Akademia Górniczo-Hutnicza
im. Stanisława Staszica w Krakowie
AGH University of Krakow

Fast simulation of the ZDC (ALICE) – update

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2025-01-08

Paper accepted for publication in *Computing and Software for Big Science*

Fast simulation of the Zero Degree Calorimeter responses with generative neural networks

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Abstract

Applying machine learning methods to high-energy physics simulations has recently emerged as a rapidly developing area. A prominent example is the Zero Degree Calorimeter (ZDC) simulation in the ALICE experiment at CERN, where substituting the traditional computationally extensive Monte Carlo methods with generative models radically reduces computation time. Although numerous studies have addressed the fast ZDC simulation, there remains significant potential for innovations. Recent developments in generative neural networks have enabled the creation of models capable of producing high-quality samples indistinguishable from real data. In this paper, we apply the latest advances to the simulation of the ZDC neutron detector and achieve a significant improvement in the Wasserstein metric compared to existing methods with a low generation time of 5 ms per sample. Our focus is on exploring novel architectures and state-of-the-art generative frameworks. We compare their performance against established methods, demonstrating competitive outcomes in speed and efficiency. The source code and hyperparameters of the models can be found at https://github.com/m-wojnar/zdc.

Keywords: generative neural networks, fast simulations, high-energy physics, zero degree calorimeter

Analysis of the ZDC neutron detector response dataset

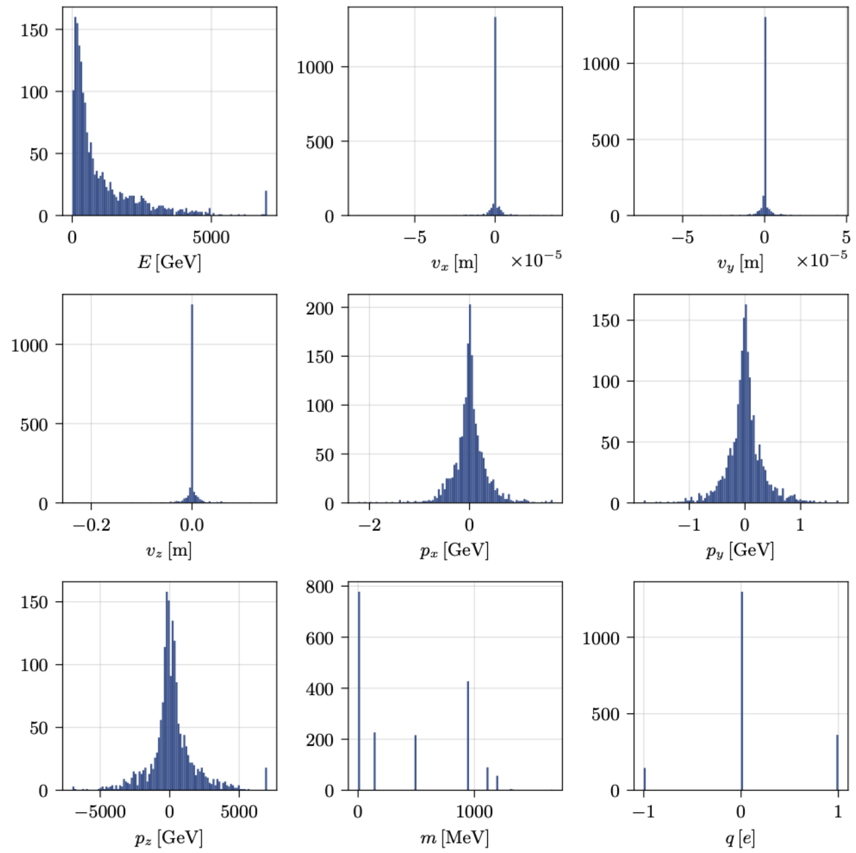


Fig. 2: Histograms of particle features. E stands for energy, v for primary vertex positions, p for momenta, m for mass, and q for charge.

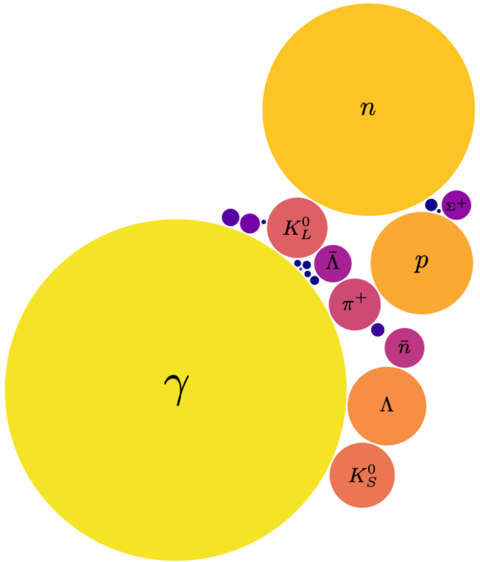


Fig. 3: Diagram depicting the distribution of particles in the dataset.

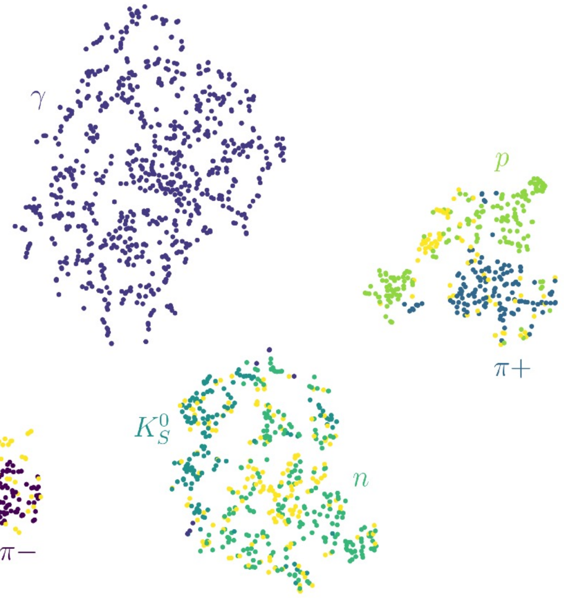
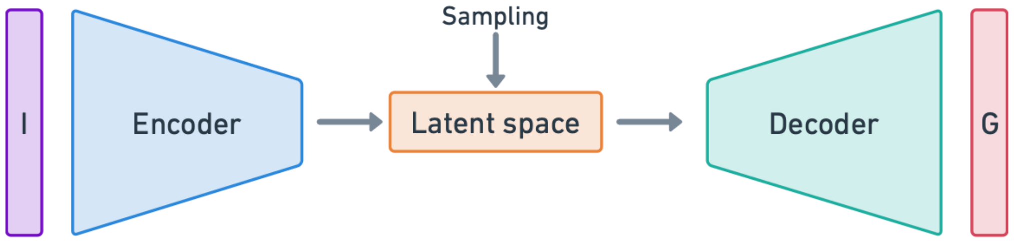
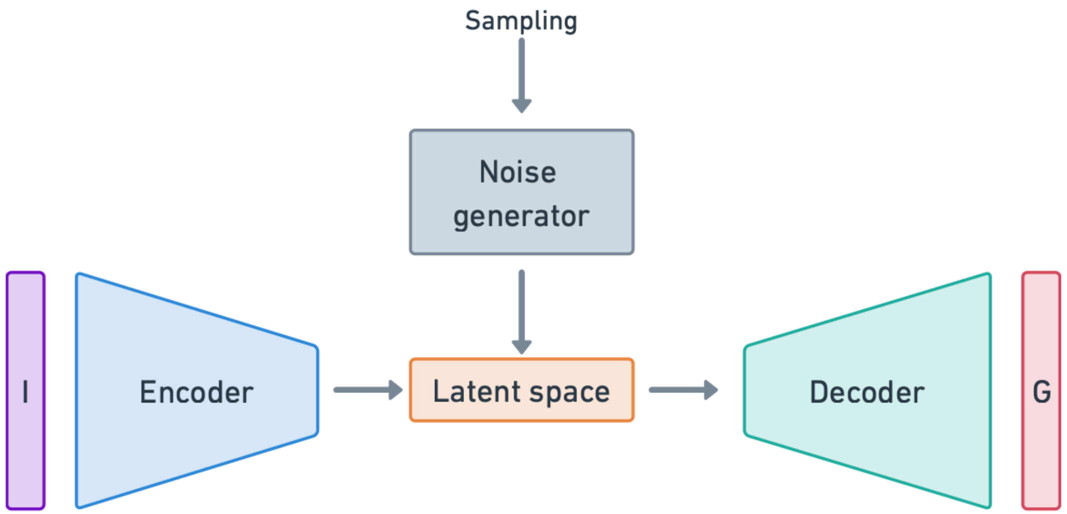


Fig. 4: Unique particle features visualization using t-SNE. The colors denote the types of the particles.

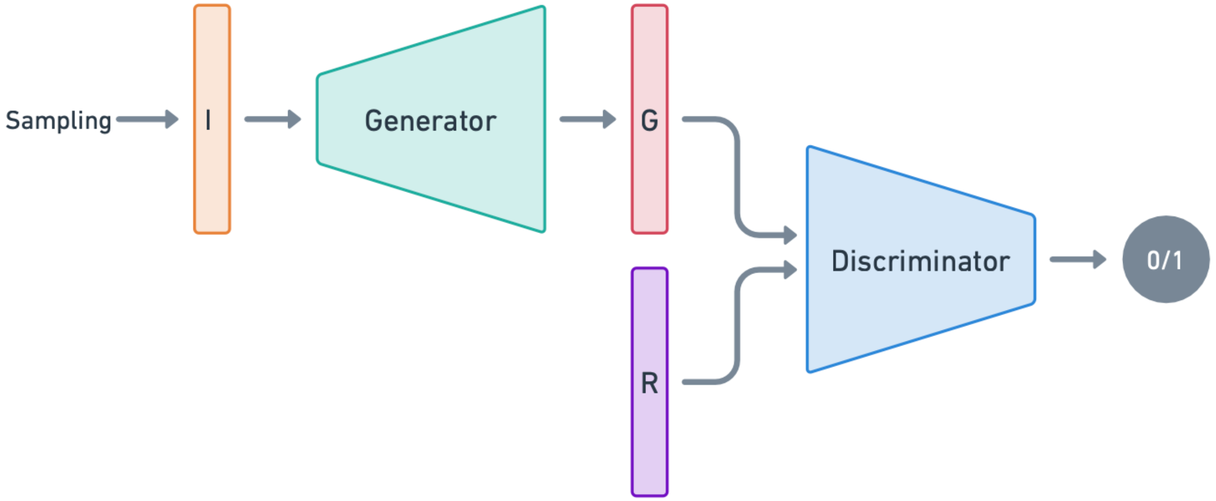
ML models implemented in the paper [previous SOTA]



Variational autoencoder (VAE)

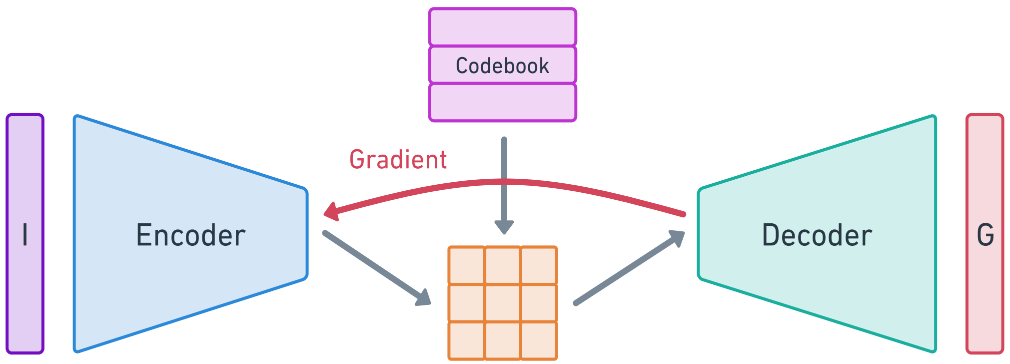


Sinkhorn autoencoder

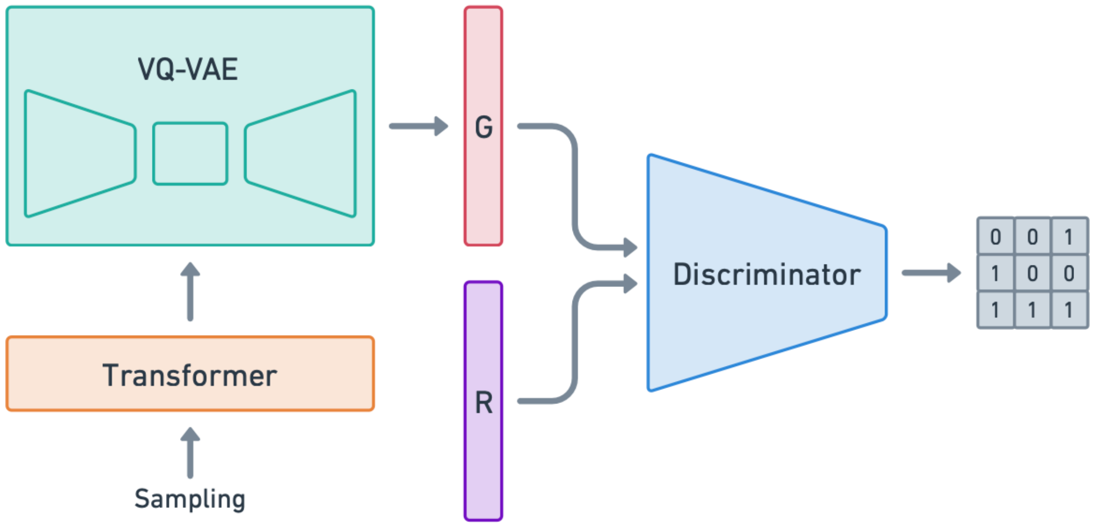


GANs

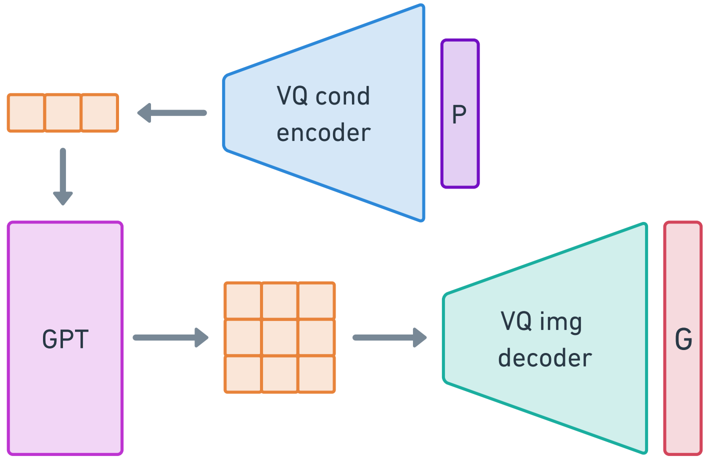
ML models implemented in the paper [ours]



Vector quantized VAE (VQ-VAE)

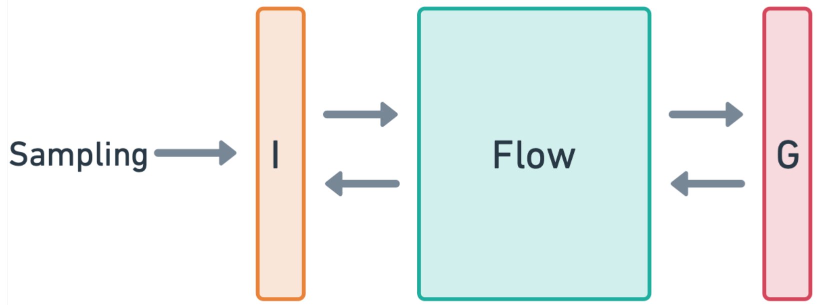


VQ-GAN

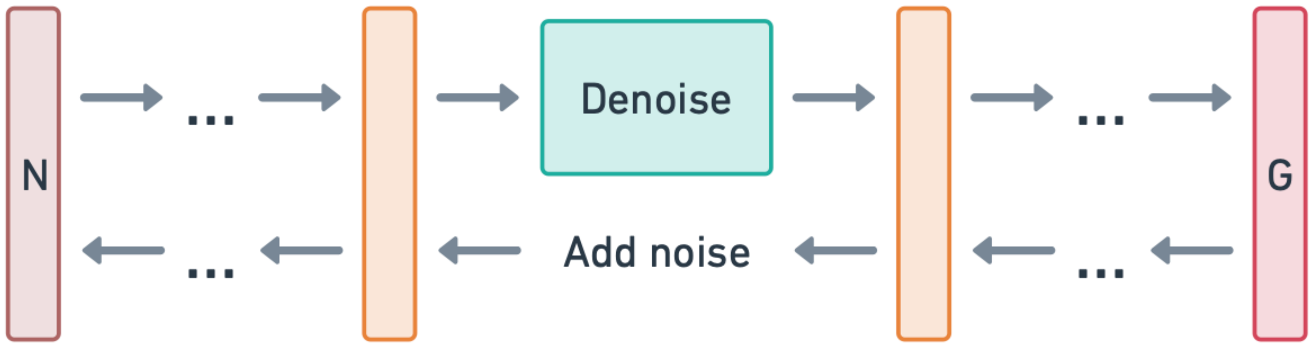


Transformer

ML models implemented in the paper [ours]



Normalizing flow



Diffusion model

ML models implemented in the paper

Model	**Wasserstein**	**MAE**	**RMSE**	**Time [ms]**
GEANT (original data)	0.53	16.41	59.87	–
Autoencoder	11.19	15.47	43.49	**0.015**
GAN	5.70	24.71	100.98	**0.023**
VQ-VAE	9.61	21.95	65.82	0.091
VQ-GAN	4.58	22.90	85.45	0.091
NF	4.11	19.36	127.22	160.0
Diffusion	**3.15**	20.10	73.58	5.360

Flow matching (FM) – new generative model

Flow Matching for Generative Modeling

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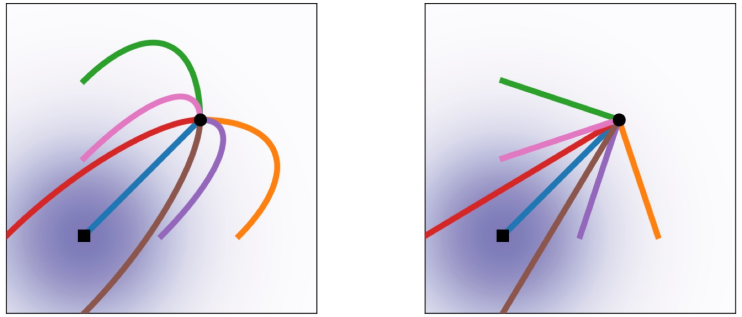


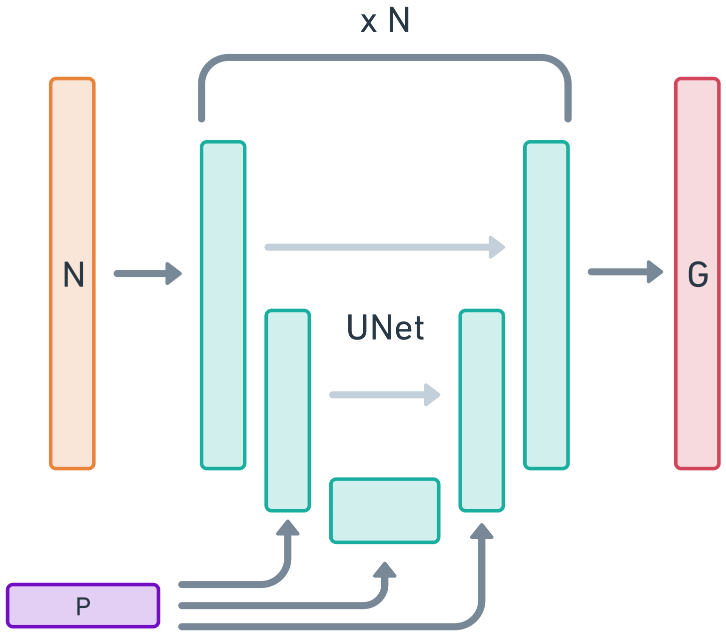
Diffusion OT

$$x_t = (1-t)x_0 + tx_1$$
$$v_t = x_1 - x_0$$
$$x_{t+\Delta t} = x_t + \Delta t \cdot v_t$$

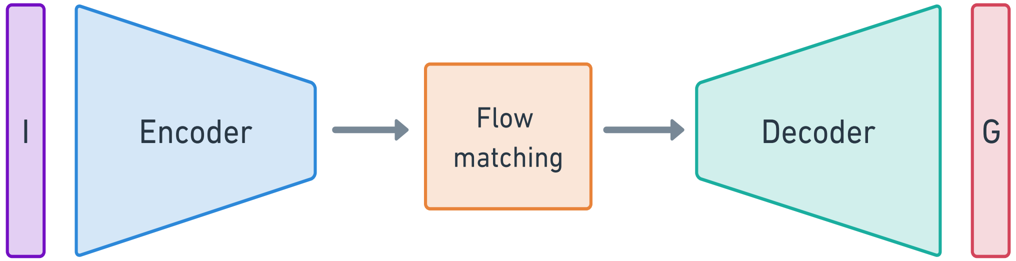
$$\mathcal{L}(\theta; x_t, v_t) = |v_\theta(x_t) - v_t|^2$$

Flow matching for fast ZDC simulation

- Presented on ML in PL 2024: [poster]

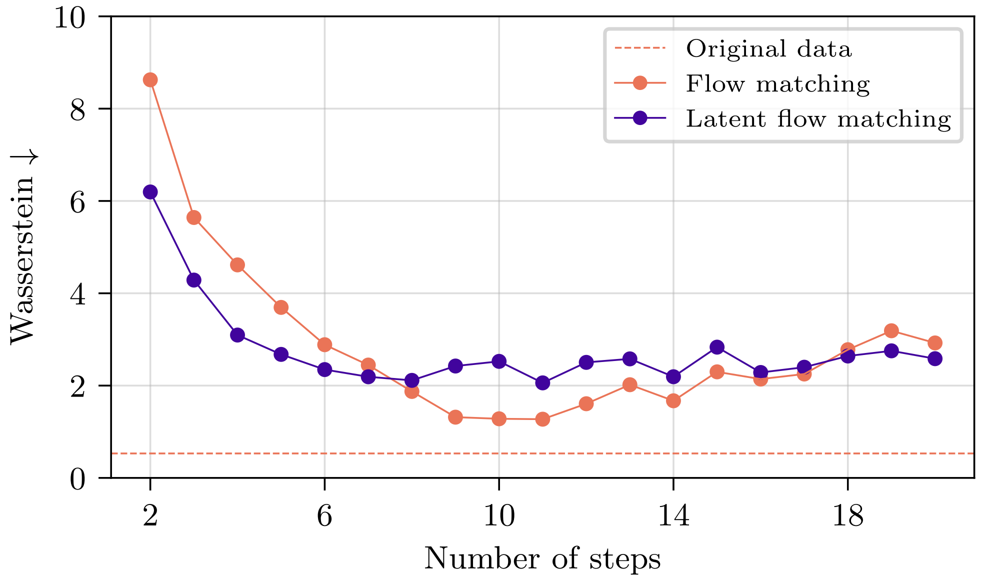


Neural network architecture – Unet



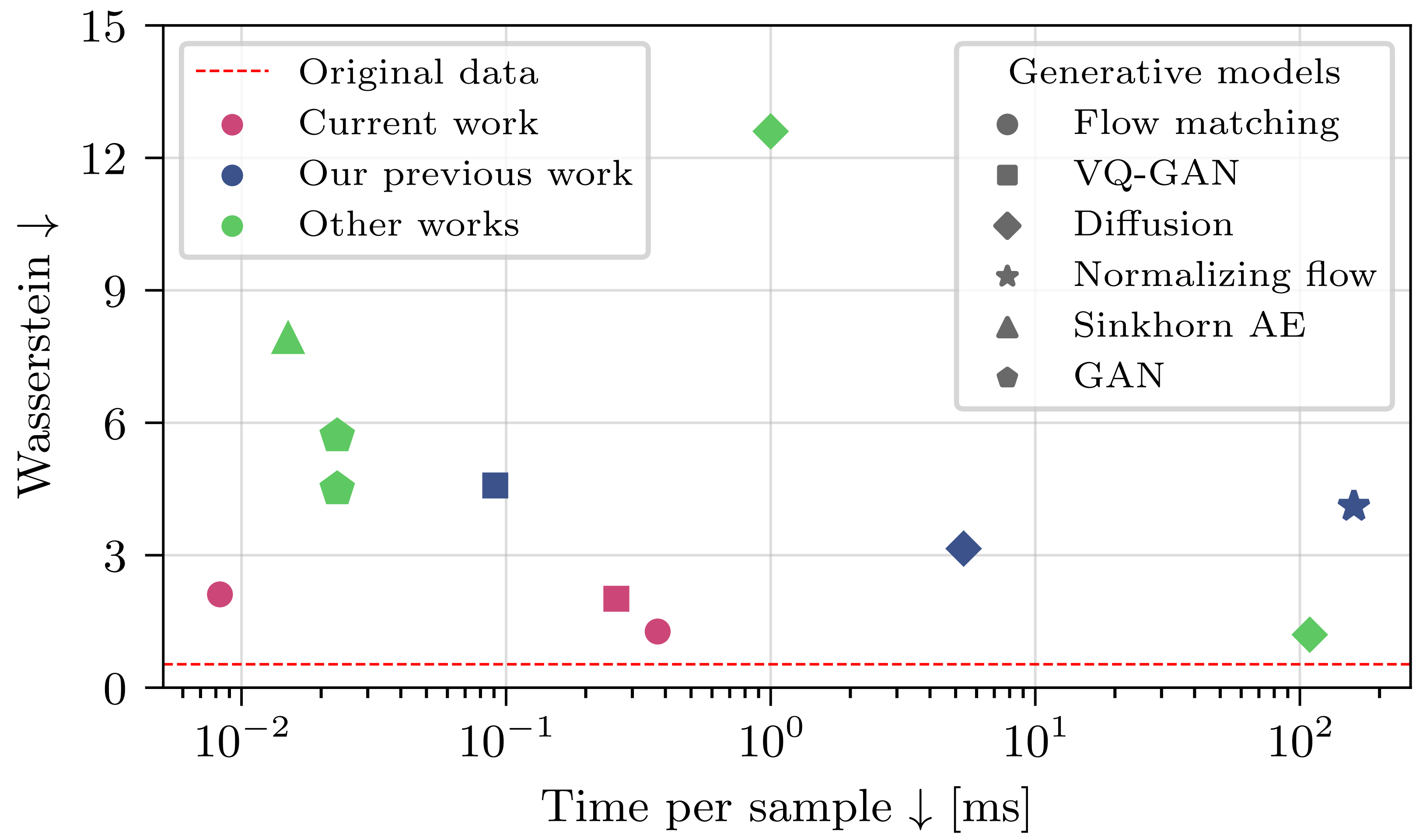
FM + VAE = Latent FM

Flow matching for fast ZDC simulation

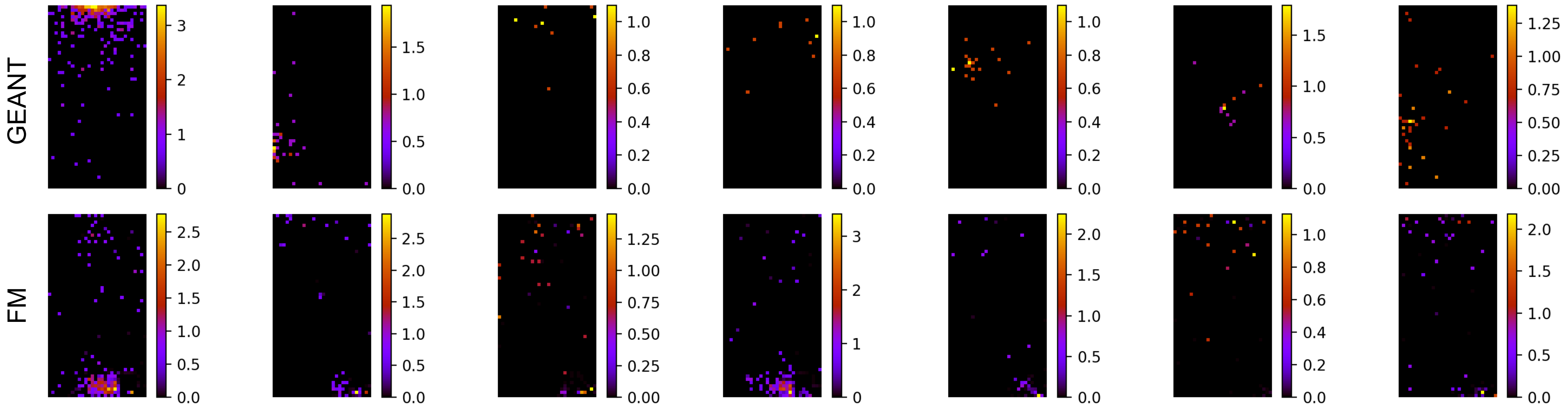


Improvement	Time ↓ [ms]	Relative change
Previous model	11.80	
Fewer num of steps (11)	2.60	-78%
Smaller model (77k)	0.62	-76%
Mixed precision (F16)	0.46	-27%
Bigger batch size (8k)	**0.37**	-18%
Latent space model	0.026	-93%
Bigger batch size (16k)	**0.008**	-63%

New SOTA for the ZDC neutron detector simulation



New SOTA for the ZDC proton detector simulation



Model	Wasserstein ↓
GAN	2.48
SDI-GAN	2.08
Flow matching	**1.30**
Latent flow matching	2.87

ZDC – transfer learning + fine-tuning

Emilia Majerz

- Presented on CHEP 2024: poster.
  - Fine-tuning of the baseline model trained on the whole data for each particle.
- Neutron detector simulation with ensemble learning.
  - Results improvement – from 2.34 +- 0.02 to 2.18 +- 0.01 (NF model).
  - The approach can be utilised for other models (GAN, VAE, diffusion, …).

Contributions and future work

- Paper on fast simulation of the ZDC accepted for publication:
  - neutron detector response dataset analysis,
  - comprehensive models comparison.
- New flow matching model:
  - SOTA for the ZDC neutron detector simulation,
  - SOTA for the ZDC proton detector simulation,
  - SOTA simulation speed among generative models (latent FM).
- Future work:
  - proton detector response dataset analysis,
  - paper on flow matching for fast ZDC simulation.