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

WMLQ 2024
4-7 June 2024, Warsaw Poland

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

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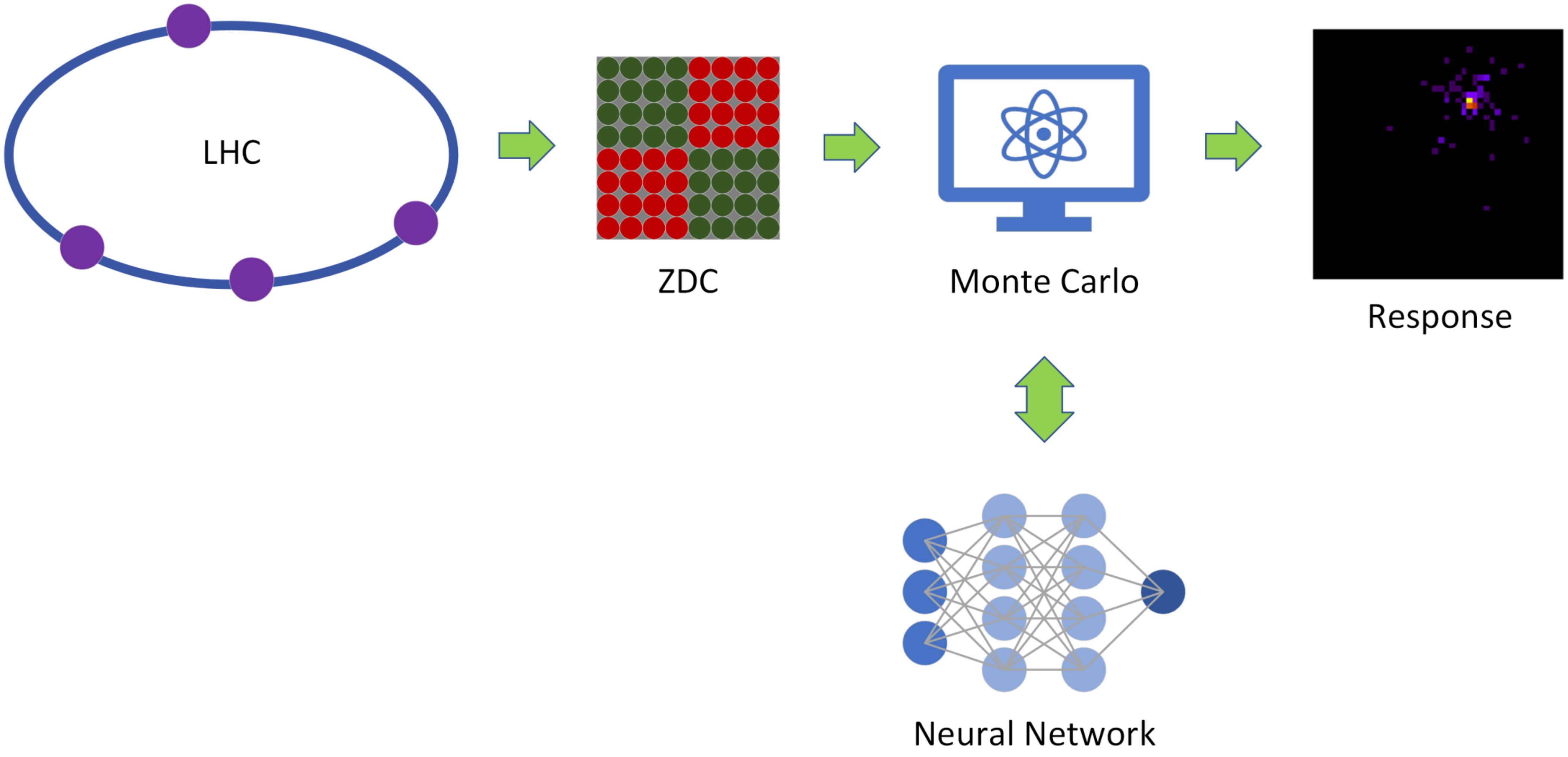
2024-06-04

What do we do?

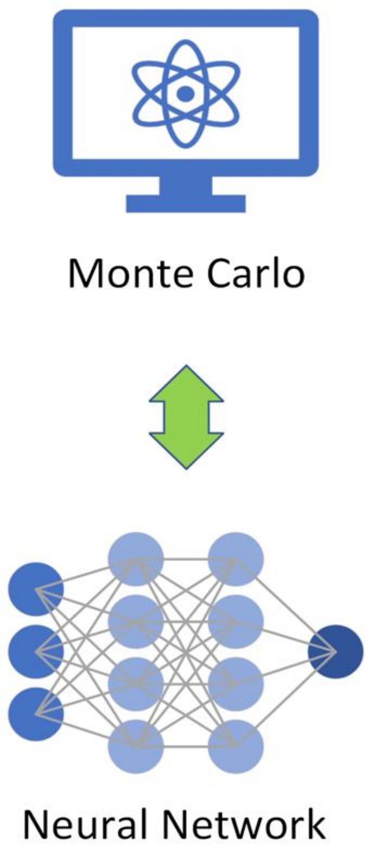


Zero Degree Calorimeter (ZDC)

- ALICE experiment.
- Detects the energy of the spectator nucleons in order to determine the overlap region in nucleus-nucleus collisions.
- Simulated using Monte Carlo approach.
  - Computationally expensive method!
- Neutron detector: 44x44 silica optical fibers grid.
  - Detection of Cherenkov light produced by charged particles in the fibers.
- Detector responses have 2-dimensional structure...
- ...making their simulation a perfect task for generative neural networks!

Fast simulations

- Using a surrogate of the whole mathematical model or its part.
  - The most computationally-intensive part -> a faster surrogate.
- Fast simulations at CERN.
  - Existing approaches at different experiments.
  - VAEs, GANs, NFs, Diffusion.
- There's still a gap to fill!
  - Research done mostly on other experiment's calorimeters.



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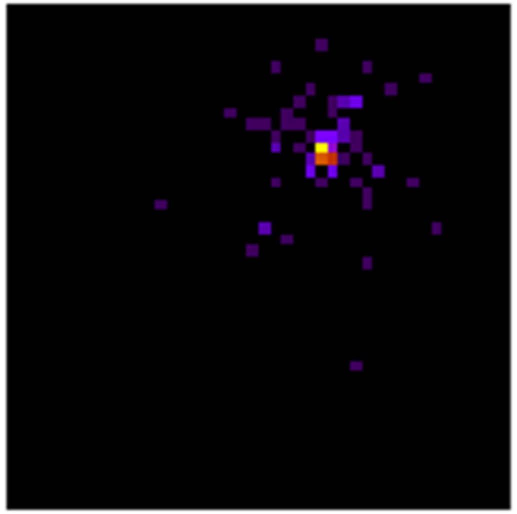
Dataset

- Tabular data + images.
  - 306780 samples.
- Simulation input – primary particle.
  - 9 features: energy, momenta (3d), primary vertex position (3d), mass, charge.
- Simulation output – detector response.
  - Only neutron detector.
  - Detector response treated as an image.
  - Responses with 10 and more photons.
- Diversity of detector responses.

10	1.5	2.3	4.1	0.1	1.4	5.6	1.0	0.0



Diverse results from the same parameters

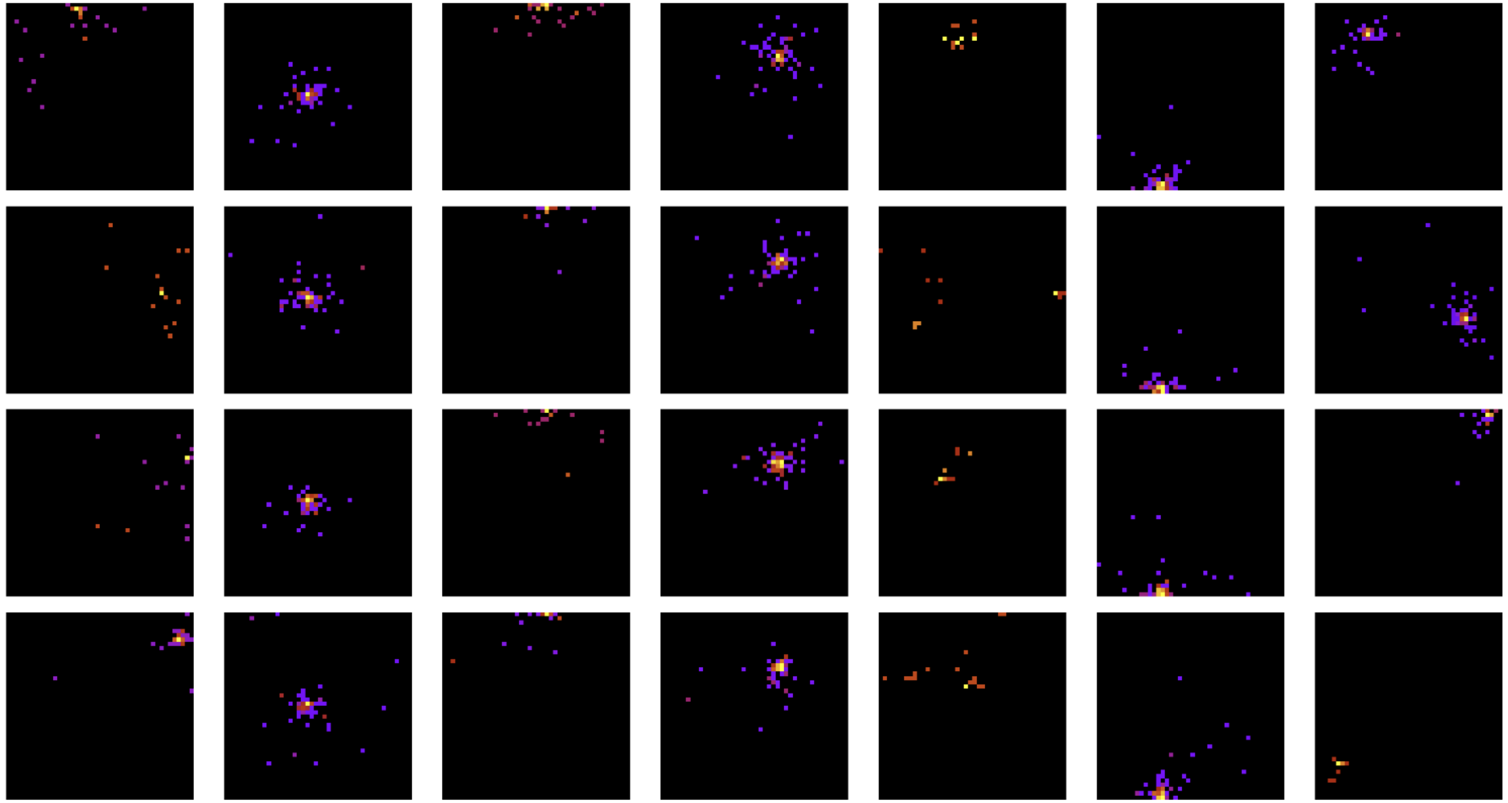
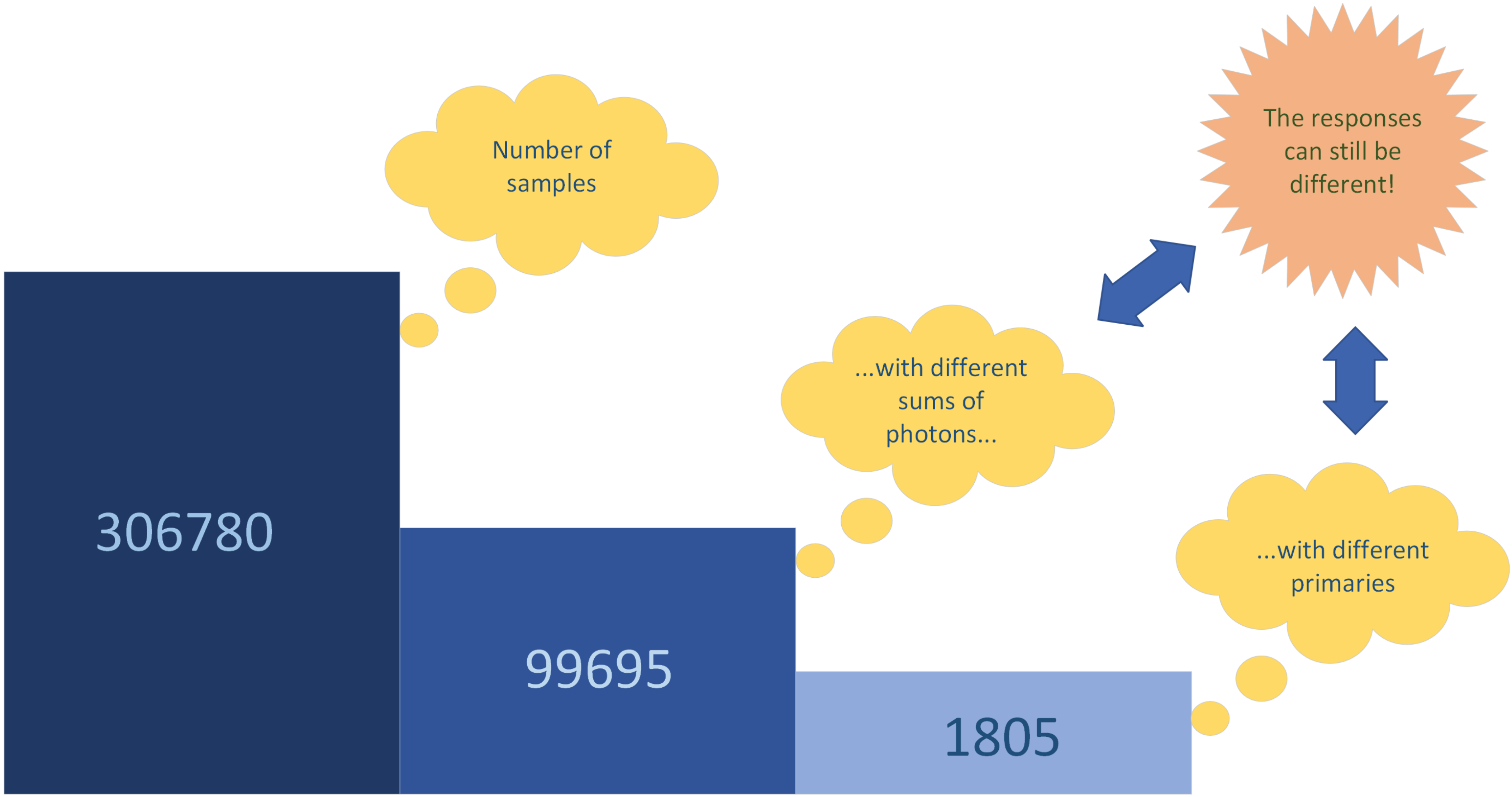


Figure 1: Example ZDC neuron detector simulations generated with GEANT software. The following columns are the responses to different particles, the first from the left is $\pi+$, followed by γ particles (the most common in this dataset), and the last is K_S^0. The rows show independent runs for the same particles.

Many samples... yet sparse data?



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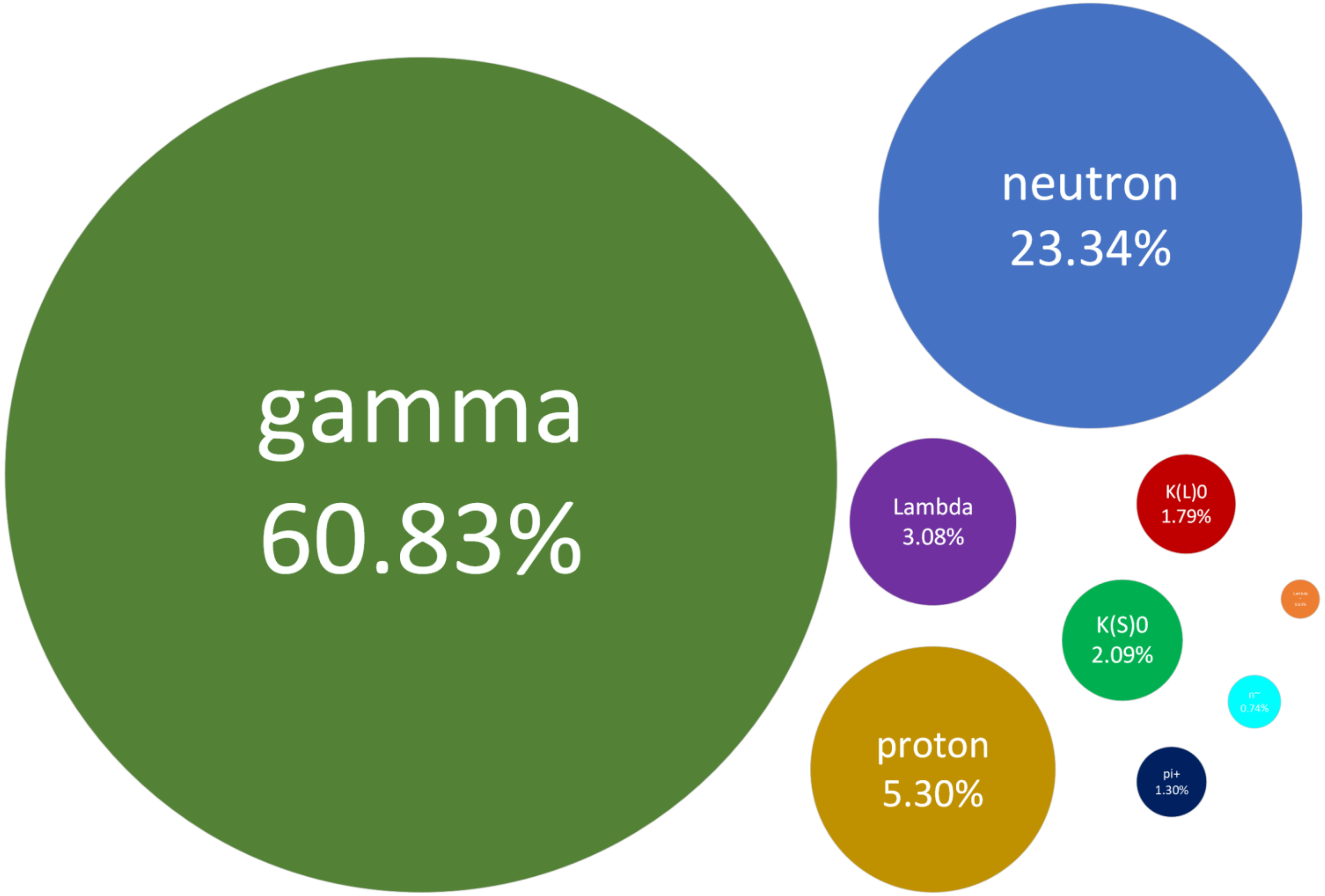
Oh no... imbalanced data!



21 different particles in total

And... we have our challenge!

Chosen generative frameworks

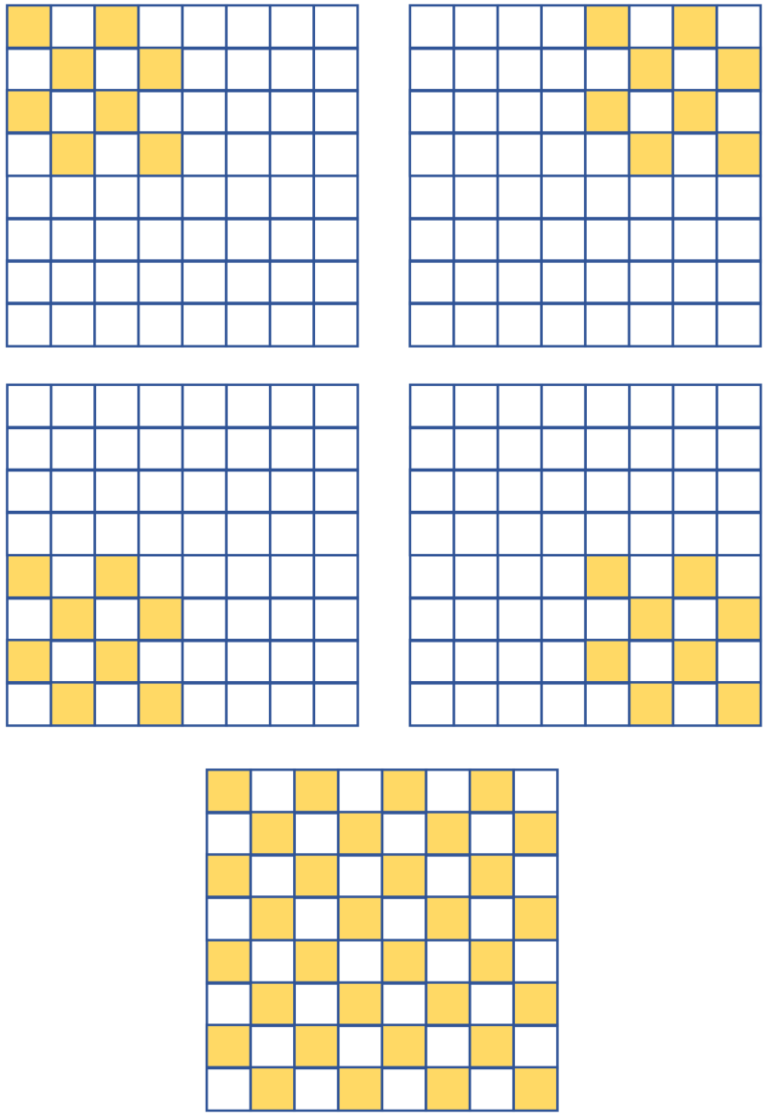
- Autoencoders
- GANs
- Vector Quantization
- Diffusion
- Normalizing Flows

Network architectures:

- CNN
- ViT
- MLP-Mixer

How do we measure the performance?

- Pixel-to-pixel comparison.
  - Can help... but not as a primary metric.
- Comparison of distributions of results.
  - ...but which distributions?
- One image -> 5 channels.
  - Wasserstein distance.
  - MAE.
- RMSE.
- Generation time.



Autoencoders

- Conditional Variational Autoencoders.
- Autoencoders with noise generator.
- Supervised autoencoders.

Architecture	CNN			ViT			MLP-Mixer		
Metric	Wasserstein	MAE	RMSE	Wasserstein	MAE	RMSE	Wasserstein	MAE	RMSE
VAE	**11.52**	17.76	50.38	11.90	18.05	49.48	12.22	18.00	49.51
Supervised AE	23.71	31.90	72.32	20.43	30.60	74.64	17.08	26.90	104.83
AE + Sinkhorn NG	26.53	29.07	66.16	**11.34**	15.88	44.17	x	x	x
AE + MSE NG	37.56	39.32	92.28	**11.19**	15.47	43.49	x	x	x

Generative Adversarial Networks (GANs)

- Conditional GANs.
- SDI-GAN.
- Postprocessing + additional loss.
- Comparison of different GAN models:

Model	Wasserstein	MAE	RMSE
GAN	7.09	25.65	104.60
GAN + postprocessing	**5.70**	24.71	100.98
GAN + l2 loss	6.44	27.37	109.24
GAN + l2 loss + postprocessing	6.07	26.78	107.07
SDI-GAN	6.57	27.01	107.82
SDI-GAN + postprocessing	6.36	26.58	105.94

Vector Quantization – the more, not always the better!

- VQ-VAE - discrete latent representations.
  - Choosing a nearest neighbor from the codebook.
- VQ-GAN - VQ-based generator.
- Medium-sized VQ-VAE achieves the best results in terms of reconstruction:

Model size	Wasserstein	MAE	RMSE
0.25M	11.54	12.96	38.46
1M	**9.86**	11.84	37.22
4M	11.73	13.78	43.54
13M	11.40	12.87	37.90
52M	12.12	13.73	39.74

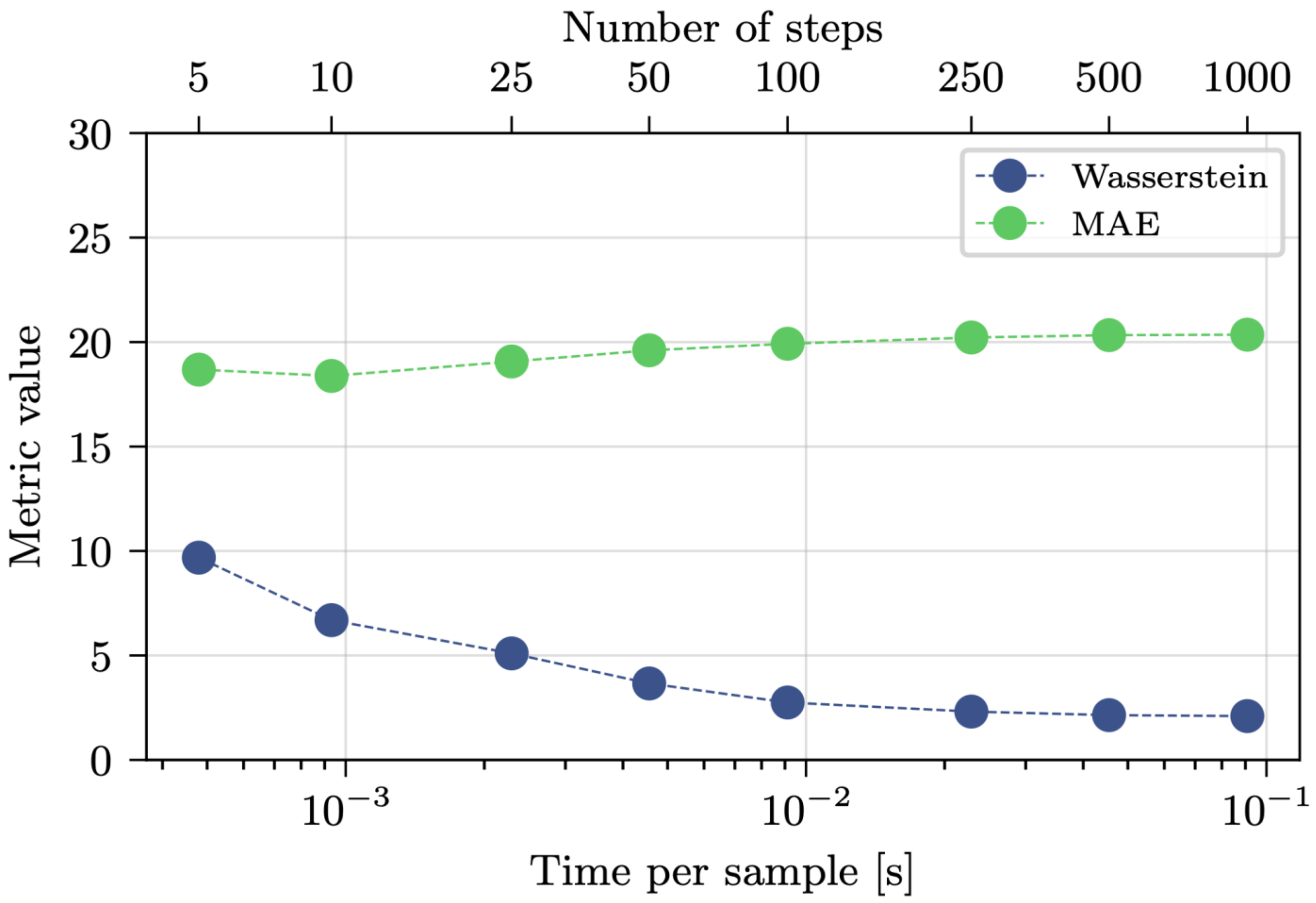
Normalizing flows

- CaloFlow-like approach.
  - Two models: one for the number of photons and one for the final result.
  - Trained independently.
- Bayesian network for the number of photons, flow as the main model.
- Adding noise to pixel values for training, removing the noise after computations.
  - Big influence on the results!
  - For one of the models:

Noise range: [0; val)	Wasserstein
1.0	12.57
0.75	6.67
0.5	**4.58**
0.1	7.10
0.01	8.10
0.001	7.39

Diffusion models

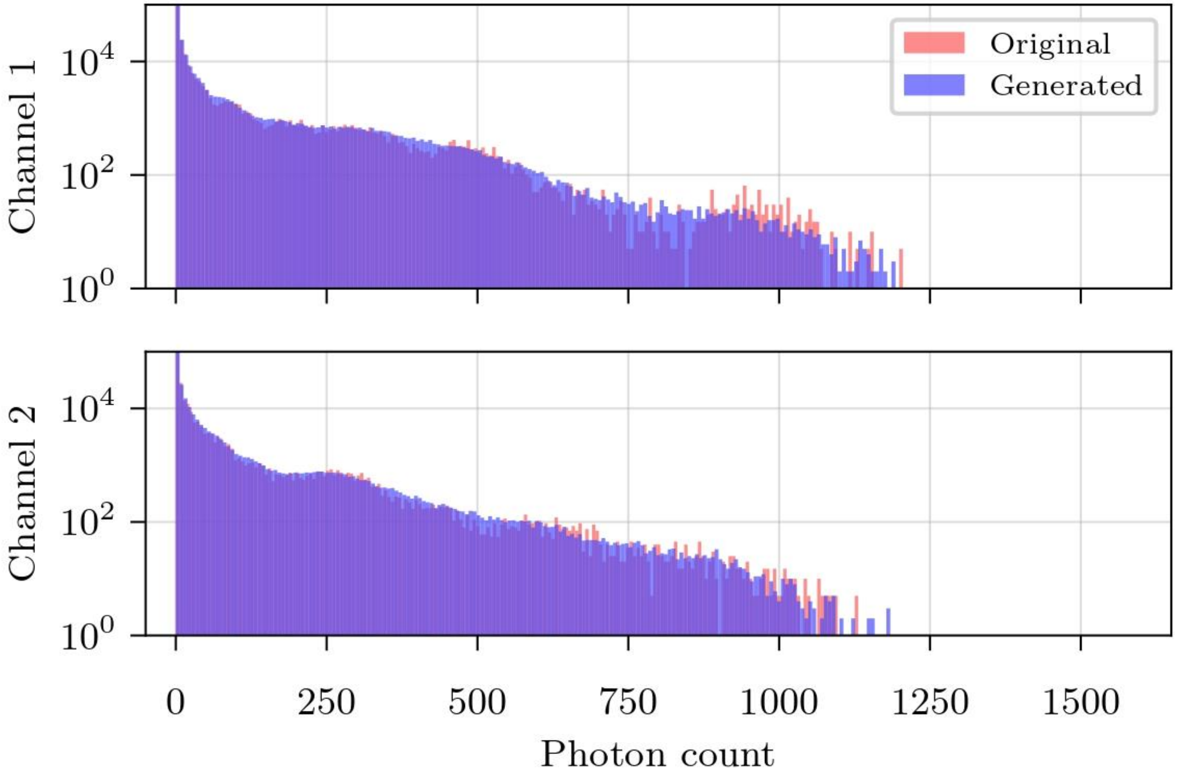
- Training a Denoising Diffusion Probabilistic Model (DDPM).
  - U-Net with convolutions and attentions.
- Sampling with a Denoising Diffusion Implicit Model (DDIM).
  - Allows for fewer steps.
- Tradeoff between generation time and the quality of the samples.

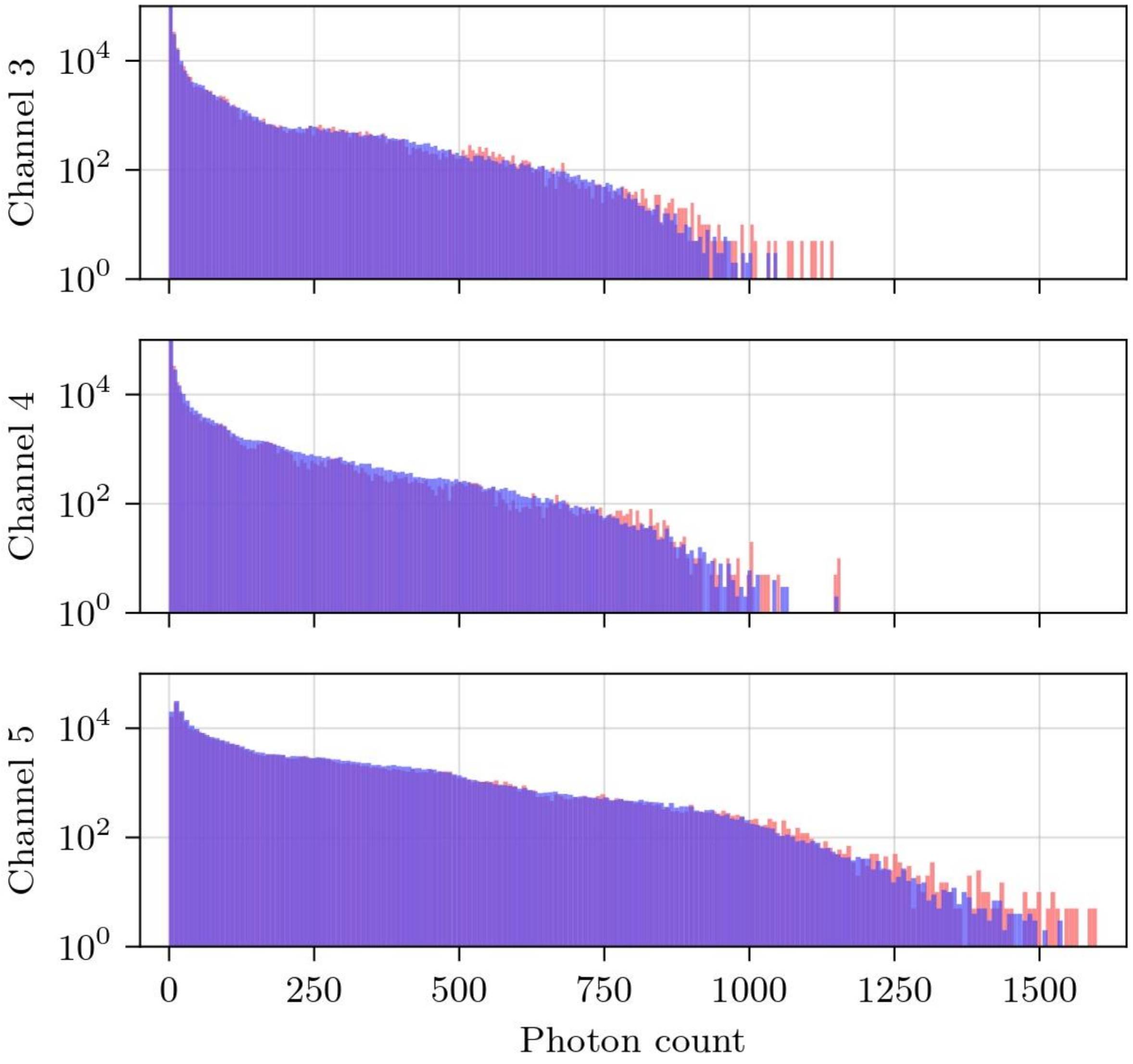


Final performance and generation time comparison

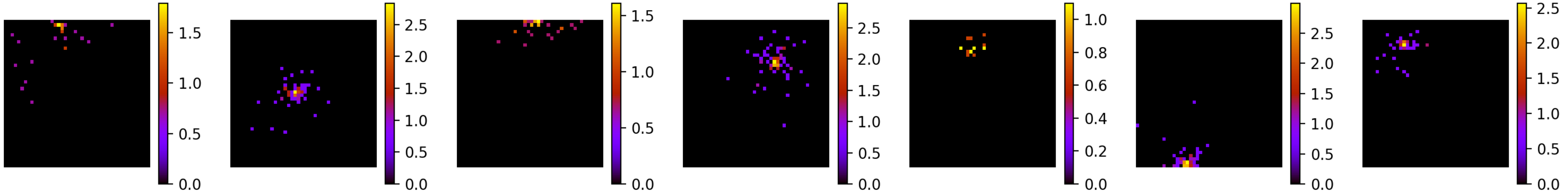
Model	Wasserstein	MAE	RMSE	Generation time [ms]
GEANT (original data)	0.53	16.41	59.87	–
Autoencoder	11.19	15.47	43.49	**0.015**
GAN	5.70	24.71	100.98	**0.023**
VQ-VAE	9.61	21.95	65.82	0.091
VQ-GAN	4.58	22.90	85.45	0.091
NF	**4.11**	19.36	127.22	160.0
Diffusion	**3.15**	20.10	73.58	5.360

Original and diffusion-generated data channels

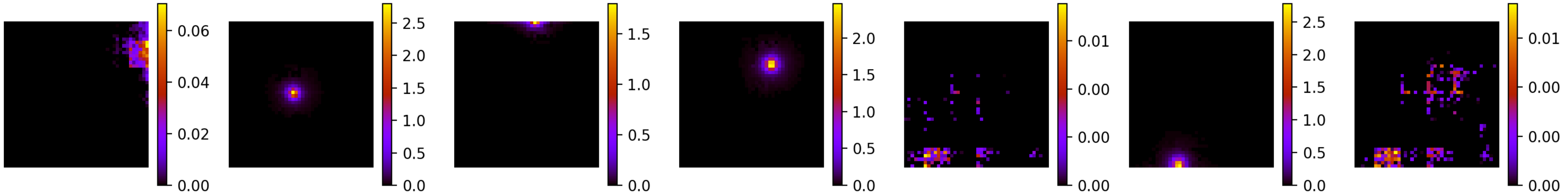




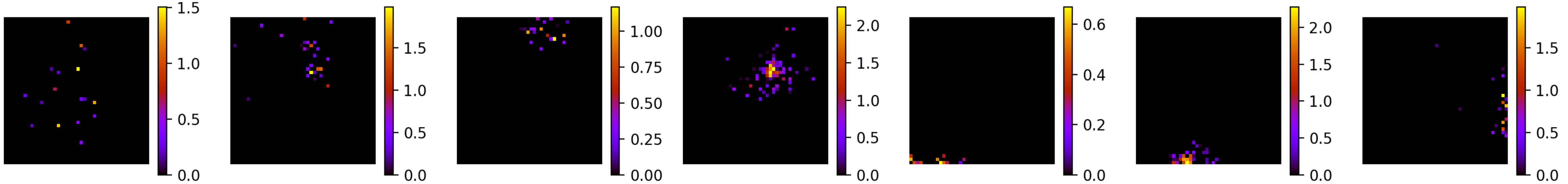
Example simulations



Reference

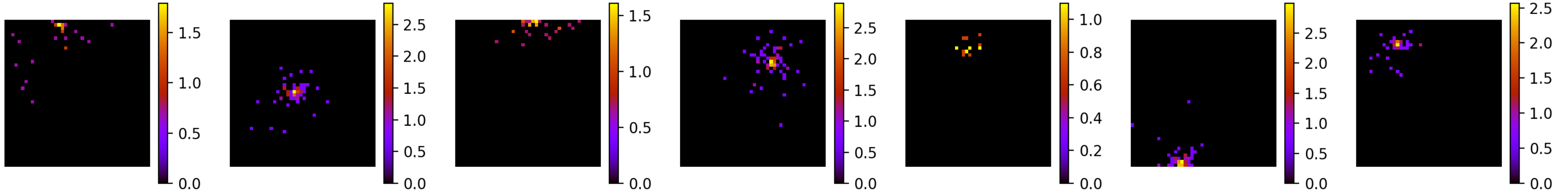


Autoencoder with a noise generator and MSE loss



GAN with a postprocessing step

Example simulations



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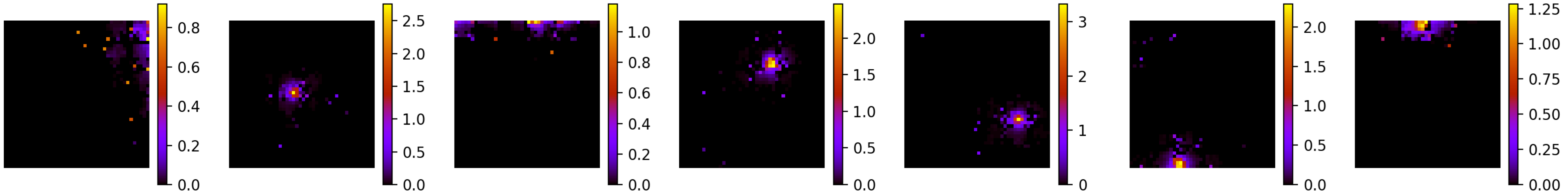
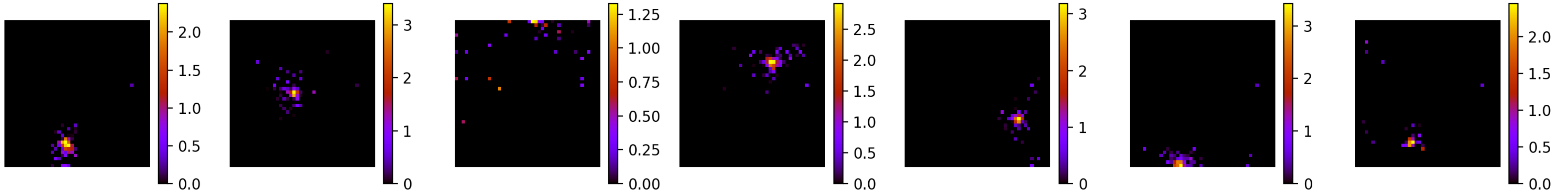
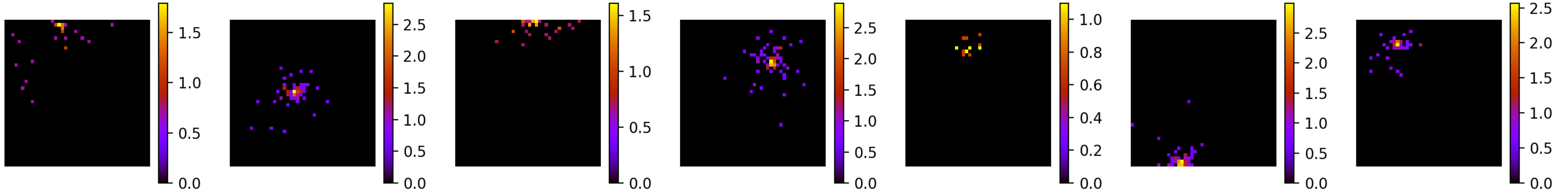


VQ-VAE with a transformer as a learnable prior and adjusted sampling temperature



VQ-GAN with a transformer as a learnable prior

Example simulations



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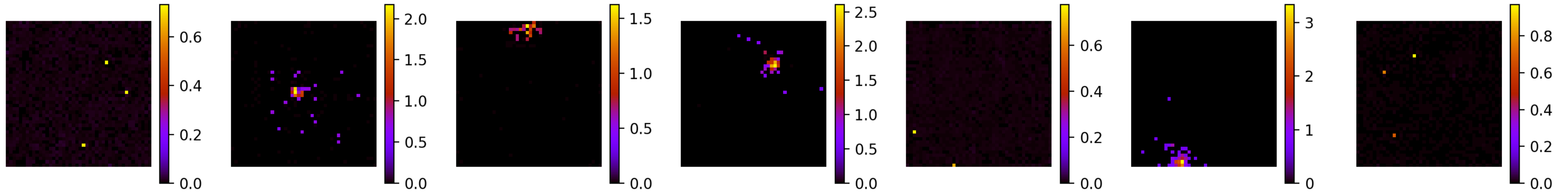
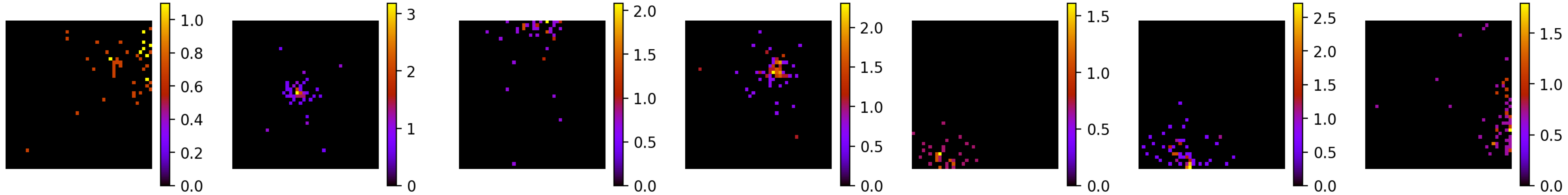


DDIM after 50 denoising steps and adjusted η parameter



NF with training noise set to 0.5

Pros & cons

	VAEs	GANs	VQs	NFs	DIFFs
Pros	• Fast generation	• Fast generation	• Pretty good metrics and a reasonable generation time	• Good metrics	• The best metrics
Cons	• Blurry outputs • Perturbated diversity	• Training stability issues	• Complicated framework	• Very slow generation*	• Slow generation

Conclusions and future directions

- ViT-based frameworks are the most effective.
- VQs, NFs and Diffusion models perform the best and are worth-developing.
    - VQs provide the best tradeoff between generation time and sample quality.
    - NFs have potential, though need to be faster.
    - Diffusion is great... but maybe can be even better?
- We want to further explore these three methods.

Code availability

https://github.com/m-wojnar/zdc

Acknowledgements

- We would like to thank Professors: Jacek Kitowski, Witold Dzwinel, Marcin Kurdziel and Jacek Otwinowski for their support in this work.
- We would also like to thank the Warsaw University of Technology's group: Jan Dubiński, Kamil Deja, PhD and Professor Tomasz Trzciński for the discussions during our meetings.
- This work is co-financed in part supported by the Ministry of Science and Higher Education (Agreement Nr 2023/WK/07) and by the program of the Ministry of Science and Higher Education entitled "PMW".
- We gratefully acknowledge Polish high-performance computing infrastructure PLGrid (HPC Centers: ACK Cyfronet AGH) for providing computer facilities and support within computational grant no. PLG/2023/016410.

Thank you!

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