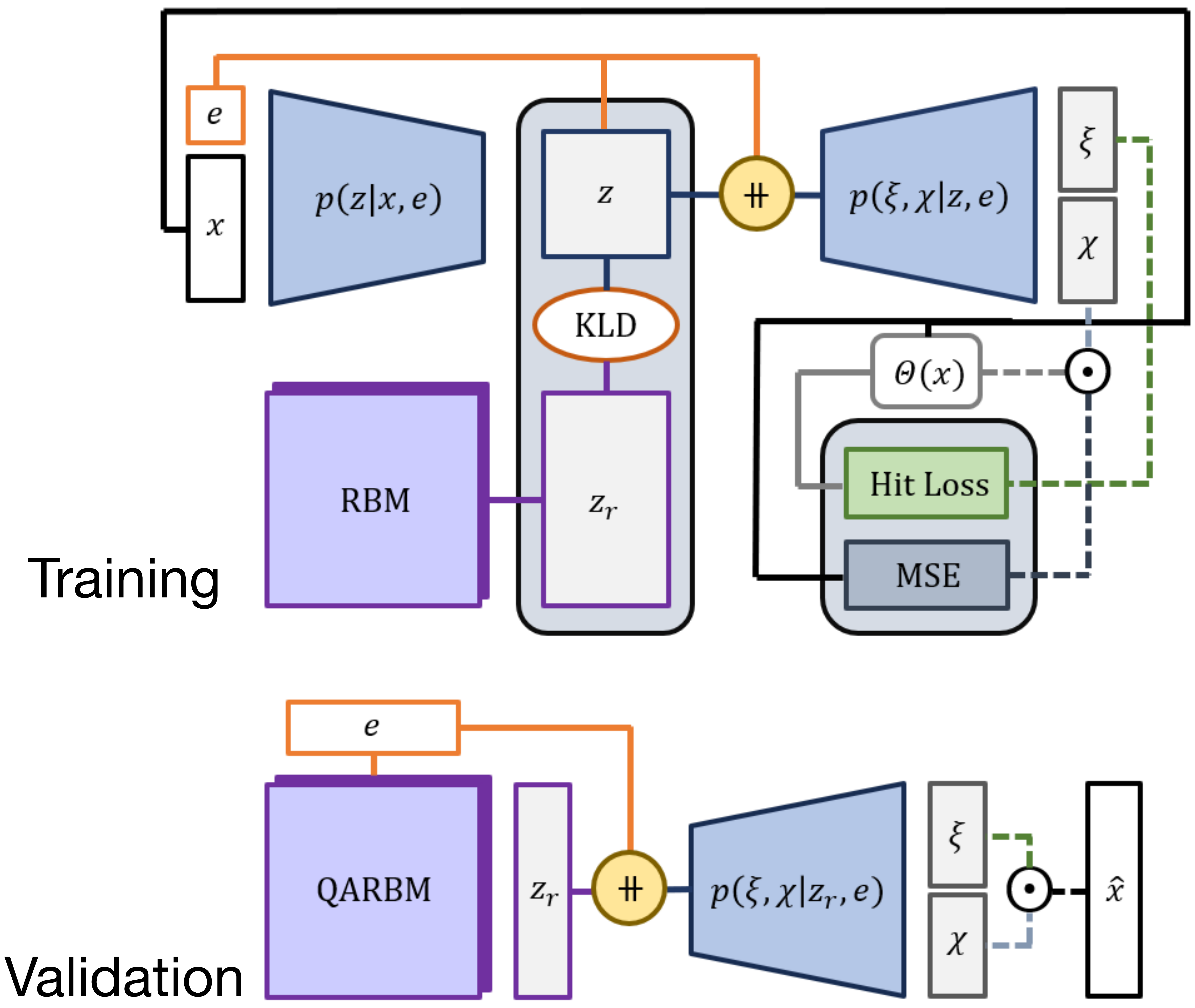
Zephyr QA

4-partite Graph

Max coord num=20



Calo4pQVAE


e
x
p(z|x,e)
z
KLD
z_r
RBM
p(ξ,χ|z,e)
ξ
χ
Θ(x)
Hit Loss
MSE
Training
e
QARBM
z_r
p(ξ,χ|z_r,e)
ξ
χ
x̂
Validation

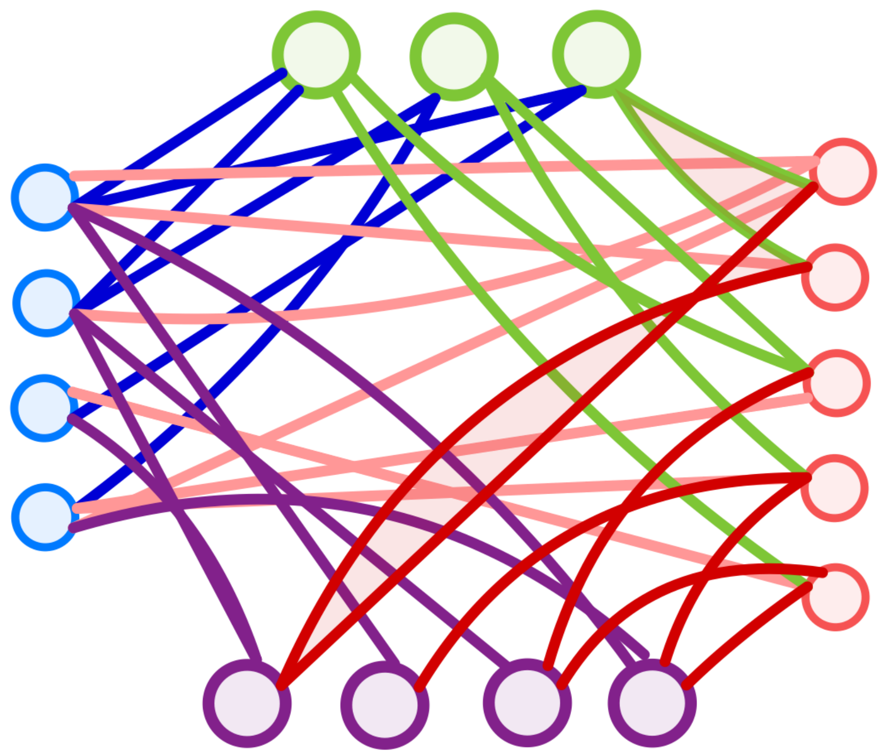
QPU conditioning

★arXiv:2410.22870

$$\sigma_z^{(i)} = \begin{cases} 1 & h_i < 0 \text{ and } |h_i| > \sum_j |J_{ij}| \\ -1 & h_i > 0 \text{ and } |h_i| > \sum_j |J_{ij}| \end{cases}$$

$k = 1,\ldots,302$ (Condition partition)

Label → f → $\sigma_z^{(k)} \in \{-1,1\}^{302}$ → g → $h_k \in \{-M, M\}^{302}$



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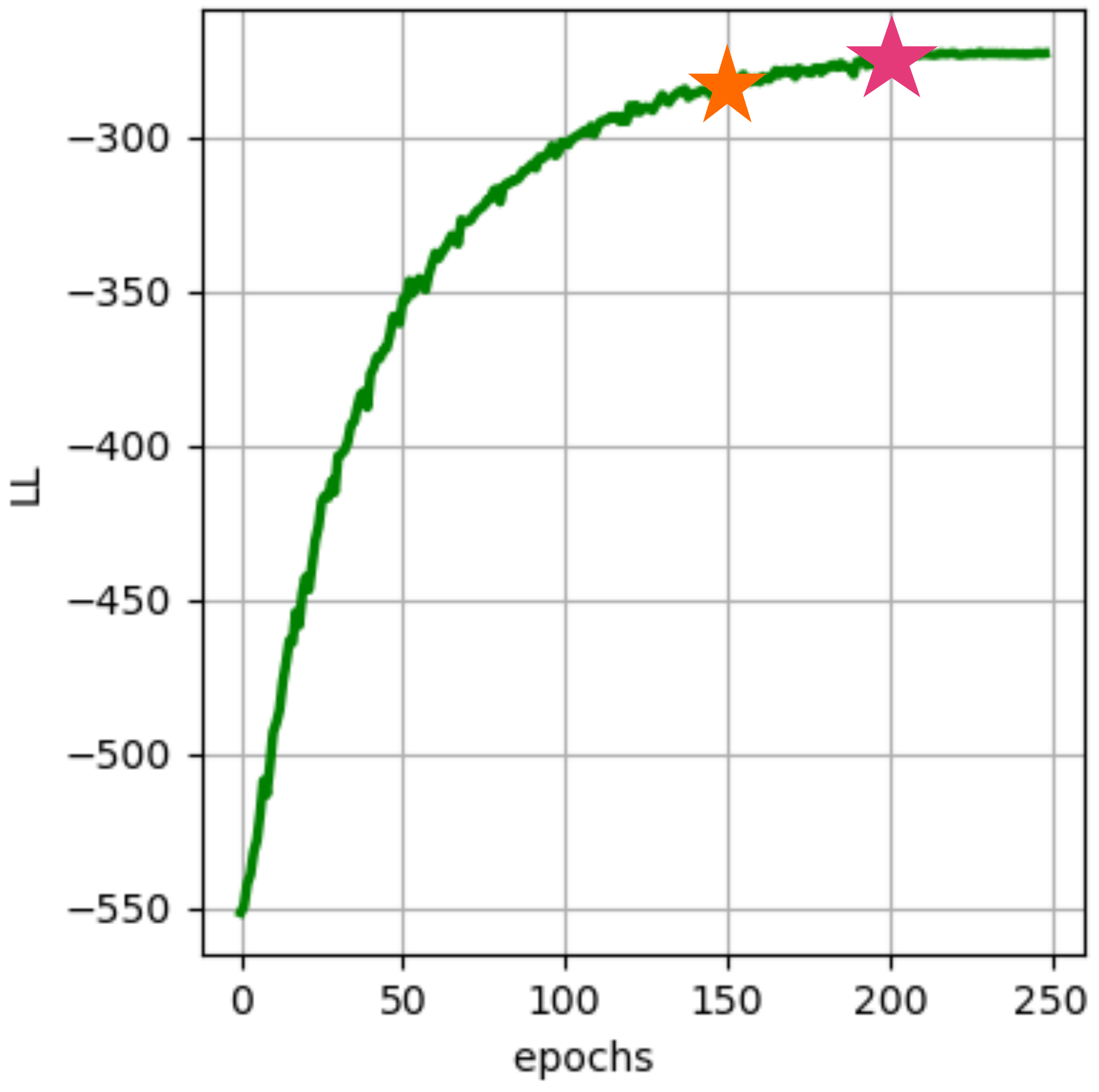
Results

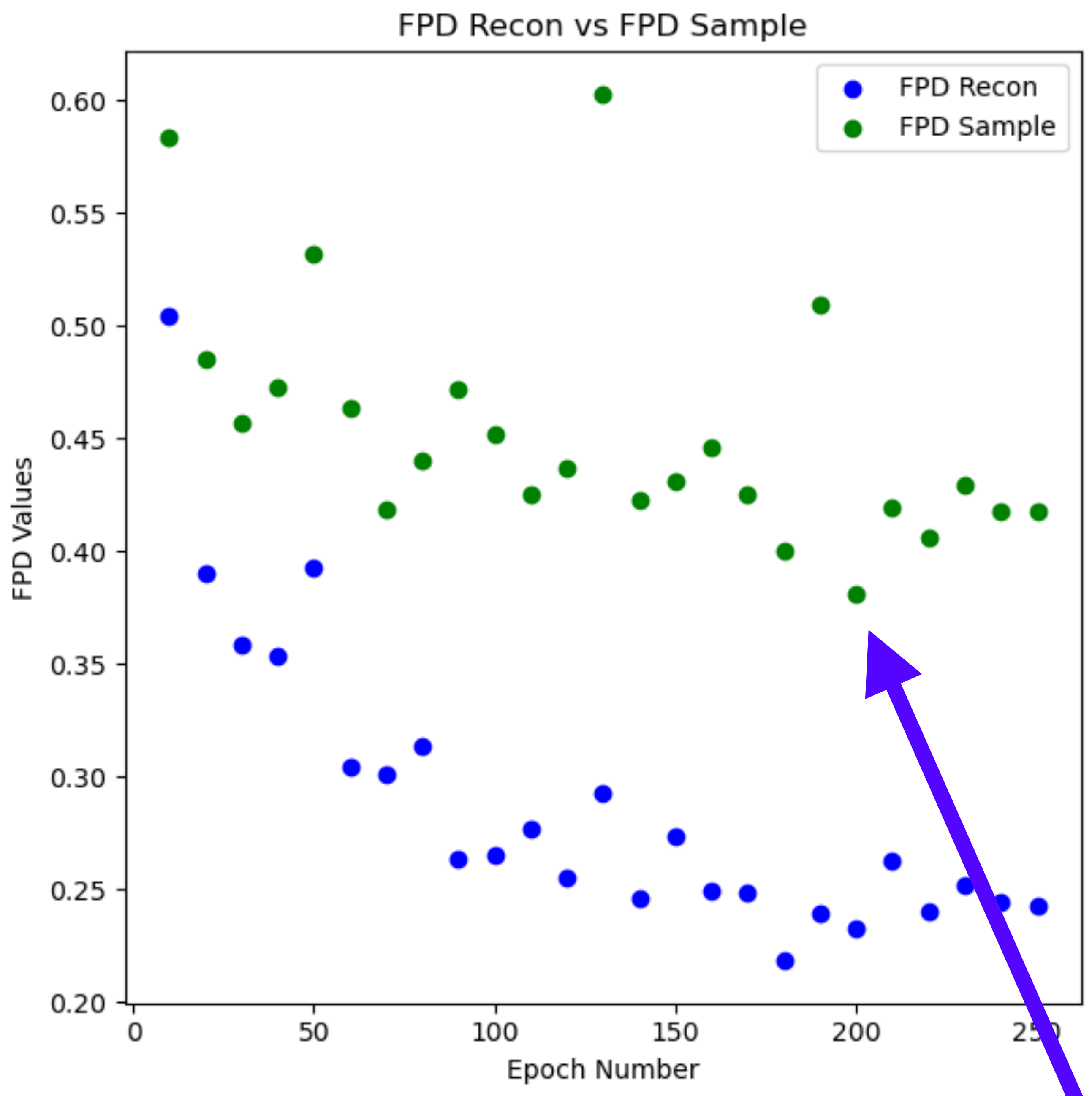
RBM Log-likelihood saturates, indicating the RBM has trained.



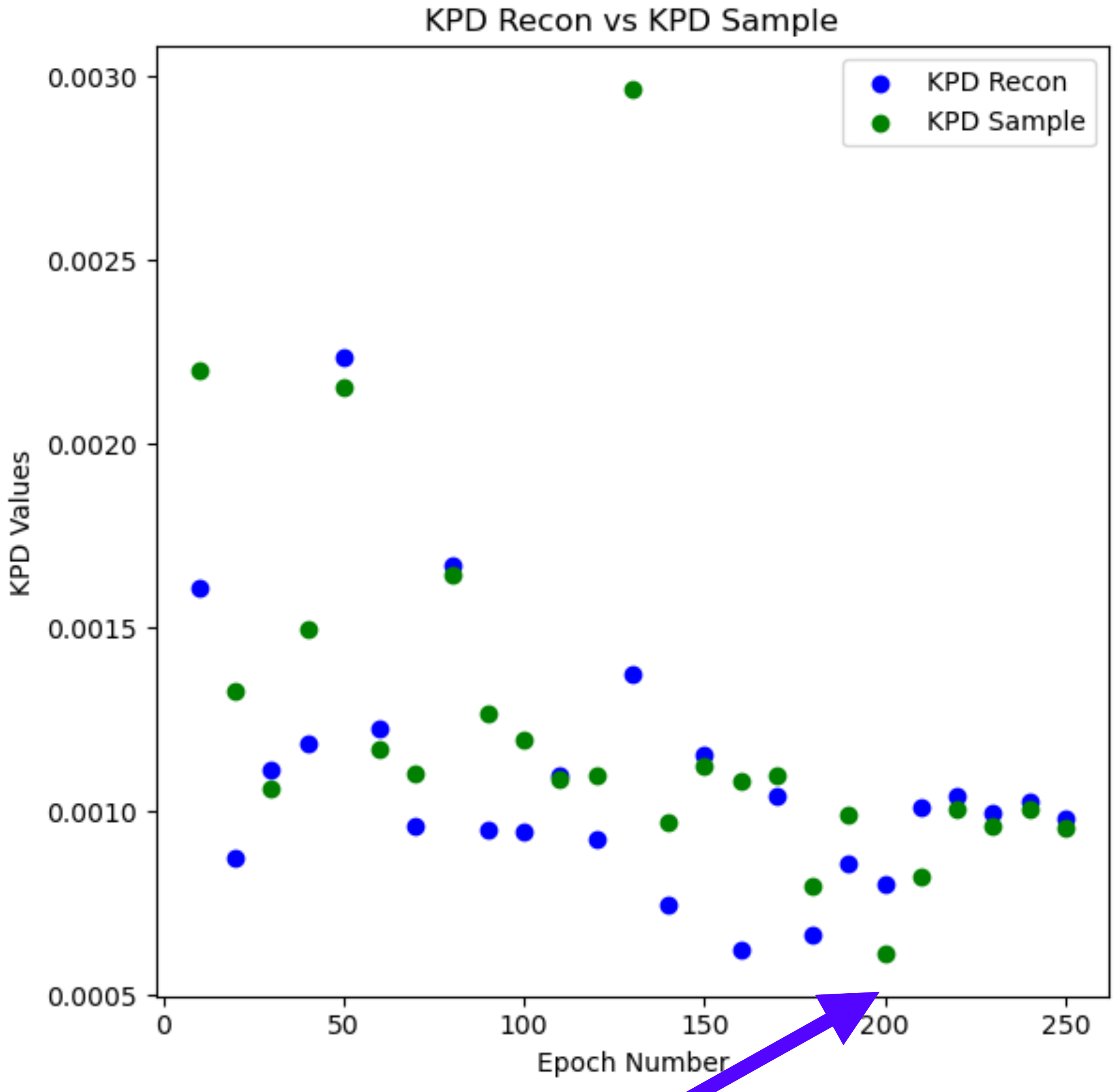
★ Slope annealing ends

★ Encoder and decoder params frozen

Frechet Particle Distance



Kernel Particle Distance



$FPD(\times 10^3) = 380.7 \pm 1.1$

$KPD(\times 10^3) = 0.61 \pm 0.06$

Following results correspond to model instance = epoch 200

Evaluating generative models in high energy physics. Physical Review D. 2023 Apr 1;107(7):076017.

Results

QA temperature estimation

★arXiv:2410.22870

System QA at Temperature $1/\beta_{QA}$

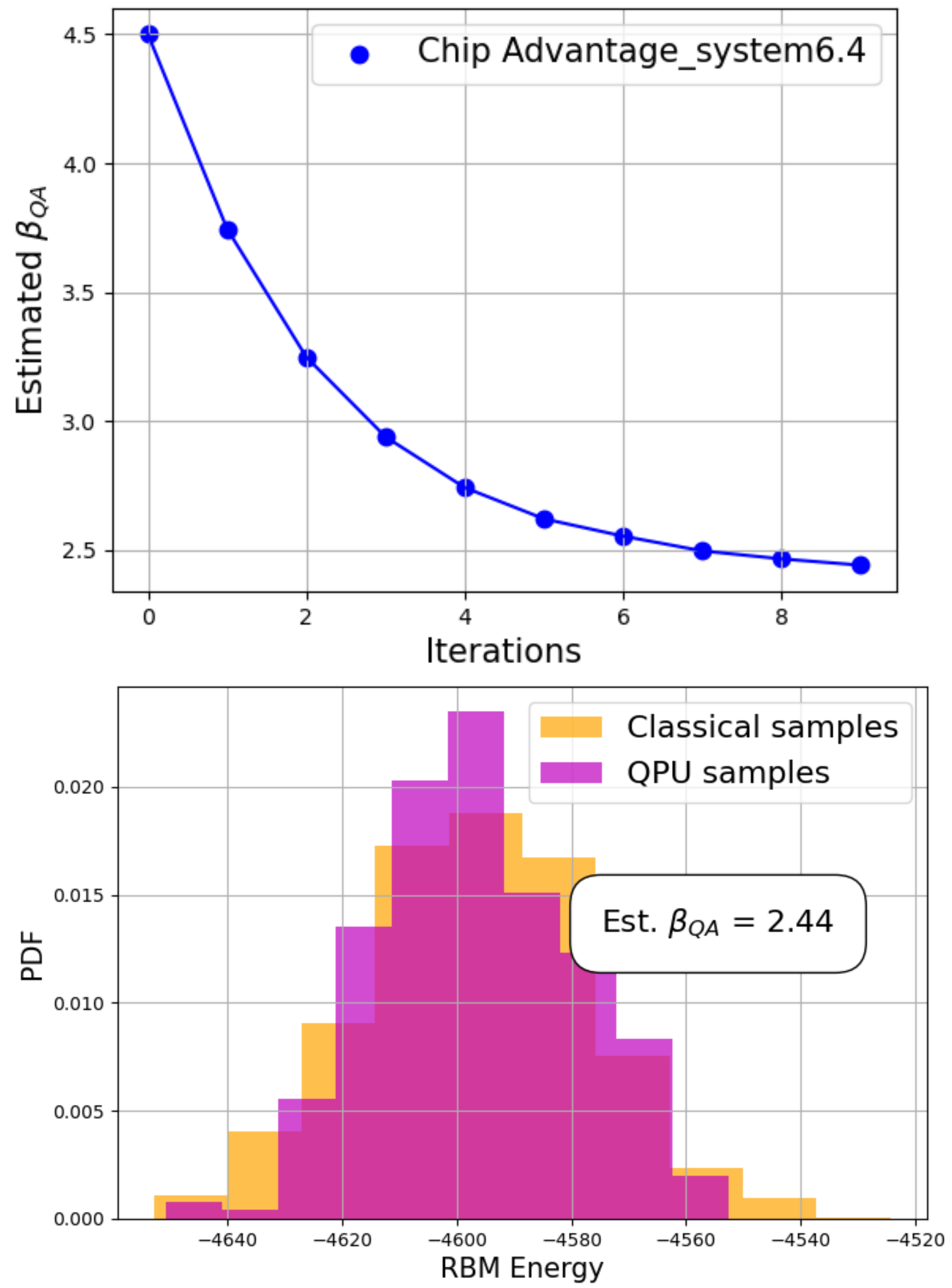
System B at Temperature $1/\beta$

$$P_{QA}(x) = \frac{e^{-\beta_{QA} H(x)}}{Z(\beta_{QA})} \qquad P_B(x) = \frac{e^{-\beta H(x)}}{Z(\beta)}$$

- Equate entropy of system QA to entropy of system B
- Assume $\beta = \beta_{QA} + \Delta\beta$

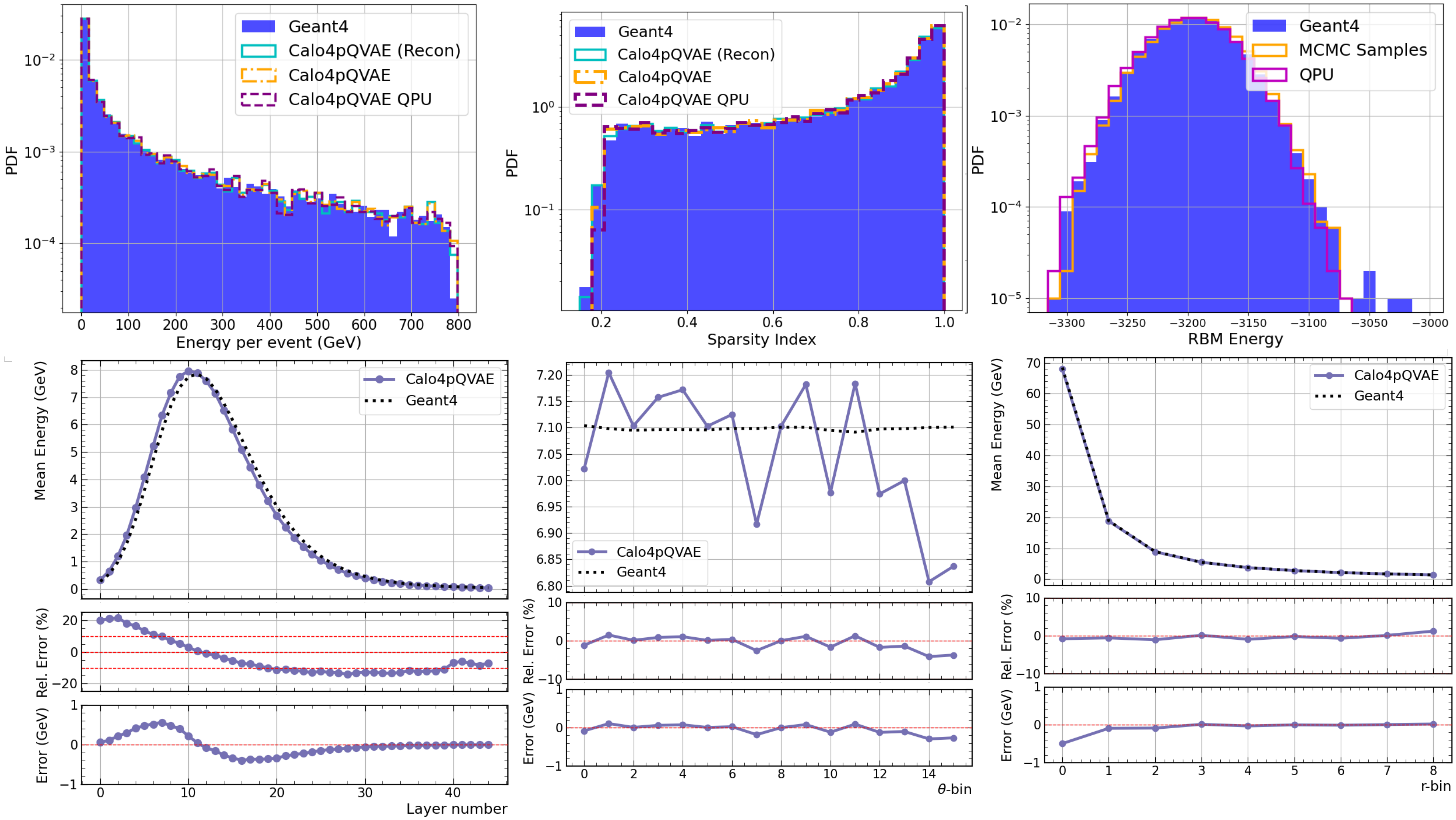
$$\beta_{t+1} = f_\delta(\beta_t) \equiv \beta_t \left(\frac{\langle H \rangle_{QA^{(r)}}}{\langle H \rangle_{B(1)}} \right)^{\delta}$$

QA inverse temperature estimation



Results

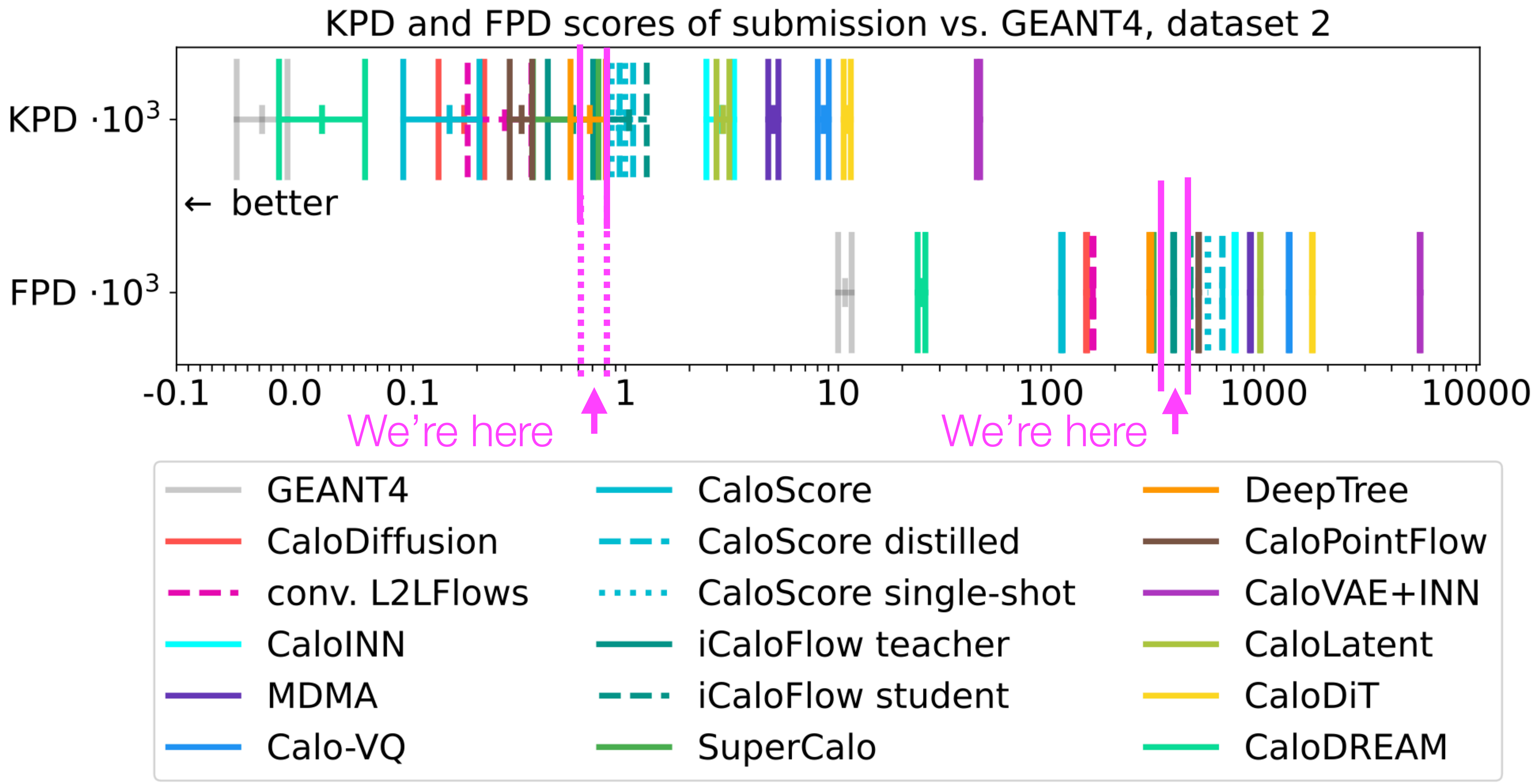
★arXiv:2410.22870



Discussion / Conclusions / Perspectives

	GEANT4	GPU (A100)	QPU	Annealing time
Time	~ 1 s	~ 2 ms	0.2 ms	~ 0.02 ms

	FPD ($\times 10^3$)	KPD ($\times 10^3$)
Pegasus	443.0 ± 2.4	0.84 ± 0.1
Zephyr	380.7 ± 1.1	0.61 ± 0.06
Zephyr	362.7 ± 1.7	0.57 ± 0.08



- ✦In the process of getting dataset from ATLAS.
- ✦Implementing hierarchical decoder.
- ✦Training using QPU.

Krause C, Giannelli MF, Kasieczka G, Nachman B, Salamani D, Shih D, Zaborowska A, Amram O, Borras K, Buckley MR, Buhmann E. CaloChallenge 2022: A Community Challenge for Fast Calorimeter Simulation. arXiv preprint arXiv:2410.21611. 2024 Oct 28.

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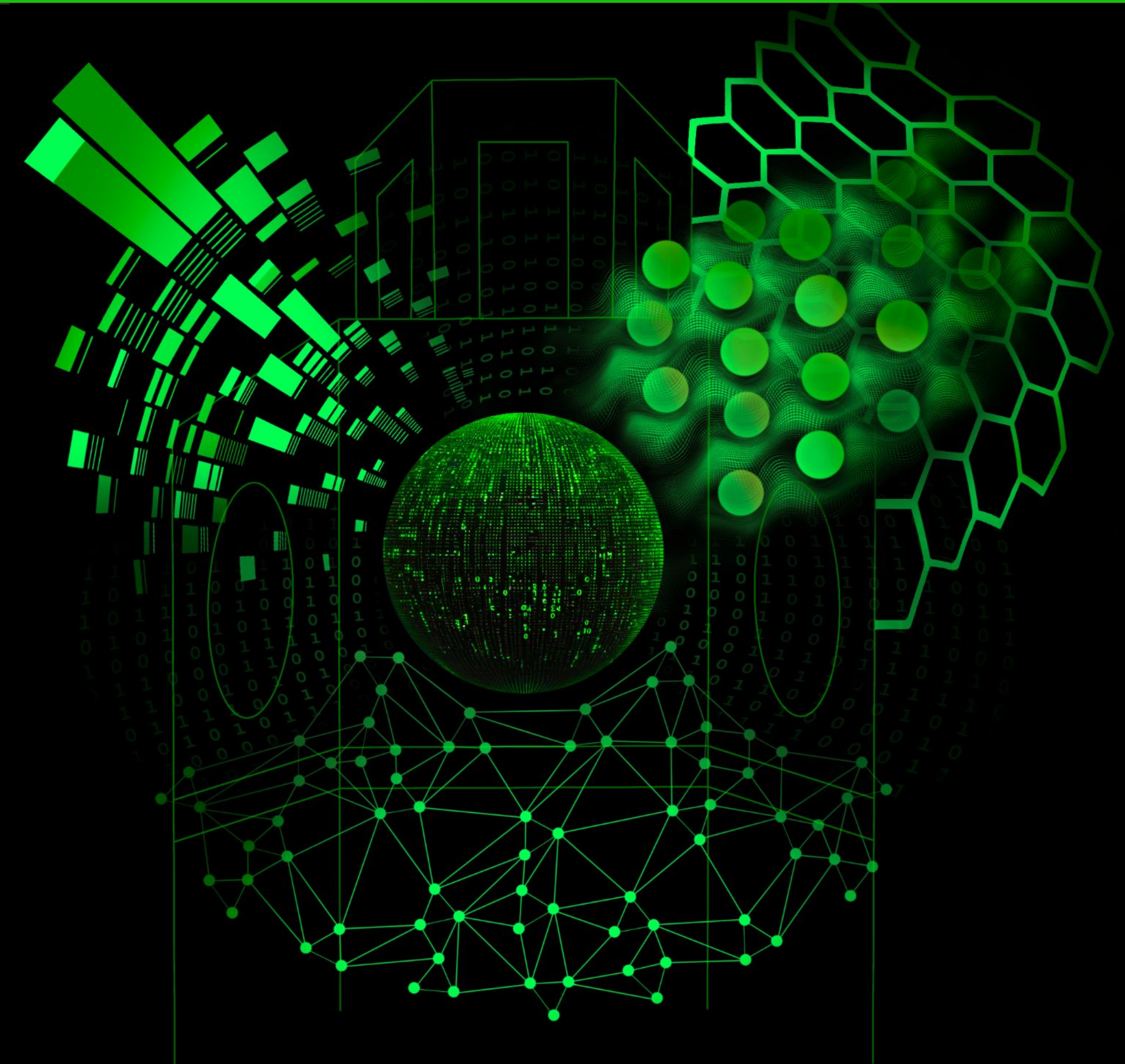
- ✳ Mitacs IT39533

- ★arXiv:2410.22870
- ★Neurips ML4Phys 2024 (accepted)
- ★IEEE-QCE QAI WS (2024)
- ★arXiv:2312.03179
- ★arXiv:2210.07430. NeurIPS 2021

Generative AI for High & Low Energy Physics



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Coordinators:
James Halverson, Jessica N. Howard*, Anindita Maiti**, Roger Melko, J. Quetzalcoatl Toledo-Marín

Scientific Advisors:
Geoffrey Fox, Eun-Ah Kim, Maximilian Swiatlowski

*Lead coordinator **Diversity coordinator

www.kitp.ucsb.edu/activities/genai25

QaloSim/CaloQVAE

jtoledo@TRIUMF.ca