HELMHOLTZAI | ARTIFICIAL INTELLIGENCE COOPERATION UNIT

SAMPLING NEUTRONS WITH ARTIFICIAL INTELLIGENCE

José I. Robledo
Jülich Supercomputing Centre (JSC)
Jülich Centre for Neutron Science (JCNS)
Forschungszentrum Jülich (FZJ)

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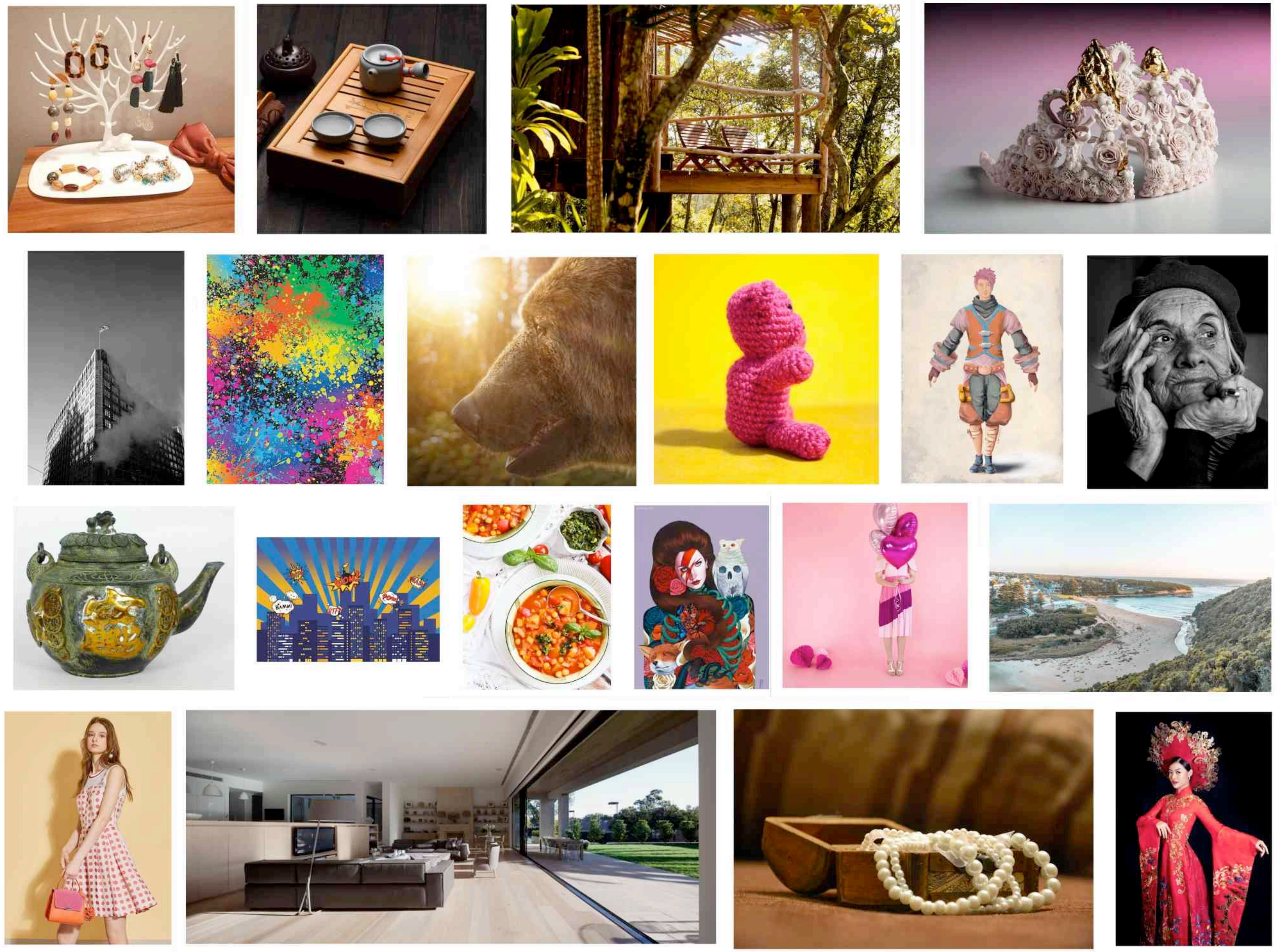
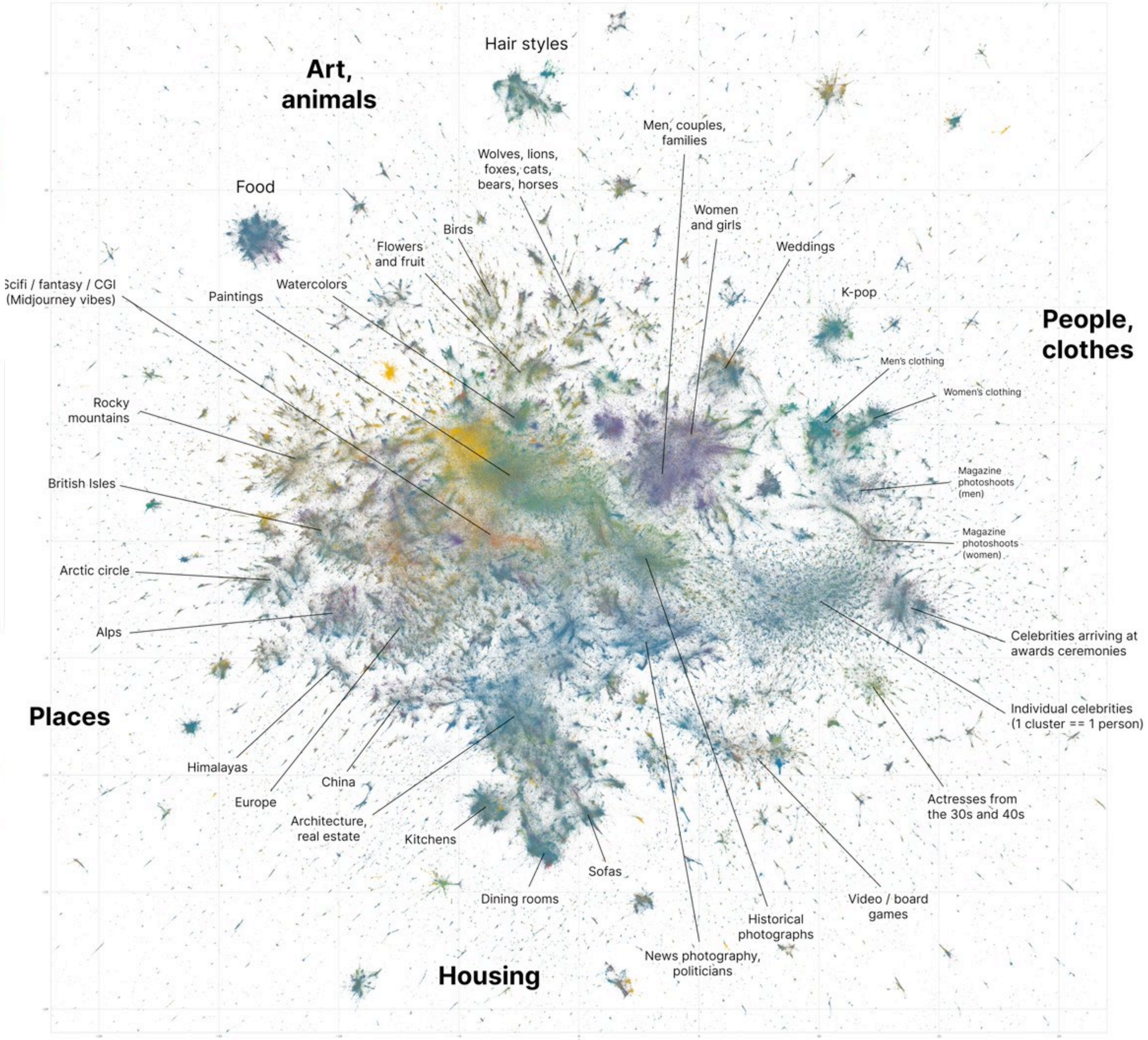
INTRODUCTION



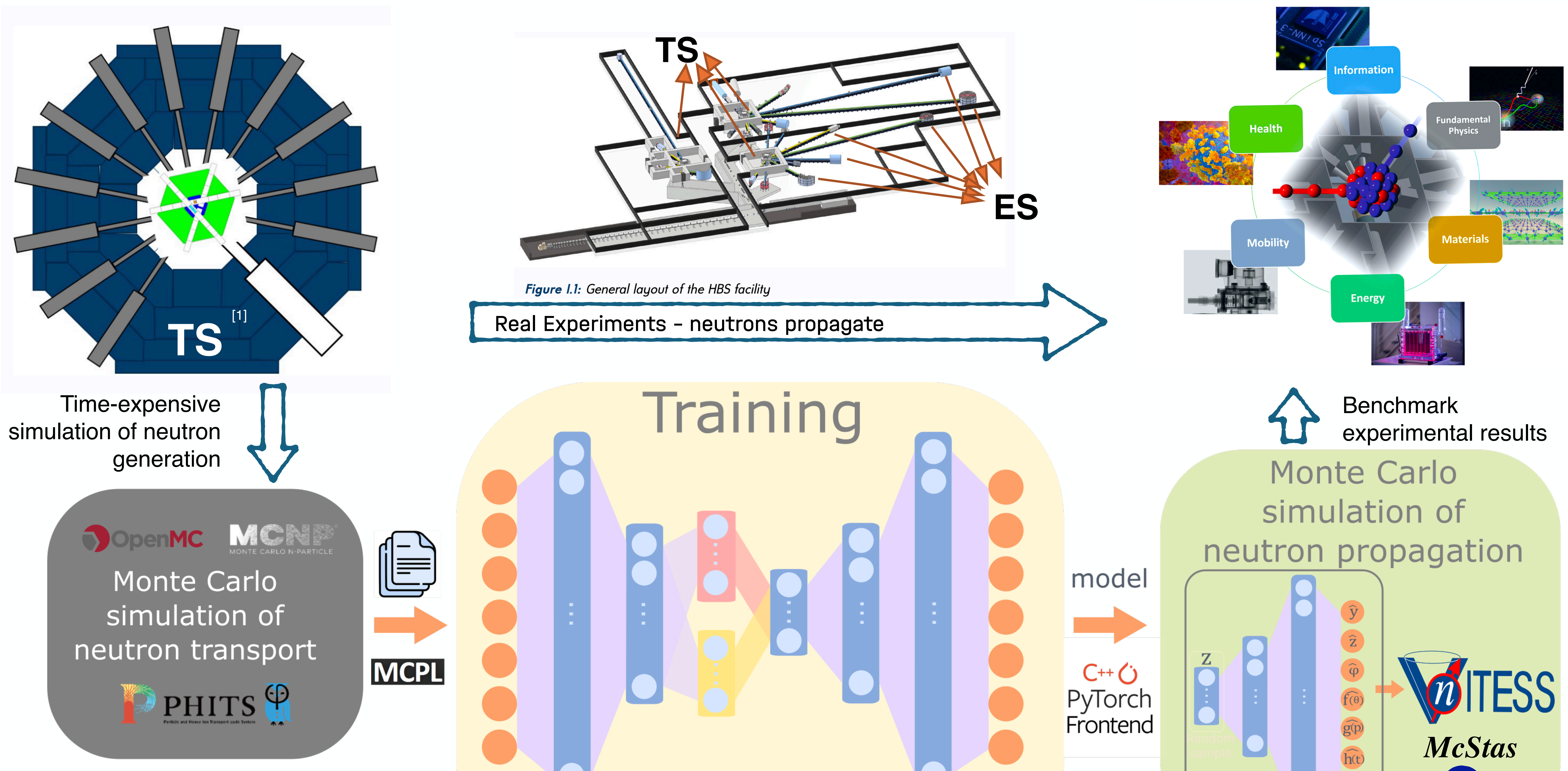
https://laion.ai/blog/laion-pop/

All captions from LAION-Aesthetics with score > 6 (n=12M)
Embedded with CLIP, UMAP to 2d



Why can't we generate neutrons?

INTRODUCTION

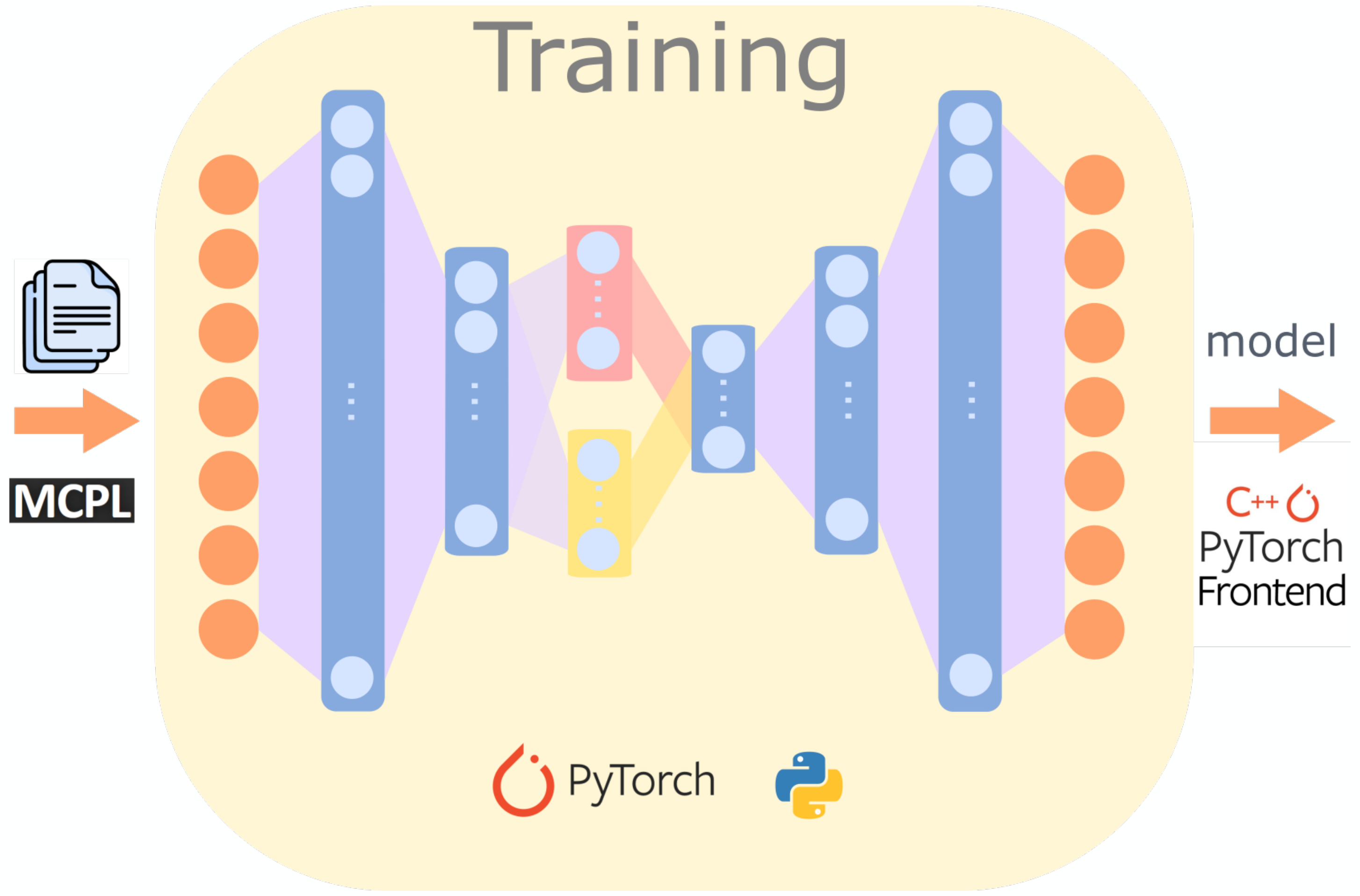


TDR MCPL file

700.000 Neutrons

https://www.fz-juelich.de/en/jcns/jcns-2/news/announcements/2023/hbs-tdr

TRAINING DATA: MCPL FILES



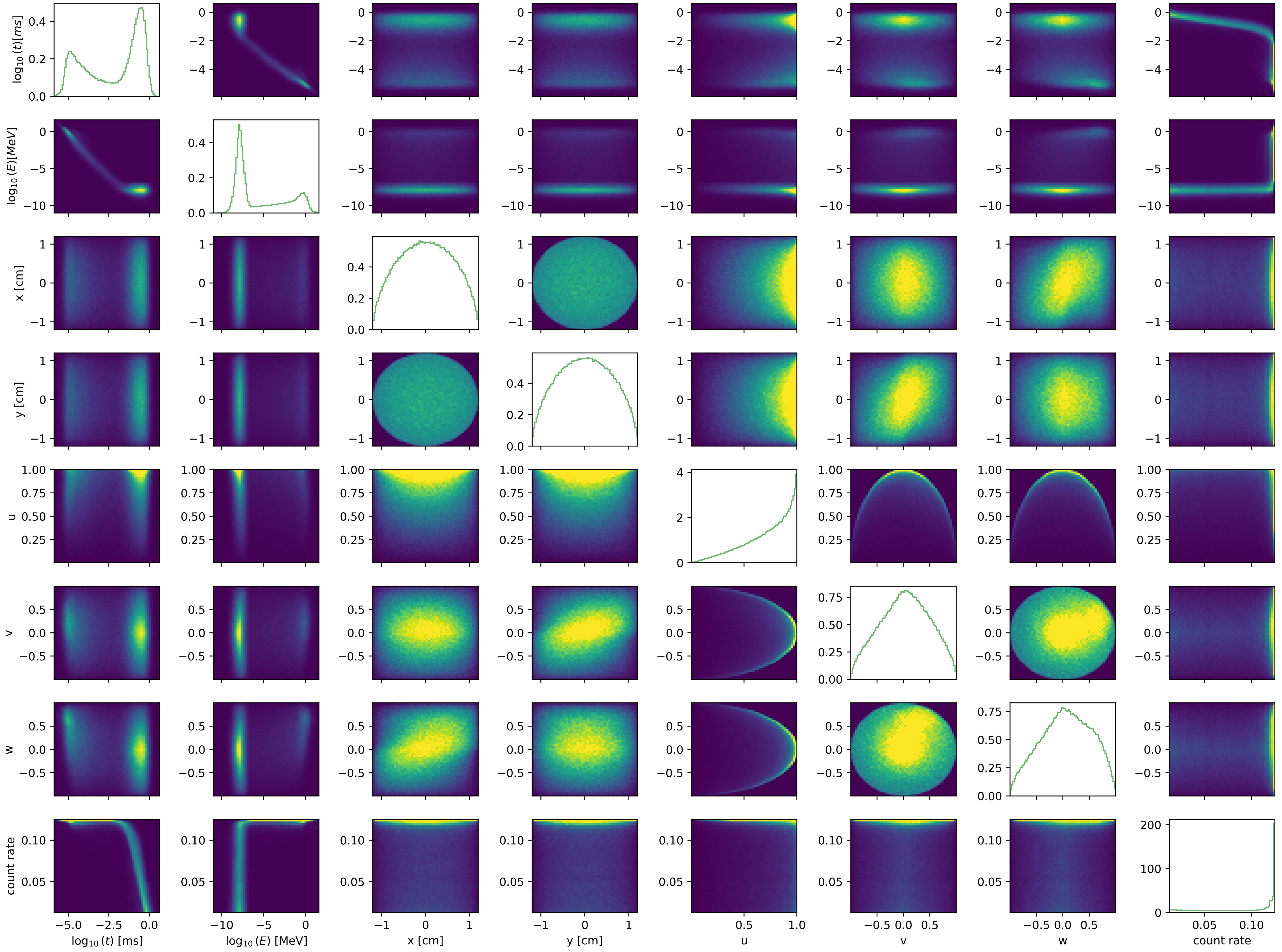
PyTorch DataLoader

Variables

- y [cm] and z [cm]
- u, v, and w
- count rate (weight)
- $\log_{10}(t)$ [ms]
- $\log_{10}(E)$ [MeV]

	pos_y	pos_z	u	v	w	count_rate	TOF	E
0	-1.157290	-0.156233	0.974585	-0.203838	-0.092924	0.124997	0.000059	9.301730e-02
1	-0.675784	0.331821	0.534119	-0.218695	0.816633	0.074287	0.157121	8.421972e-08
2	0.598687	-0.840697	0.647142	0.740285	-0.182169	0.074748	0.156539	8.232719e-08
3	0.775426	-0.258992	0.508785	0.752556	0.418089	0.075199	0.156472	1.423273e-07
4	-0.778382	0.114899	0.702195	-0.399447	-0.589376	0.122384	0.007535	5.222545e-08
...	...	...	...	...	...	...	...	...
676553	-0.711618	-0.400495	0.916834	-0.103239	-0.385690	0.124989	0.000039	8.381045e-03
676554	-0.052427	0.881021	0.818265	0.572754	-0.048949	0.124998	0.000005	2.565348e-01
676555	-0.042421	0.981967	0.545910	-0.667388	0.506533	0.025299	1.222780	2.869063e-09
676556	0.244454	-0.181313	0.743137	-0.051606	0.667146	0.080170	0.105039	2.322999e-08
676557	-1.063570	-0.350045	0.633484	-0.657062	-0.408617	0.032235	0.657213	6.777769e-09

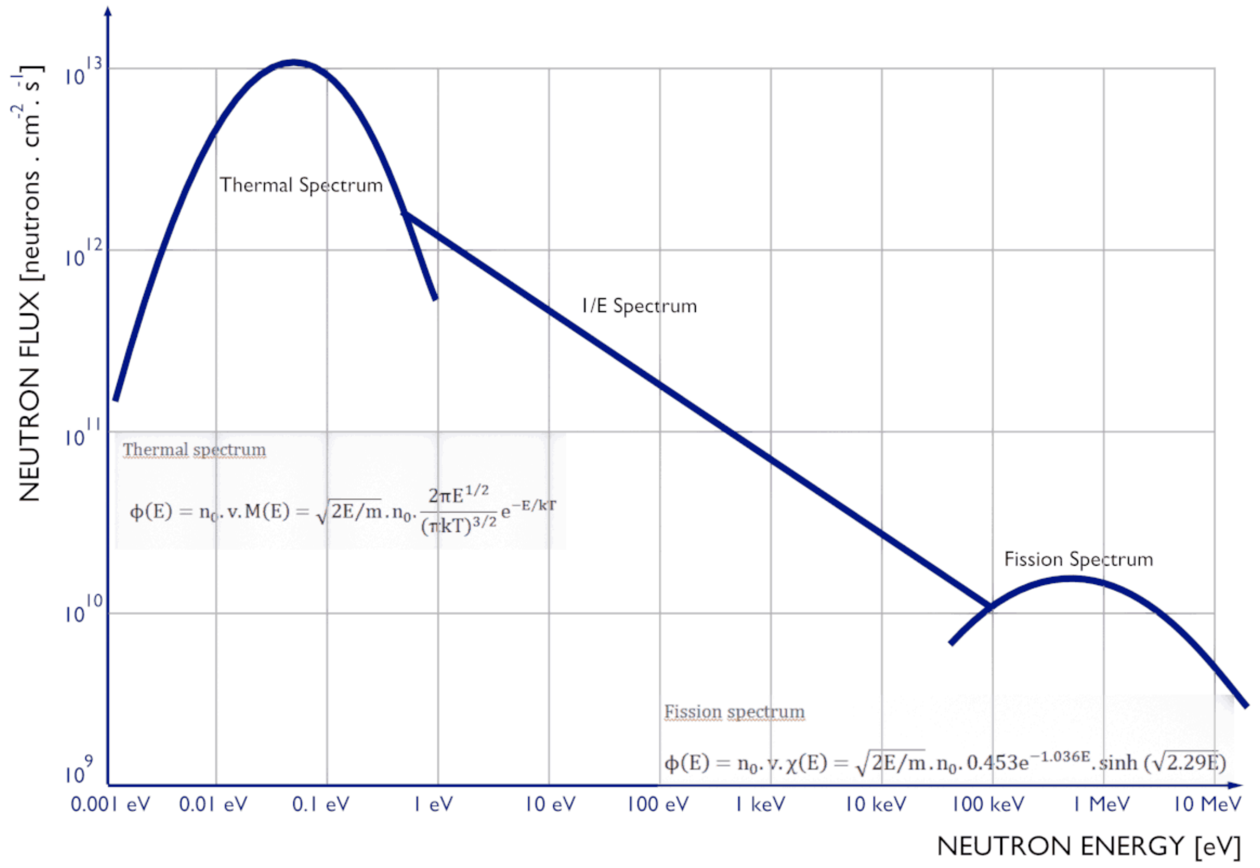
676558 rows × 8 columns

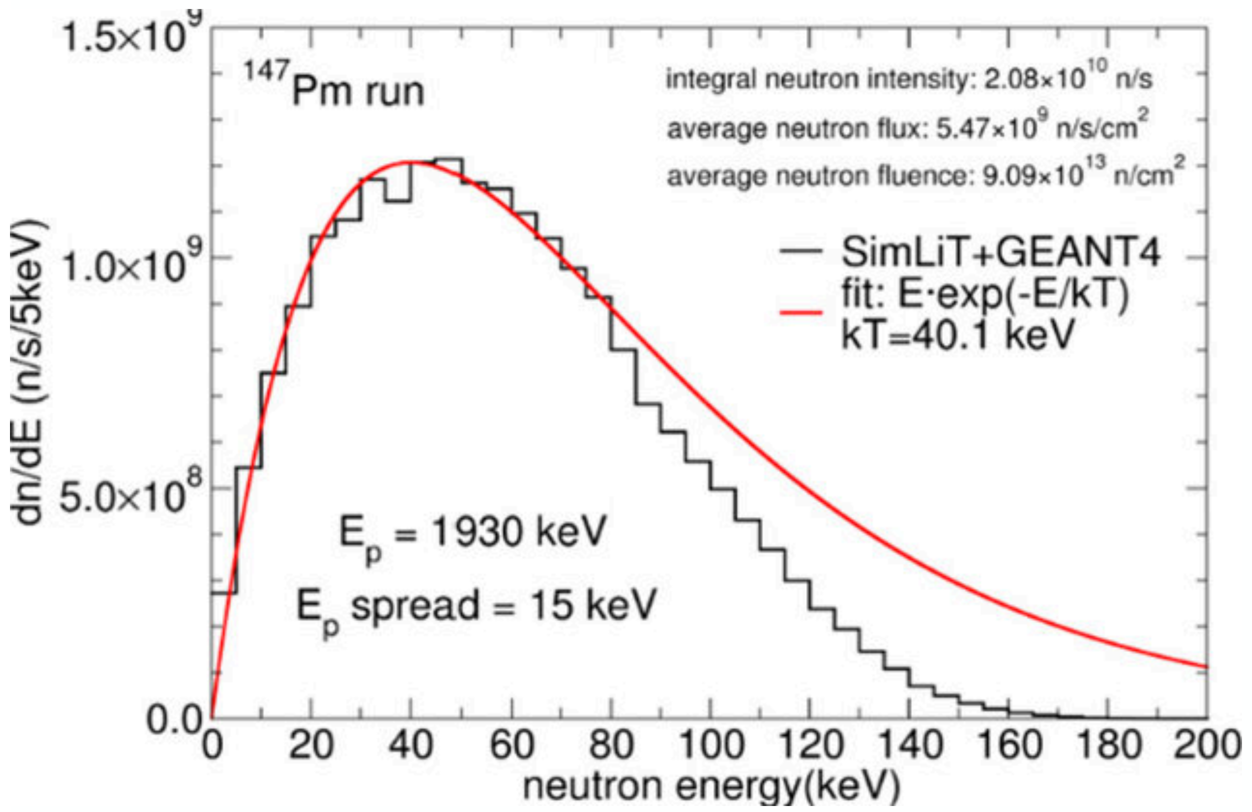


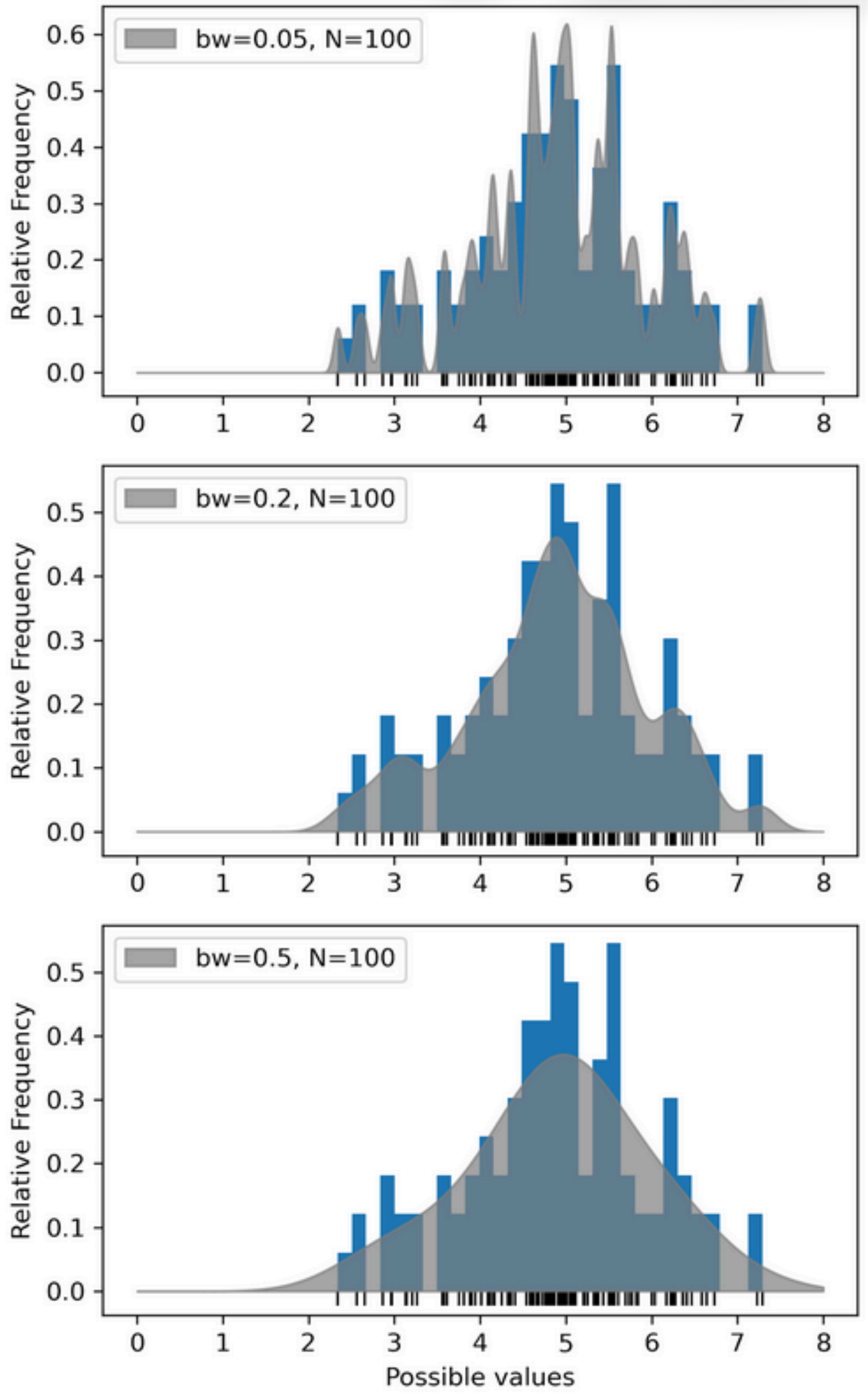
T. Kittelmann et al. Monte Carlo particle lists: MCPL. *Computer Physics Communications*, *218*, 17-42.

CURRENT APPROACHES TO SOURCE ESTIMATION

- Analytical approximation based on theory / fitting to observed data







- Kernel Density Estimation

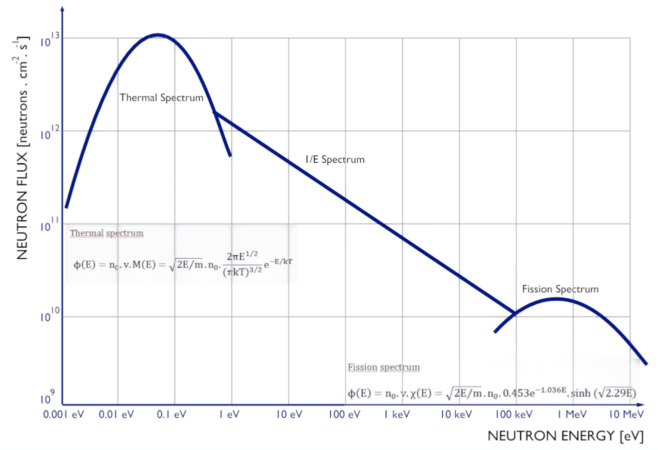
KDSource

$$\hat{f}(\mathbf{x}) = \hat{f}(x_1, x_2, \ldots, x_D) = \sum_{\mathrm{i}=1}^{N} w_{\mathrm{i}} \left\{ \prod_{\mathrm{j}=1}^{D} \frac{1}{h} K\left(\frac{x_{\mathrm{j}} - (\tilde{p}_{\mathrm{i}})_{\mathrm{j}}}{h} \right) \right\}$$

Schmidt, N. S. et al. (2022), KDSource, a tool for the generation of Monte Carlo particle sources using kernel density estimation. *Annals of nuclear energy*, *177*, 109309.

PROS & CONS

- Analytical approximation based on theory / fitting to observed data
  - Reliable when assumptions are adequate (Theoretical foundation)
  - It is an approximation and assumptions are needed
  - simple and fast for sampling
  - lack features specific to individual cases
  - Fitting parameters are characteristic of the distribution (interpretability)



- Kernel Density Estimation
  - Non-parametric approach, making it adaptable (flexibility)
  - Although, hyper-parameter: Bandwidth and kernel
  - Data-driven, potentially providing a better representation of the distribution
  - Computational cost for high dimensional spaces
  - Fast sampling
  - **Data dependency for sampling**

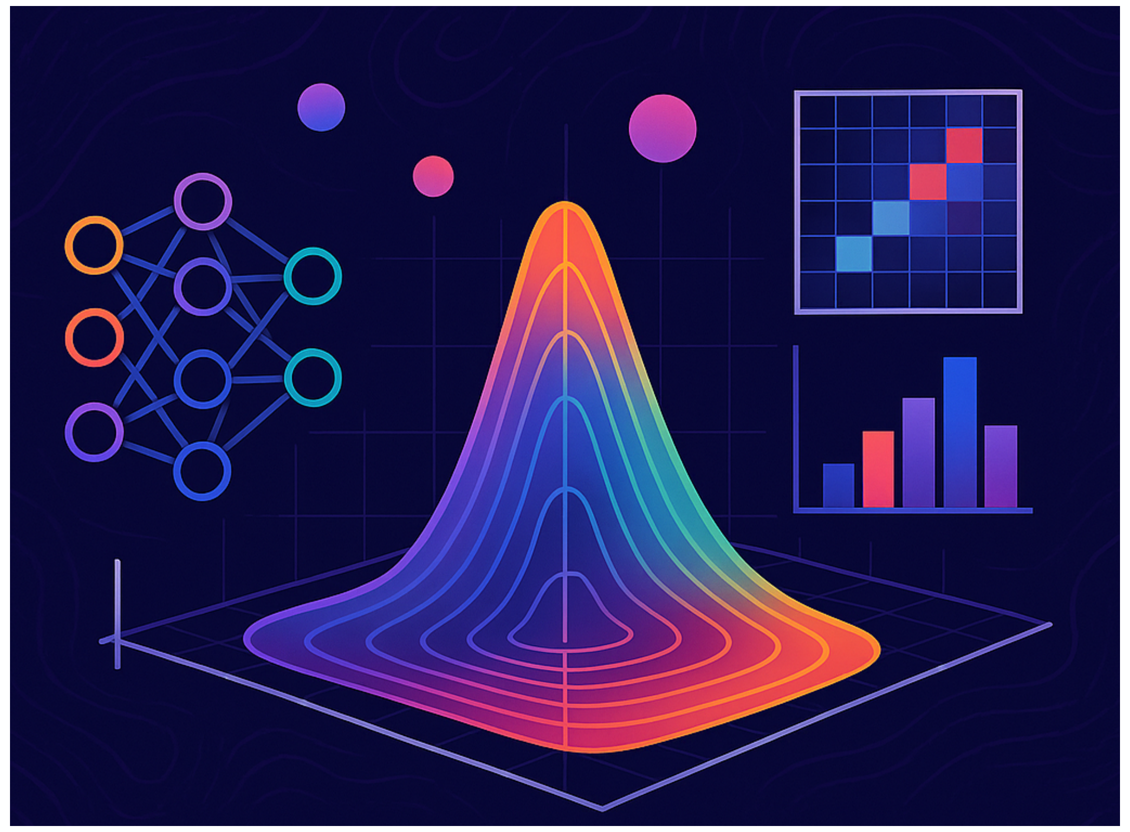
KDSource

GENERATIVE MODELS

- **Objective:** Learn the underlying patterns and distributions of a dataset and generate new data points that resemble the original

We can use generative models to learn the multivariate phase-space distribution of neutrons from a Monte Carlo Particle List (MCPL file)

- *Easy to generate new neutrons to propagate inside tracing software.*
- *capable of learning and generating data with complex patterns and structures between phase-space variables! (High fidelity and realism)*
- *Not limited to specific types of data (Flexibility)*
- ***Once trained, no need to keep the original dataset used to train it.***
- *High-computational cost for training*
- *Large datasets*
- *Lack of interpretability*
- *Depending on model size, slow for sampling*

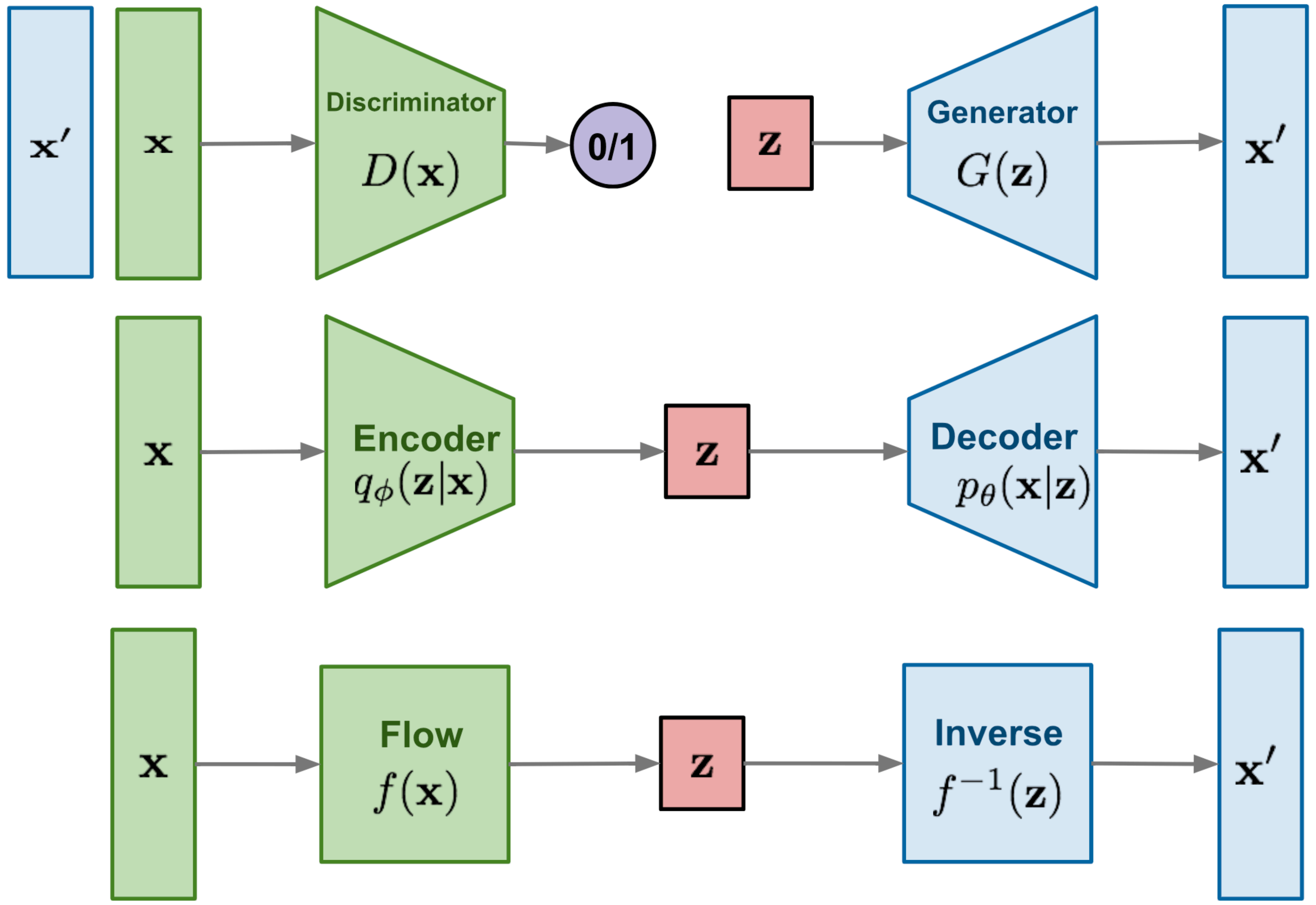


GENERATIVE MODELS

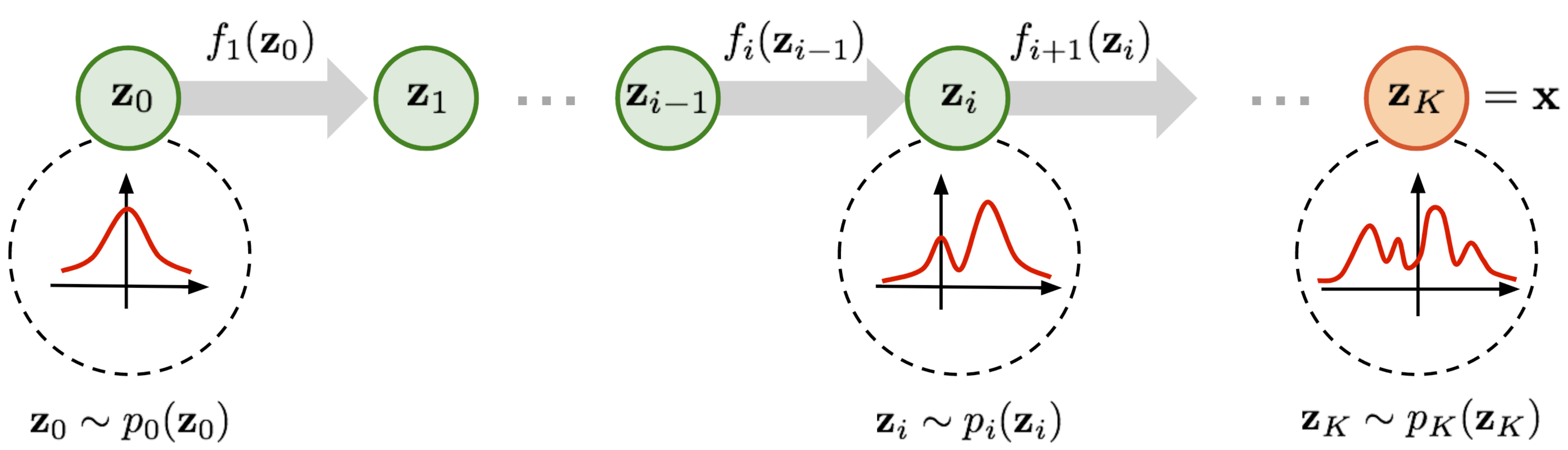
GAN: minimax the classification error loss.

VAE: maximize ELBO.

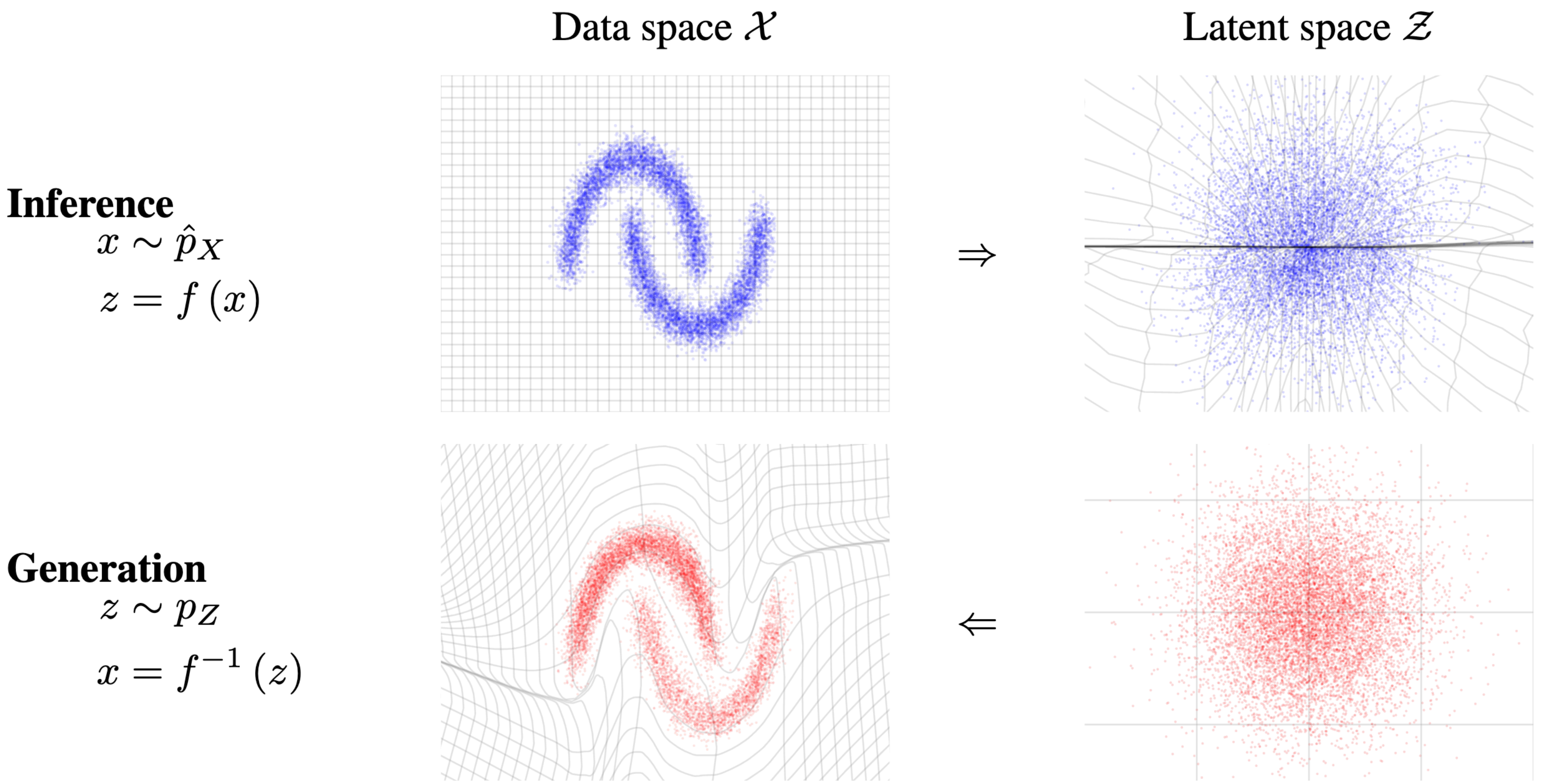
Flow-based generative models: minimize the negative log-likelihood



Normalizing Flows



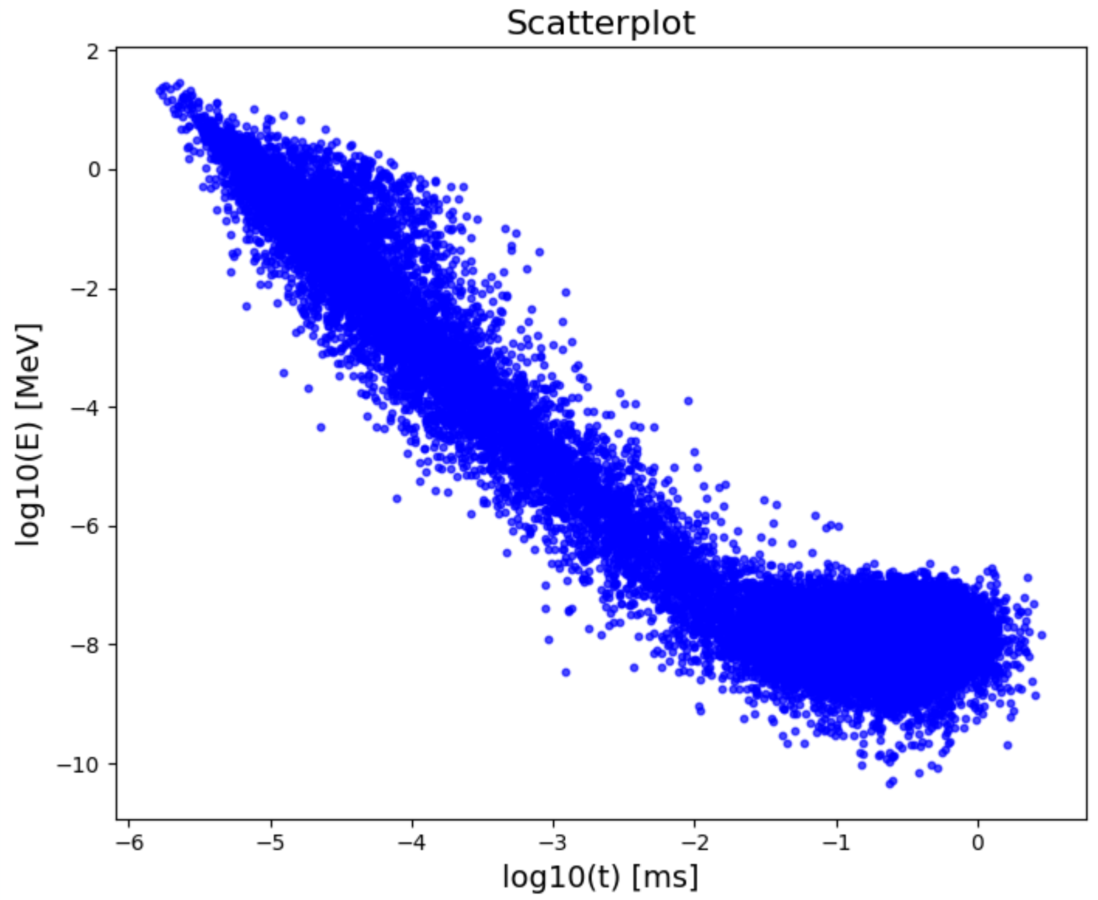
$$p_x(x) = p_z(z)\left|\frac{dz}{dx}\right|$$

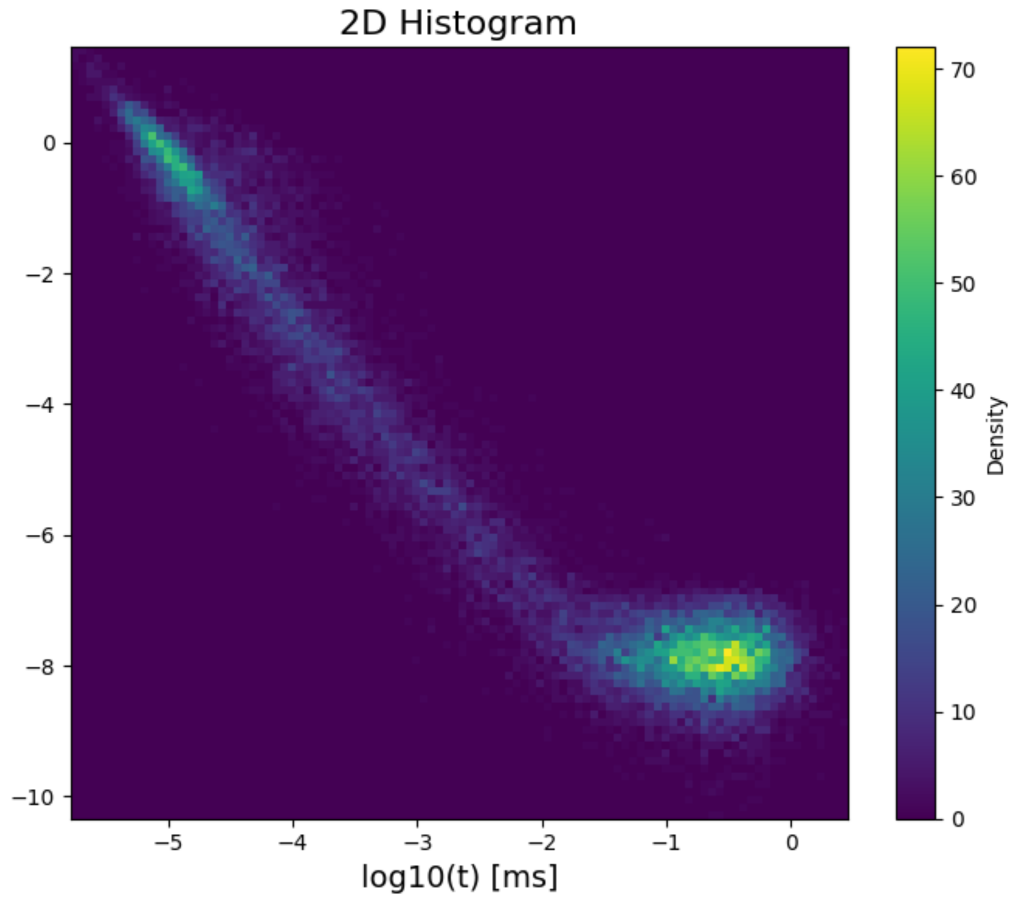


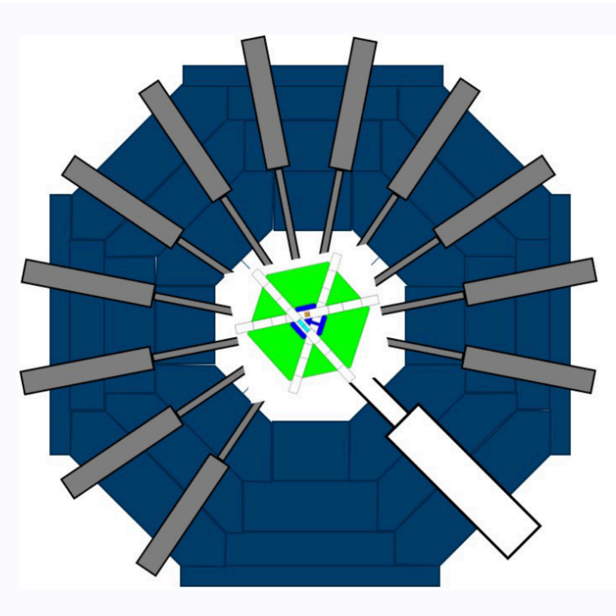
https://uvadlc-notebooks.readthedocs.io/en/latest/tutorial_notebooks/tutorial11/NF_image_modeling.html

TOY EXAMPLE ON 2D

20.000 neutrons, only time and energy

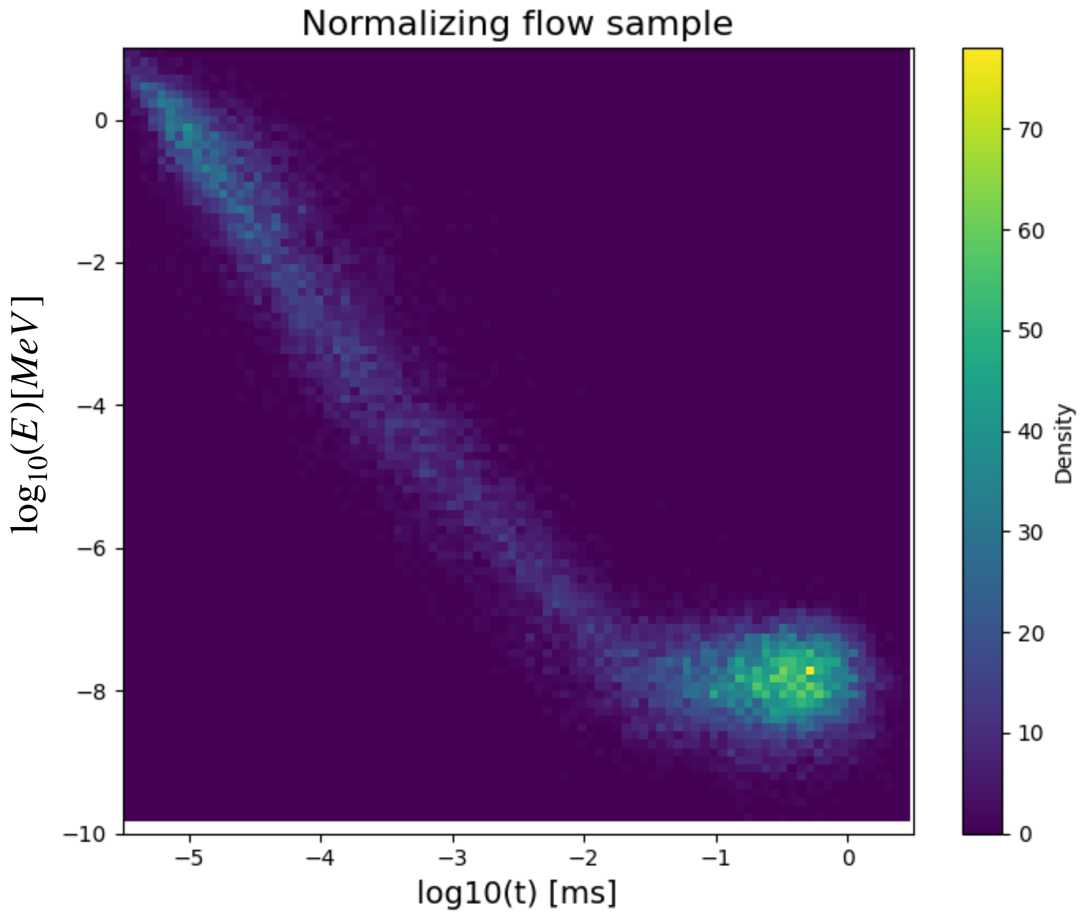


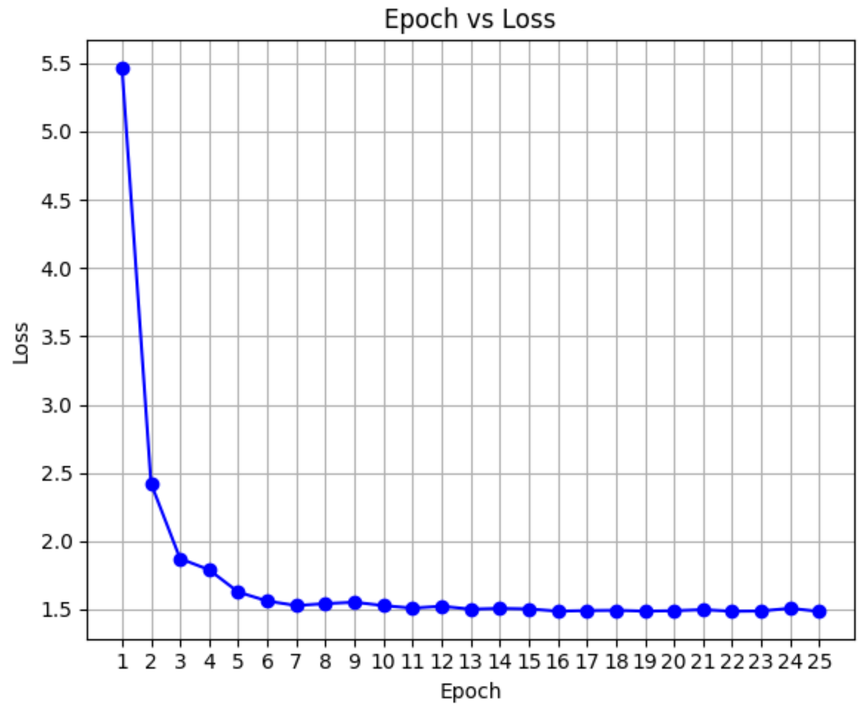




After 25 epochs

Sampling 20000

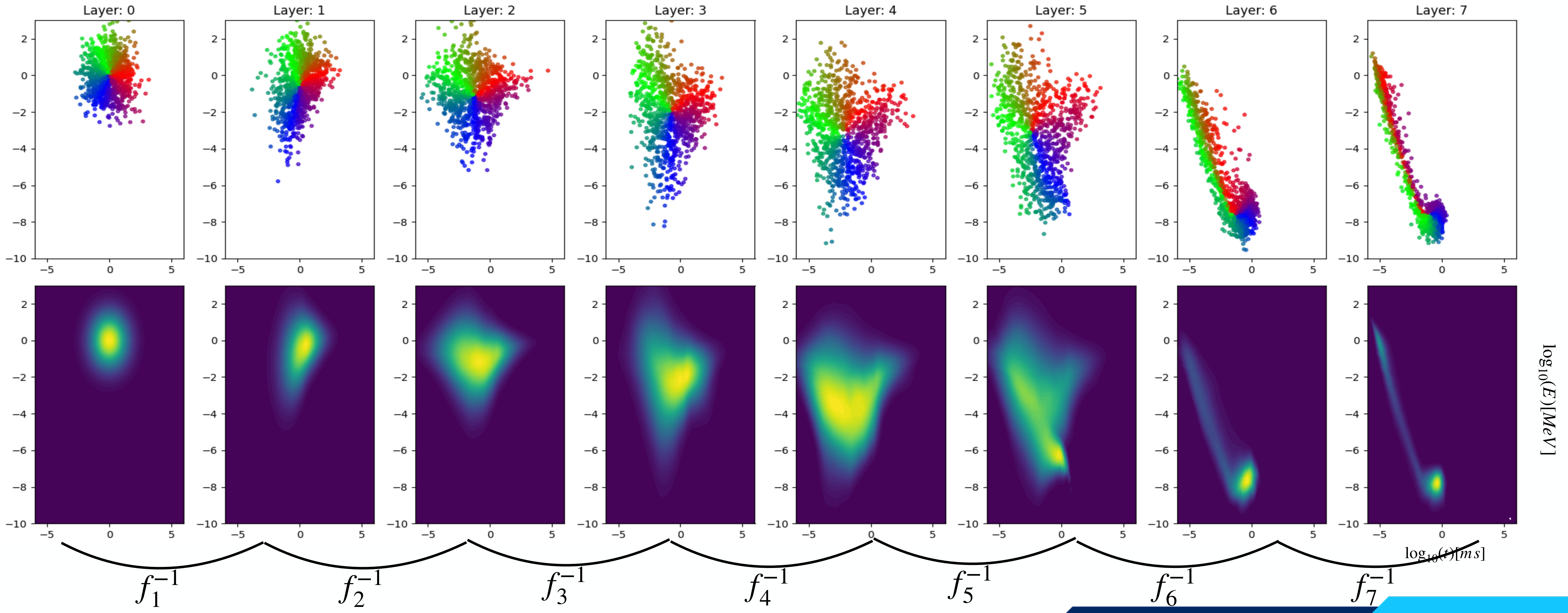




Invertible transformations

2D Normal distribution

Easy to sample



Artificial sample

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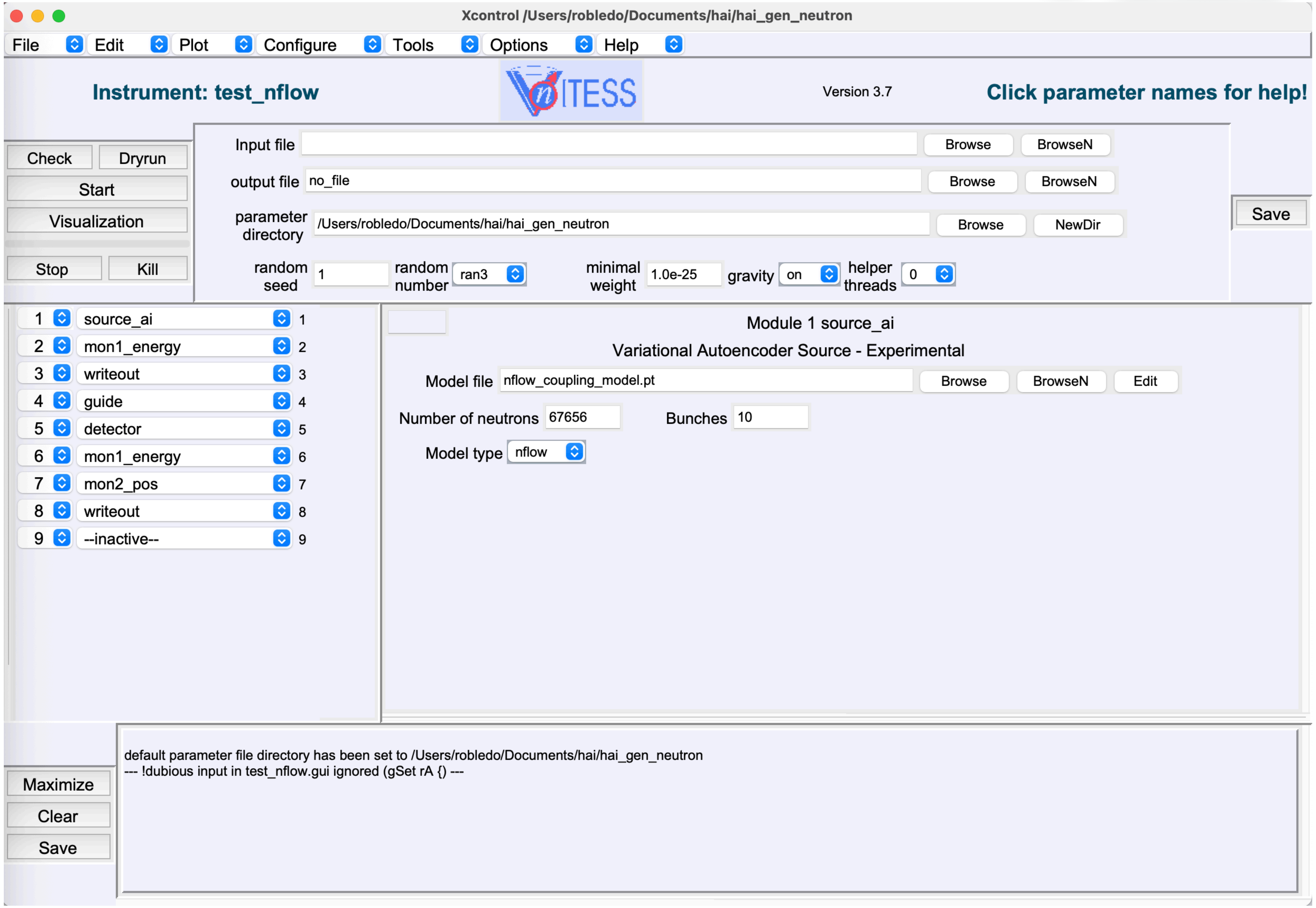
VITESS

New source_AI module

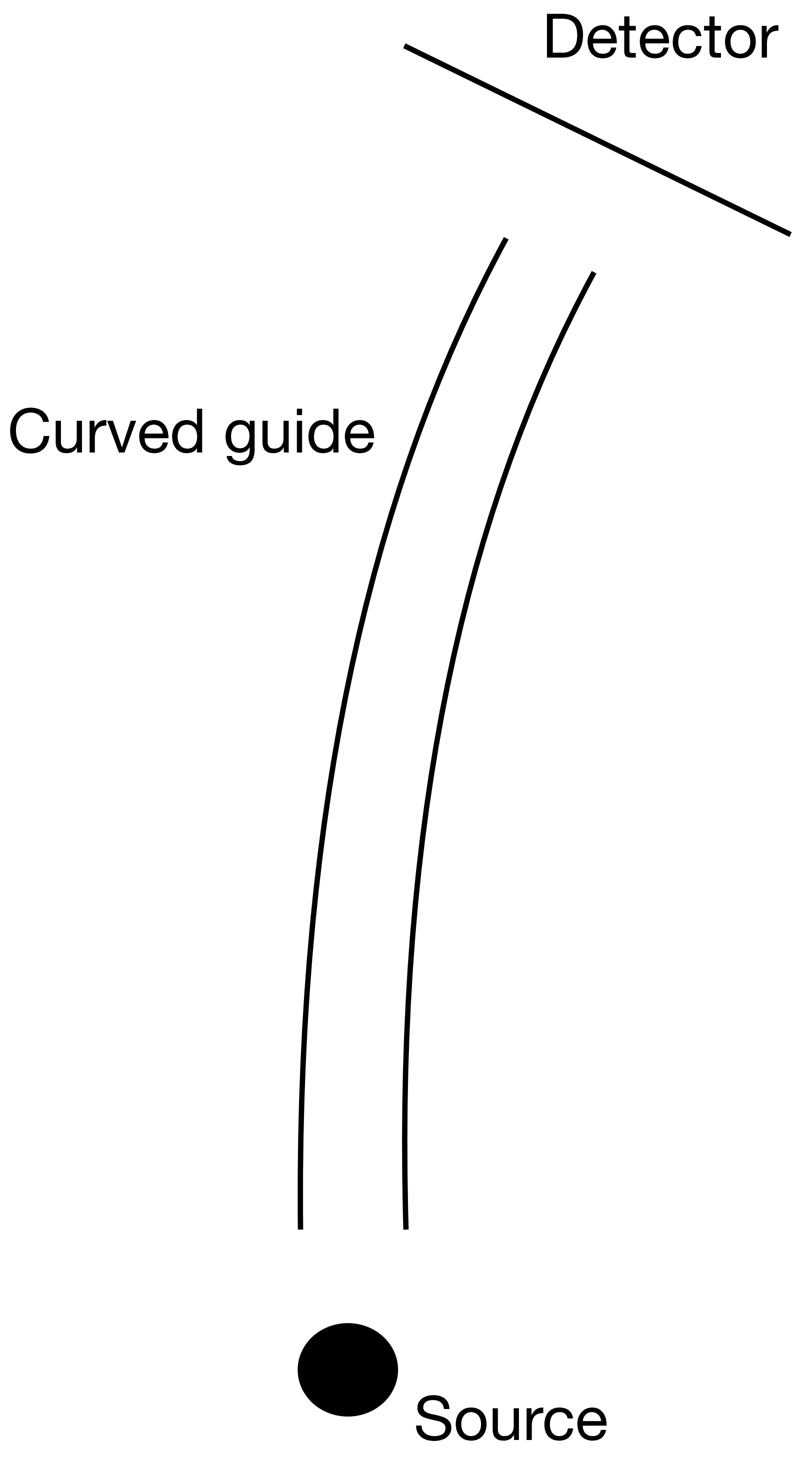
PyTorch

C++ Frontend

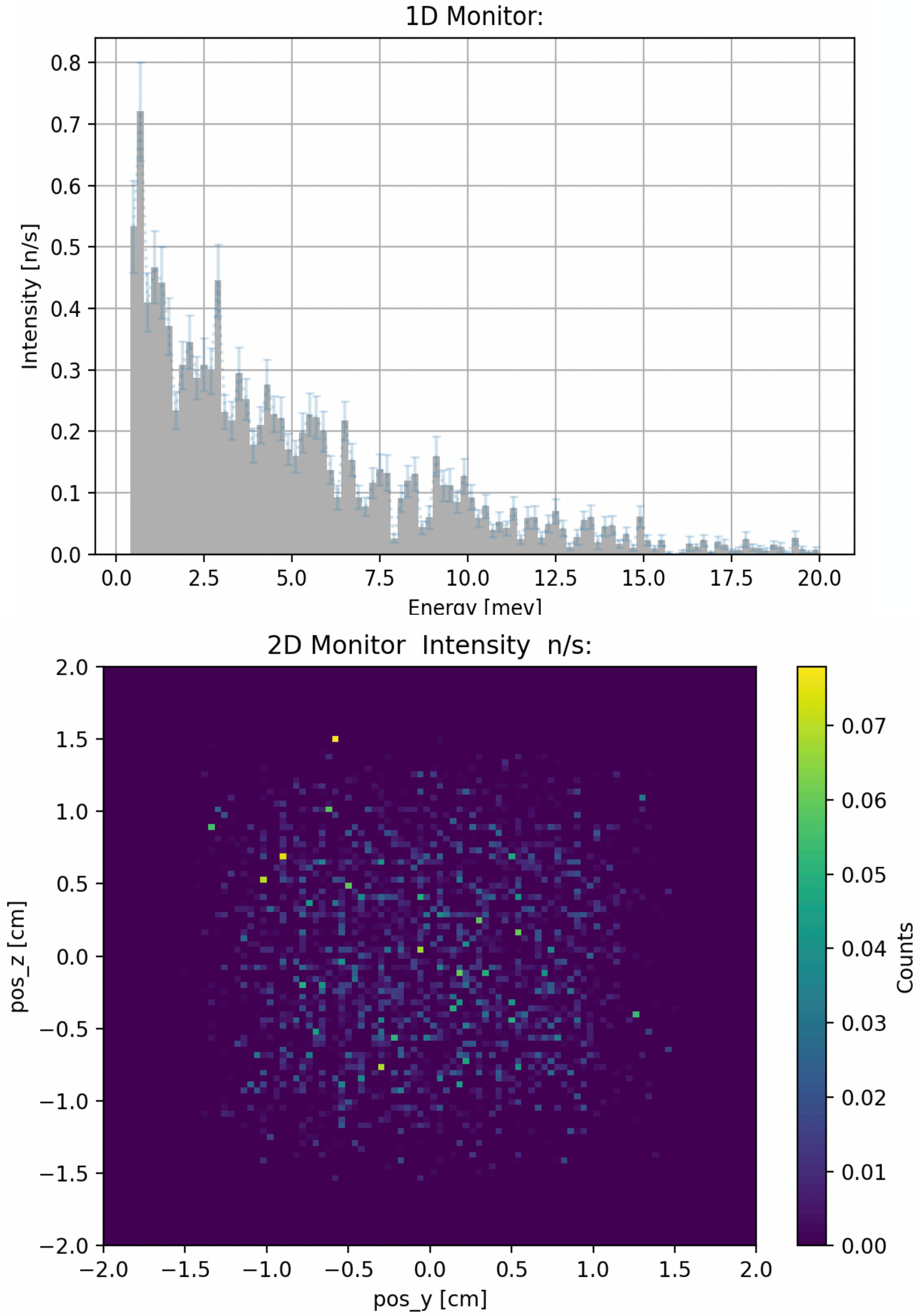
Model needs to be jit compiled



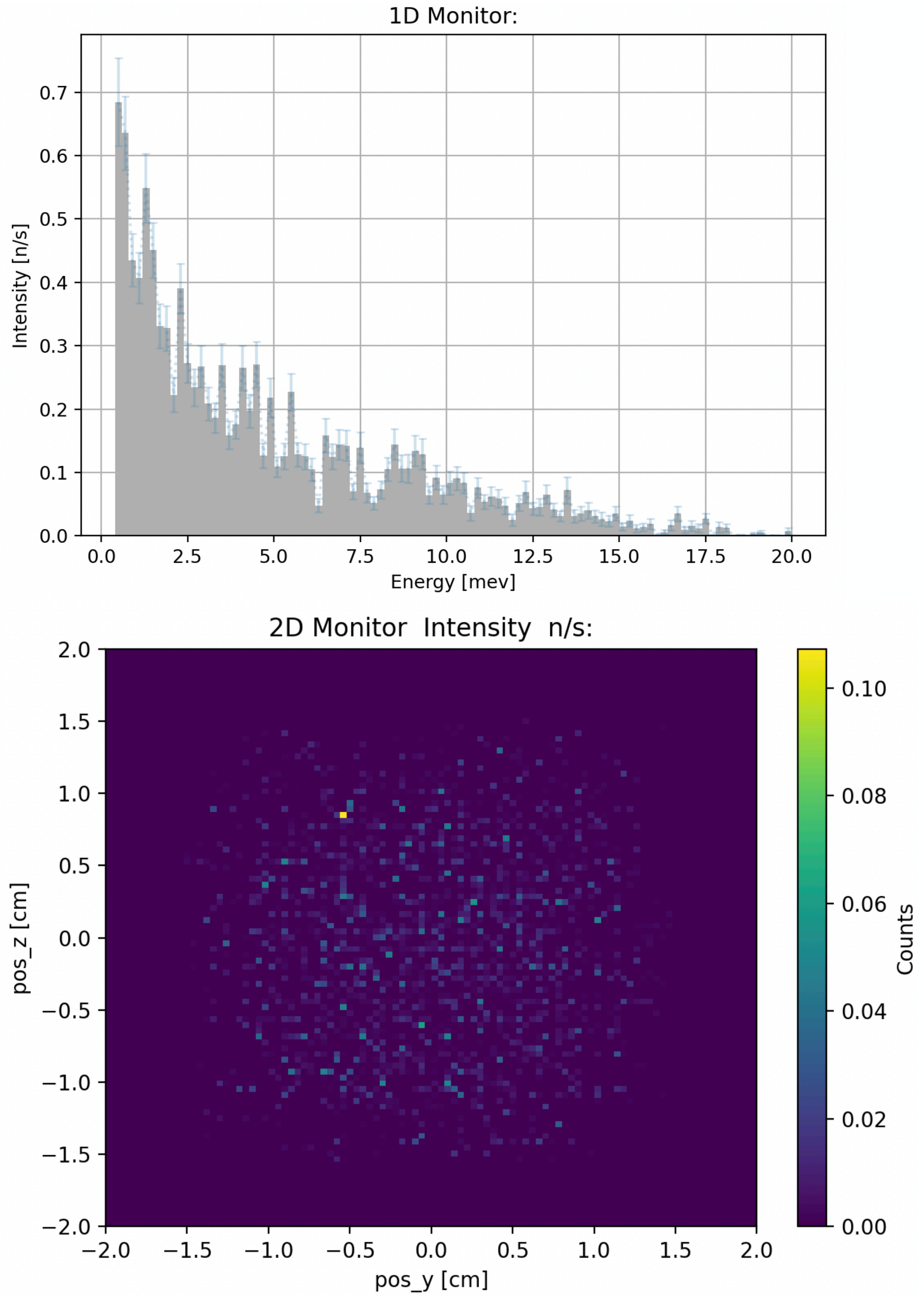
SAMPLING ON VITESS



mcpl

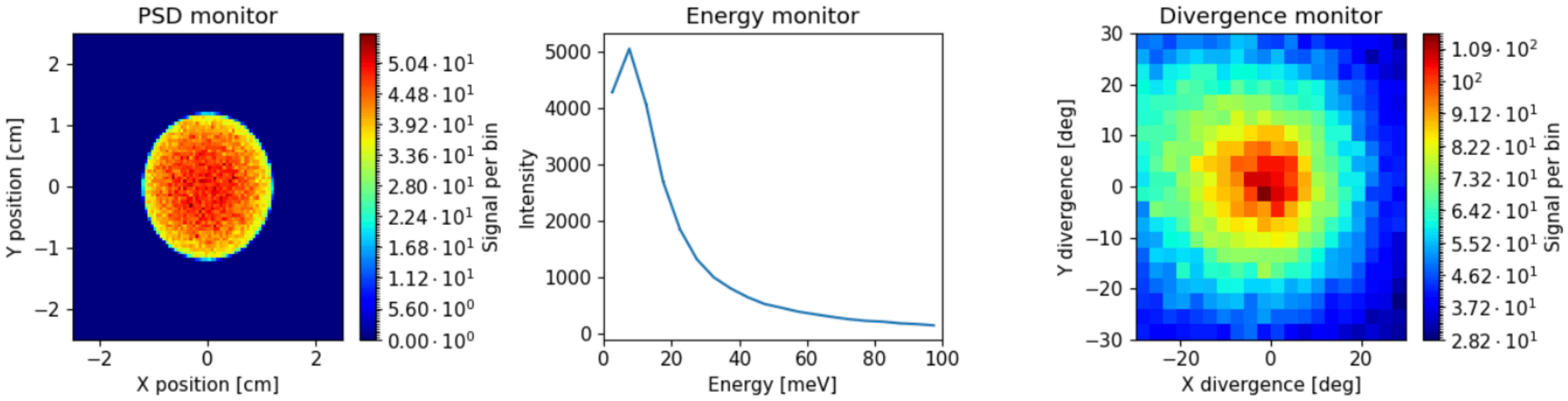


NFlow



MCSTAS

```python
import np2mcpl

# Load model
model = torch.load("nflows_model.model", map_location=torch.device('cpu'), weights_only=False)

# sample model
samples = model.sample(int(1e7))

# Transform to adapt to mcpl format if necessary

...

# Save data
np2mcpl.save("output", samples)

# Load data
import mcstasscript as ms
instrument = ms.McStas_instr("sample_normalizing_flow")
source = instrument.add_component("source", "MCPL_input")
source.filename = '"output.mcpl.gz"'

PSD = instrument.add_component("PSD", "PSD_monitor")
PSD.set_AT([0, 0, 0.2], RELATIVE=source)
PSD.set_parameters(xwidth=1, yheight = 1, filename='"PSD.dat"')
data = instrument.backengine()
ms.make_sub_plot(data)
```

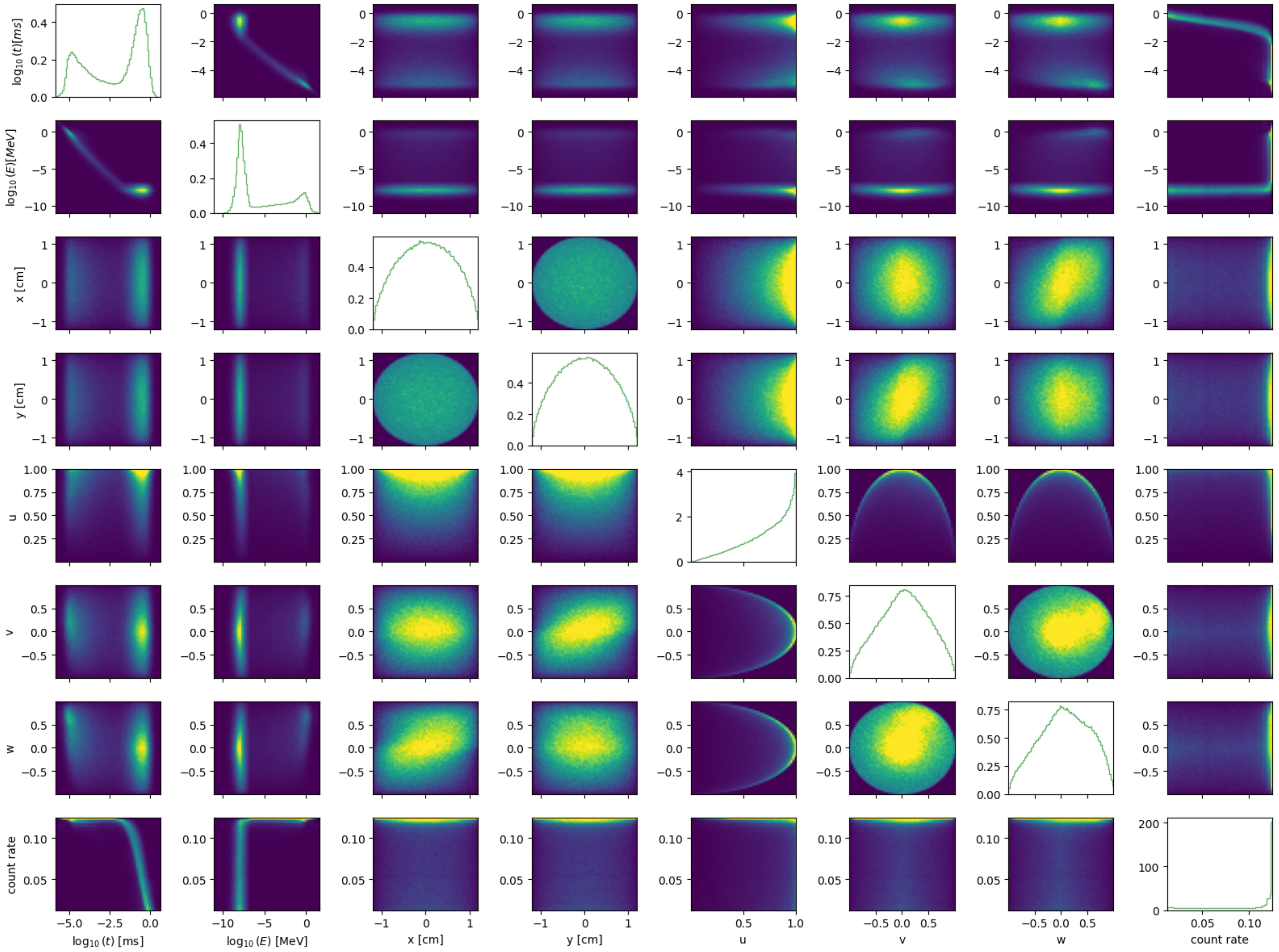


*Same procedure can be done in **vitess-python***

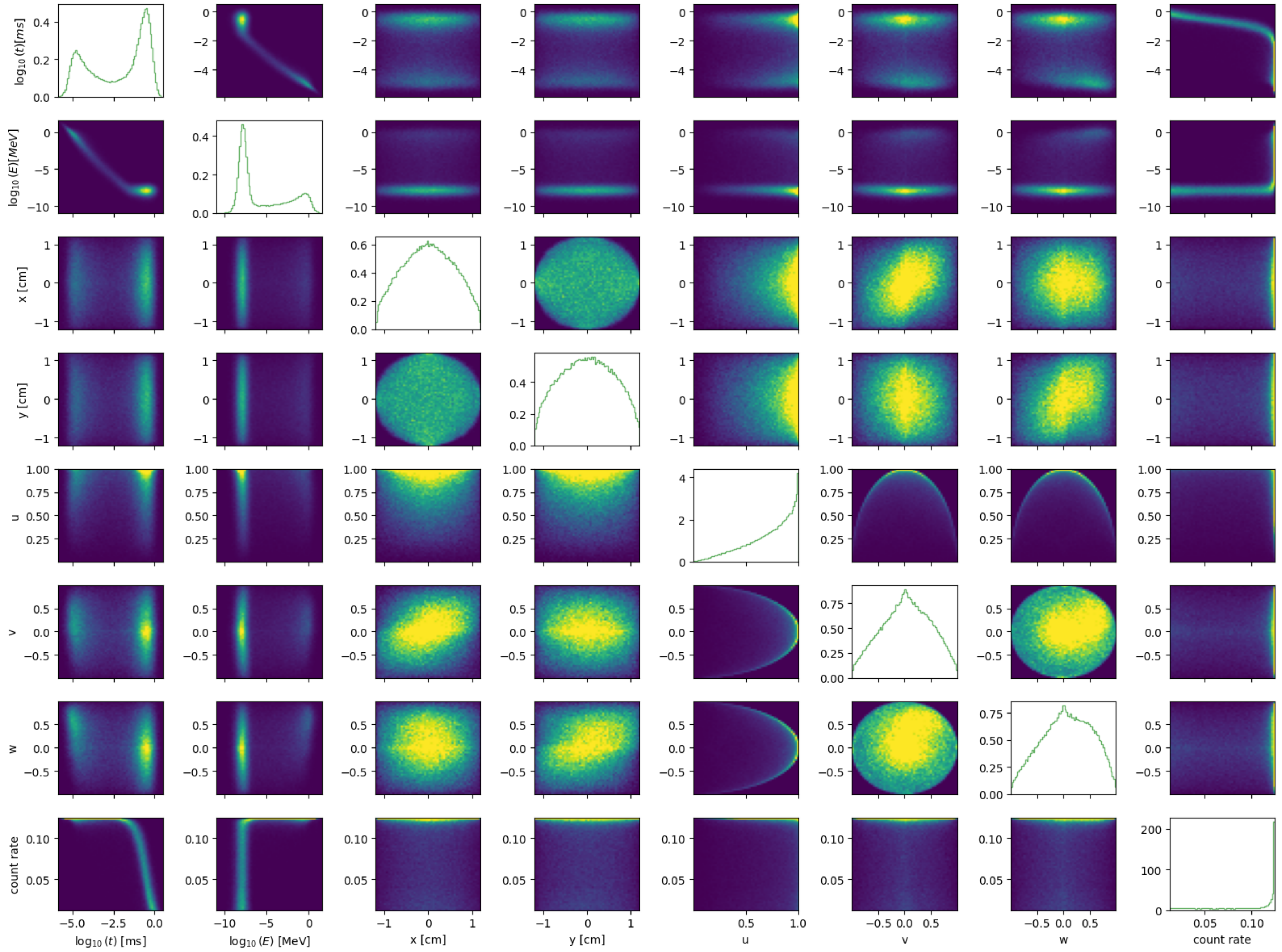
*Poster: "**Vitess-Python: A Python API for VITESS Instruments**" - Fabian Beule*

Comparison between NFlow and MCPL

MCPL histograms



NFlow histograms



Comparison between NFlow and MCPL

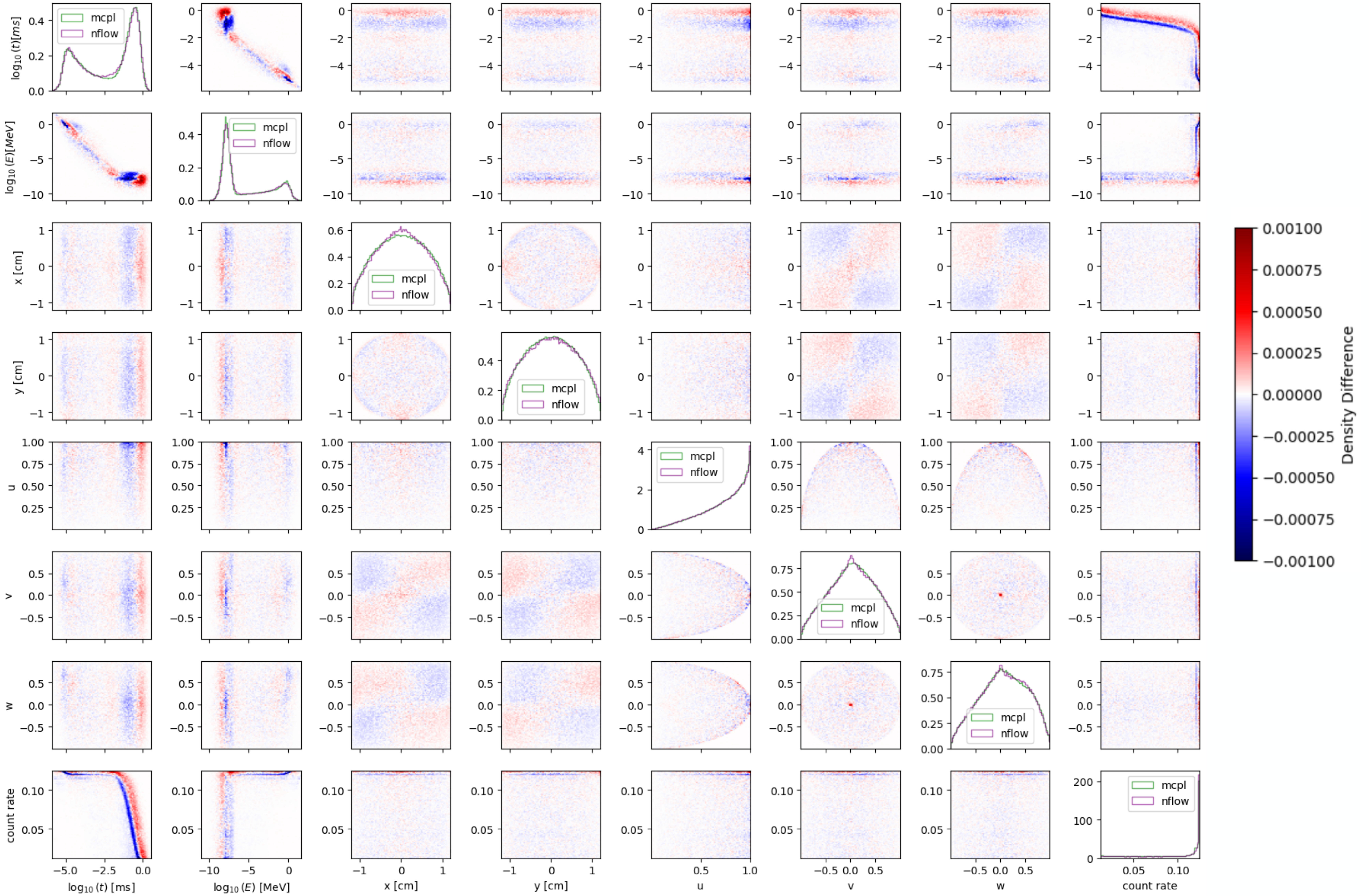
Blue: under-estimate

Red: over-estimate

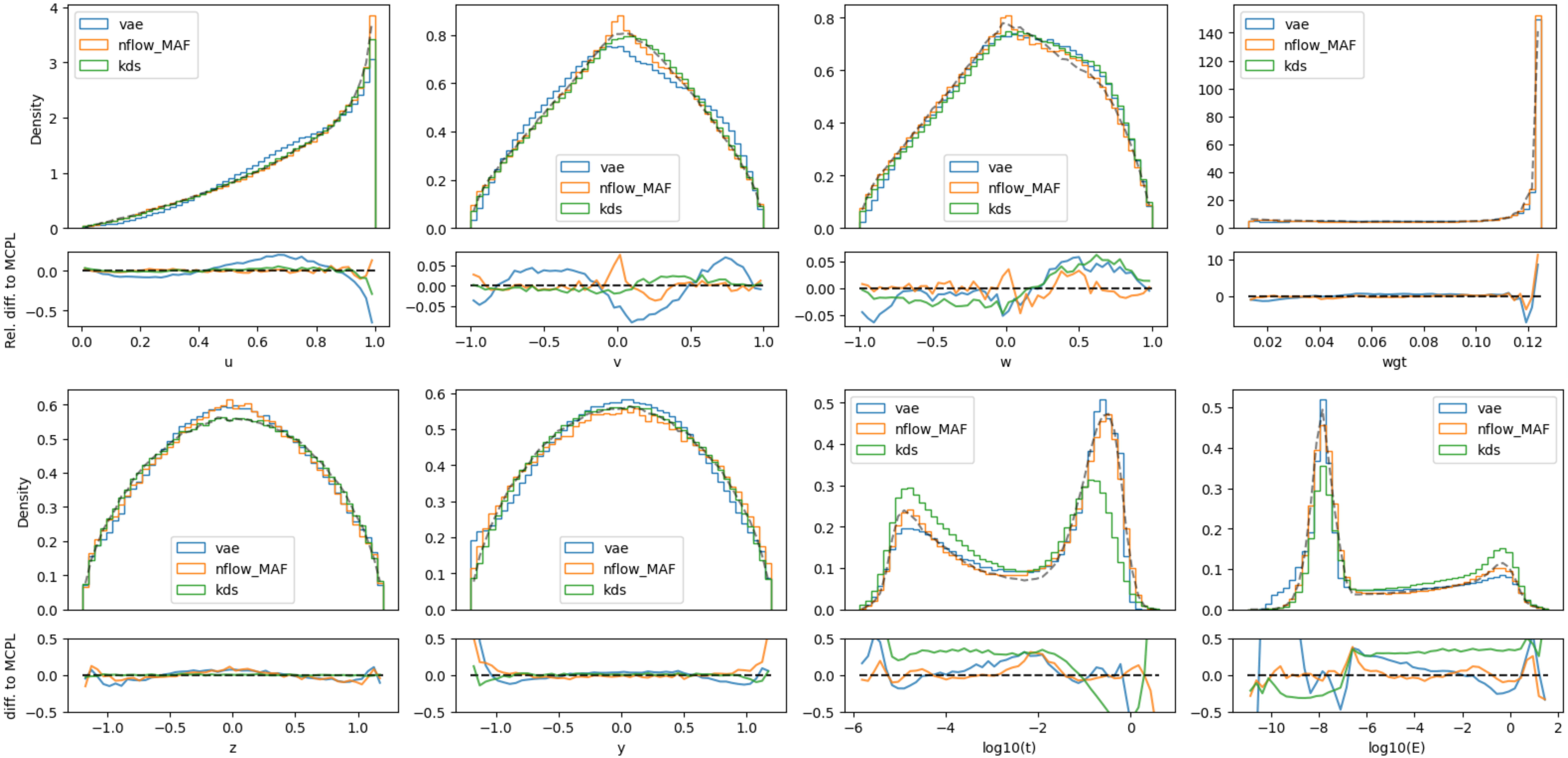
model can be stored in a file consisting of **few KB**

easily loadable through PyTorch API

we can sample from the latent space



COMPARISON BETWEEN MODELS



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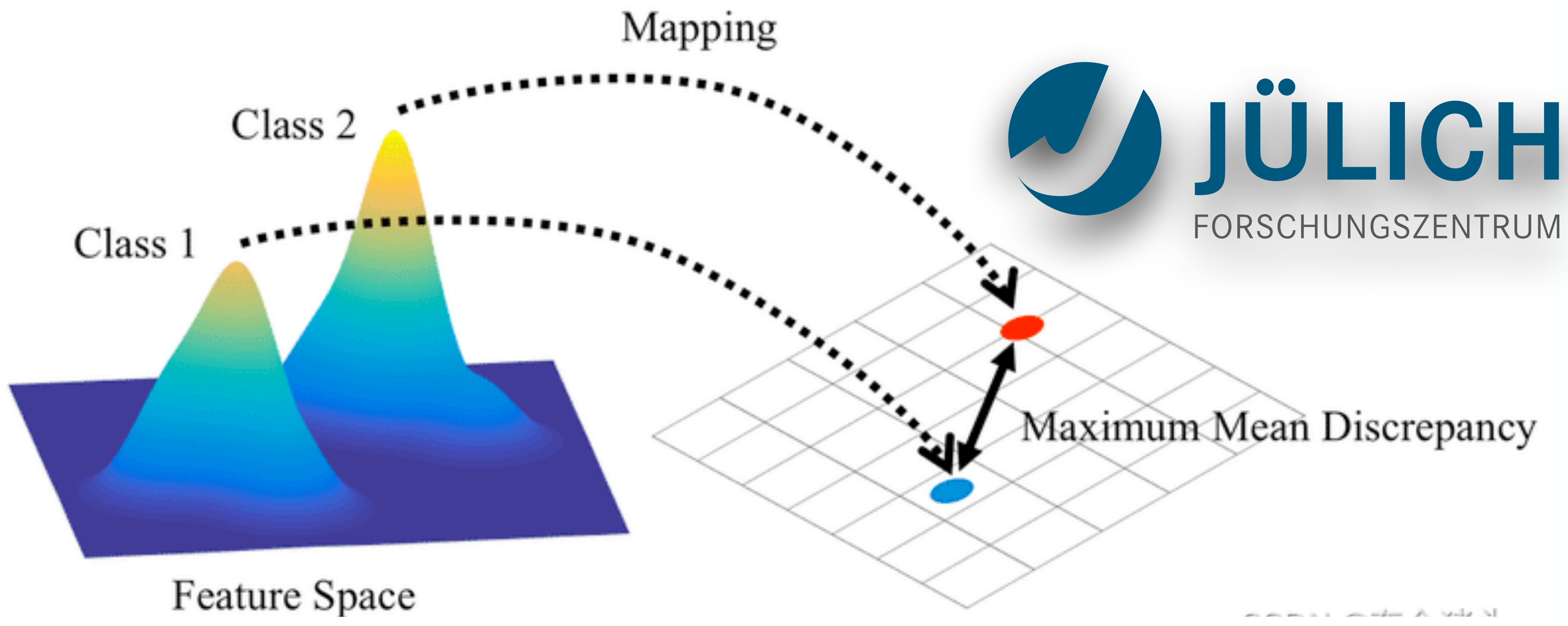
QUANTIFYING DIFFERENCES



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Statistical measure: Maximum mean discrepancy (MMD)

Determine if two datasets are likely to have been drawn from the same distribution by embedding probability distributions into a Reproducing Kernel Hilbert Space (RKHS) and then calculating the distance between the means of these embeddings.

Model	Average MMD *
MCPL	0.00015 ± 0.00016
MAF NFlow	**0.00053 ± 0.00010**
Coupling Flow	0.00171 ± 0.00015
VAE	0.00308 ± 0.00017
KDSource	0.08014 ± 0.00143
Uniform	0.15231 ± 0.00149

* sample size = 10000, average over 10 samples

Model	Sampling time / 700.000 n (s)
KDSource	2
VAE	8
NFlow	7

SUMMARY

- Generative models can learn multivariate probability distributions from data
- MCPL files make great training data!
- Normalizing Flows show great potential in learning neutron phase-space variable distributions, but they can estimate poorly if distributions have sharp features.
- These sources can already be used in Vitess and McStas, and are easily extensible to other Monte Carlo software.
- There are multiple architectures of NFs, as well as VAEs and GANs. Exploring which model does best is still an art. Physical constraints can be added inside the loss function.
- Metrics for comparing multivariate distributions should be taken into account for model selection.

Thank you for your attention! Questions?

Jose Robledo

Forschungszentrum Jülich