Calo4pQVAE: A calorimeter surrogate for high energy particle-calorimeter interactions using D-wave's Zephyr topology

★arXiv:2410.22870

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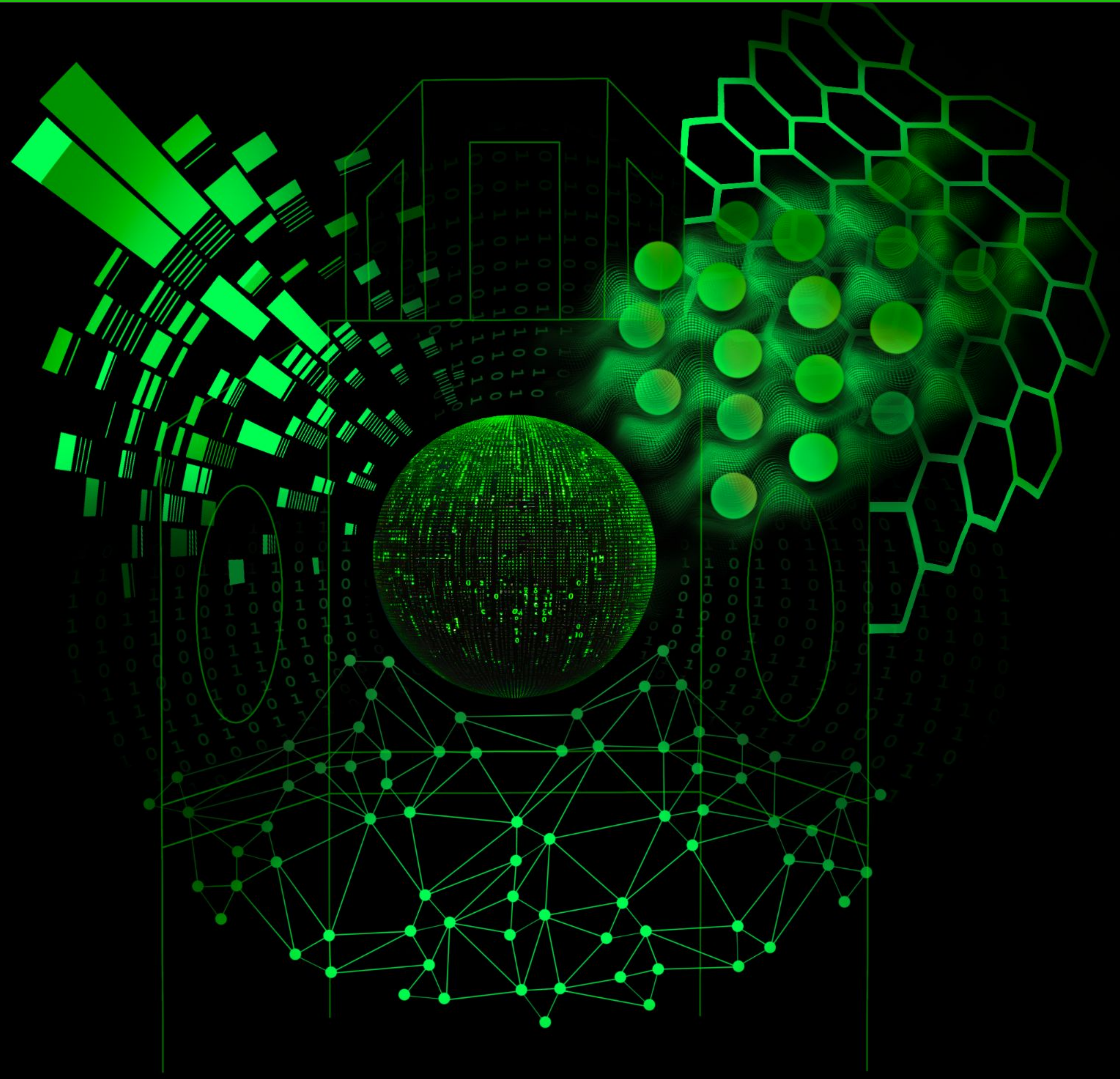
Generative AI for
High & Low Energy Physics

UC SANTA BARBARA
Kavli Institute for
Theoretical Physics



Generative AI has been broadly adopted to meet the growing need for complex simulations in high energy and condensed matter physics. However, scientific simulations require assurances of uncertainty quantification and interpretability; aspects which are comparatively lacking in current methods. This seven-week program at the Kavli Institute for Theoretical Physics will bring together experts from high energy and condensed matter physics, computer science, and industry to work towards developing effective, robust, and interpretable generative AI methods for physics simulations.

Nov. 03, 2025 - Dec. 19, 2025

Application deadline: Dec. 8, 2024

www.kitp.ucsb.edu/activities/genai25

Coordinators:

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

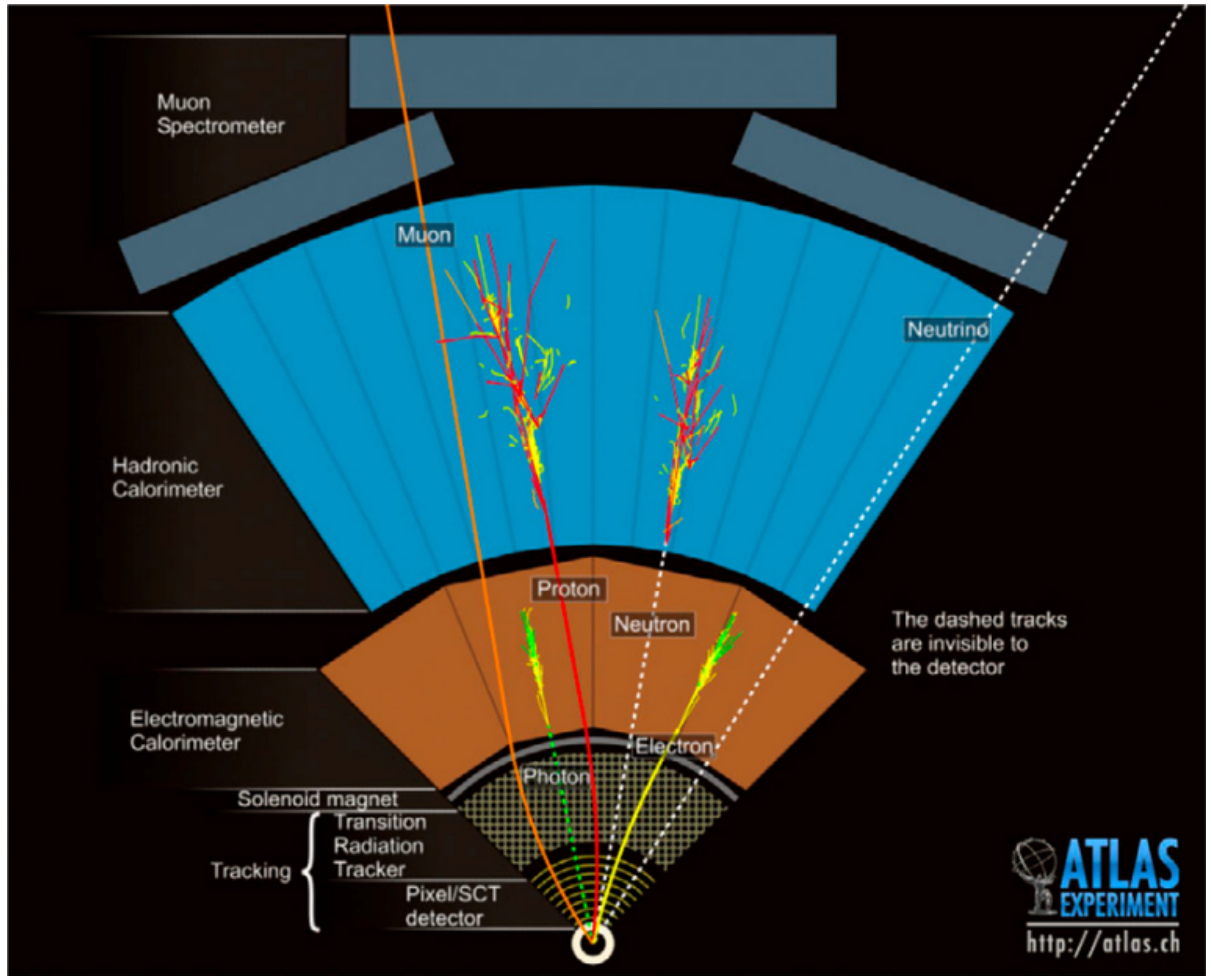
Scientific Advisors:

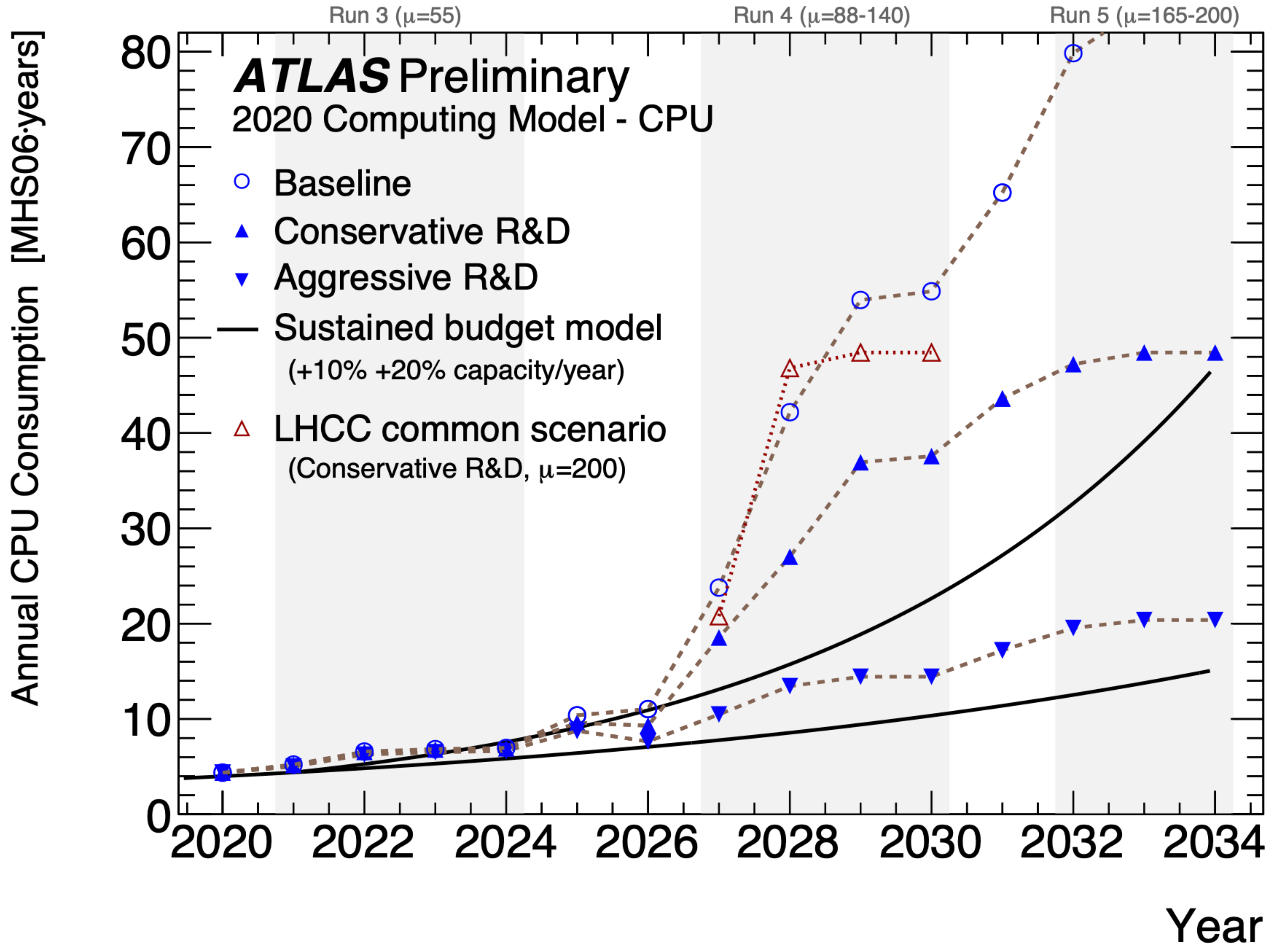
Geoffrey Fox, Eun-Ah Kim, Maximilian Swiatlowski

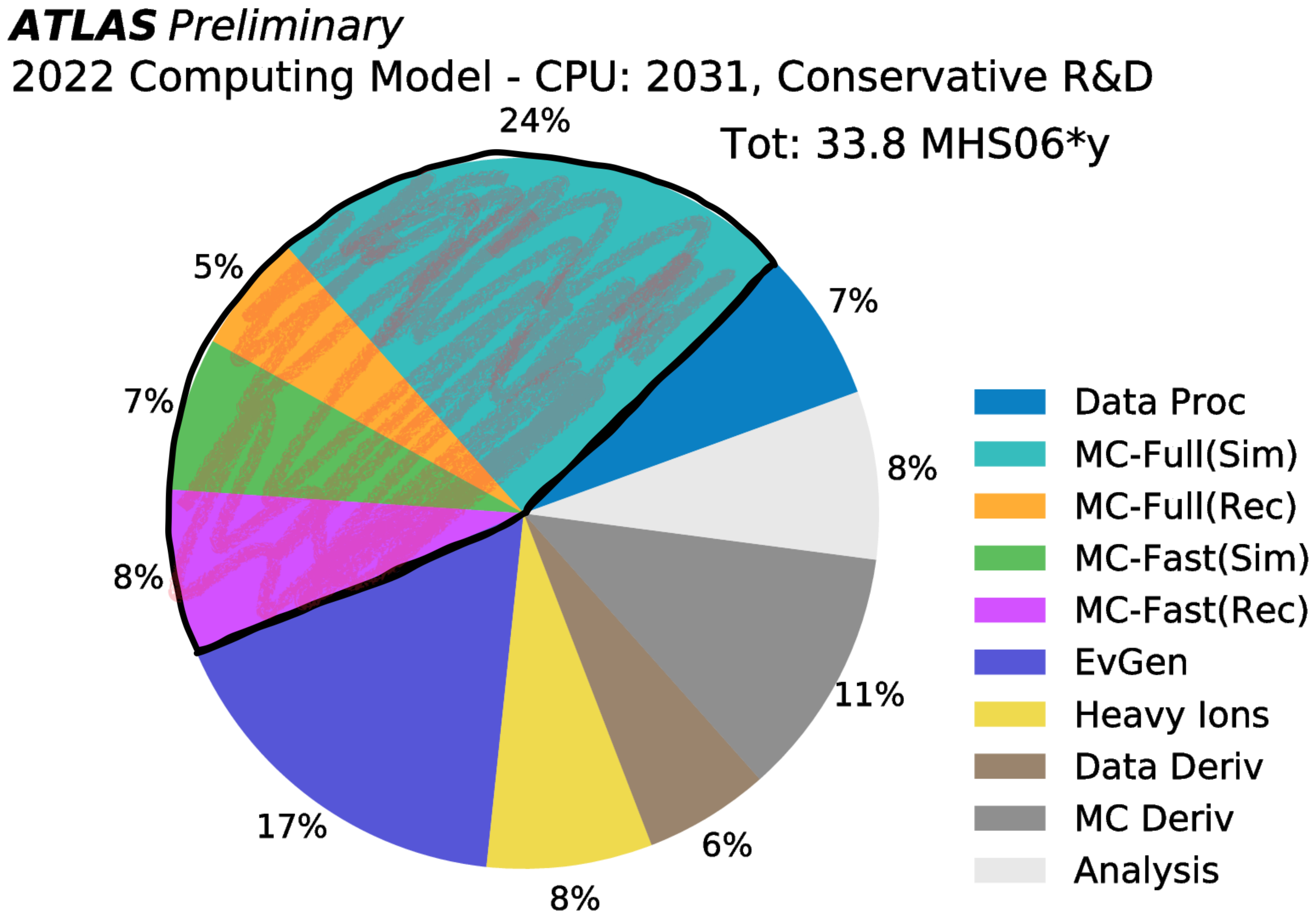
*Lead coordinator **Diversity coordinator

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.

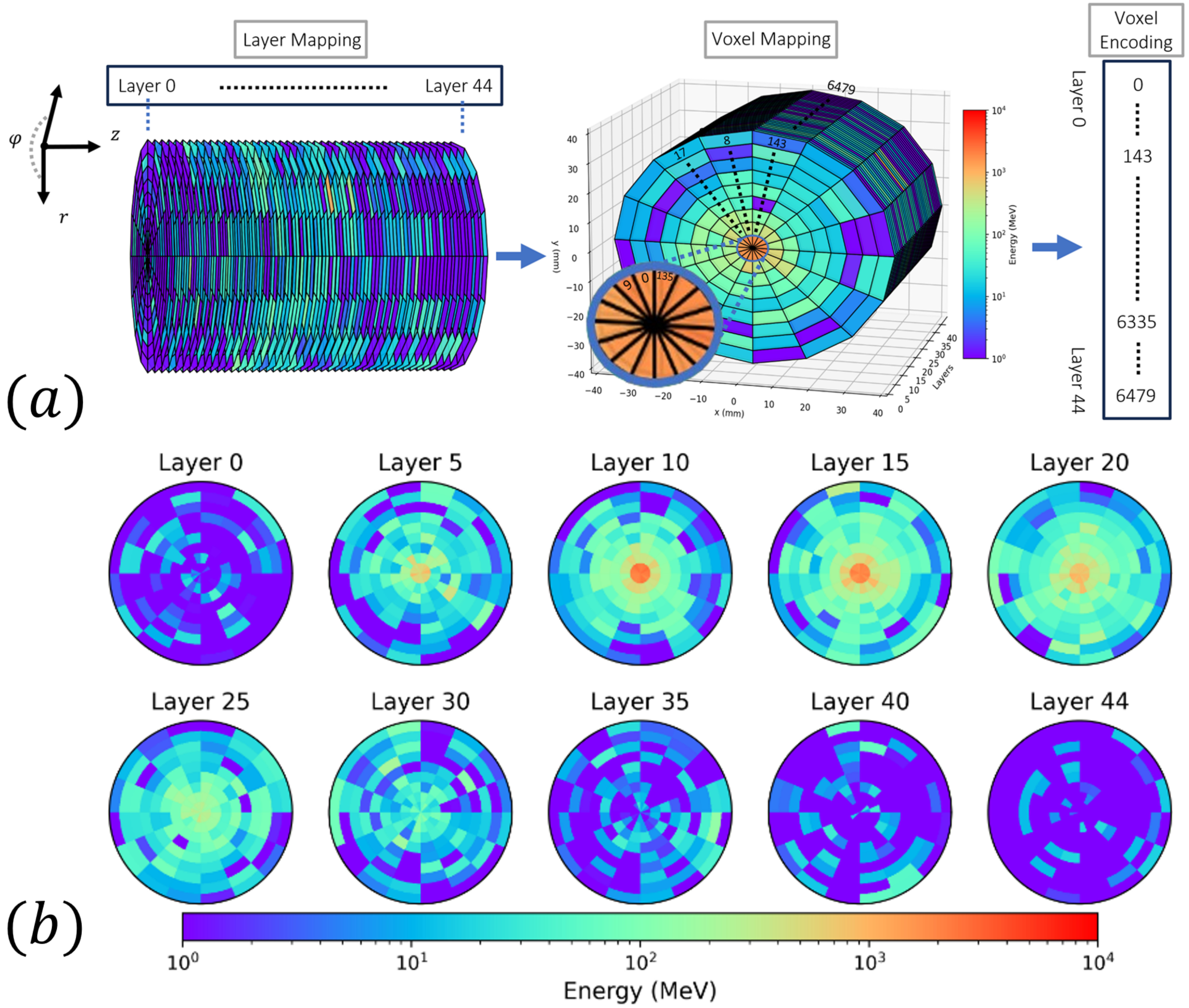






Scientific Data Lake for High Luminosity LHC project and other data-intensive particle and astro-particle physics experiments. InJournal of Physics: Conference Series 2020 Dec 1 (Vol. 1690, No. 1, p. 012166). IOP Publishing.

CaloChallenge

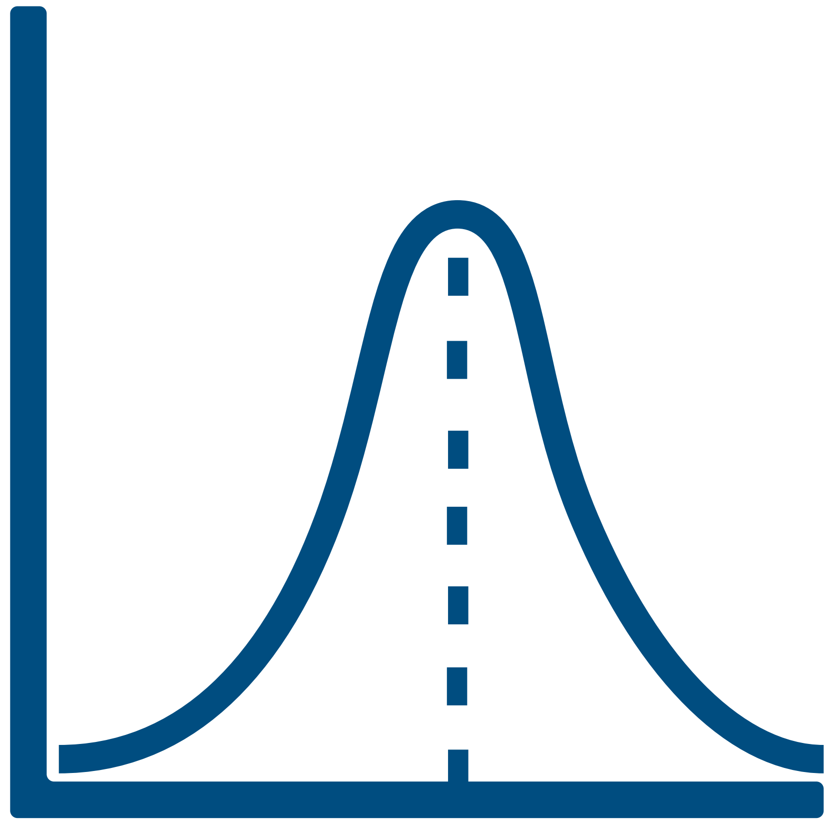


	Dataset
Particle type	Electron showers
Layers	45
Voxels per layer	9 radial * 16 angular
Incident energies	Log-uniform distribution (1GeV-1TeV)
N. of events	100,000

Generative Models

Simplest Example: Box-Muller Method

Gaussian Distribution



Generative Models

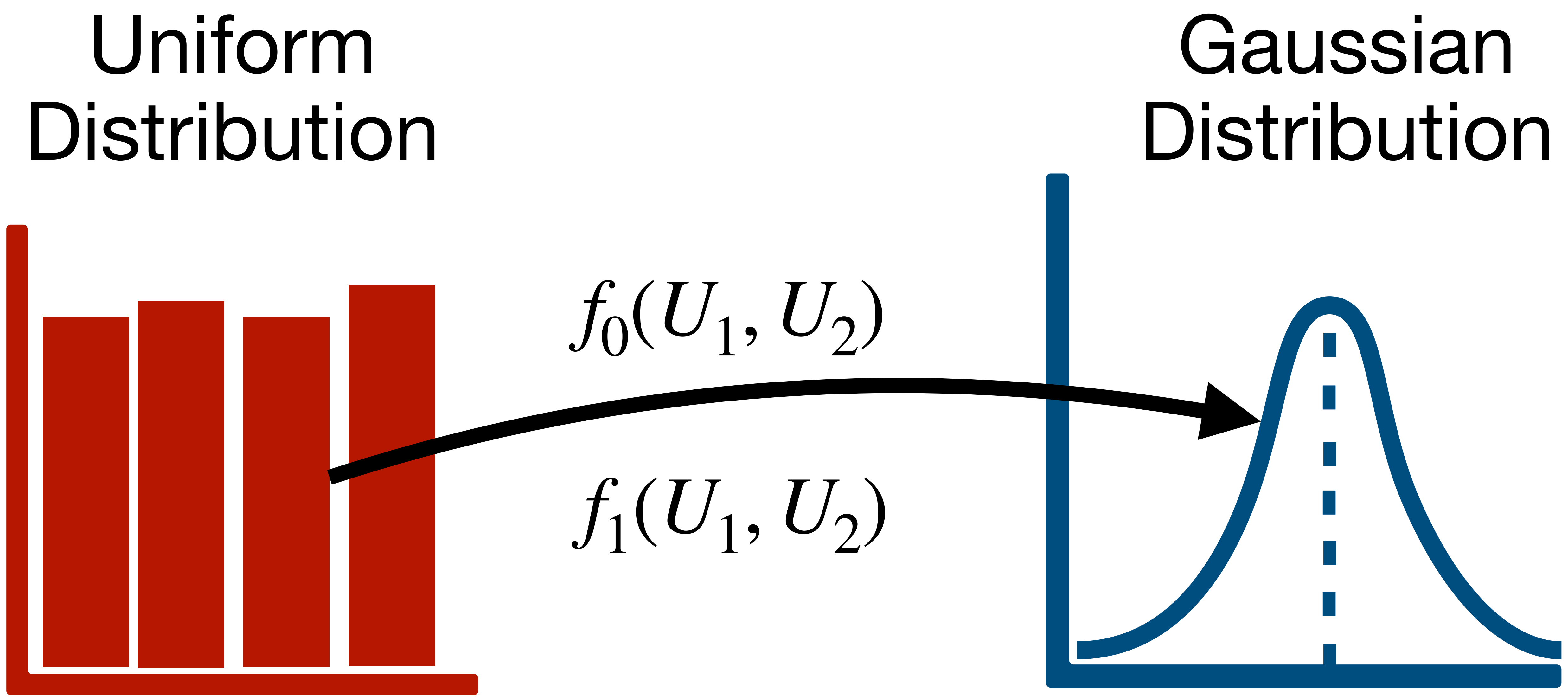
Simplest Example: Box-Muller Method

Uniform Distribution

Gaussian Distribution

Generative Models

Simplest Example: Box-Muller Method



Recipe:

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

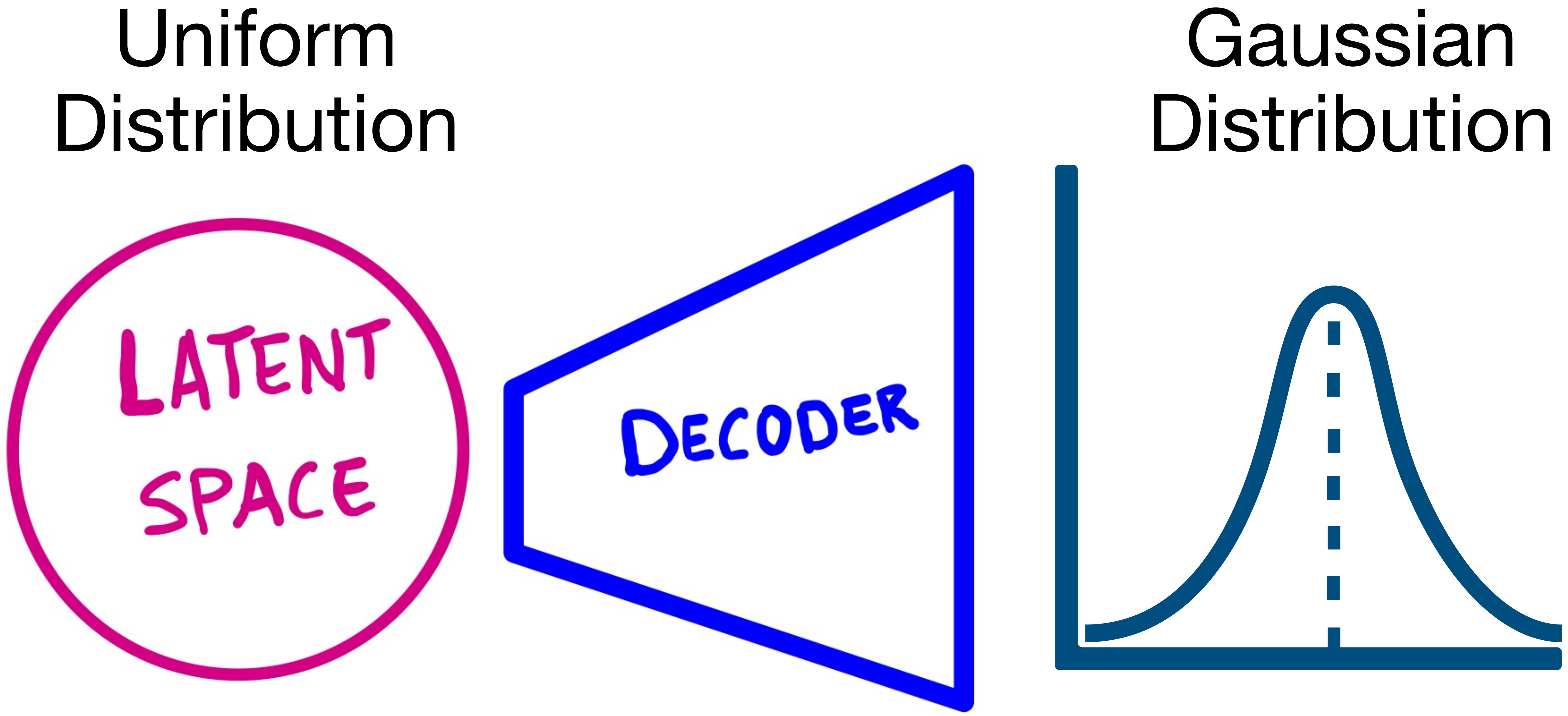
2. Substitute in:

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

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

Generative Models

Simplest Example: Box-Muller Method



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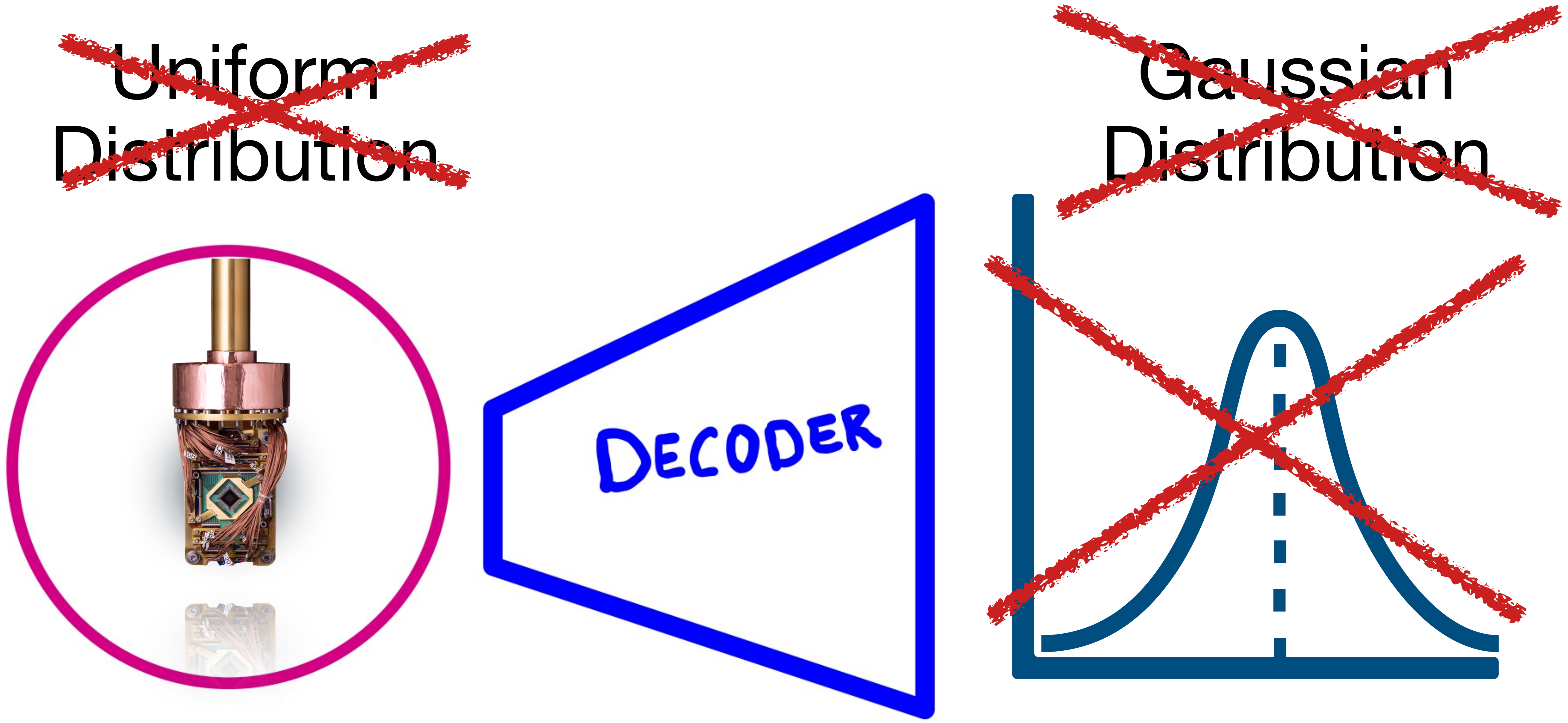
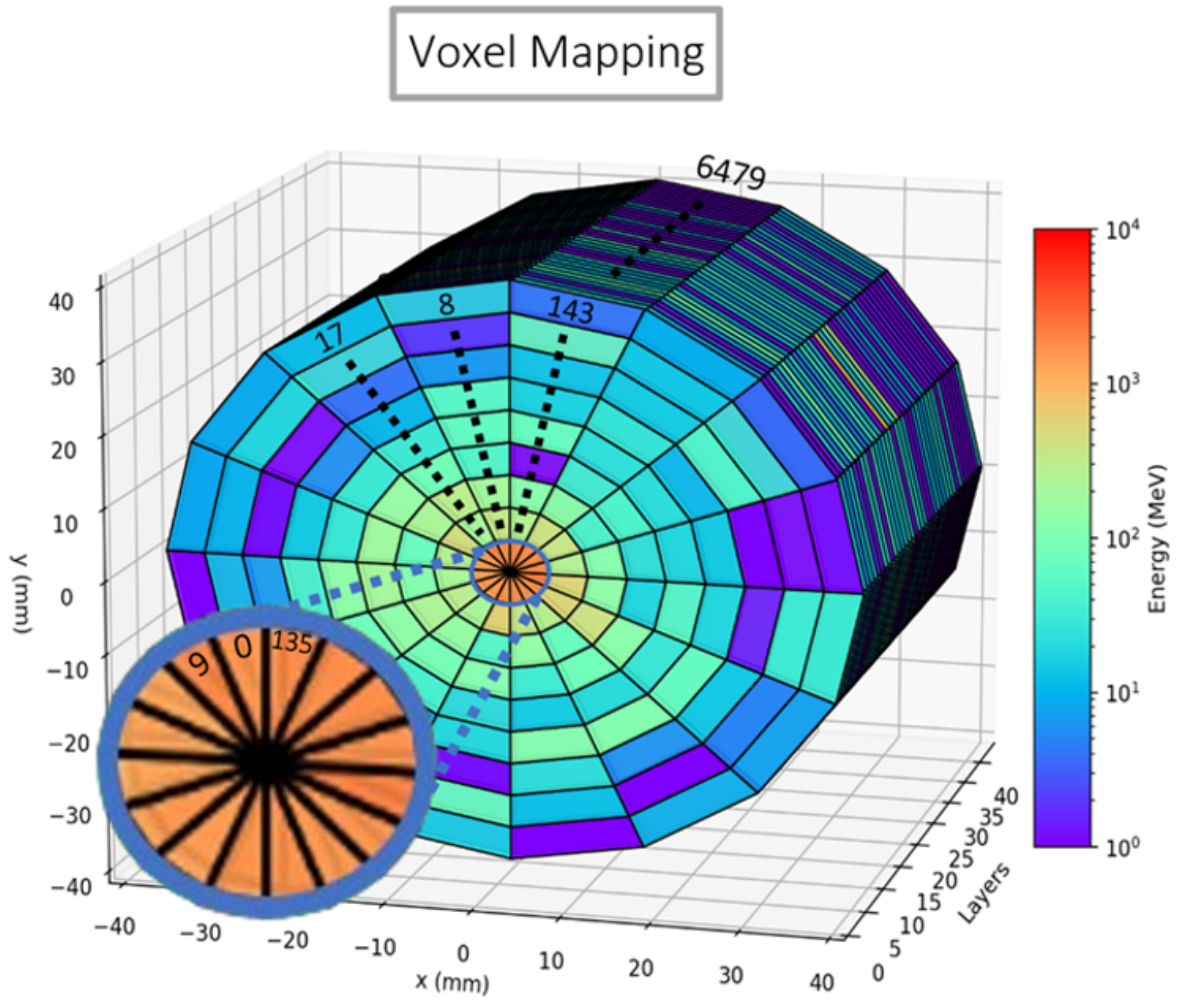
Generative Models

For particle-calorimeter interactions + quantum-assisted



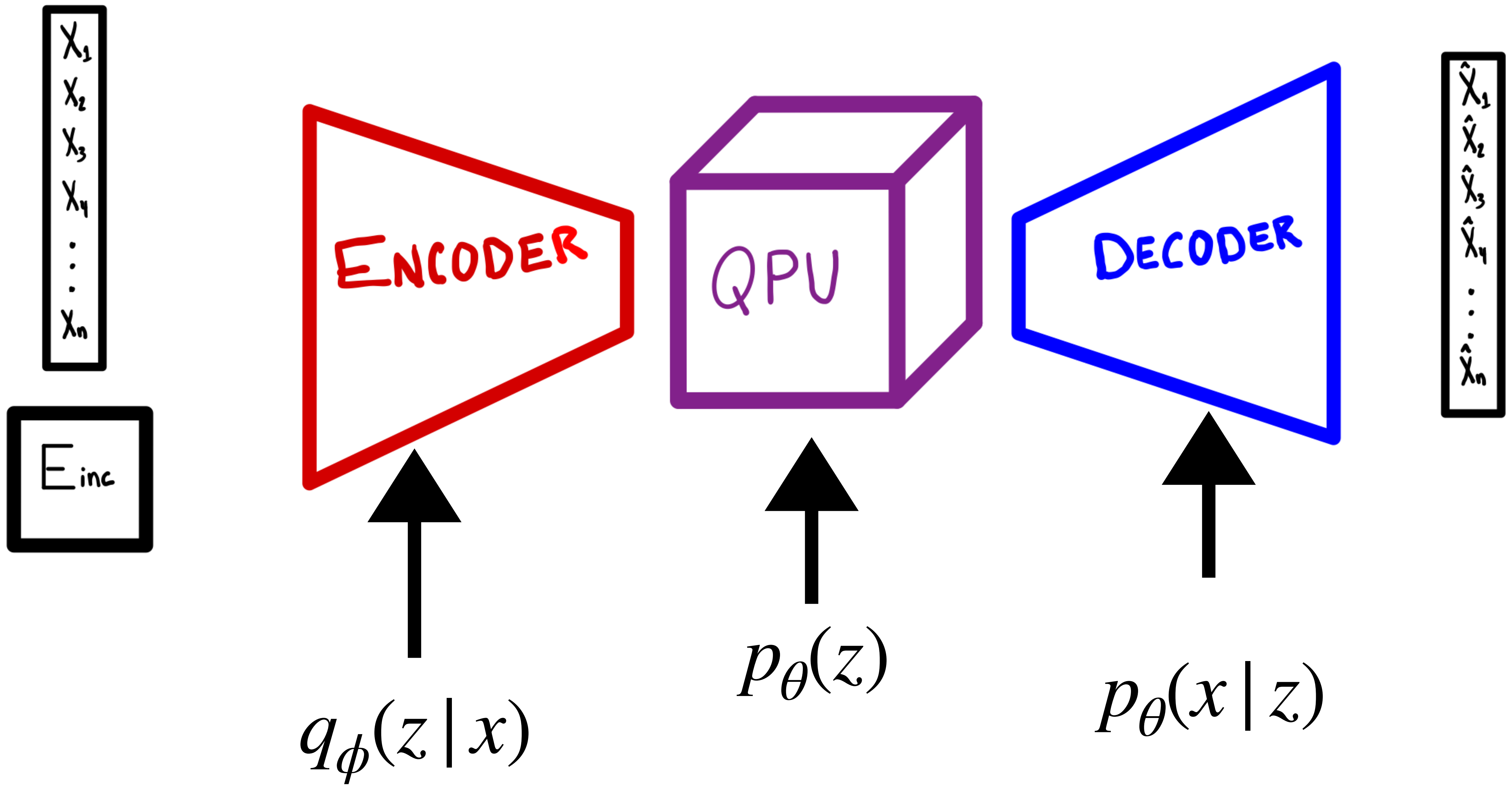
~~Uniform Distribution~~

~~Gaussian Distribution~~



Quantum-Assisted Discrete VAE

DIY



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

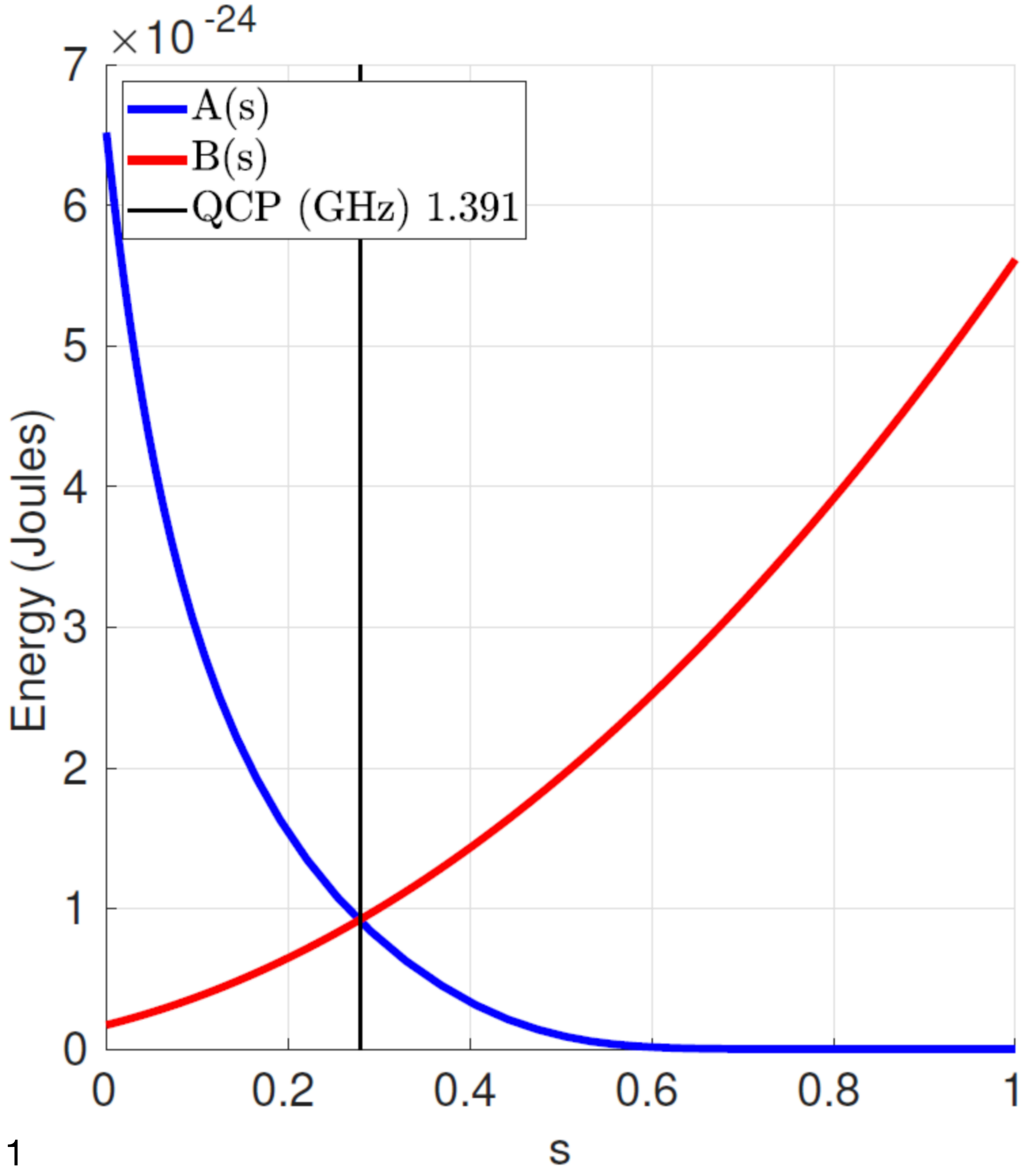
- ✦ Start with a VAE
- ✦ Replace Gaussian prior with Boltzmann prior.
- ✦ Use the QA as an RBM surrogate.

Quantum Annealer

Basics

$$\mathcal{H}_{ising} = \underbrace{-\frac{A(s)}{2}\left(\sum_i \hat{\sigma}_x^{(i)}\right)}_{\substack{\text{Initial Hamiltonian}\\ H_1}} + \underbrace{\frac{B(s)}{2}\left(\sum_i c_i\,\hat{\sigma}_z^{(i)} + \sum_{i>j} J_{i,j}\hat{\sigma}_z^{(i)}\hat{\sigma}_z^{(j)}\right)}_{\substack{\text{Final Hamiltonian}\\ H_0}}$$

- 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***.



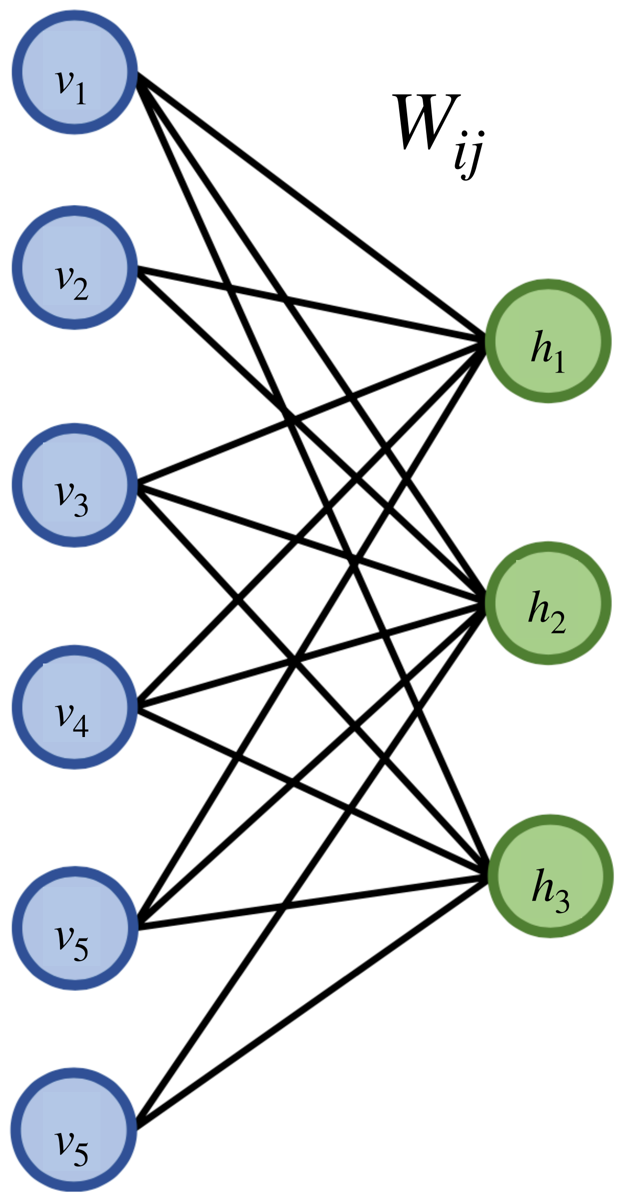
Amin MH. Searching for quantum speedup in quasistatic quantum annealers. Physical Review A. 2015 Nov 19;92(5):052323.

Quantum Annealer

Topologies

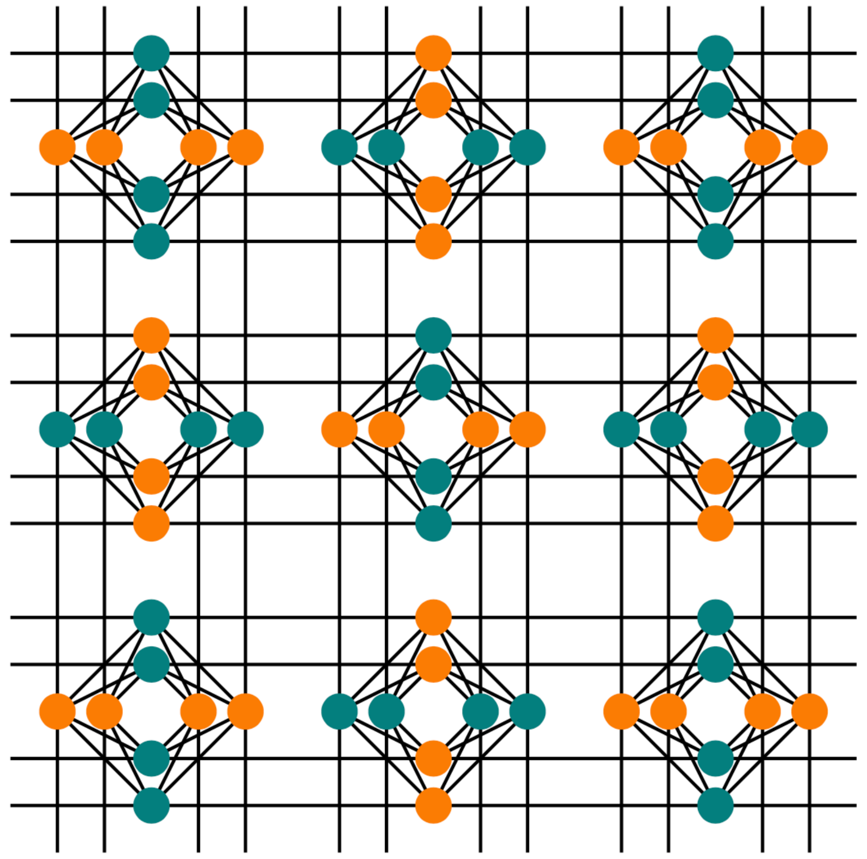
Fully Connected RBM

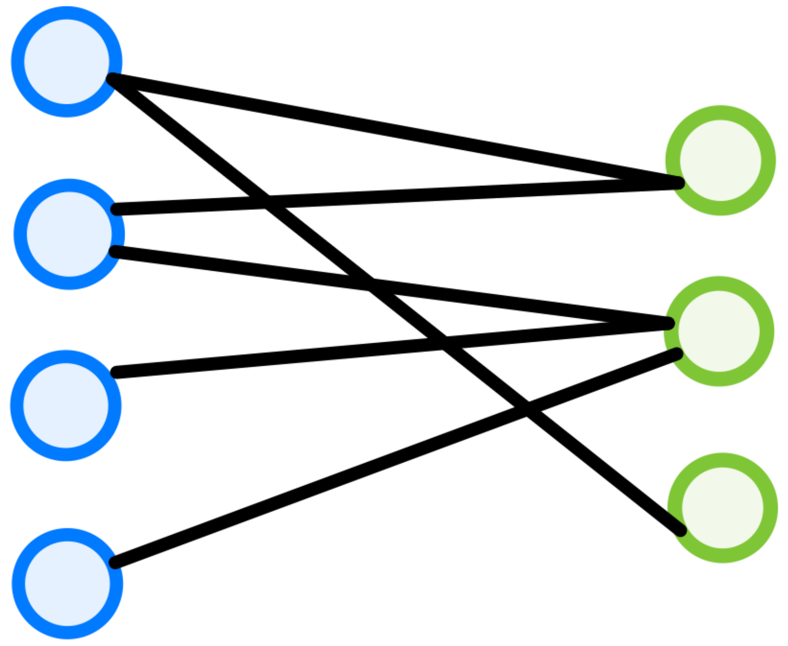
2-partite Graph



Chimera QA

2-partite Graph

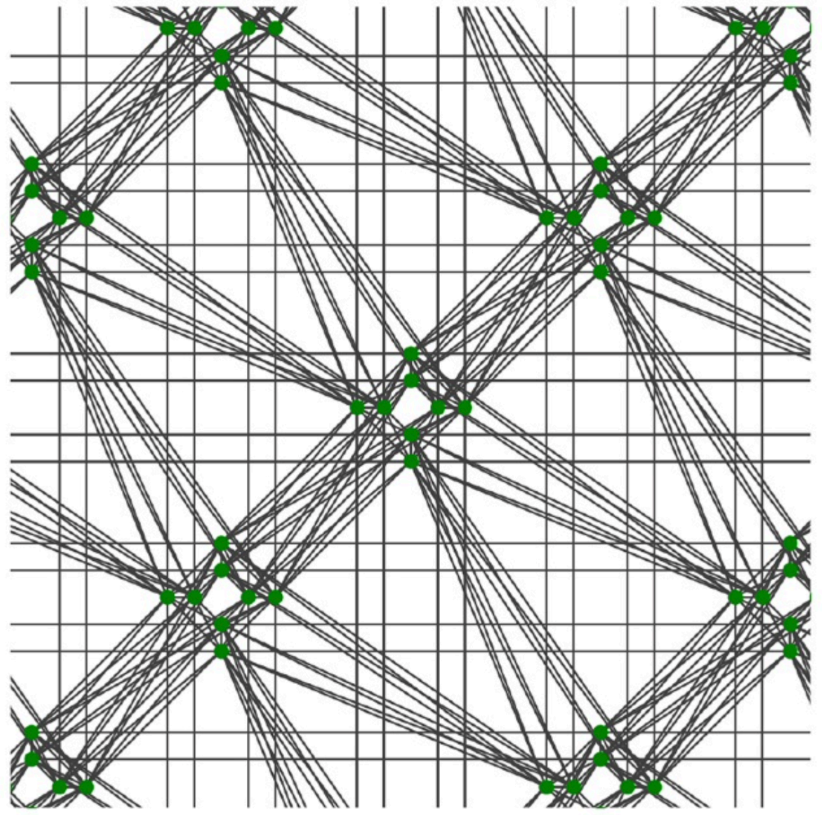




Pegasus QA

4-partite Graph

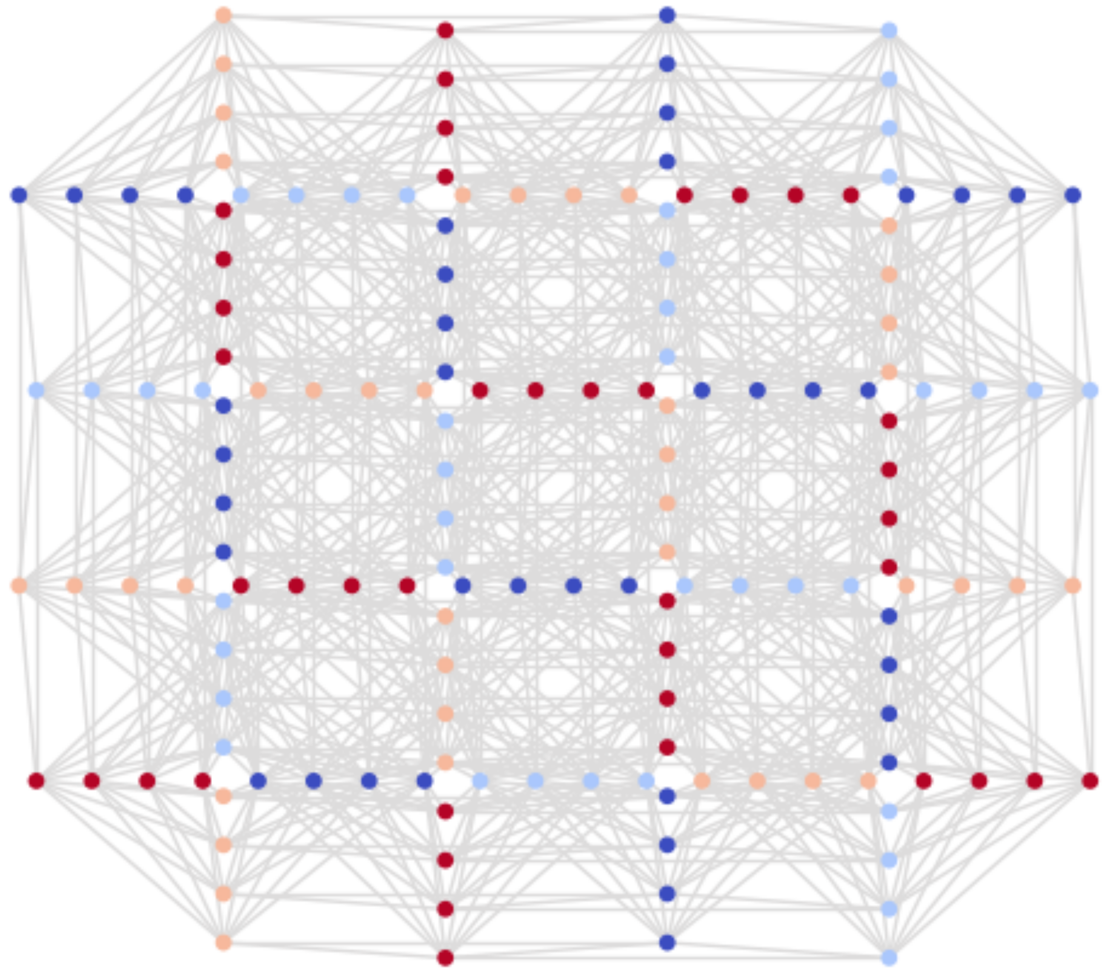
Max coord num=15

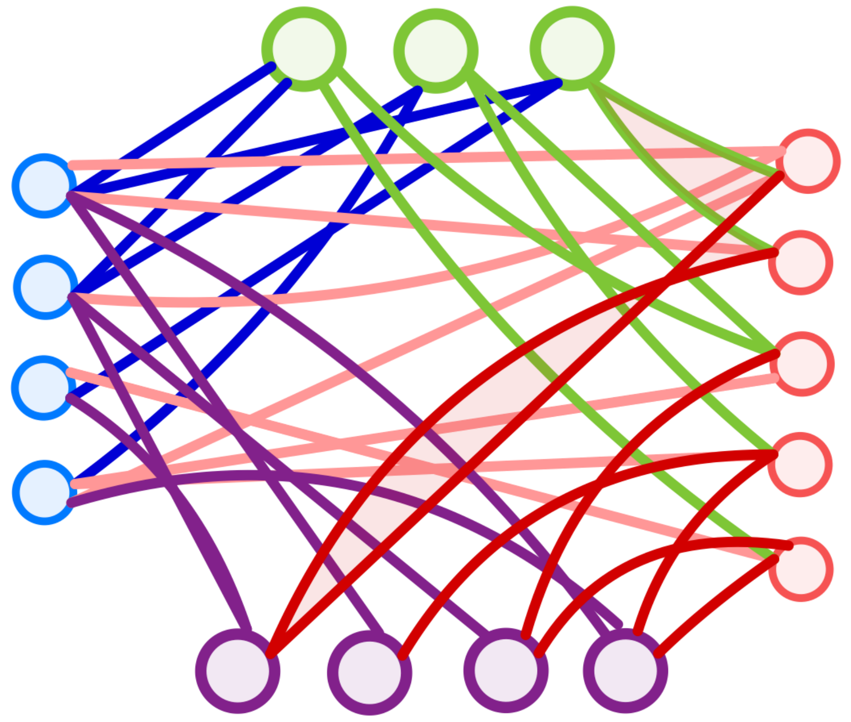


Zephyr QA

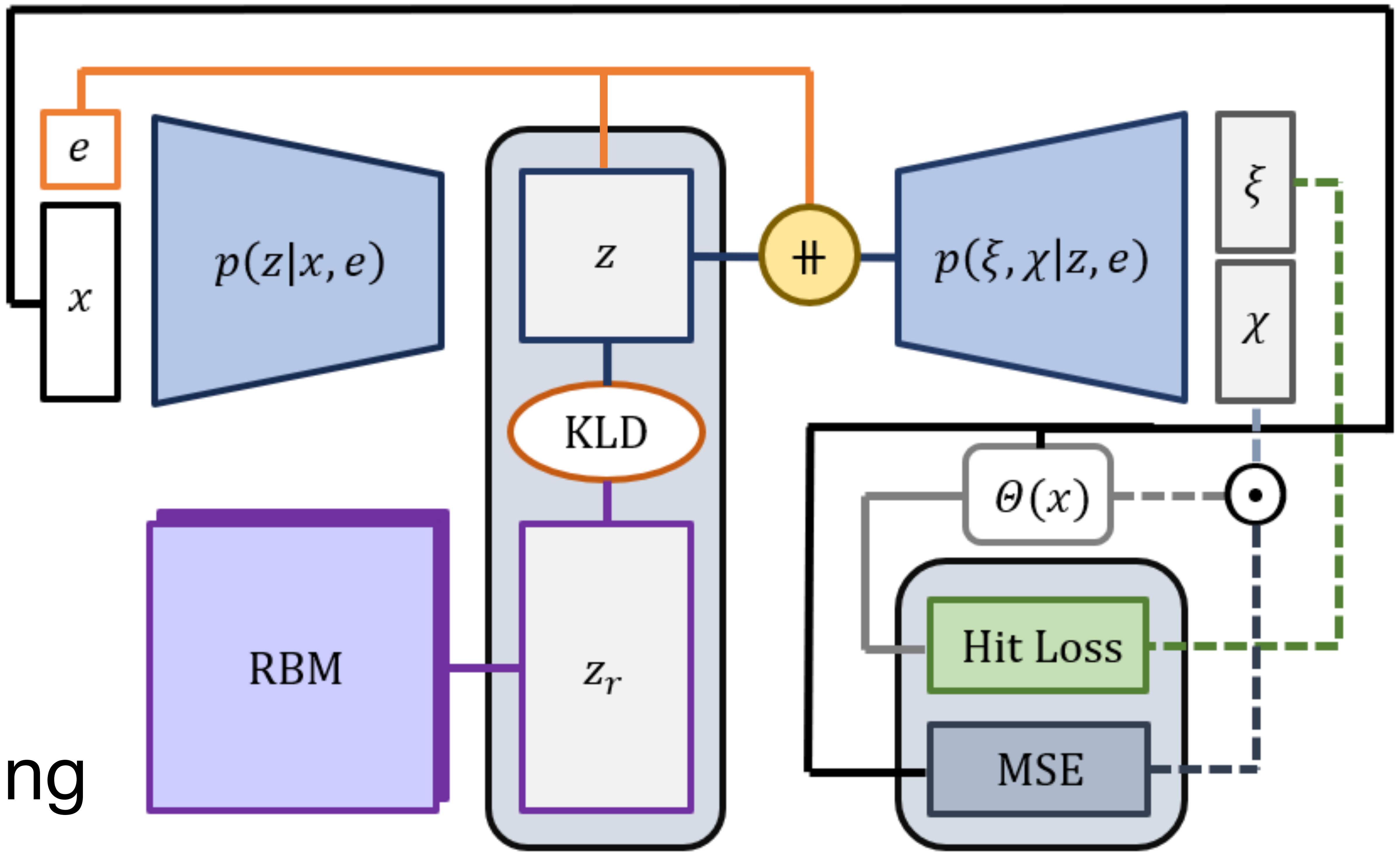
4-partite Graph

Max coord num=20

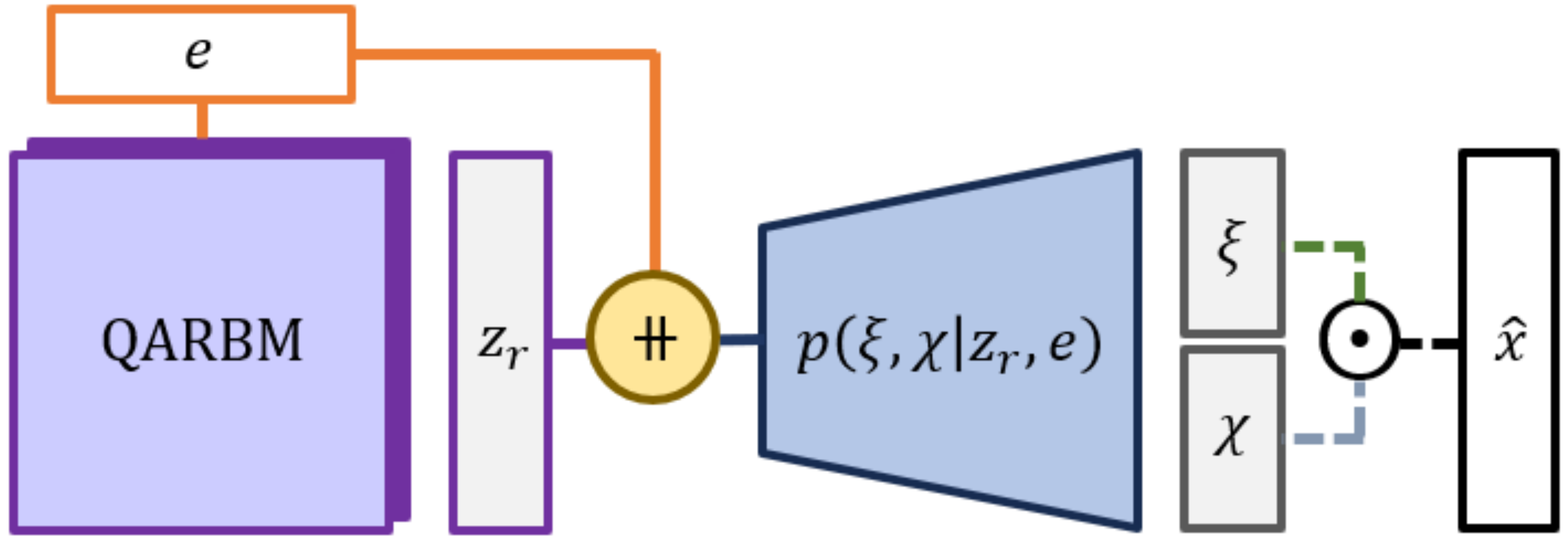




Calo4pQVAE



Training



Validation

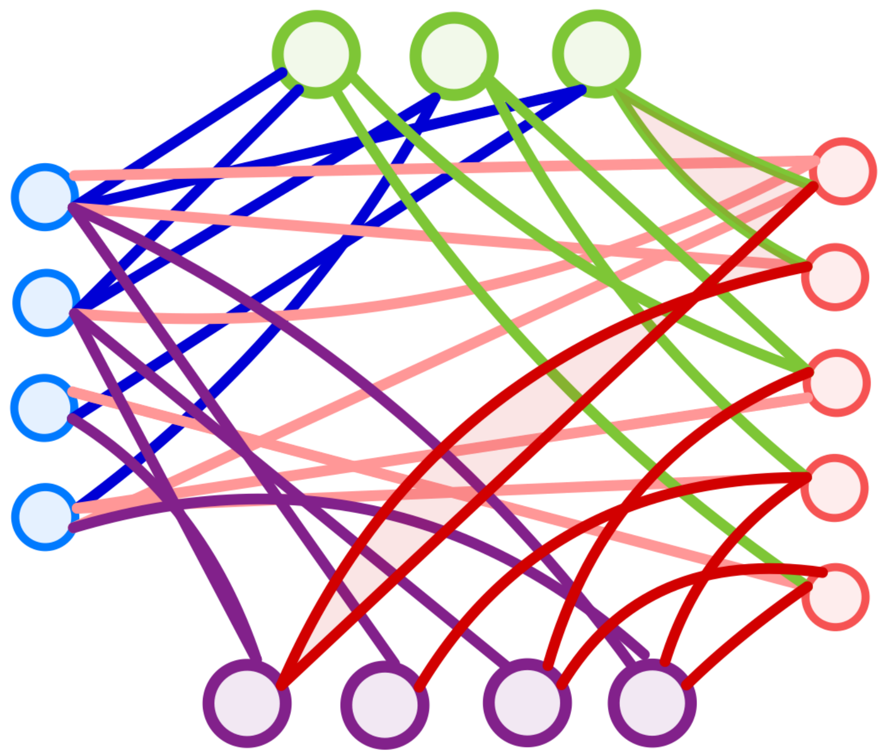
QPU conditioning

★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)

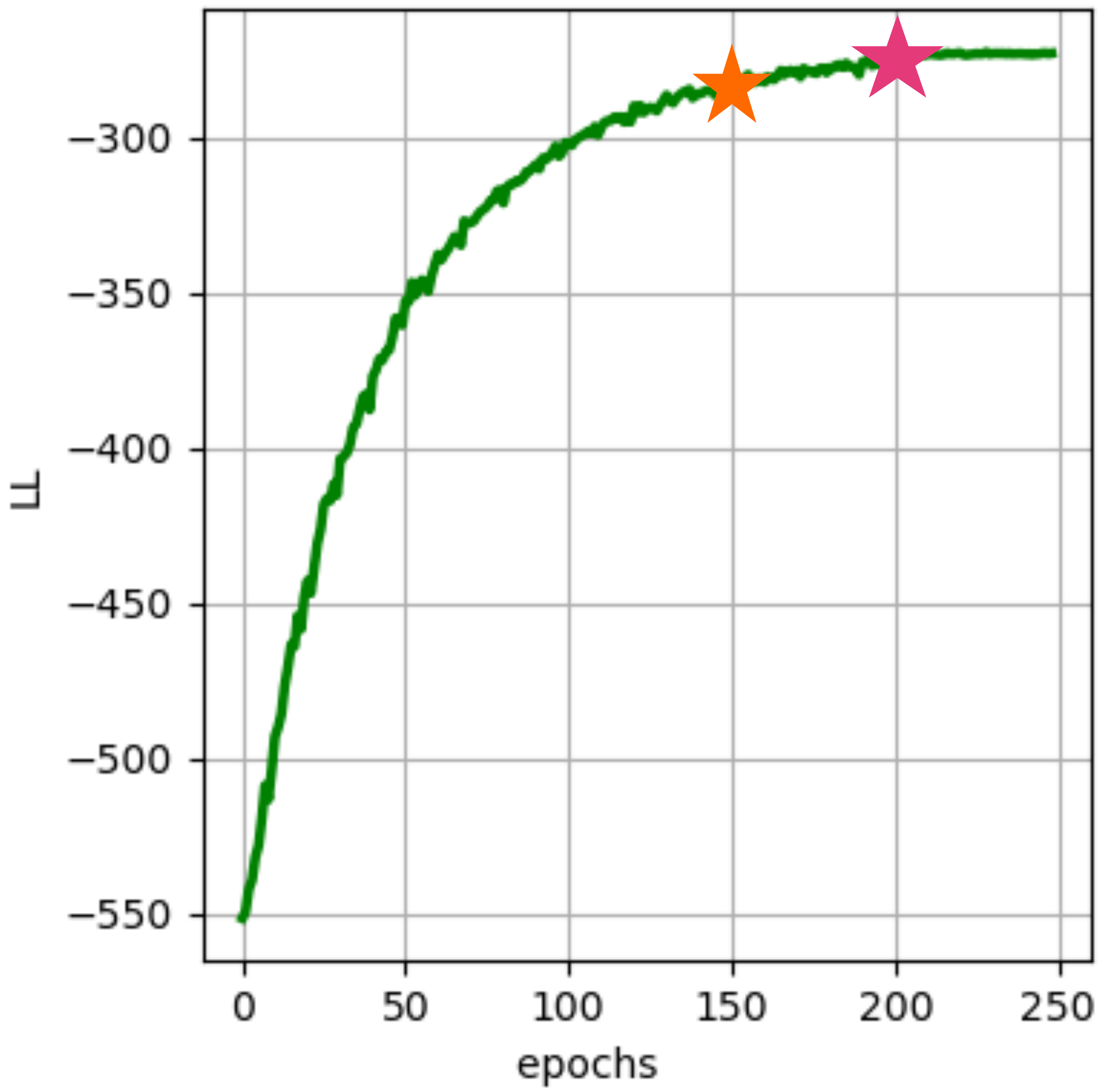
$$\boxed{\text{Label}} \xrightarrow{f} \boxed{\sigma_z^{(k)} \in \{-1,1\}^{302}} \xrightarrow{g} \boxed{h_k \in \{-M,M\}^{302}}$$



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

Results

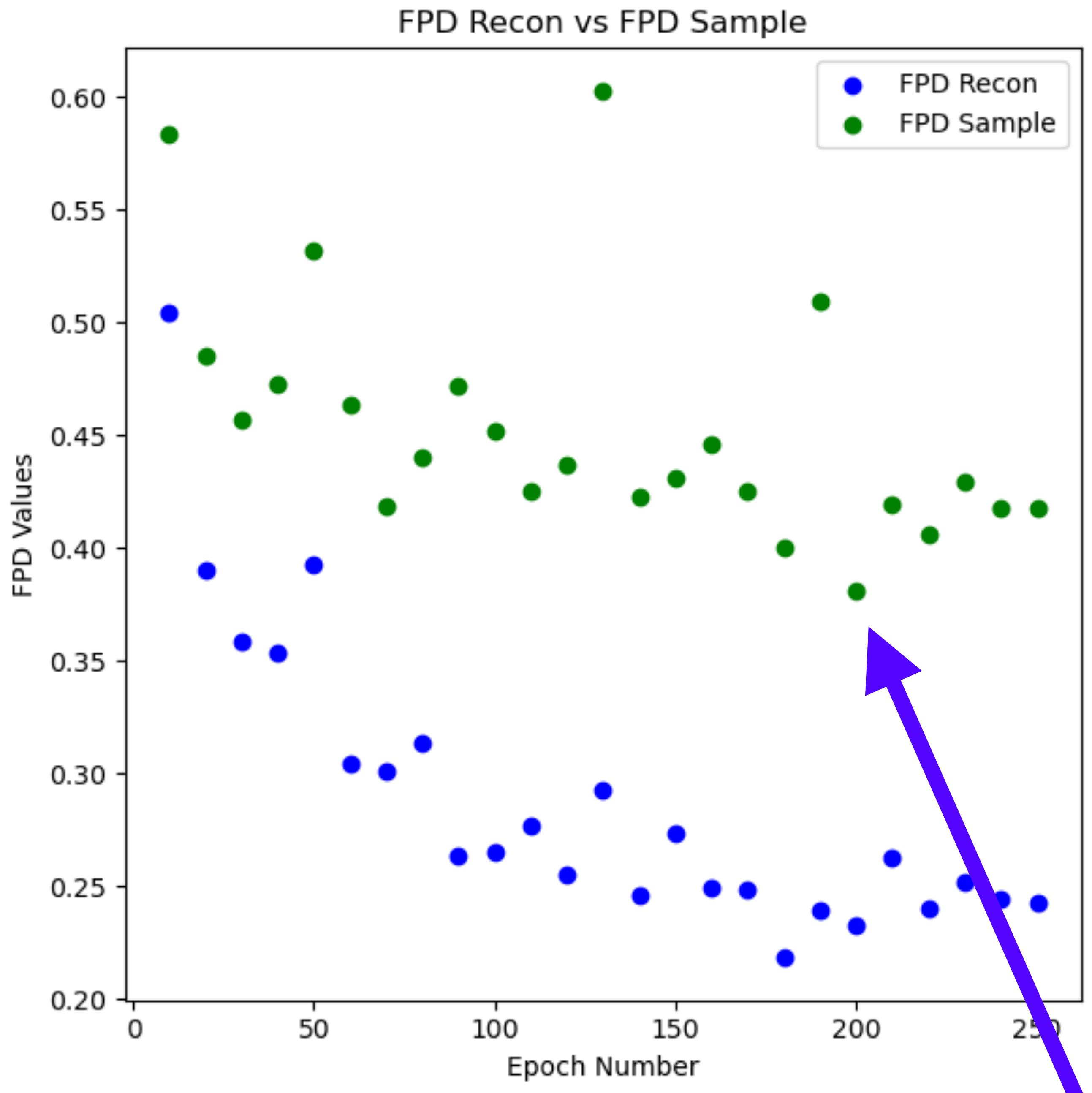
RBM Log-likelihood saturates, indicating the RBM has trained.



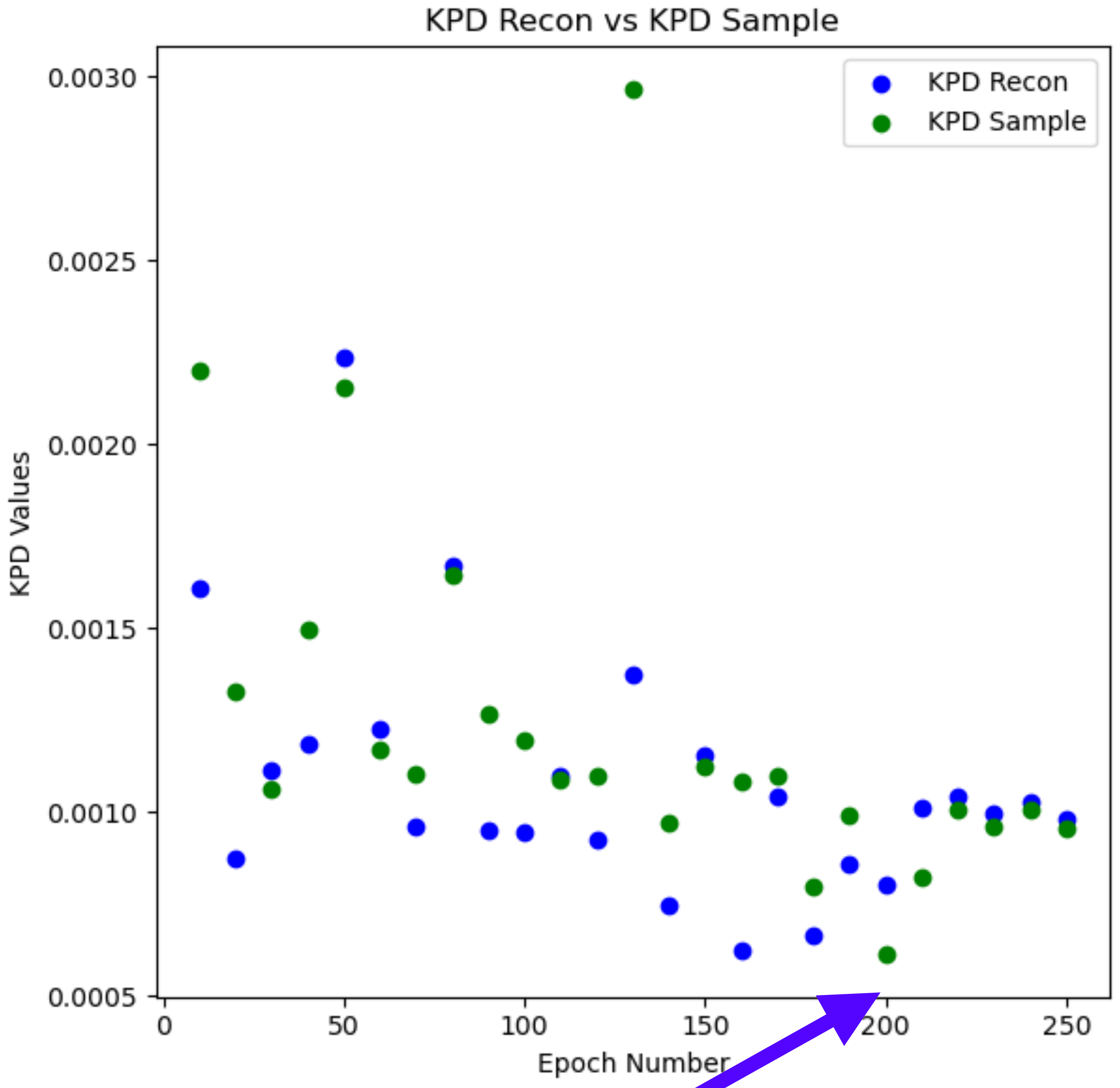
★ Slope annealing ends

★ 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 $1/\beta$

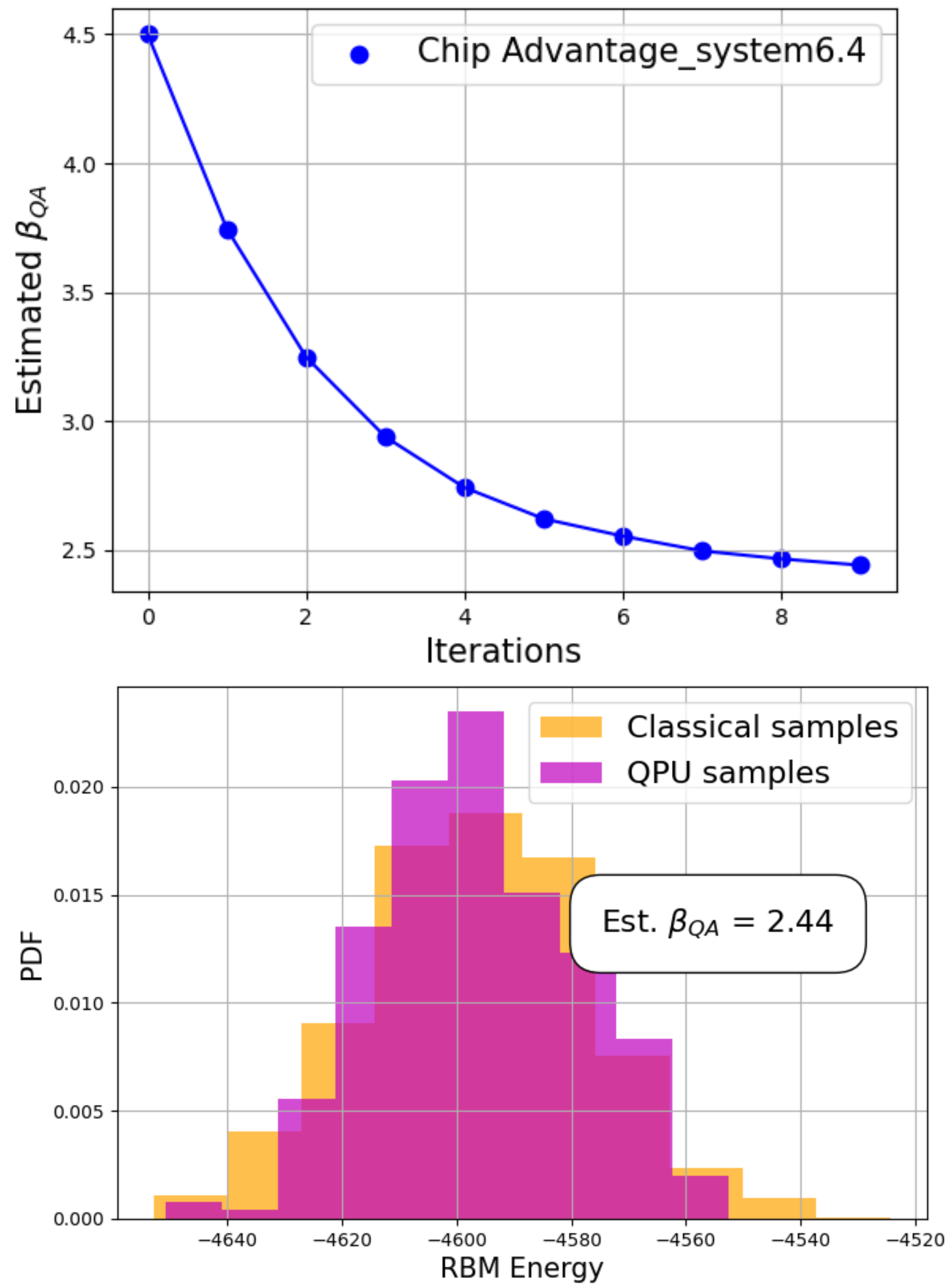
$$P_{QA}(x) = \frac{e^{-\beta_{QA}H(x)}}{Z(\beta_{QA})}$$

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

- 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

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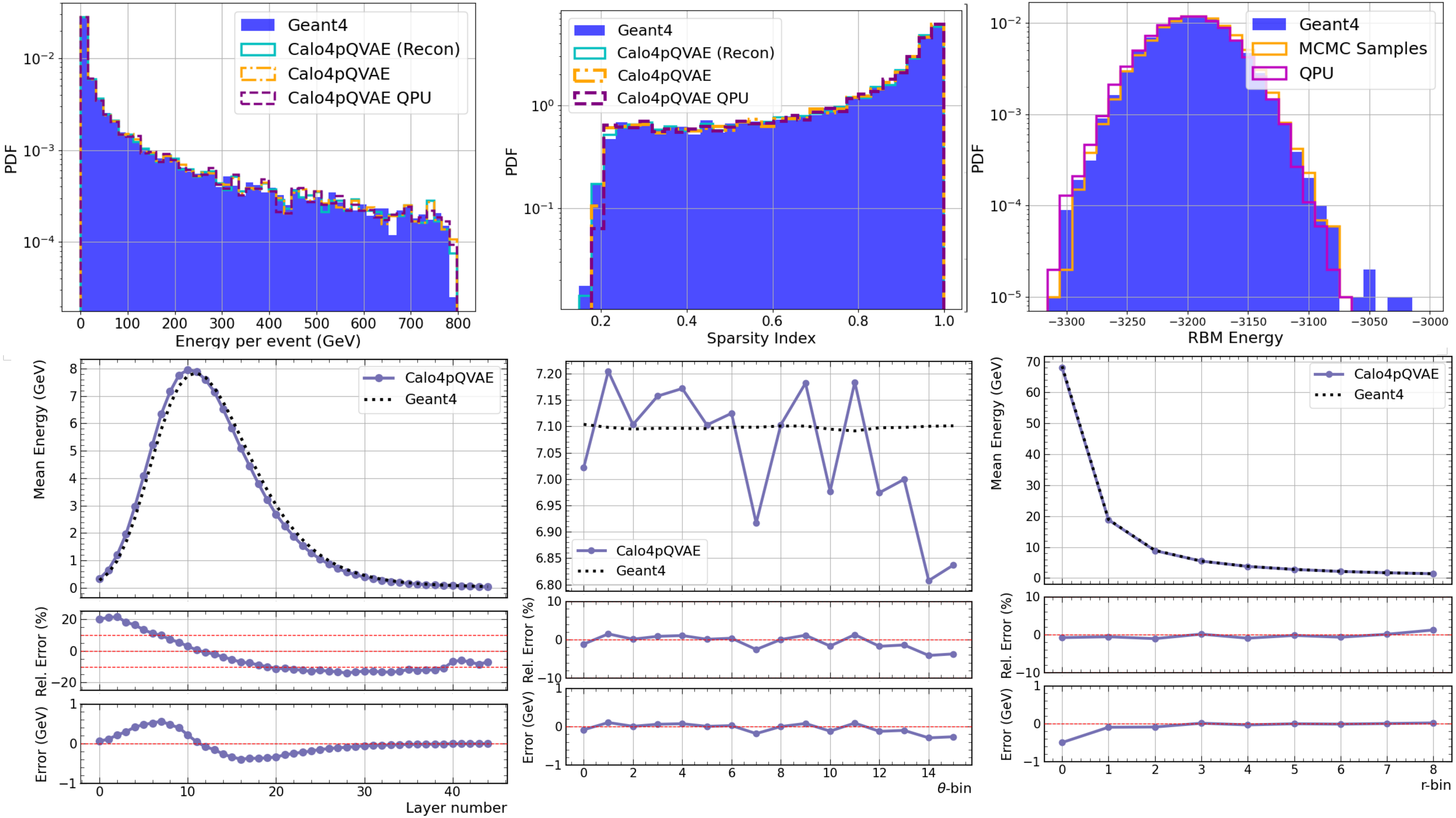
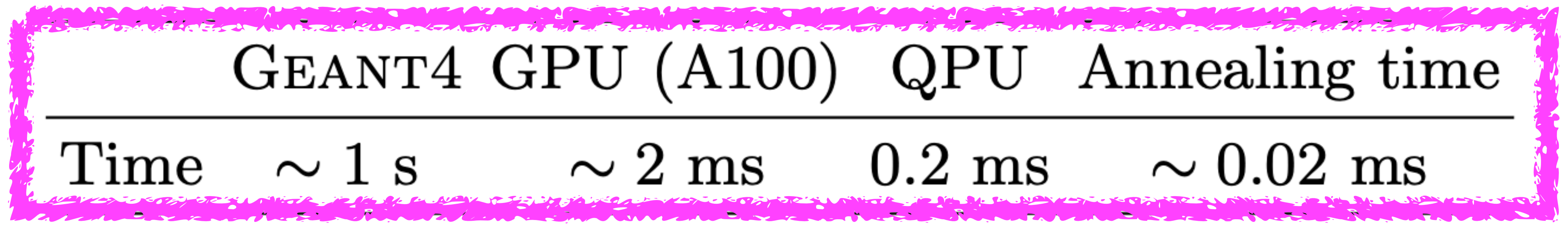
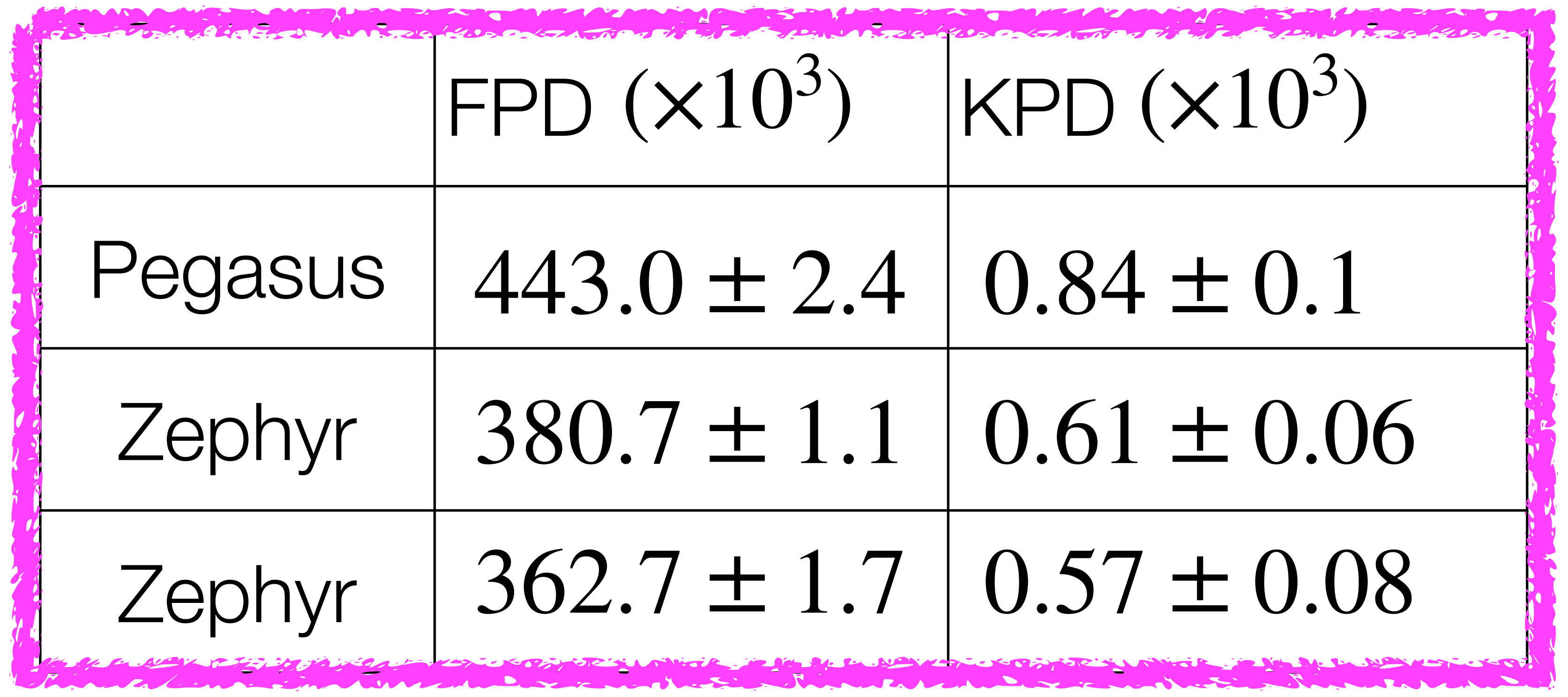


Discussion / Conclusions / Perspectives



	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.

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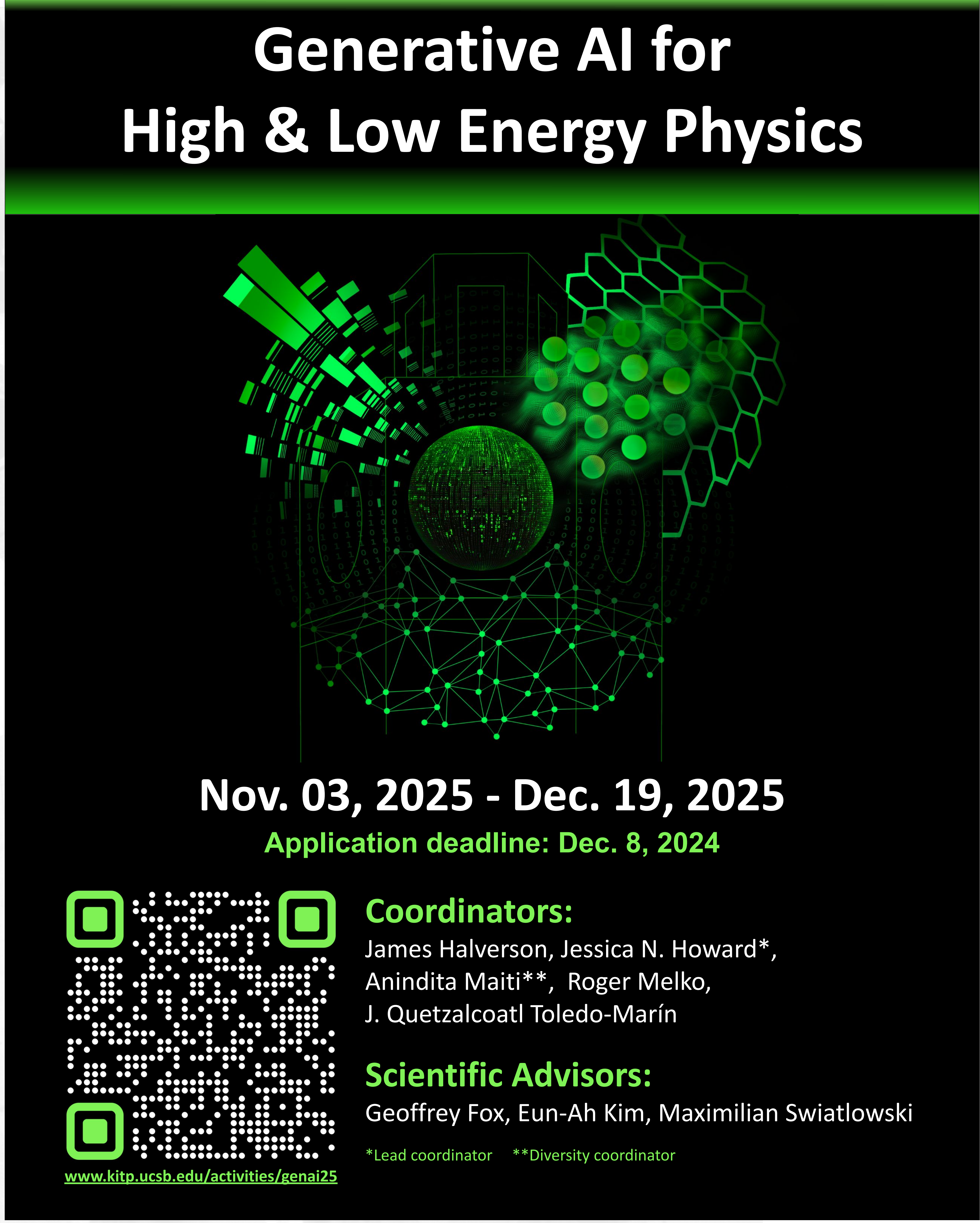
★arXiv:2312.03179
★arXiv:2210.07430. NeurIPS 2021



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QaloSim/CaloQVAE

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