Emulating low energy nuclear interactions with Deep Learning

Emulating BLOB with Variational Autoencoders and perspectives

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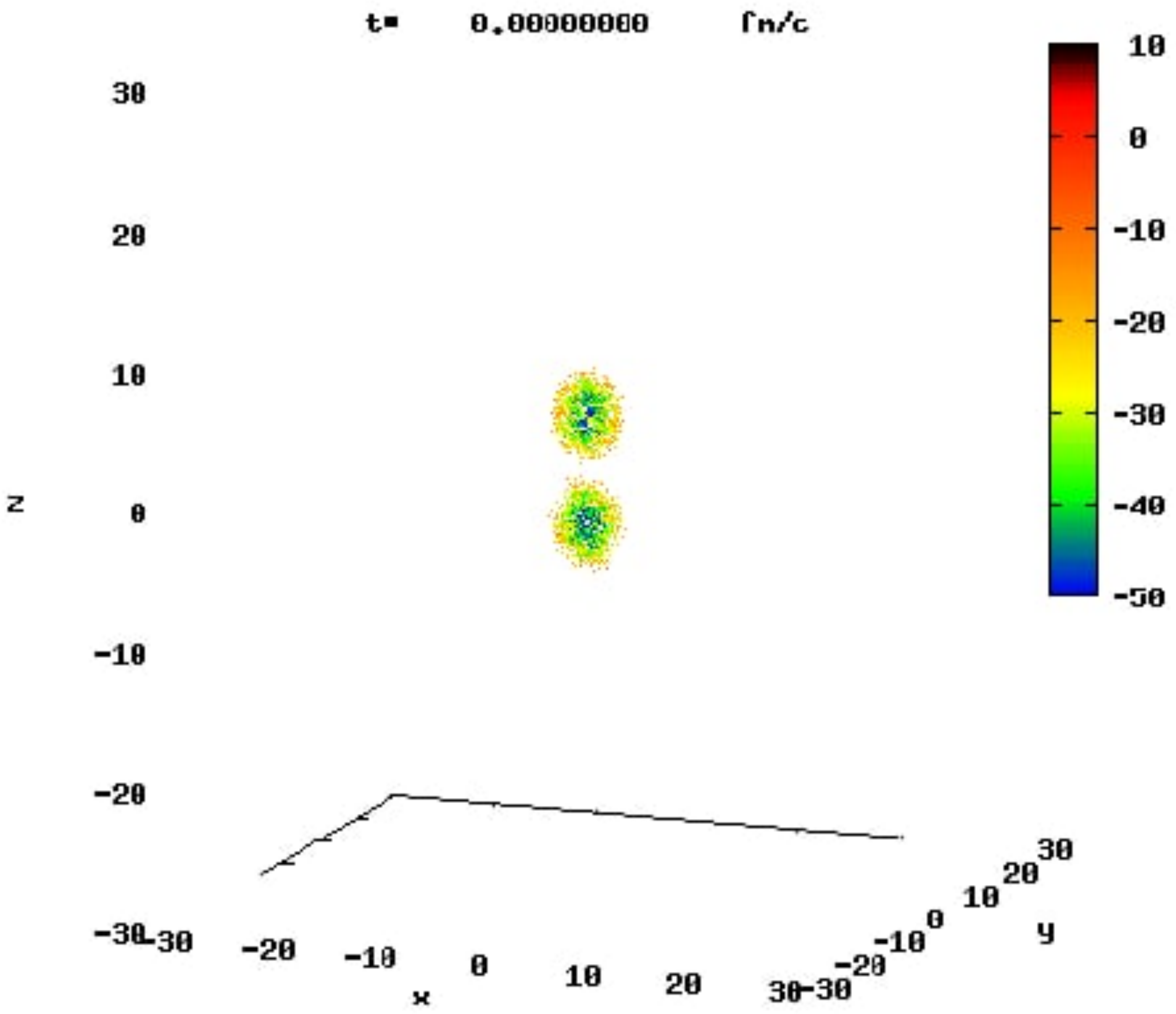
BLOB

(Boltzmann Langevin One Body)

- BLOB describes the time evolution of the one-particle density (of a nucleon in the phase space) by solving numerically a semi-classical, one-body transport equation;
- Nucleons interactions are modeled as two-body inelastic collisions;
- To solve the transport equation, BLOB samples the density distribution in phase space with test particles;
- Test particles are under the action of an effective Mean Field nuclear potential;
- The BLOB final state (output) is a probability density function (PDF) of finding a nucleon in a point of the phase space. This PDF is built starting from the coordinates of the test particles at the end of the reaction.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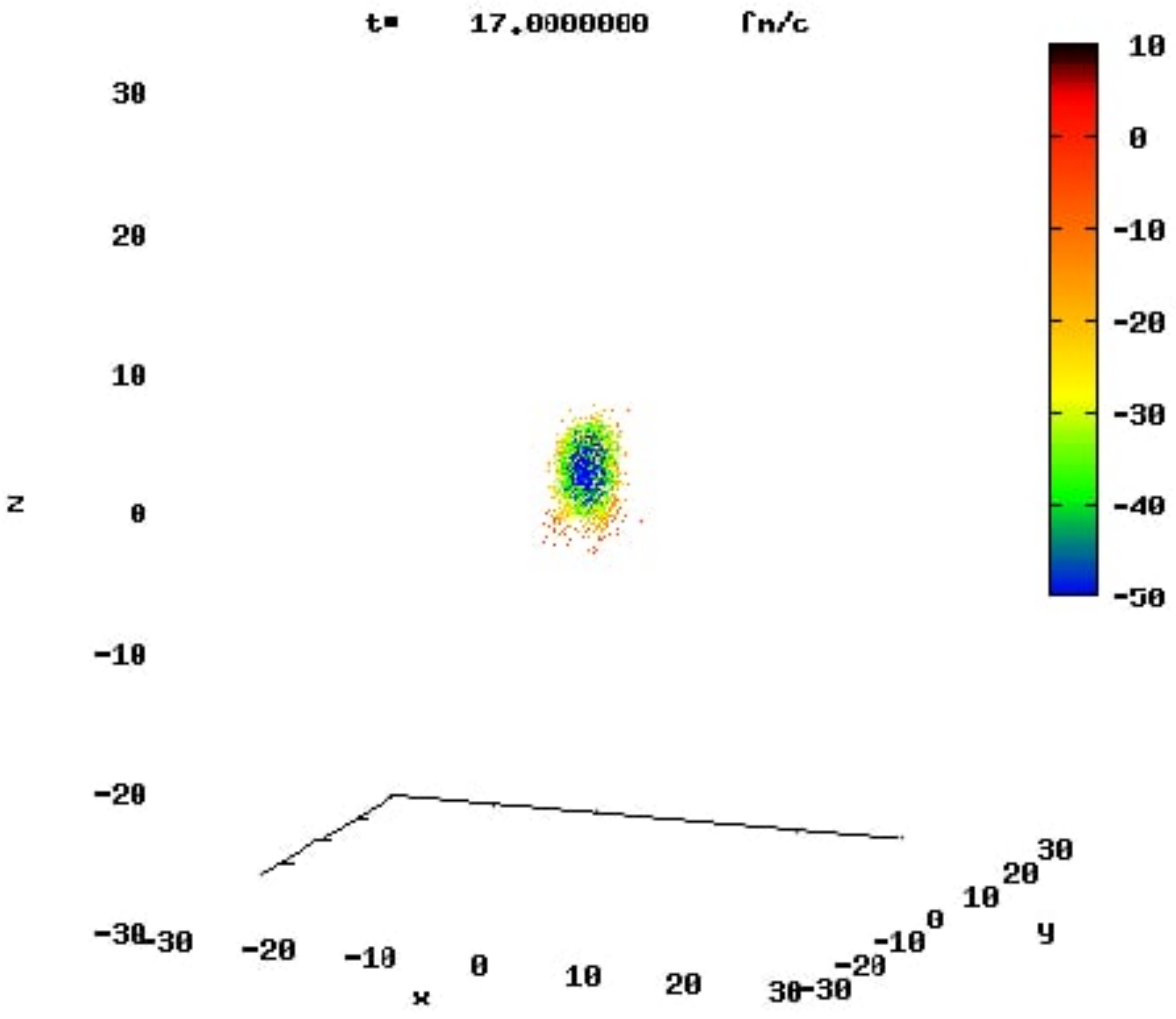

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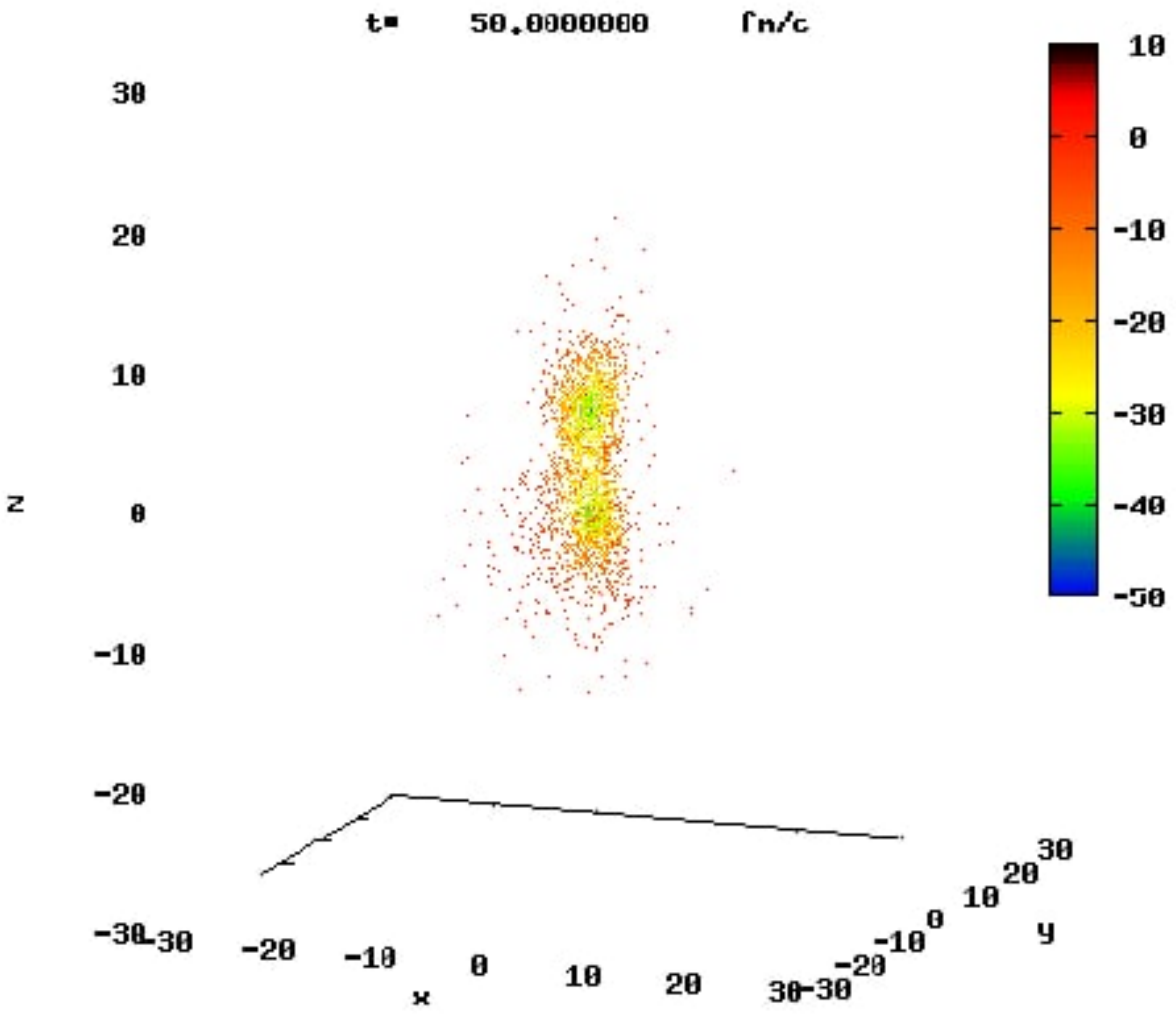
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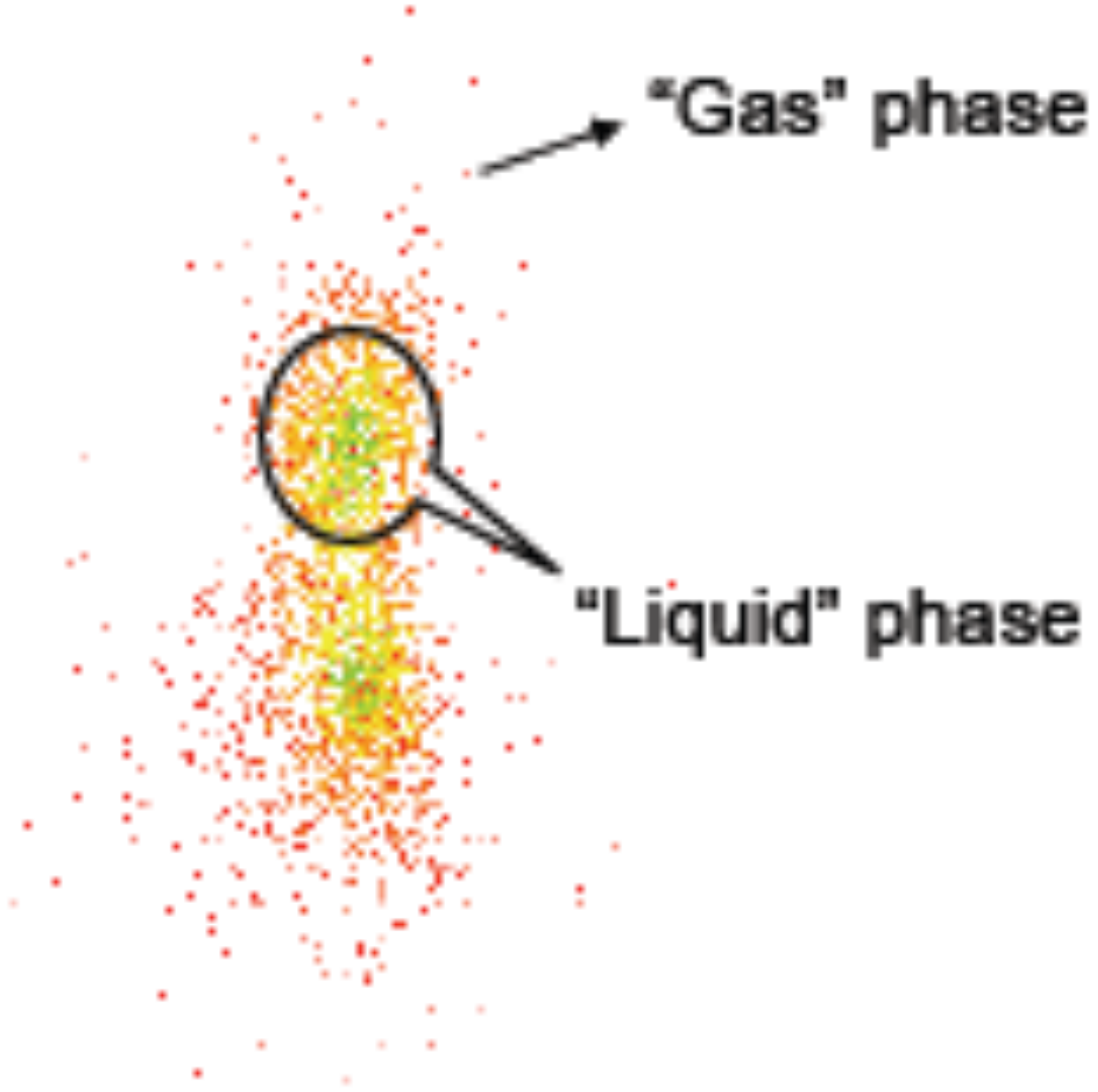
BLOB

(Boltzmann Langevin One Body)

- A “liquid” and a “gas” phase are defined by applying a clustering procedure to the output PDF;
- Each liquid phase neighborhoods stands for a large fragment. The rest of the test particles, the gas phase, represents the nucleons emitted in the first part of the reaction.
- Depending on the impact parameter b, one can have up to 3 large fragments.



Dataset

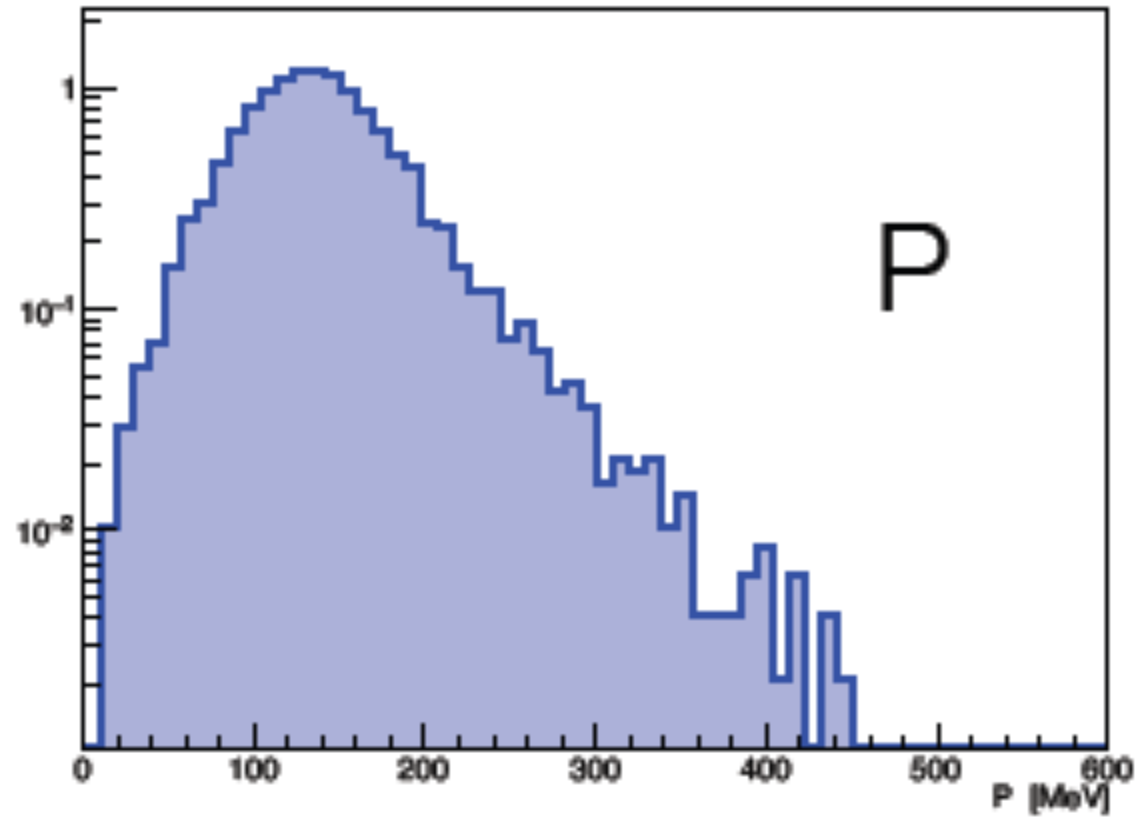
Dimensionality reduction

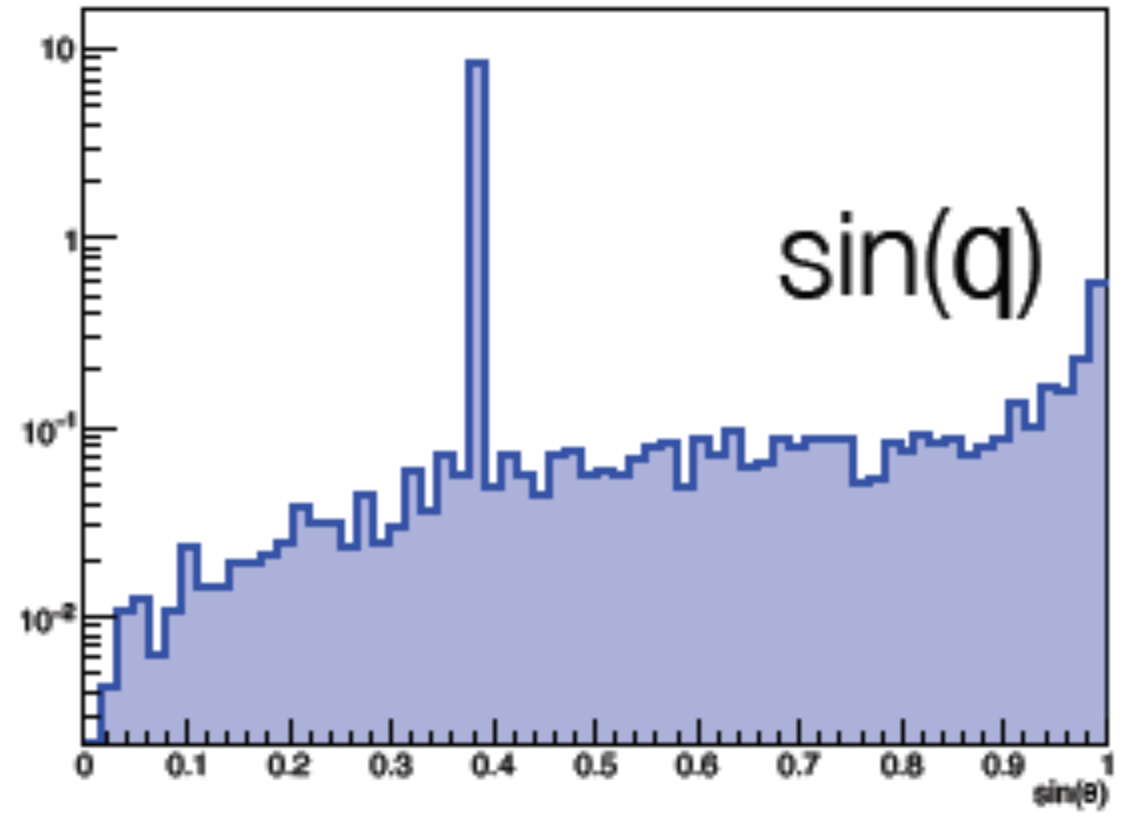
- BLOB output consists of two six dimensional (phase space) distributions: one for protons and one for neutrons;
- Such an output can be discretized binning the phase space;
- Premade 6D Convolutional Layers are not available: we reduce the dimensionality of the data to 3 DoF;
- The information loss of this process doesn’t invalidate our method, but the resulting “images” are sparse and not smooth;

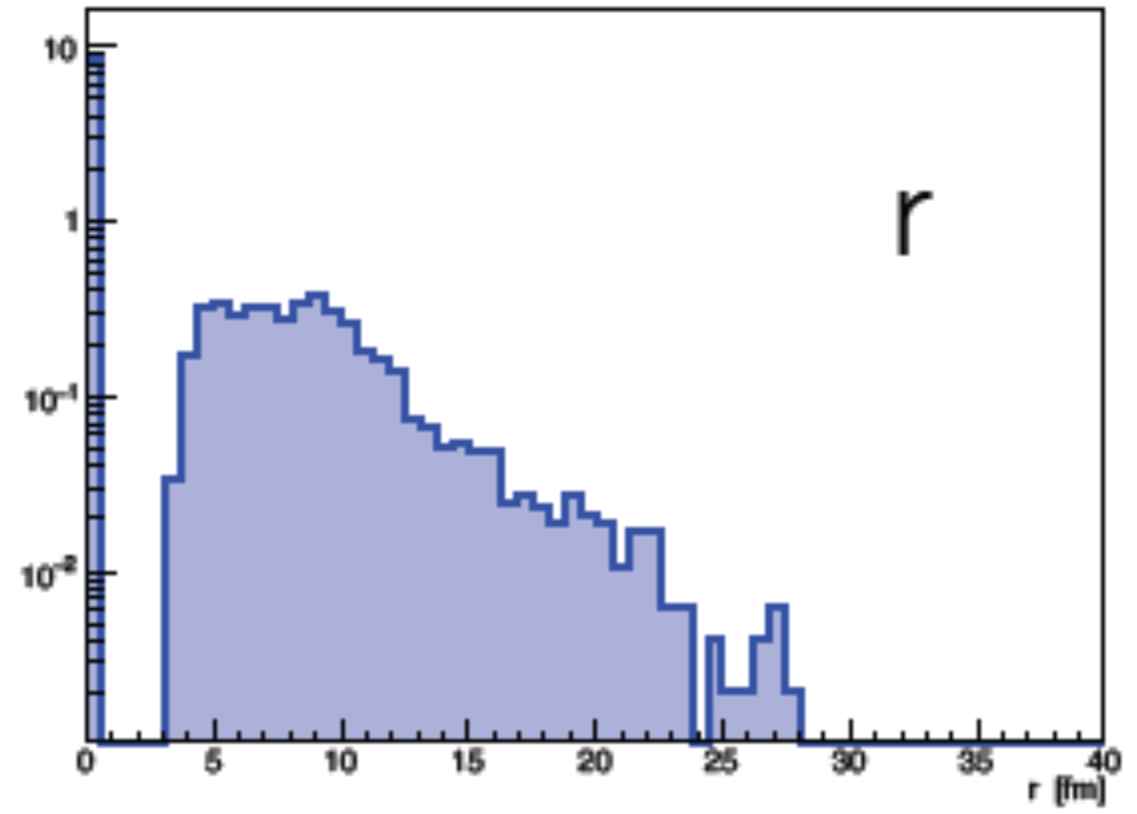
Dataset

Dimensionality reduction

- For each test particle, we consider only:
  - P = the modulus of its momentum,
  - q = its angle with the collision axis,
  - r = its distance from the closest large fragment center;
- Large fragments are represented by 500*A test particles. All the particles belonging to a fragment have r=0 and same q;
- The momentum p of each test particle is sampled from a gaussian distribution (with mean = large fragment momentum and sigma = excitation energy).
- The test particles are divided into 3 groups, one for each large fragment. Each group is “assigned” to a single color channel (RGB);

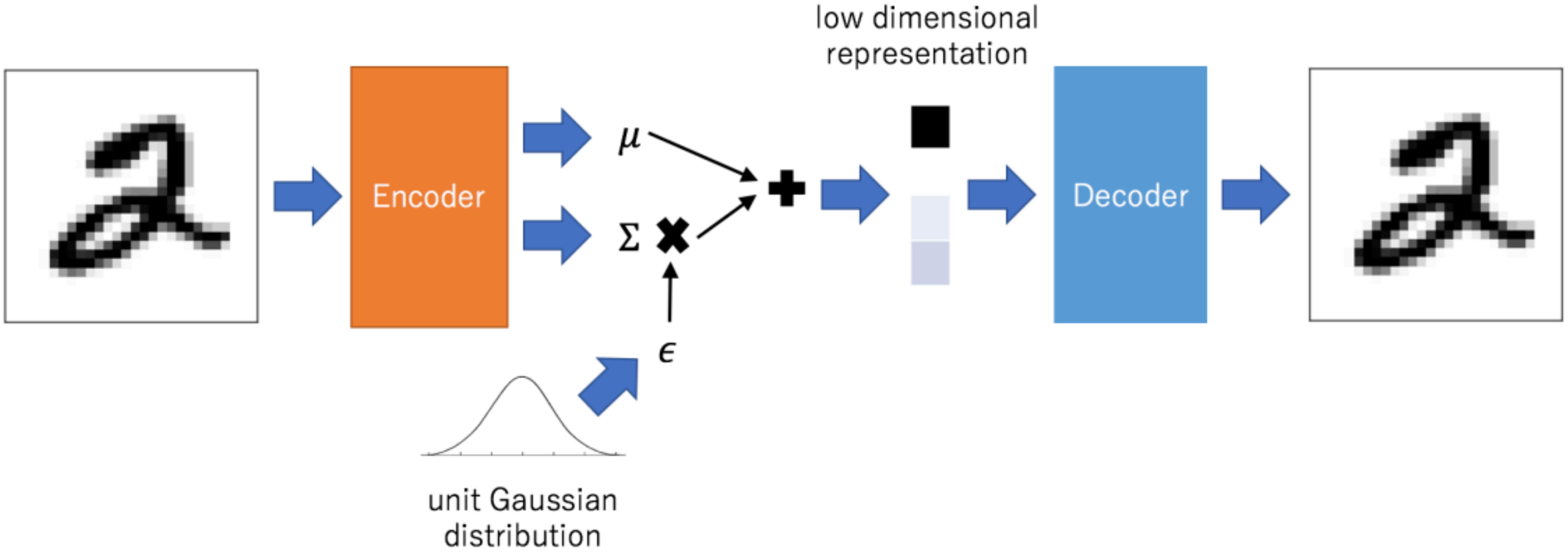






Variational Autoencoder

The basics



Variational Autoencoder

Our initial goal

- Our initial idea was to build a Deep NN that could “understand” the physics behind the BLOB model (“all the information is contained in b”);
- We hoped that the VAE would encode each image in its b and autonomously organize the latent space according to b (unsupervised approach);
- To this aim:
  - we made a preliminary study of the dataset (PCA) to understand how to compress it, but there was no subset of features that could adequately describe the variability of the dataset;
  - we designed the encoder (3D CNN) to predict the b of a given image,
  - we tested 1D latent space,
  - we developed a symmetic decoder to generate synthetic data.

Variational Autoencoder

New attempt

- Unfortunately, our model could not emulate the PDFs;
- Probably, given the characteristics of the dataset, the encoder compression was too high;
- Therefore, we switched to a 2D latent space;
- Nevertheless, this new latent space was not disentangled and often collapsed;
- To solve these problems, we added a new task: a Predictor (regression task, z vs b) forcing the latent space to organize itself according to b (semi-supervised approach);
- Hypertuning (VGG-like conv blocks, number of filters) + asymmetric decoder to further improve the quality of the reconstructed PDFs.

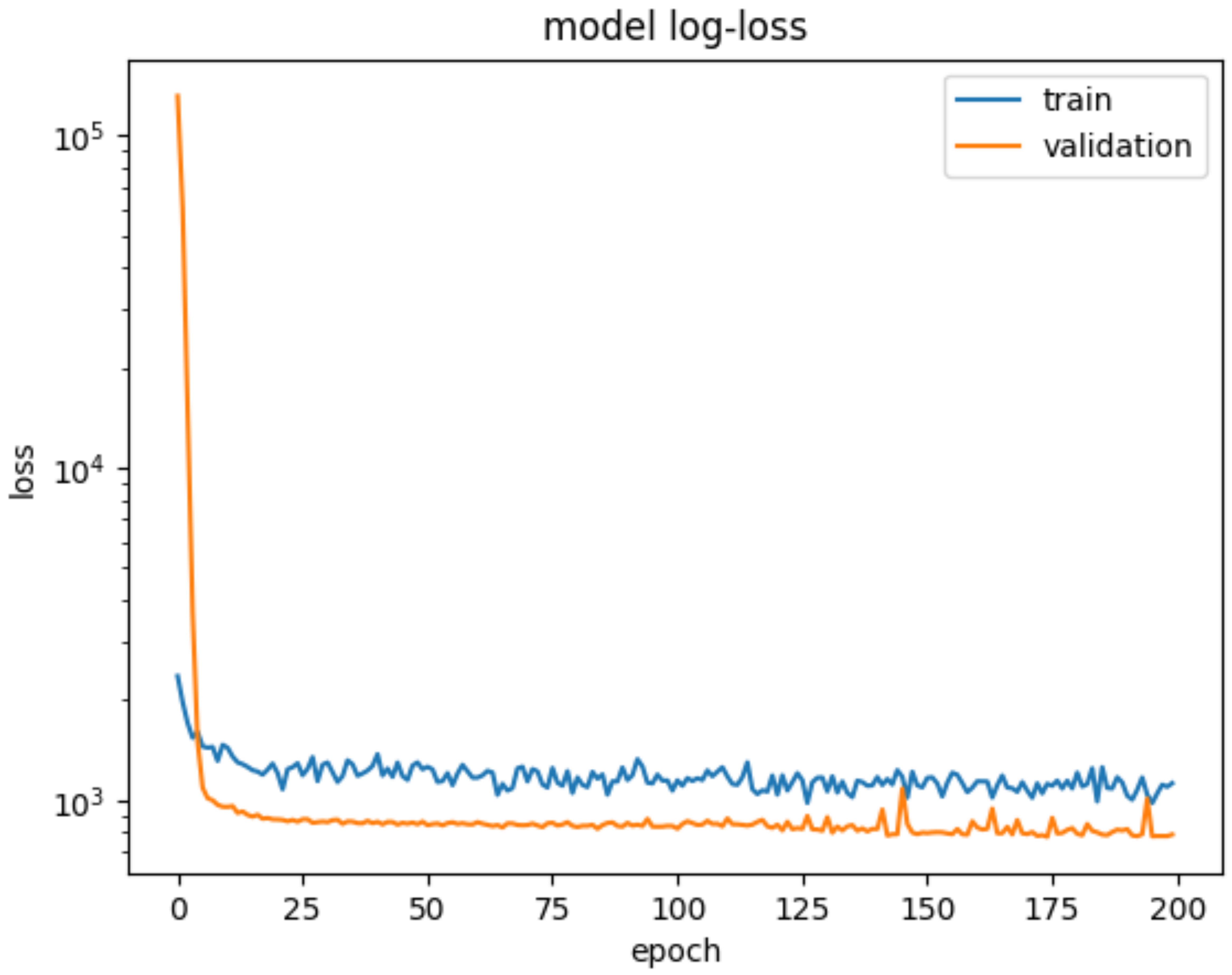
Variational Autoencoder

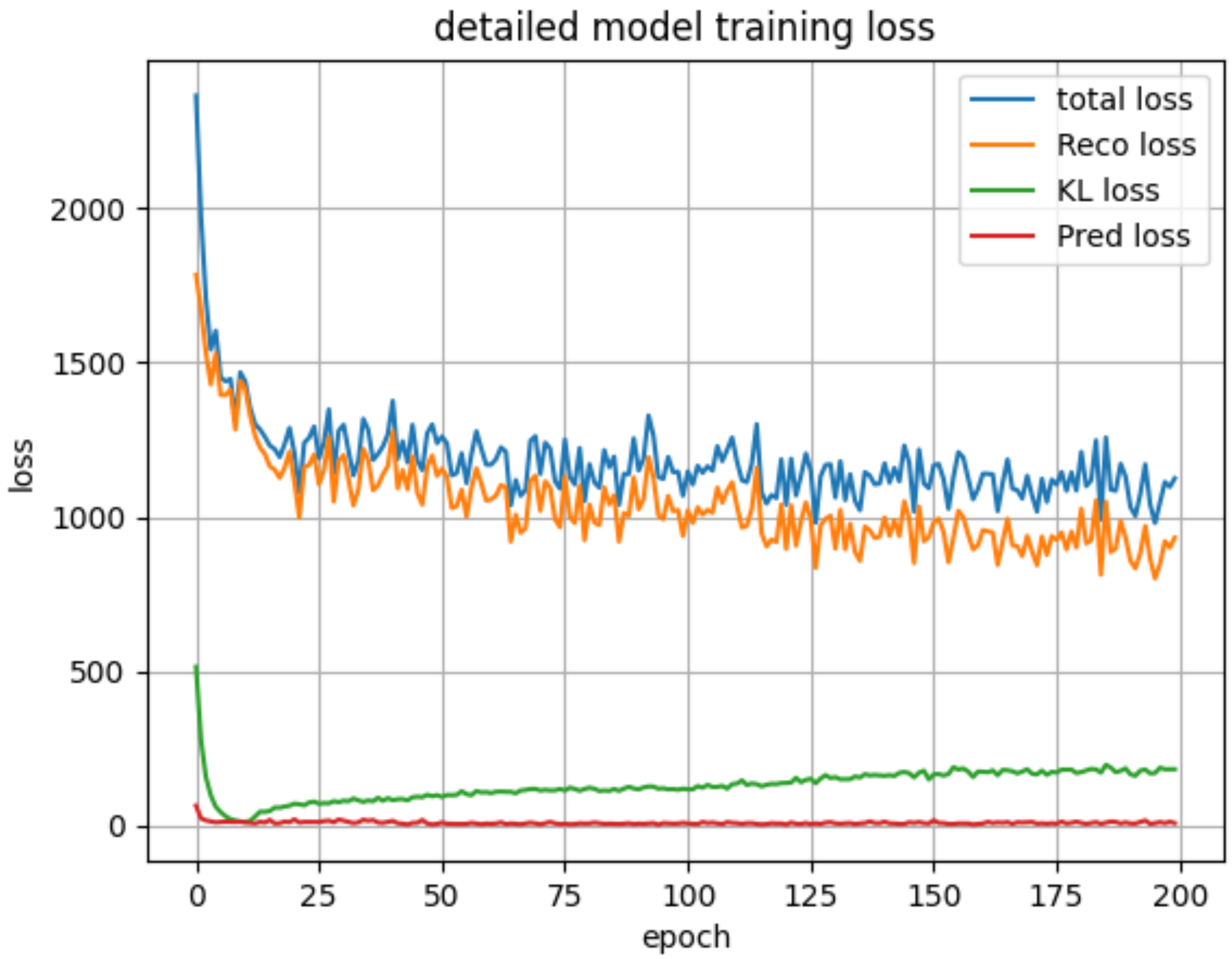
The final working model

- Input tensors: shape (32, 32, 32, 3), each labelled with its impact parameter (we are working with a downsized dataset because the training is easier and faster);
- 3D Convolutional encoder;
- 2D latent space;
- Predictor (regression task, latent vector vs b) to force latent space disentangling;
- Asymmetric decoder.

Variational Autoencoder

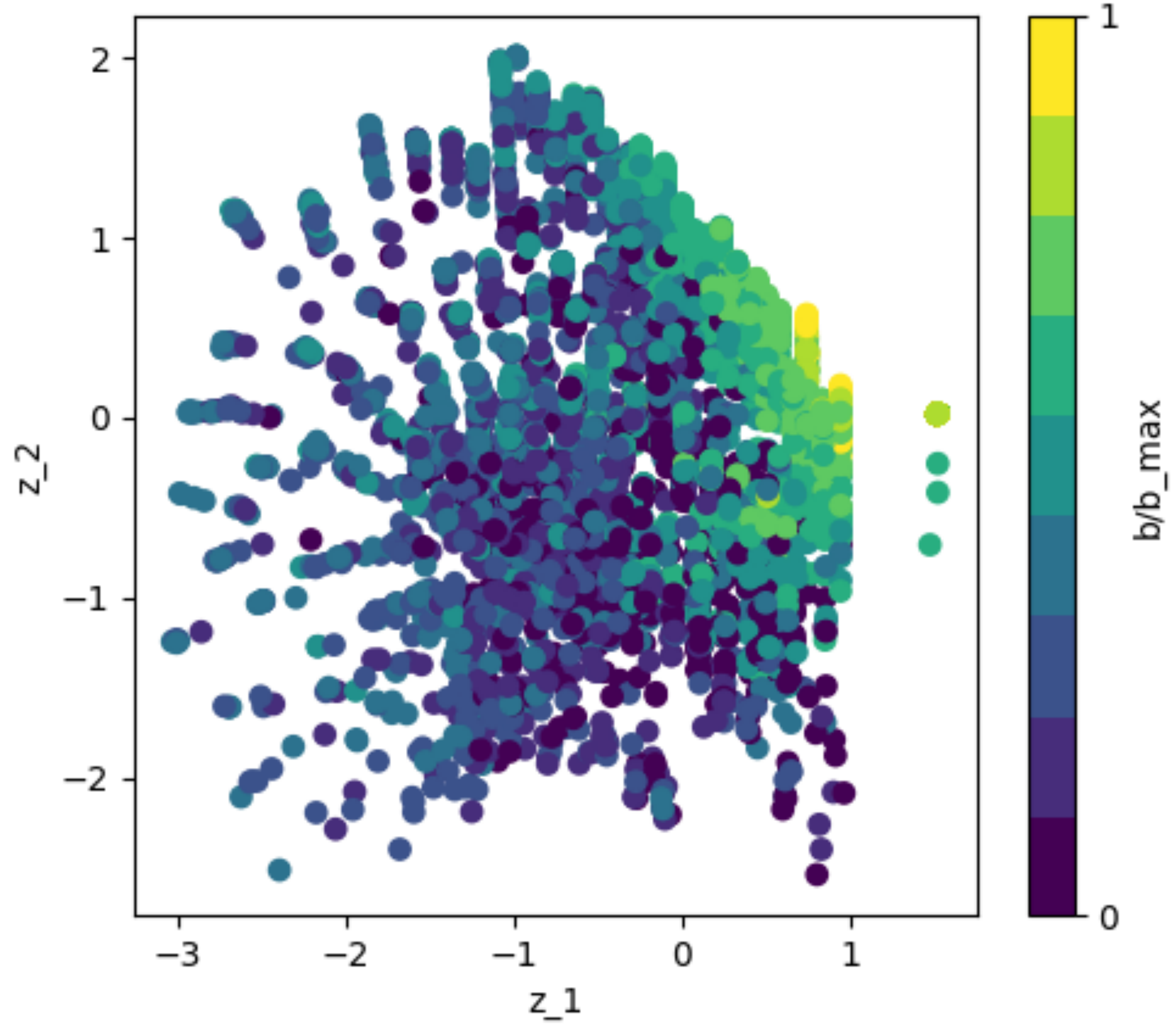
Our results: learning curves





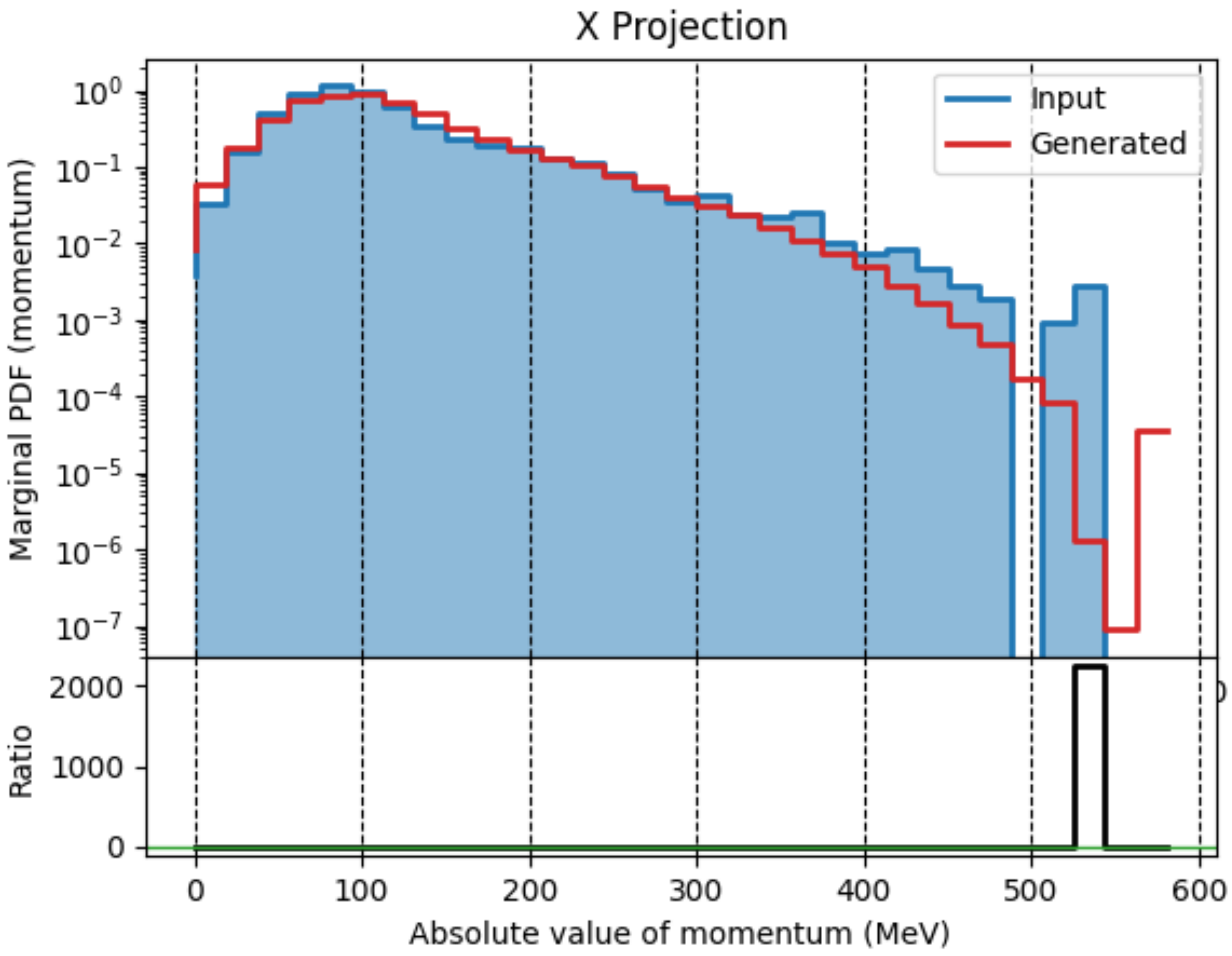
Variational Autoencoder

Our results: 2D latent space



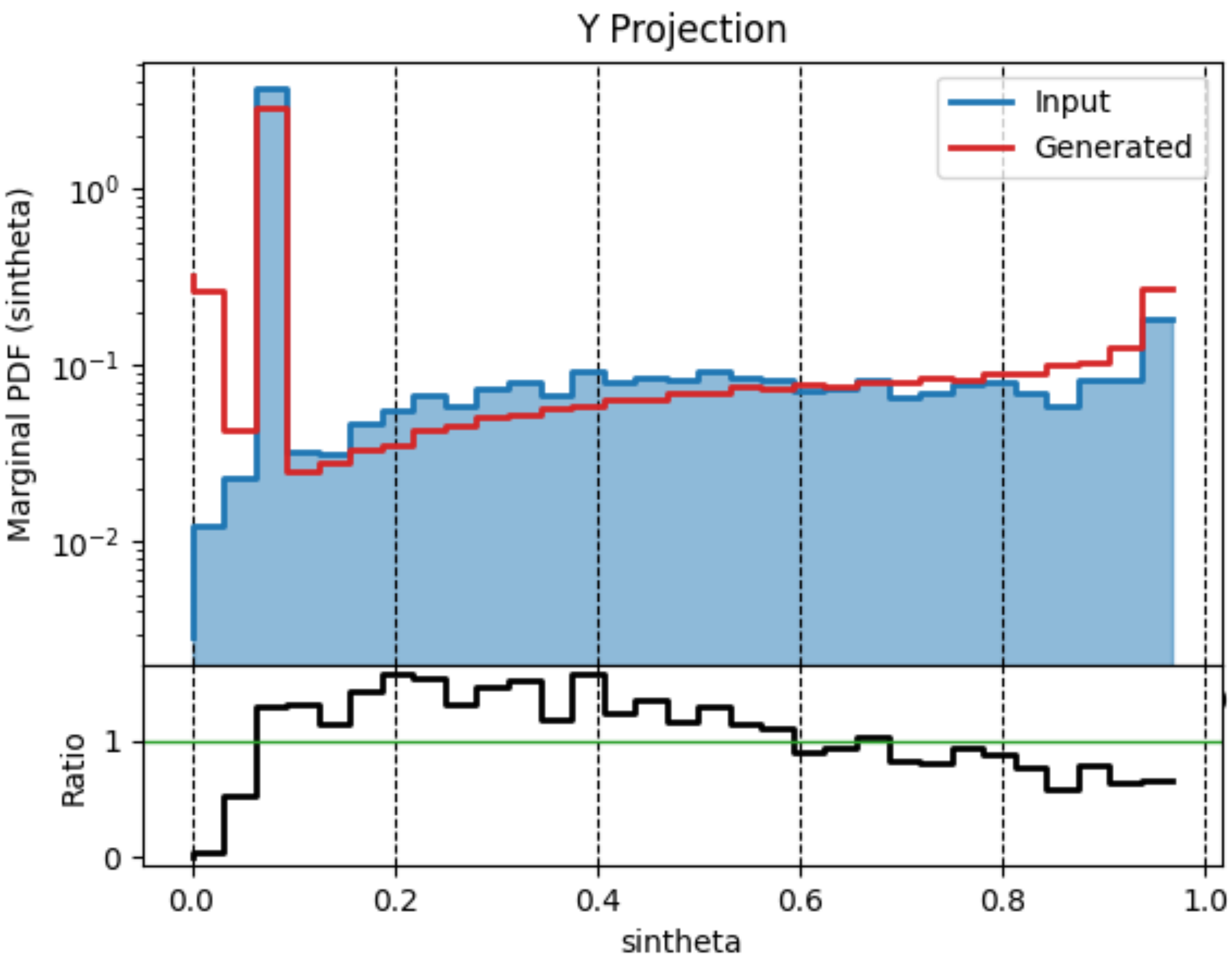
Variational Autoencoder

Our results: momentum modulus P



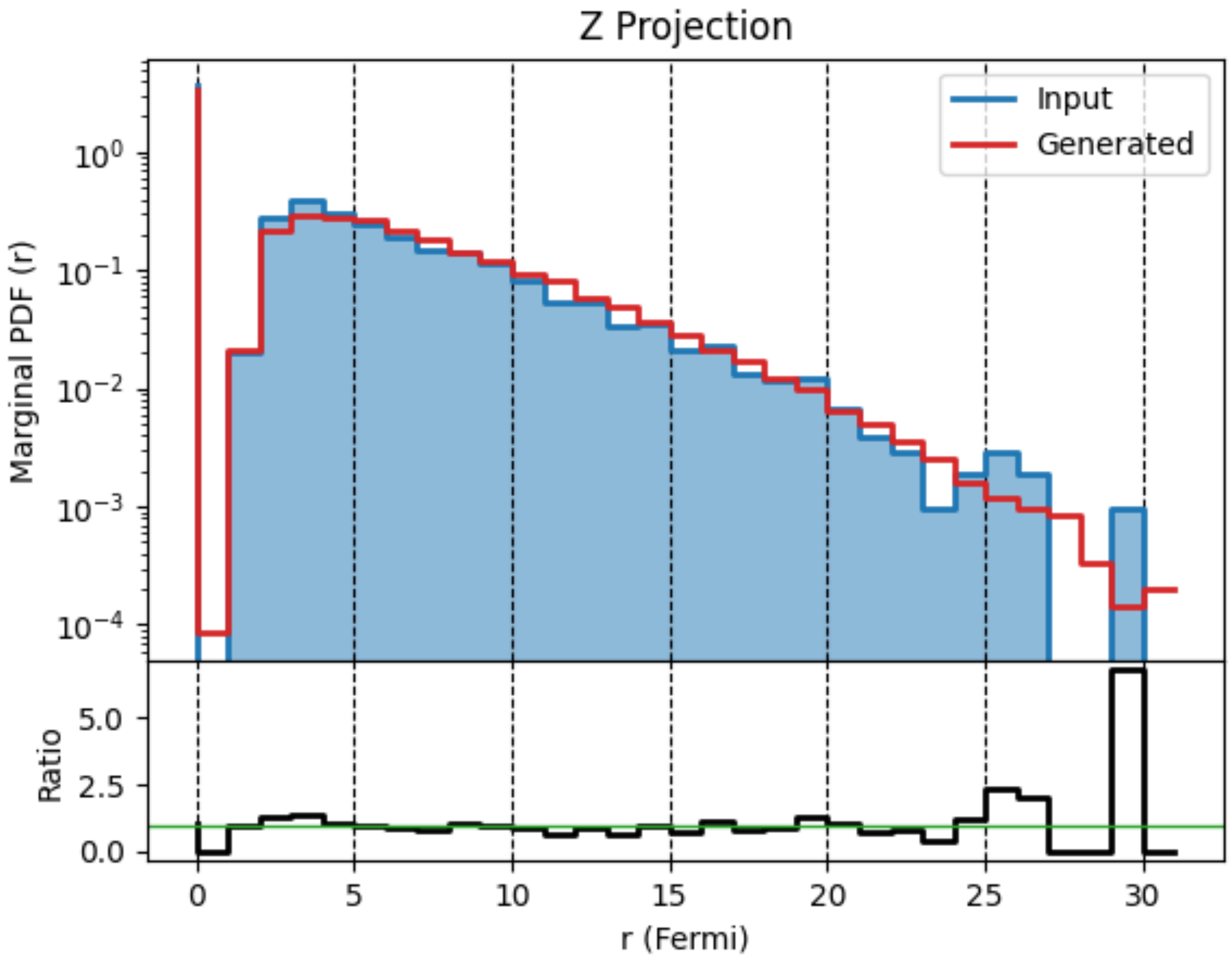
Variational Autoencoder

Our results: sin(q)



Variational Autoencoder

Our results: r



Perspectives

VAE, GAN and Graph Neural Networks

- Short-term goals:
  - Porting our model in C++ to interface it with Geant4;
  - Adding the interaction energy as an input for the VAE;

- Mid-term goals:
  - adding A and Z of the target as inputs for the VAE

- Long term goal:
  - Graph Neural Network (to simulate the whole nuclear reaction).

- + feasibility study: GAN (avoid the collapse of our network);

Summary

- **Final goal:** design a Deep Generative Model to emulate the results of BLOB in order to interface its trained decoder to Geant4;
- **1st attempt:** unsupervised learning with a “physical” interpretation of the learning process. Unsuccessful;
- **Subsequent approaches**: data-driven, “unphysical” optimization of the VAE + semisupervised learning;
- Satisfactory reconstruction results, but still too little control over the generative phase to finalize the model.

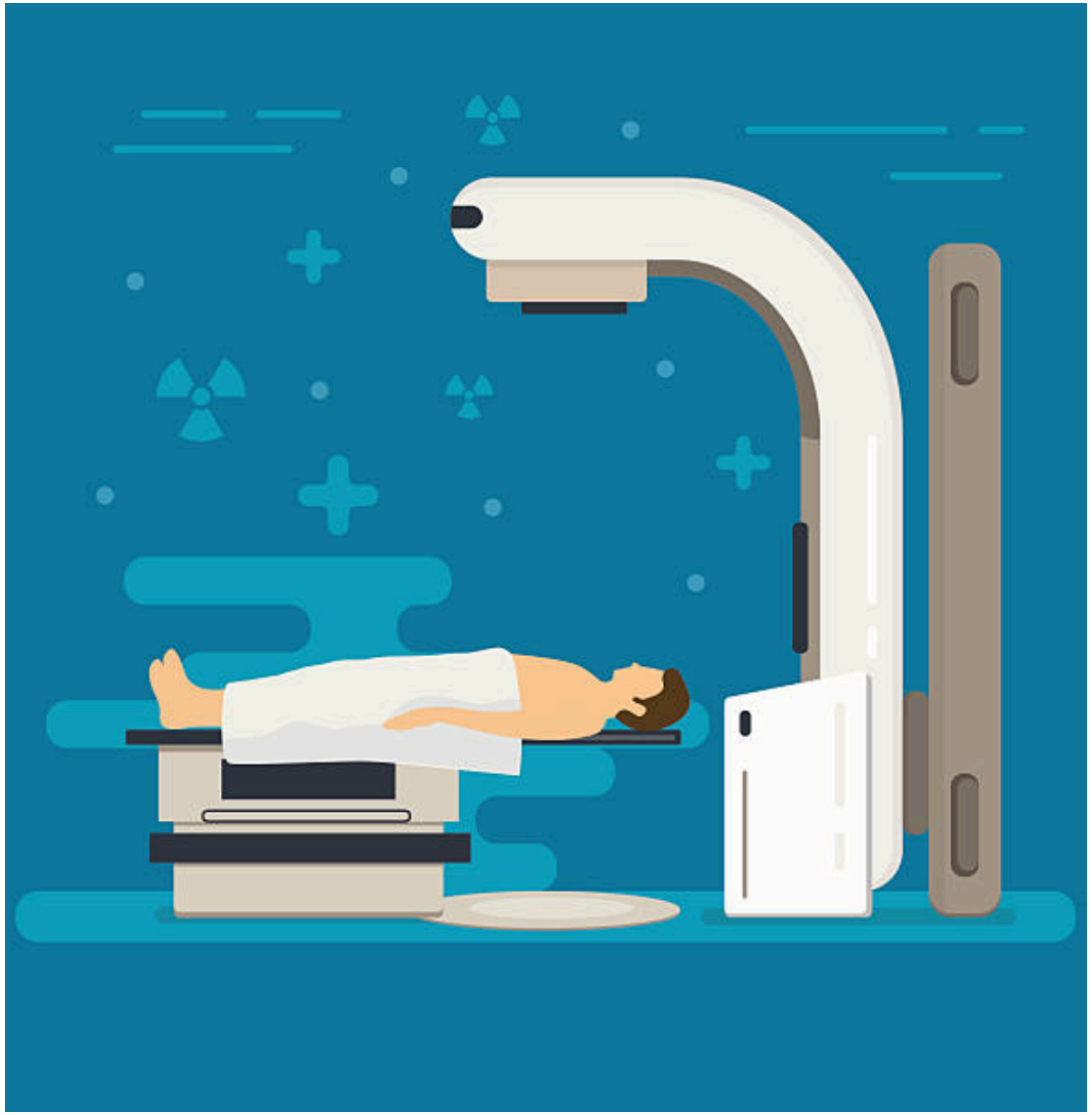
Thank you for your attention!

Backup

Hadrontherapy

and Monte Carlo (MC) simulations

- *Hadrontherapy*: a form of radiation therapy that involves the use of proton and carbon ions ("hadrons");
- Hadrons are heavier and have more energy than electrons. Consequently, they are more effective in destroying cancer cells;
- *MC codes* are used to initialize and validate treatment planning algorithms (*dosimetric calculations*).



Geant4 for dosimetric calculations

Limitations at low energies

- Geant4 is a Monte Carlo toolkit;
- Geant4 can simulate the body of a patient by importing his Computed Tomography scan in DICOM format;
- Several models for electromagnetic interactions are implemented in Geant4 but there is no dedicated model to describe inelastic nuclear reactions below 100 MeV/u;
- *Solution*: interface Geant4 with BLOB (Boltzmann Langevin One Body), a numerical model developed to simulate heavy ions collisions.

Using Deep Learning

To work around BLOB limitations

- Problem: BLOB computation time is too large for any practical application;

- Idea:
  - Bin the PDF outputs of BLOB to form a dataset of 3D “images”;
  - Feed this dataset to some Deep Generative Neural Network;
  - Use the Trained NN to generate BLOB-like outputs.