# Towards the emulation of BLOB, a nuclear interaction model, with Deep Learning

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Mon Oct 24, 2022
IV Geant4 International User Conference
at the physics-medicine-biology frontier
Naples, Italy

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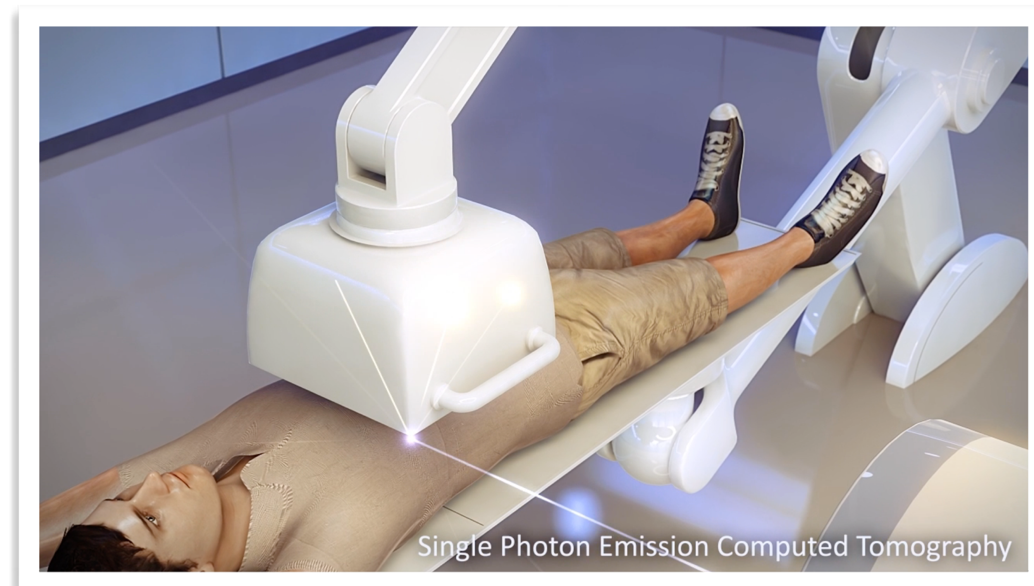
# Hadrontherapy and Monte Carlo

- Hadrontherapy:
  - External radiation therapy using strongly interacting particles to treat mainly tumour
  - Mainly with p and C ions




- MC codes are used to:
  - Generate input parameters of the treatment planning algorithms
  - Validate the dose calculation of such algorithms
  - Estimate the production of **b** emitters, such as $^{11}$C and $^{15}$O
  - Link the production of prompt **g** with the dose distribution

# Problems in Geant4 below 100 MeV/u

- Despite the numerous and relevant application would use it, there is no dedicated model to nuclear interaction below 100 MeV/u in Geant4

- Many papers showed the difficulties of Geant4 in this energy domain:

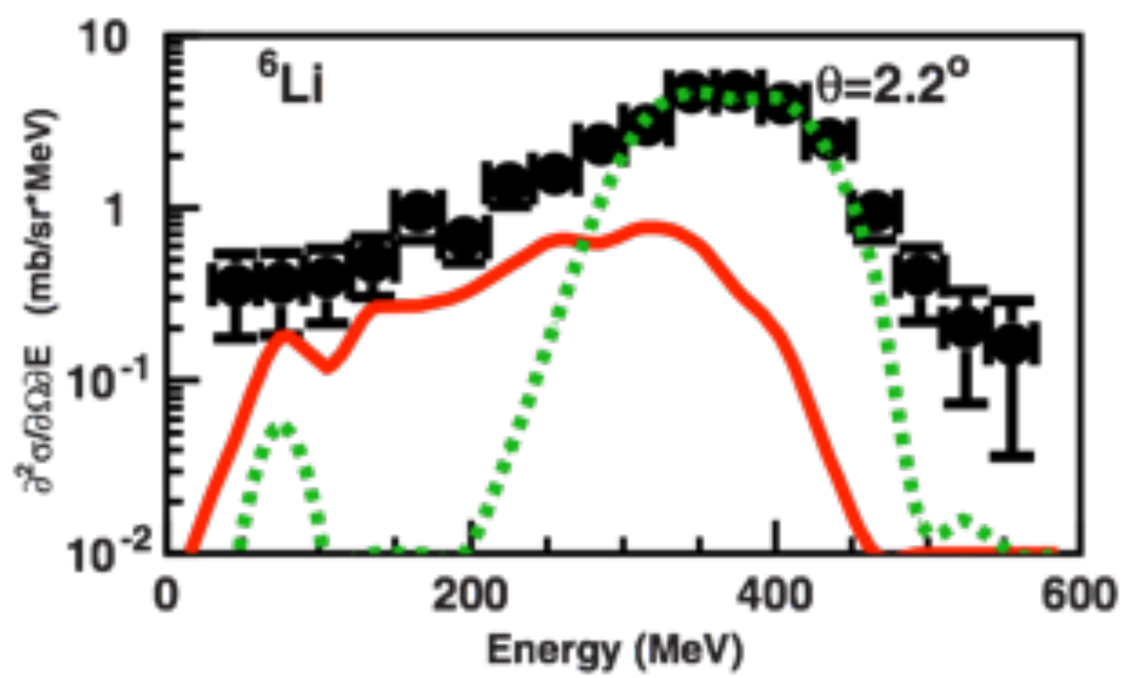
    - Braunn et al. have shown discrepancies up to one order of magnitude in $^{12}C$ fragmentation at 95 MeV/u on thick PMMA target

    - De Napoli et al. showed discrepancy specially on angular distribution of the secondaries emitted in the interaction of 62 MeV/u $^{12}C$ on thin carbon target

    - Dudouet et al. found similar results with a 95 MeV/u $^{12}C$ beam on H, C, O, Al and Ti targets

- **Exp. data**
- **G4-BIC**
- **G4-QMD**

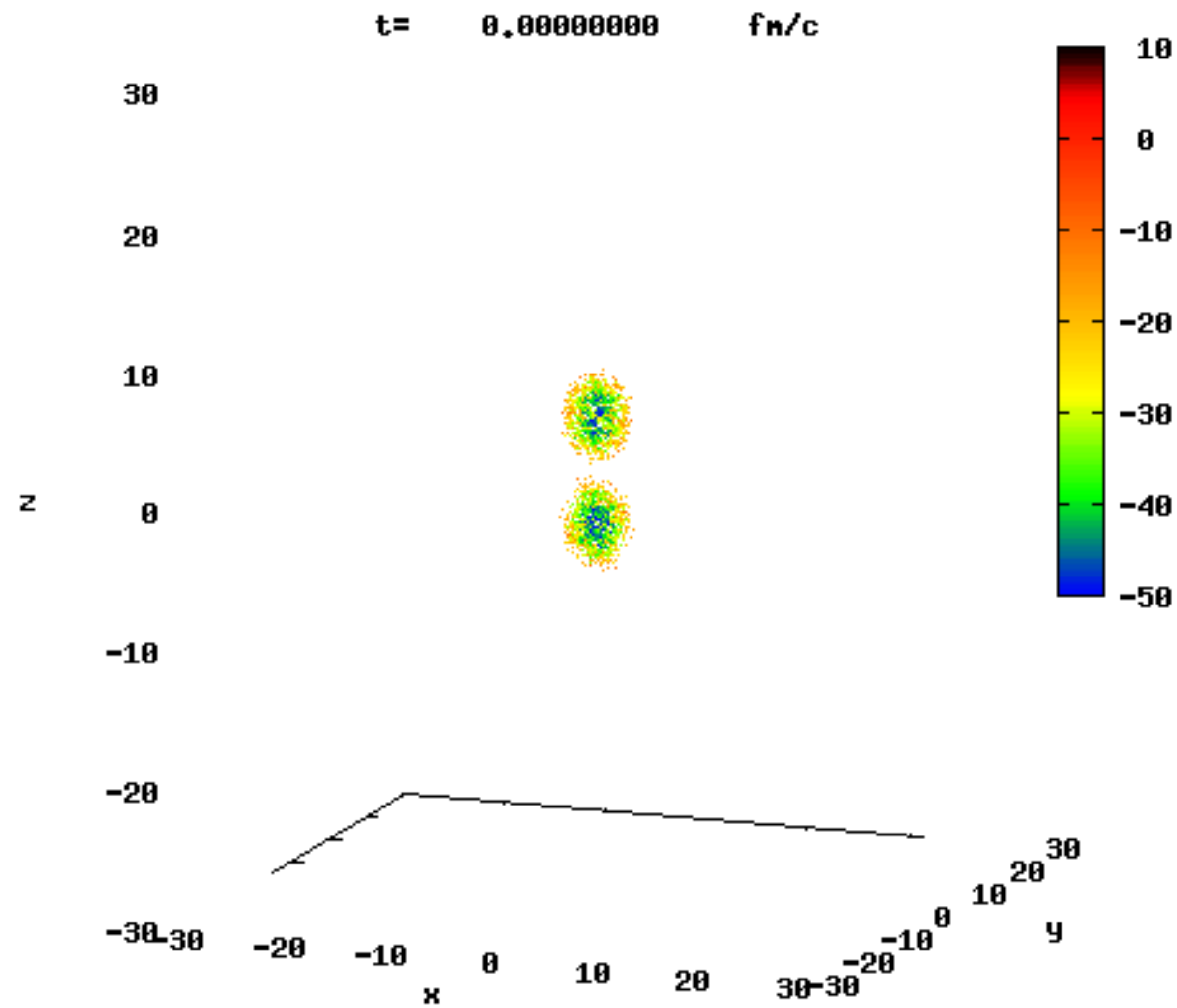
[Plot from De Napoli et al. Phys. Med. Biol., vol. 57, no. 22, pp. 7651–7671, Nov. 2012]




Cross section of the $^6$Li production at 2.2 degree in a $^{12}C$ on $^{nat}C$ reaction at 62 MeV/u.

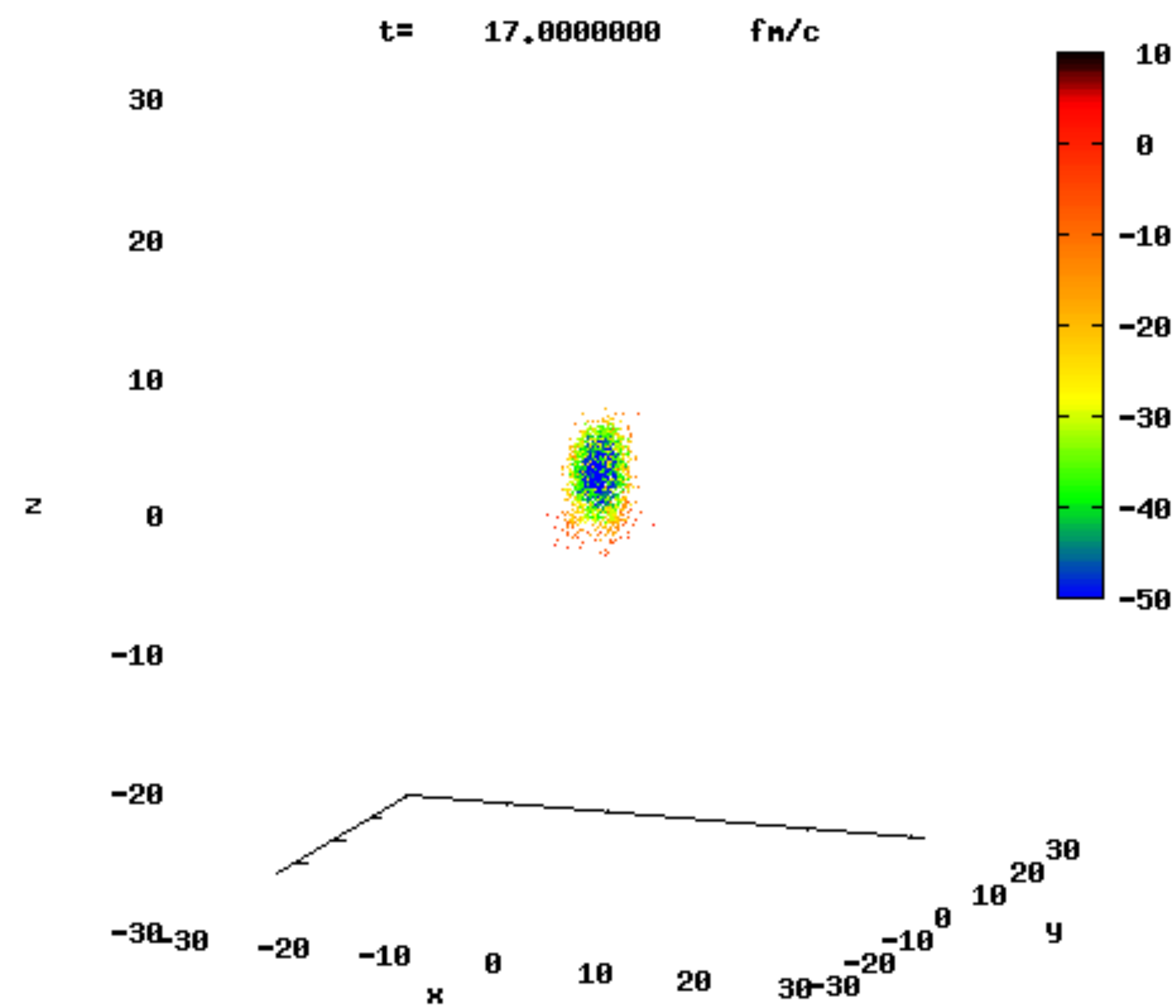
# BLOB (Boltzmann-Lagevein One Body)

- describes the time evolution of the density distribution
- it uses the test particles approach
- 500 test particles per nucleon in this simulation



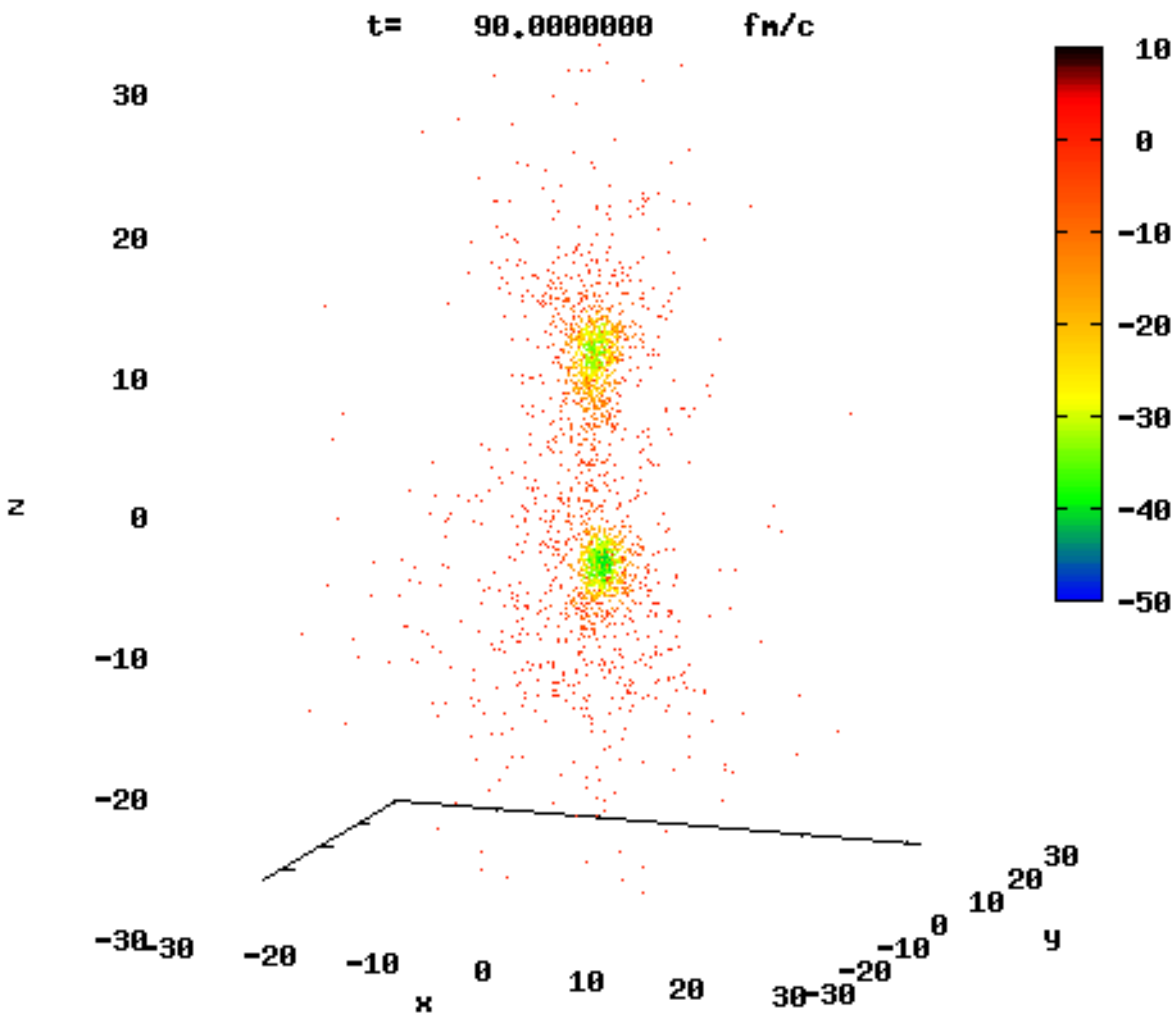
# BLOB (Boltzmann-Lagevein One Body)

- involves the implementation of an effective attractive mean-field nuclear interaction
- mean-field is self-consistent, depends on the density
- two body interactions are explicitly treated as test particles collisions



# BLOB (Boltzmann-Lagevein One Body)

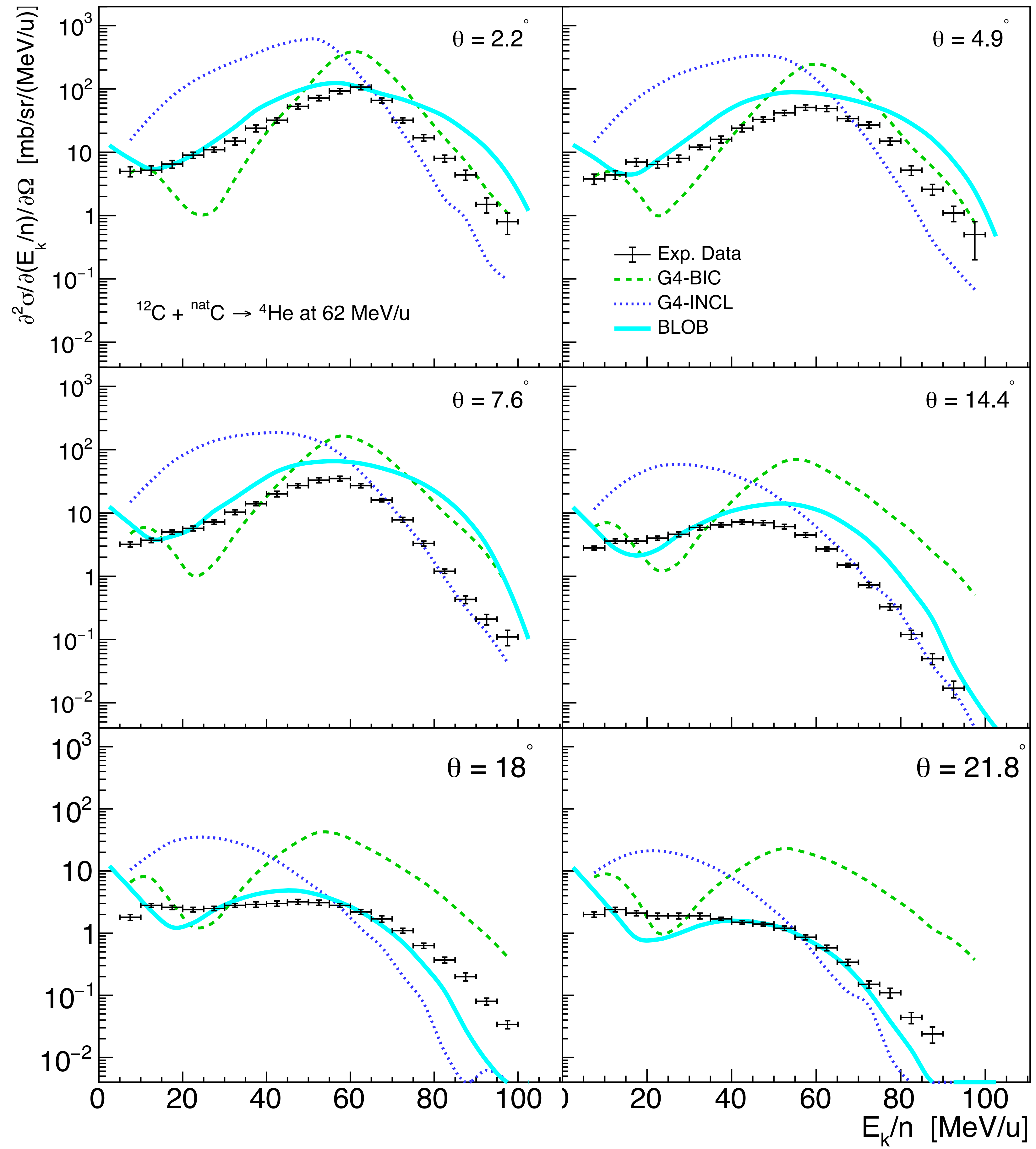
- the final state is a distribution probability of finding a nucleon in a position of the phase space
- from which the physical state has to be sampled



# BLOB and Geant4

- We interfaced BLOB with Geant4 and its de-excitation model

- obtaining promising results




Is everything fine?

# Emulating BLOB with Deep Learning

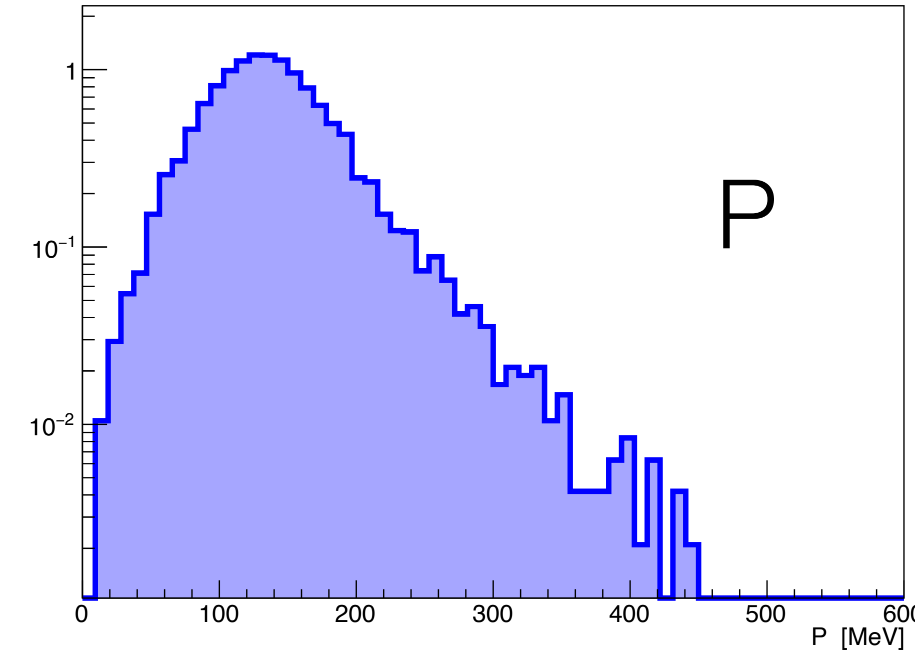
- BLOB running time is too large for practical applications

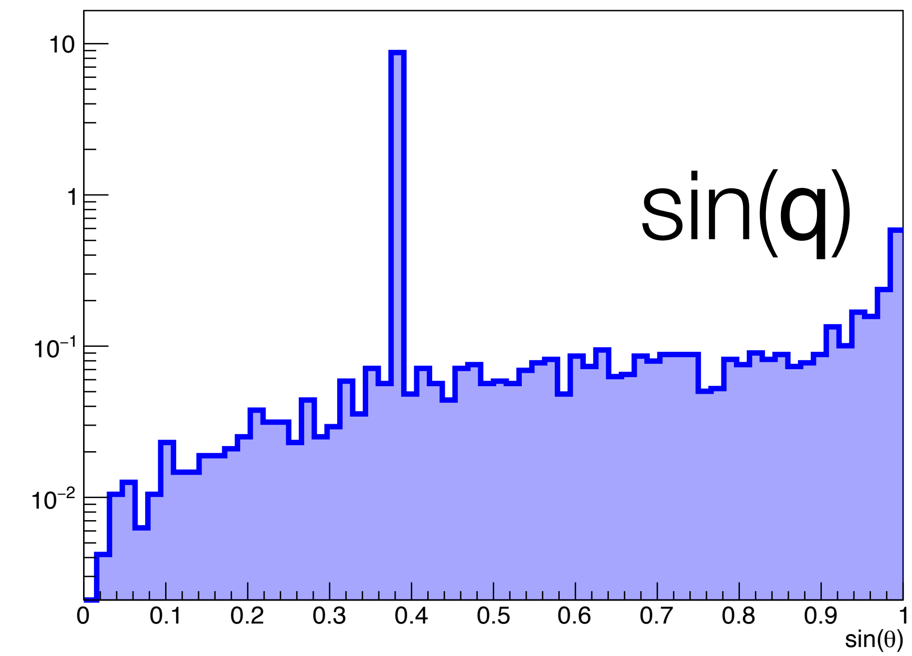
**Up to 10 min per interaction!**

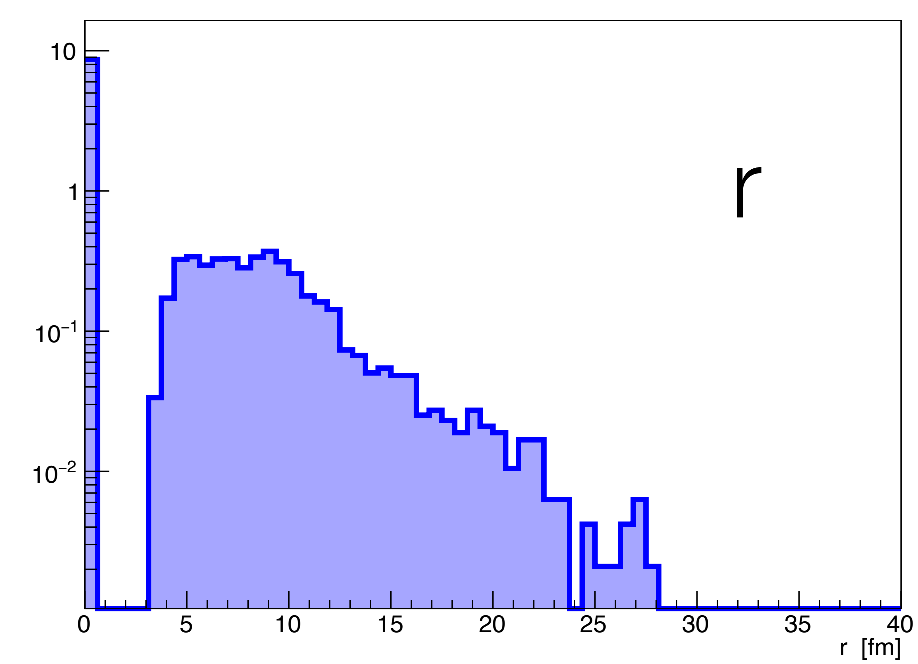
- The idea:
  - Bin the PDF output of BLOB
  - Creating a 3D “image” to use existing Keras library
  - Train a Variational Auto Encoder (VAE)
    to reproduce such “images”
  - Condition the VAE to the impact parameter

# Reducing dimensionality

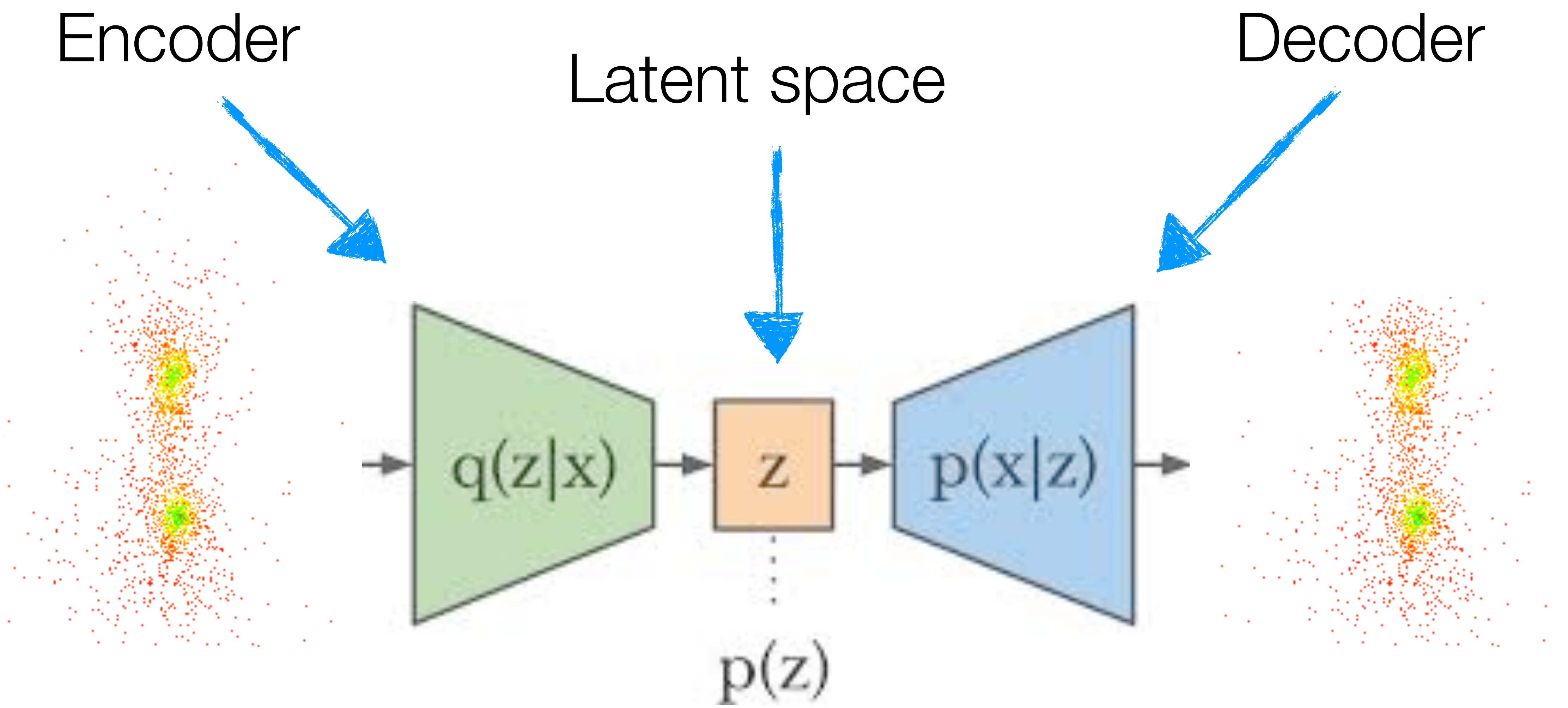
- To reduce the dimensionality and use the Keras 3D kernels
- We consider only:
  - The modulus of the momentum
  - its angle with the collision axis
  - The distance of each test particle with the fragment center
- We divided the test particles in three samples (one for each possible large fragment):
  - To use the color channels



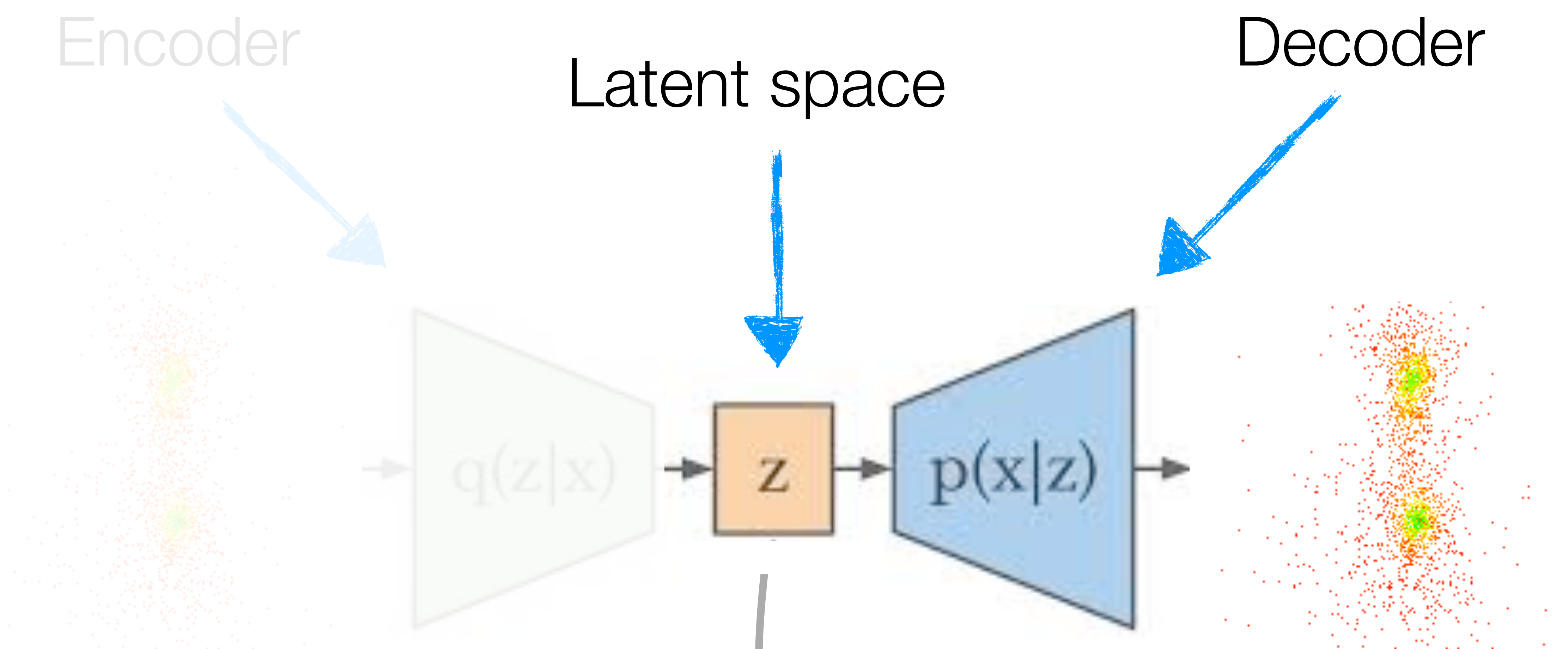



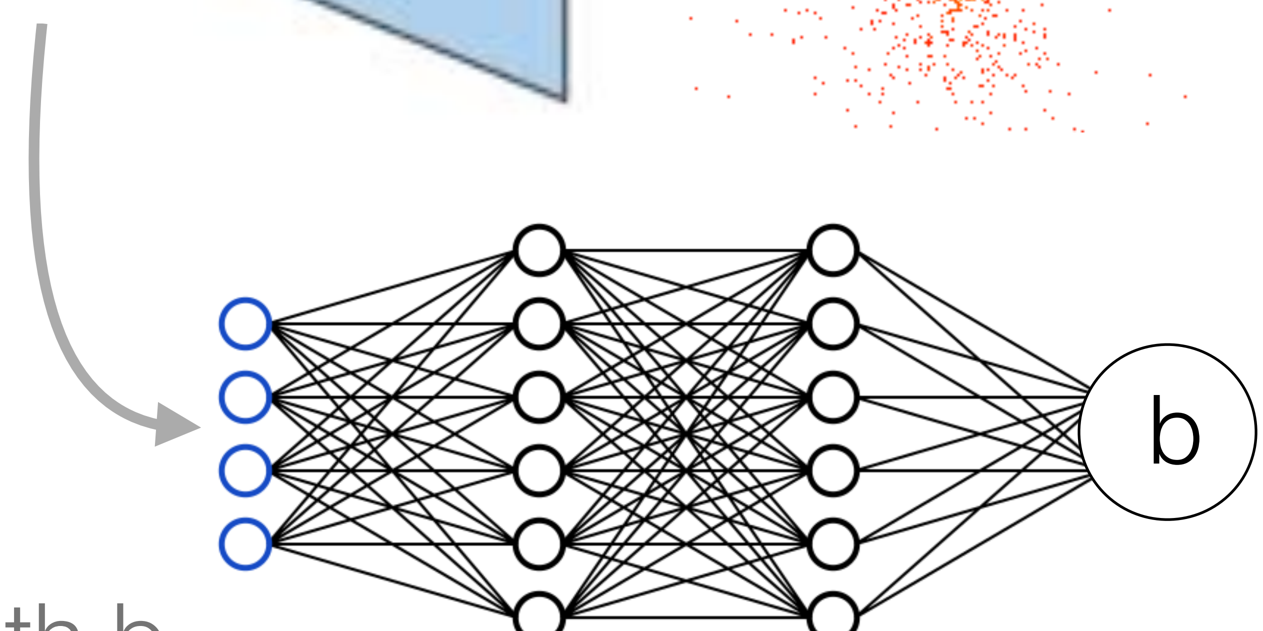
# Variational Auto Encoder for BLOB



# Variational Auto Encoder for BLOB




Train a predictor from latent space to impact parameter b

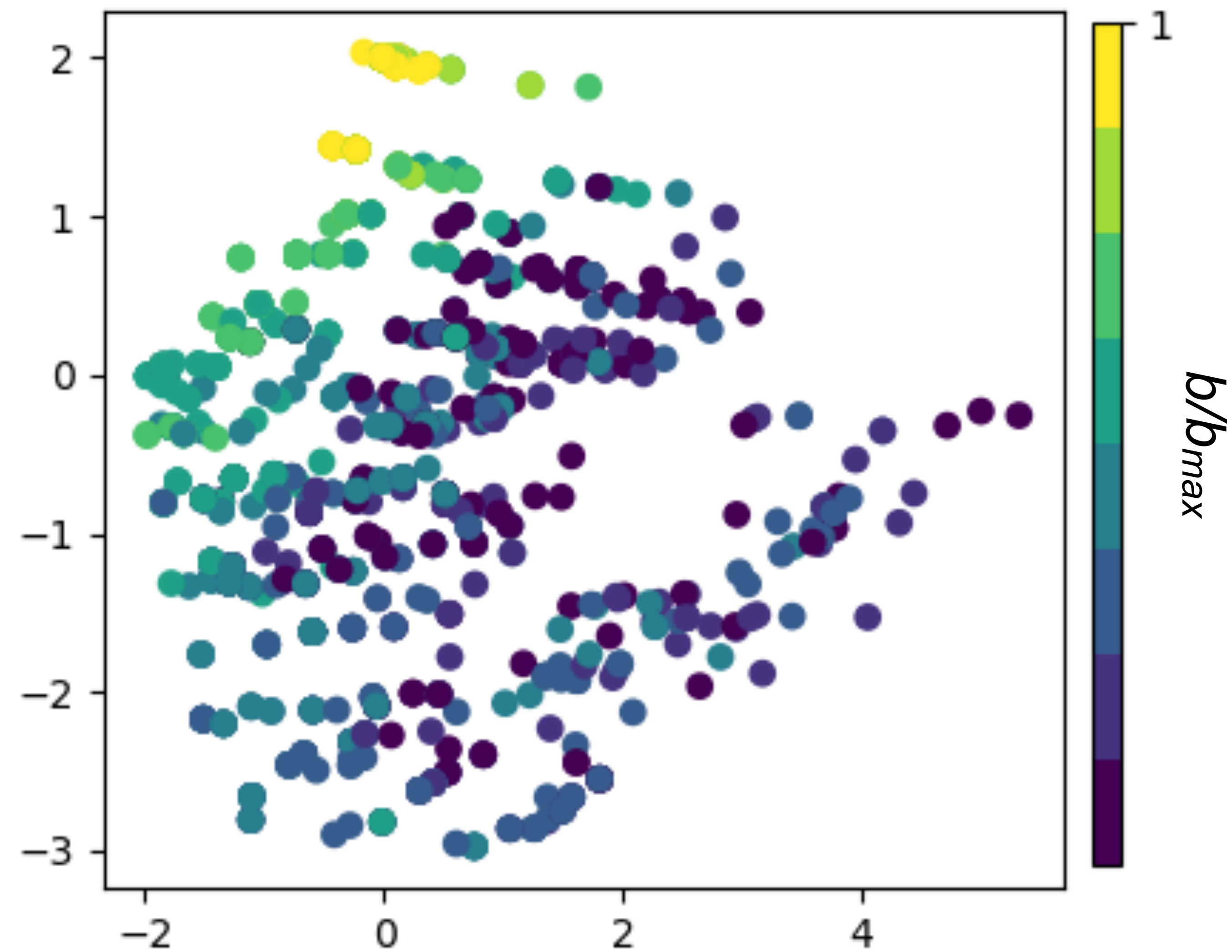



Gómez-Bombarelli at al. arXiv:1610.02415]

Z will be correlated with b

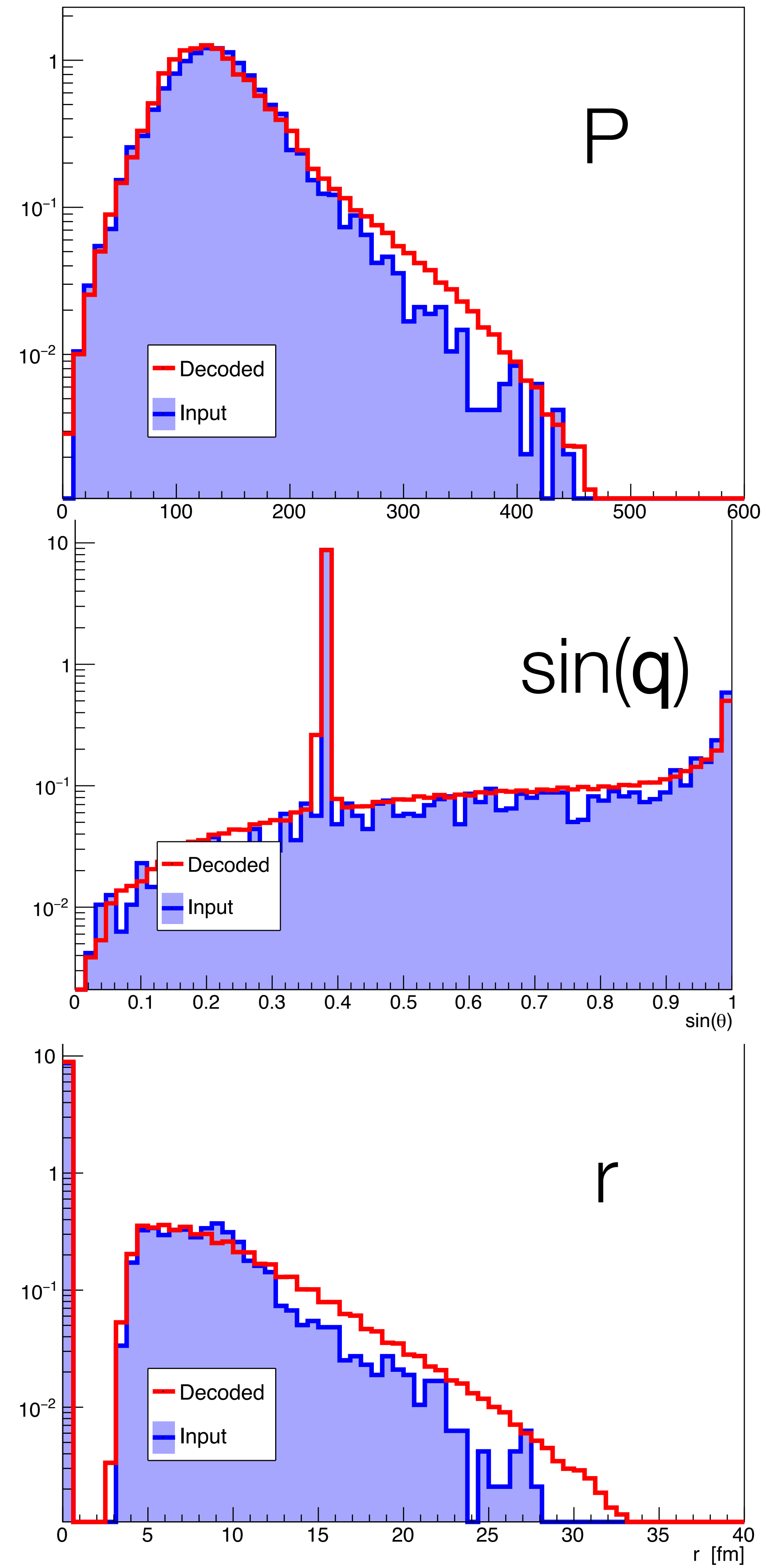
# Latent space

- 600 epochs of training
- Events with similar impact parameters are close in latent space
- Especially the events with very large impact parameters



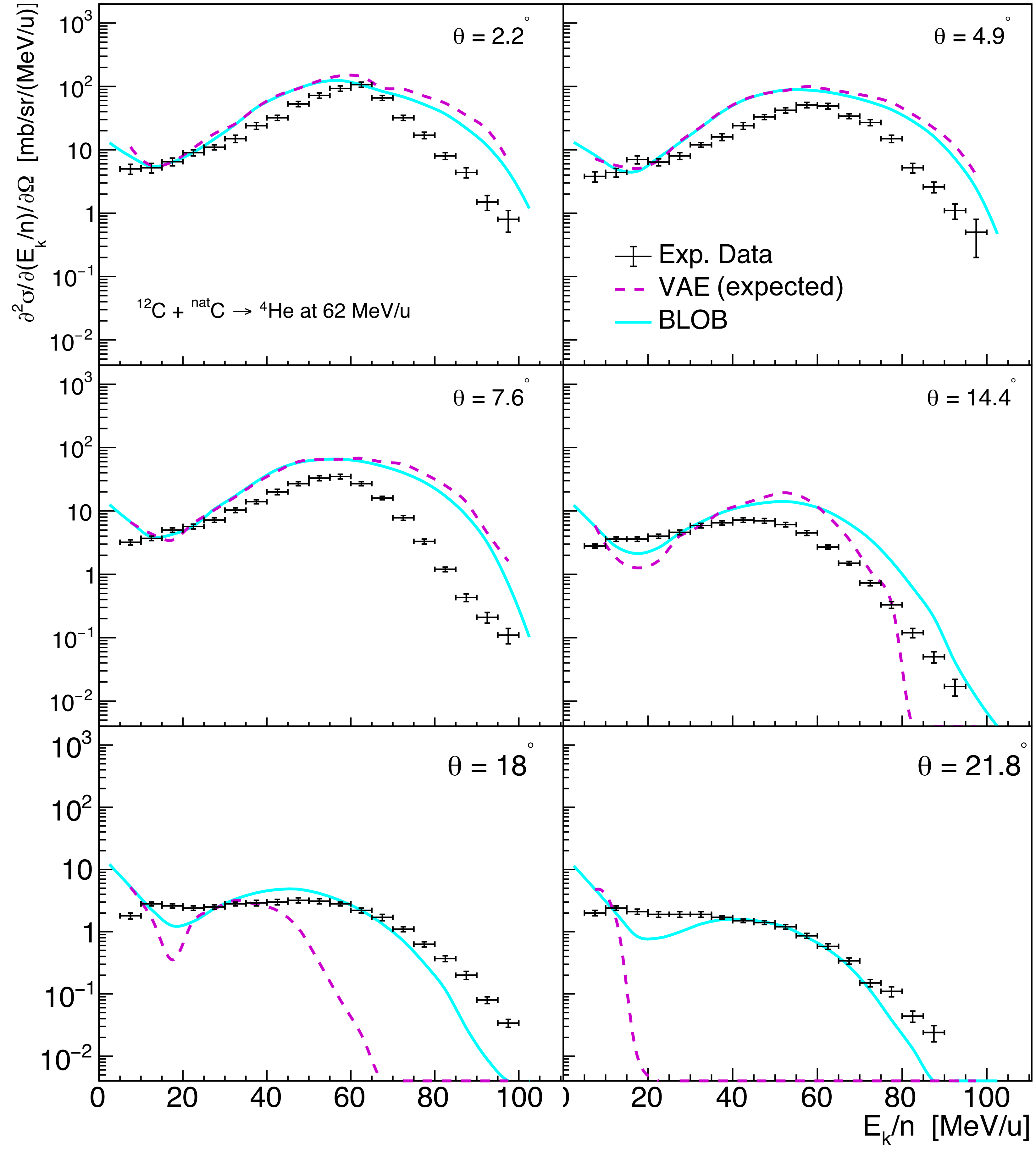
# Output distributions

- The generated distributions (red) looks similar to the input  (blue)
- The generated event has been generated from the same position in latent space of the input
- Input from training dataset



# Testing reconstruction

- Model written in pytorch
- Exported in ONNX
- VAE directly interfaced with Geant4 and its de-exitation model



## Final remarks

- Proof-of-concept work
- Errors can mainly come from compression from 6D to 3D

## Future plans

- Build 6D Convolutional Neural Networks
- Try Graph Neural Networks

# Summary

- An interface between BLOB and Geant4 has been developed
- The agreement with experimental data is good
  but the running time is too large
- We are exploring the possibility of using a cVAE
  to emulate the model
- Preliminary results are encouraging

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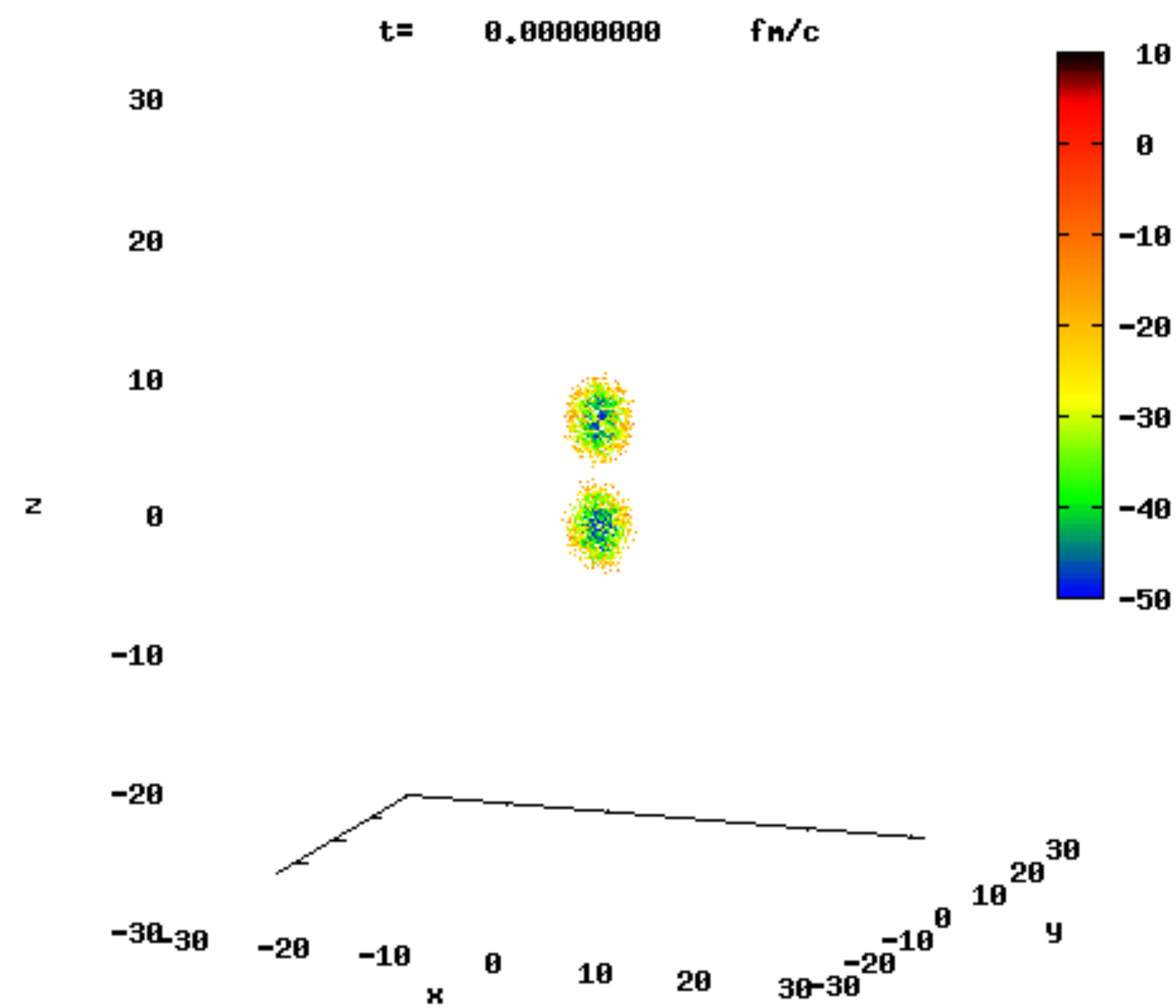
# BLOB - Details of numerical implementation

- Test particle method: each nucleon is represented by a collection of test particles Total number of test particles: $N_{tot} = N_{test} * A$

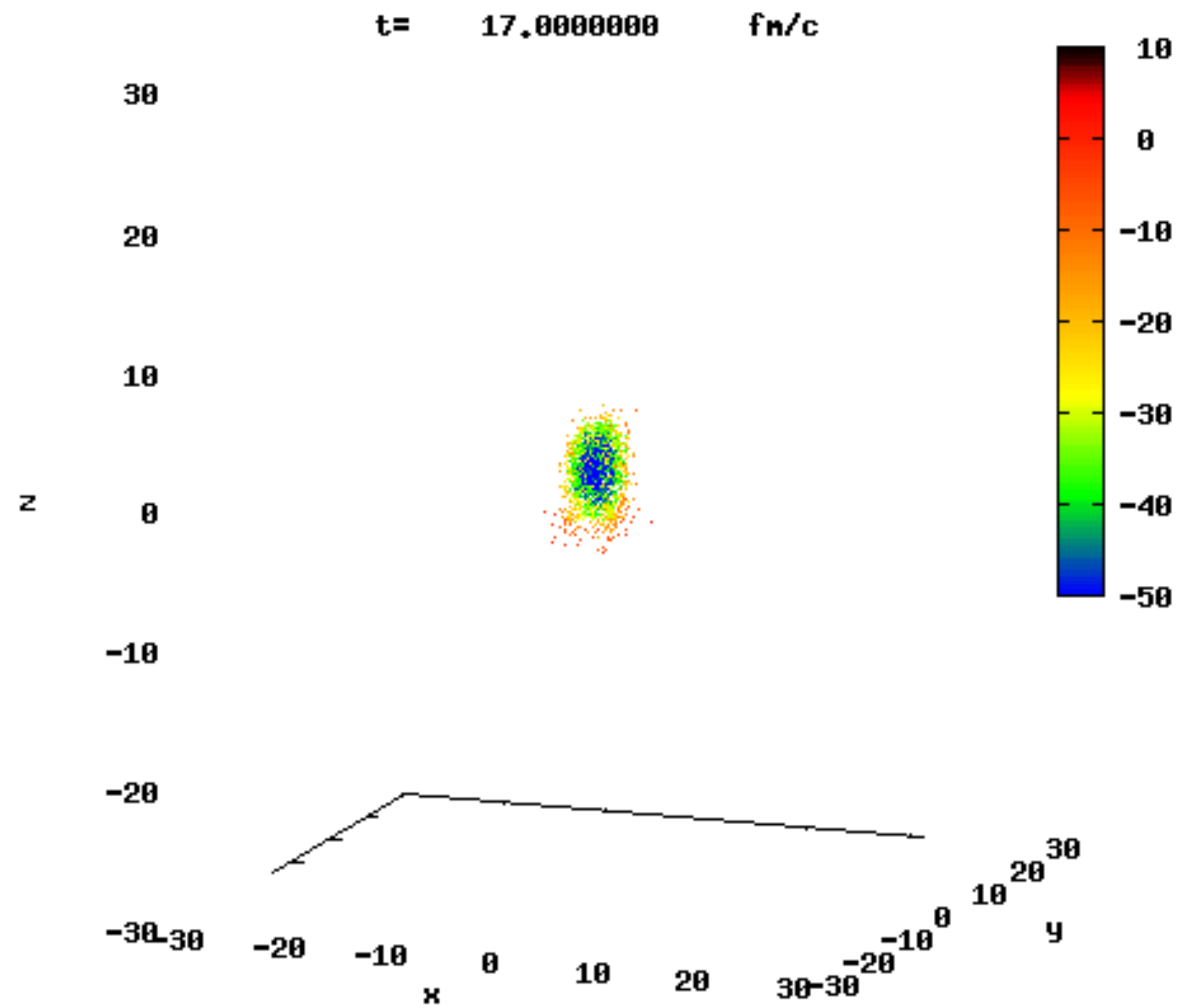
- Vlasov dynamics: Test particle positions and momenta
are propagated according to the Hamilton equations (non relativistic)

- Monte Carlo method to solve the collision integral, with
free n-p and p-p cross sections,
with a maximum cutoff of 50 mb



# BLOB - Fluctuations

- Implemented in full phase space
- Clouds of test particles (nucleons) are moved once a collision happens
- Shape modulation of the packet ensures Pauli blocking is respected



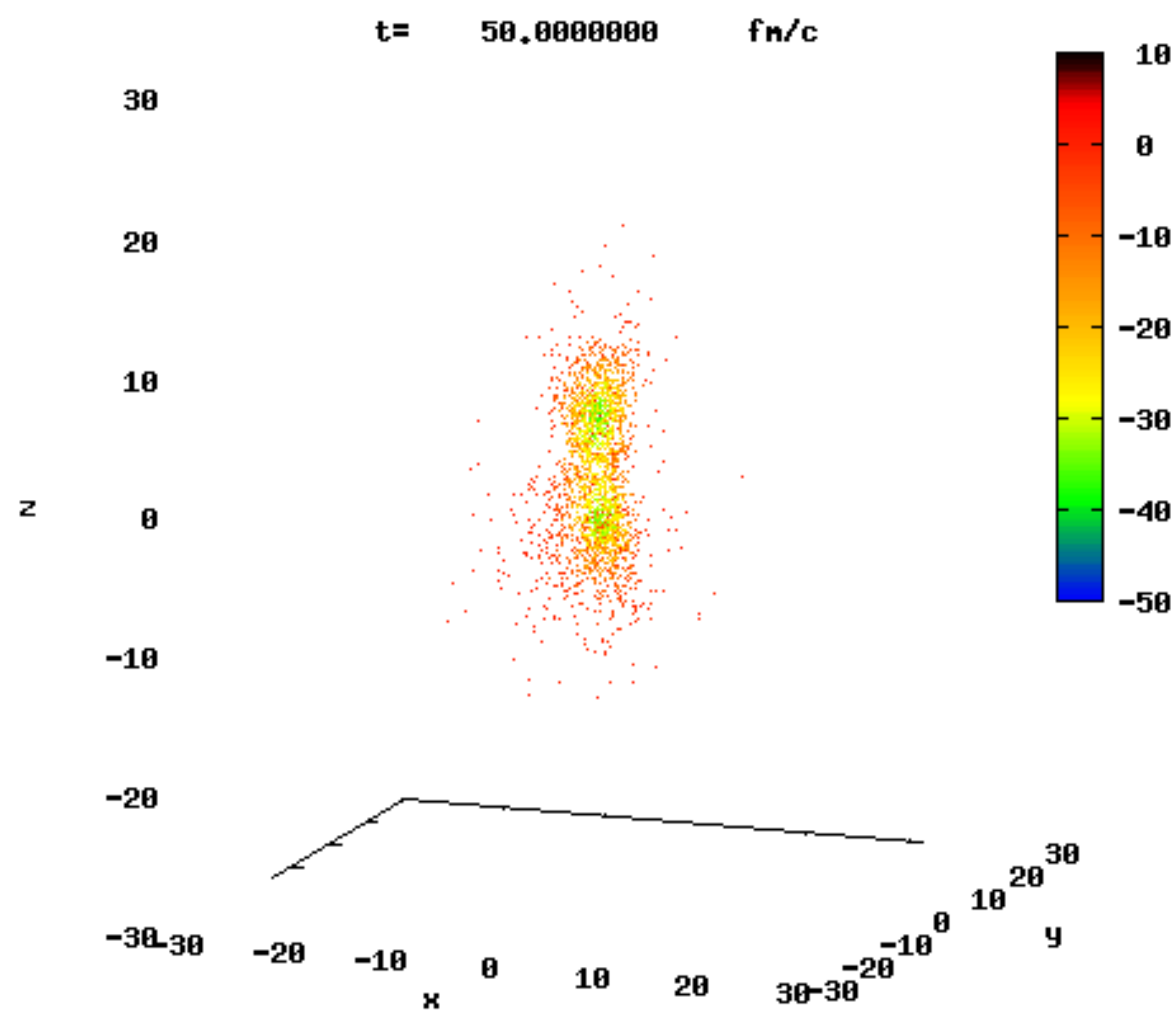

[Rizzo,Chomaz,Colonna, NPA 806,40(2008)]
[Napolitani and Colonna, PLB 726,382(2013)]

# BLOB - Final state

- Density threshold to isolate the “liquid” matter from the evaporated nucleons: $\rho > 0.03 \text{ fm}^{-3}$

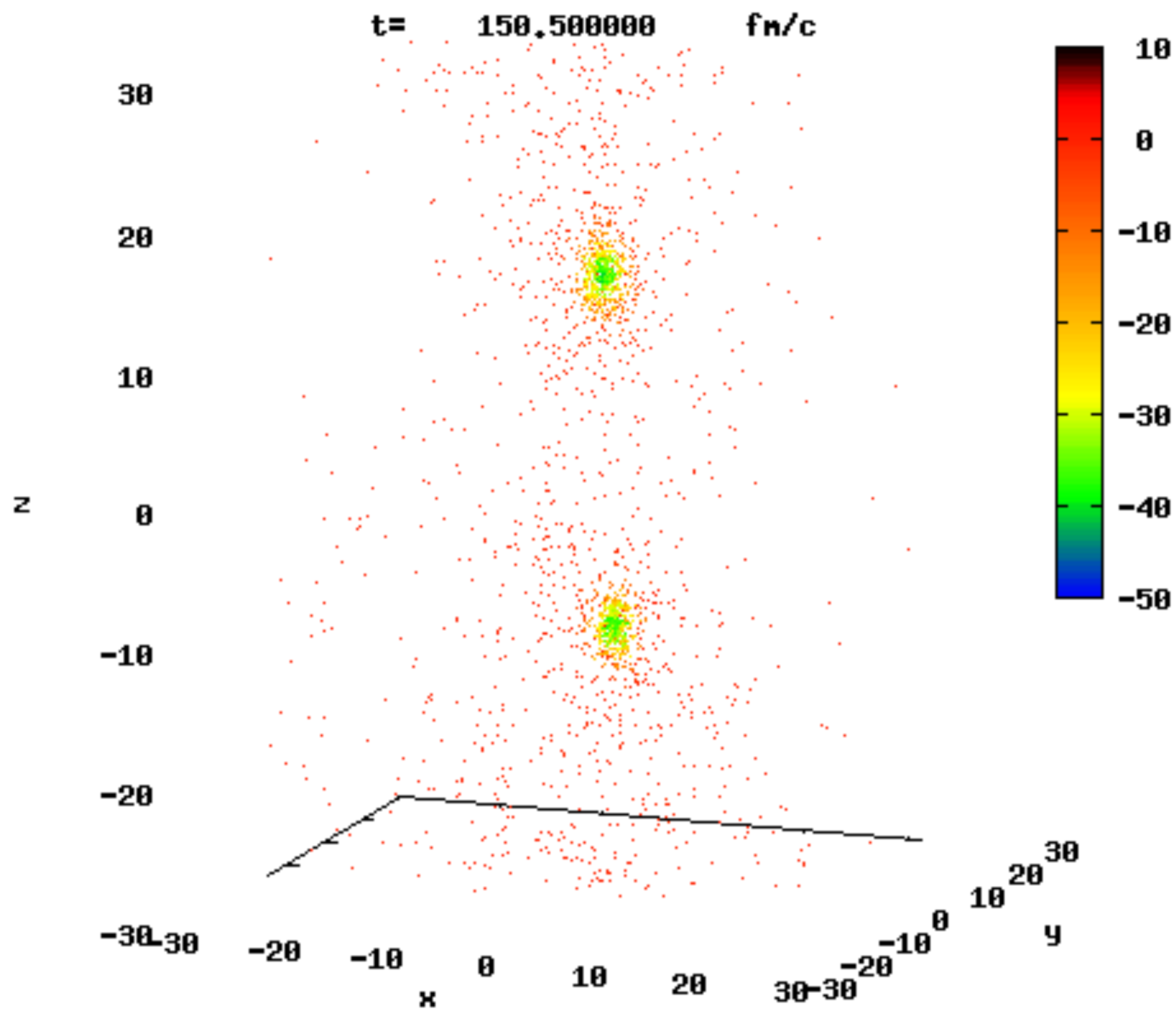
- Full information in coordinate and momentum space for all fragments

- Fragments are excited nuclear drops



# BLOB - Geant4 interface

- Developed as a G4-model
- Imports the BLOB output
- Samples the physical final state
    - Fragments mass and charge
    - Gas particles emitted
- Applies Geant4 de-excitation to excited fragments



# Conditioning to *b*

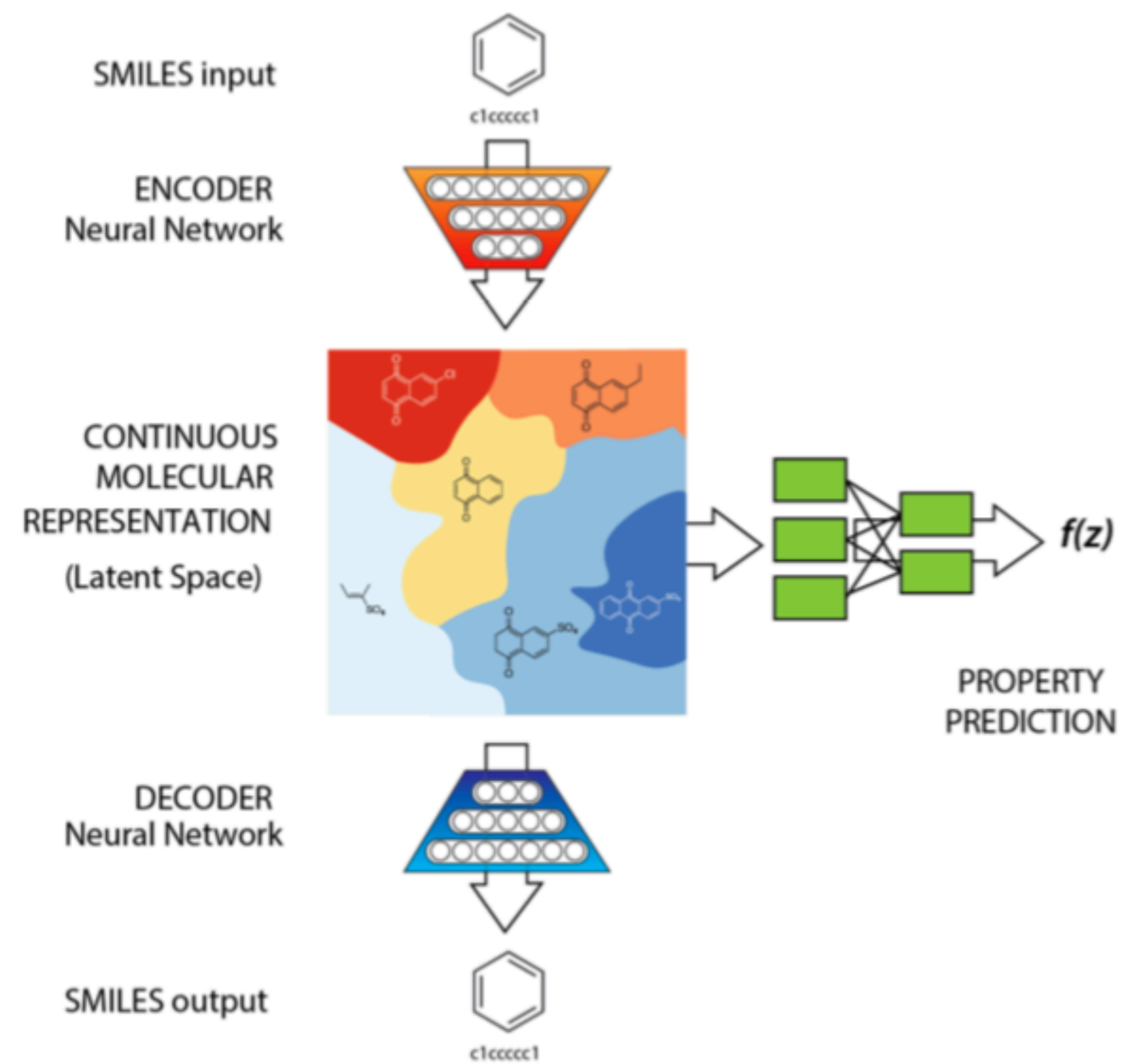
- Taking inspiration from:

[Automatic chemical design using a data-driven continuous representation of molecules, Gómez-Bombarelli at al. arXiv:1610.02415]

- VAE for generating new chemical compounds with properties that are of interest for drug discovery

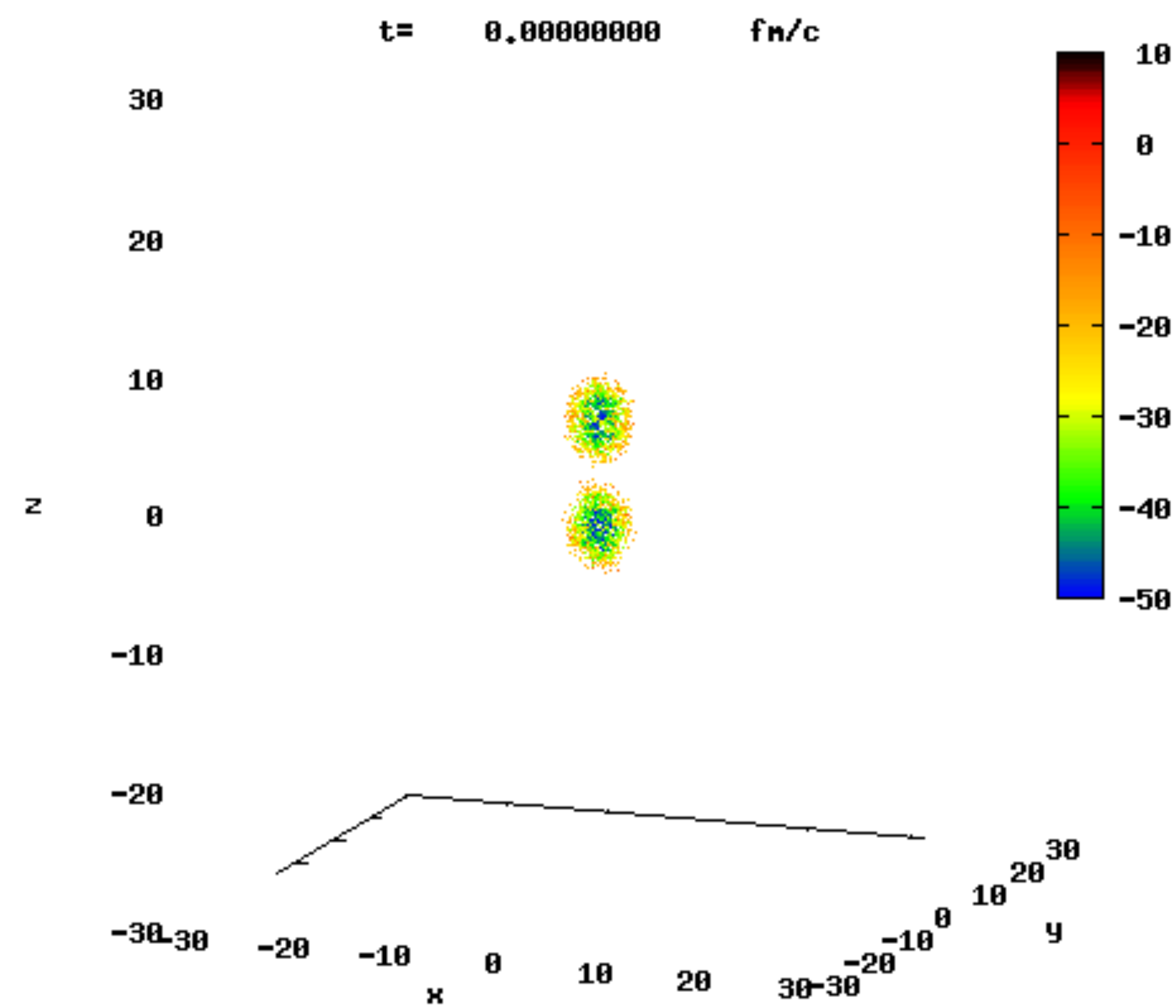
- To organise latent space w.r.t chemical properties they jointly trained the VAE with a predictor

- It predicts these properties from latent space representations



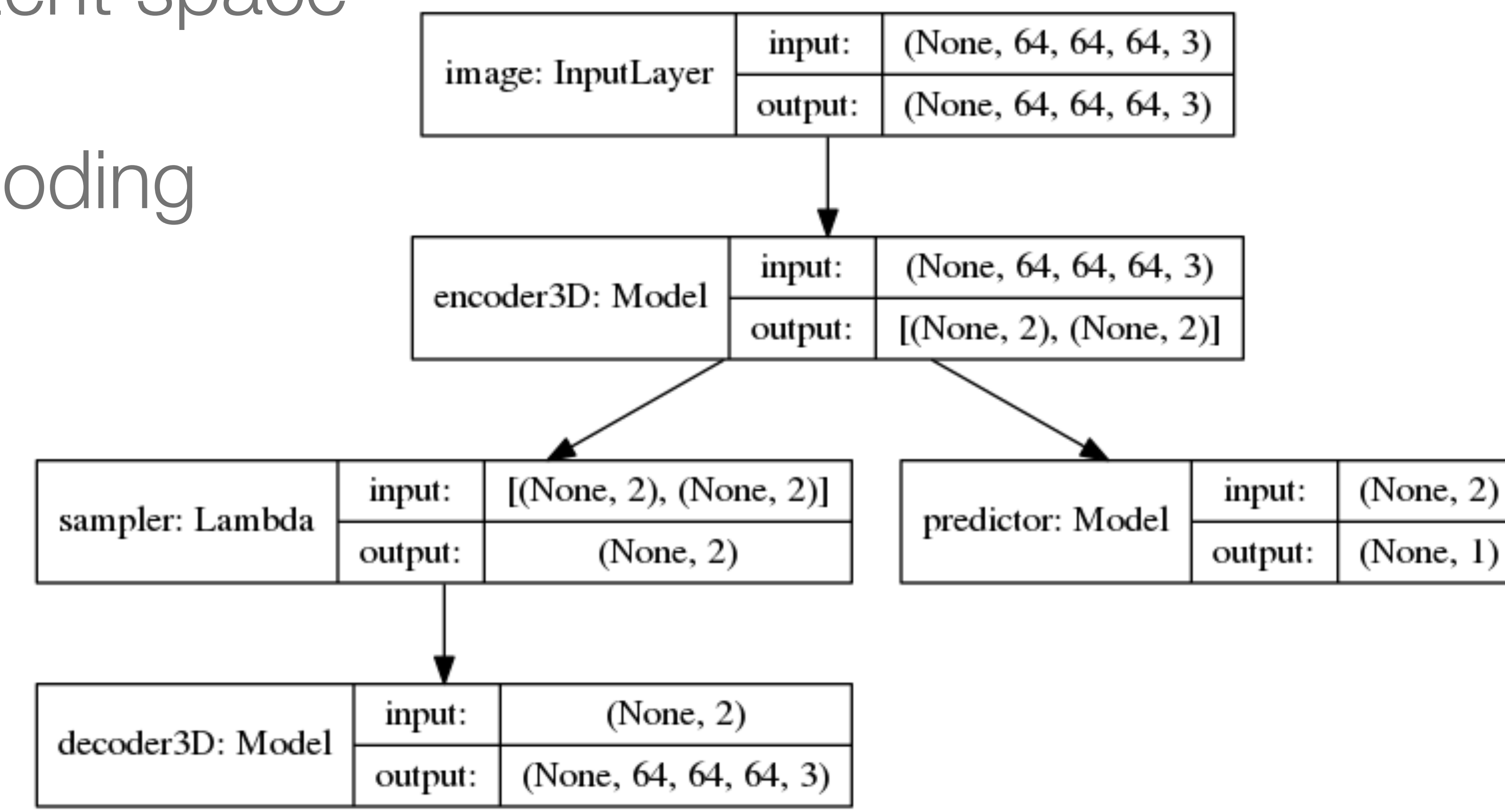
# BLOB (Boltzmann-Lagevein One Body)

- Simulates the evolution of the PDF of nucleons in the phase space
- Test particle approach:
  - 500 particles x nucleon
  - self-consistent mean-field
  - two-body interactions (particles collisions)



# Conditional VAE

- Convolutional 3D encoding
- Conditioned latent space
- Symmetric decoding

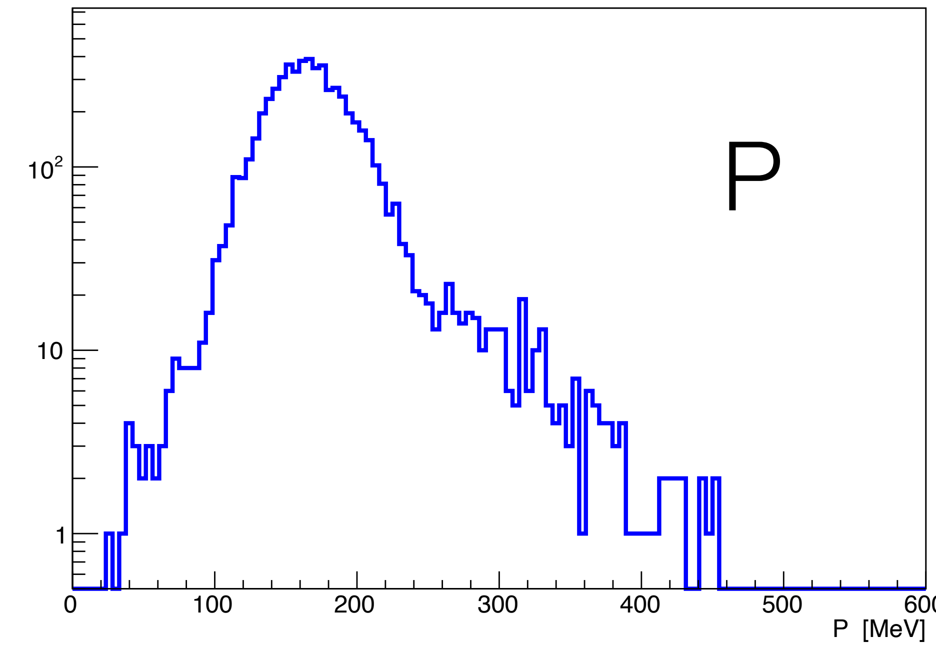


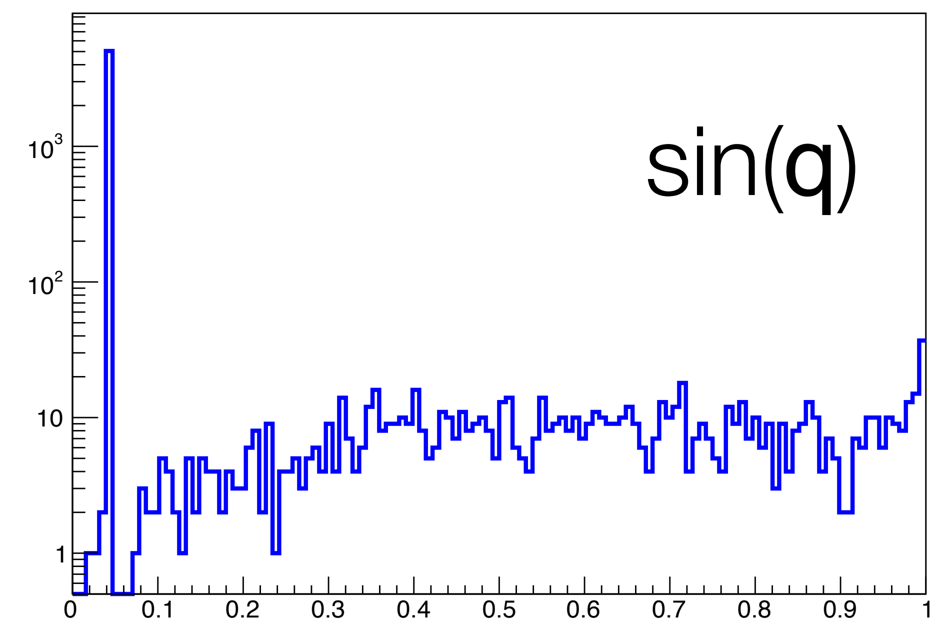
# Training dataset

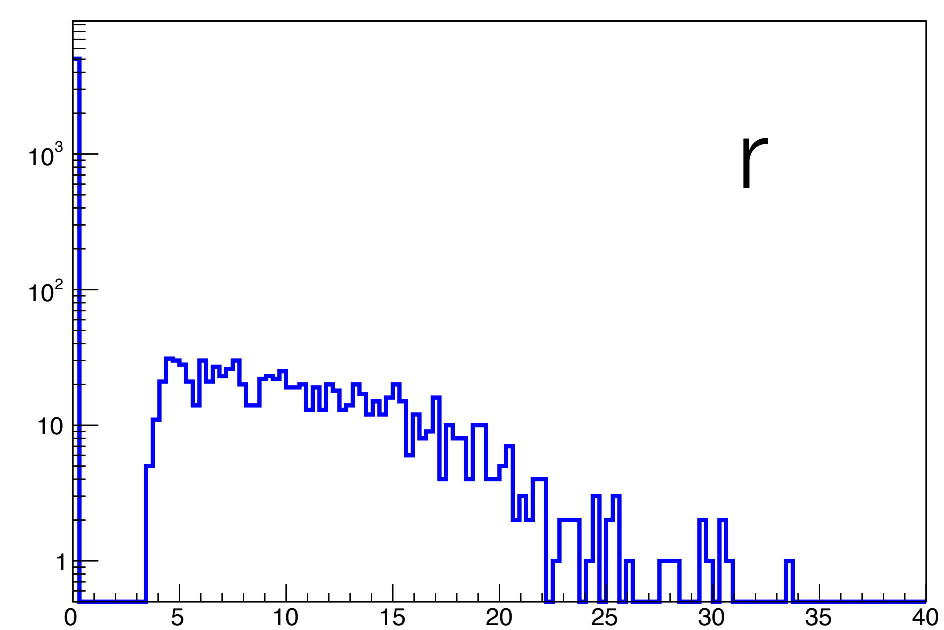
- The BLOB final state is a list with the position in the phase space of fragments and gas particles
- Fragments: A and Z (real), P, Q and Excitation energy
- Gas particles: Z, P and Q. Each represent a 1/500 probability of having a nucleon in that position of phase space
- 2000 events
- Generated with uniform impact parameter
- 1500 of them for training and 500 for testing

# Reducing dimensionality

- We divided the test particles in three samples:
    - To use the color channels
- sin(**q**) instead of **q** to:
    - have same sign
    - enhance small angles

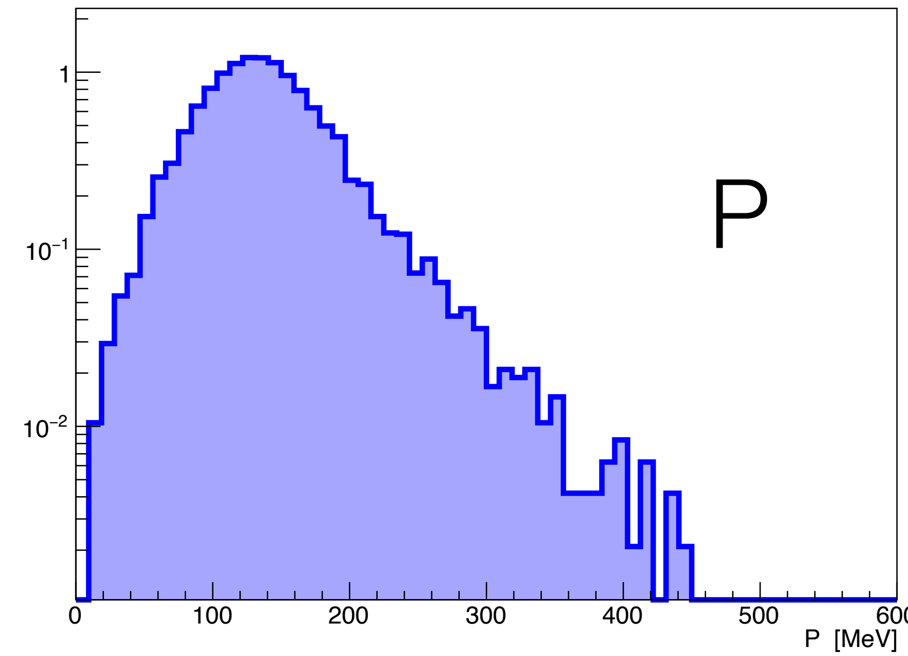


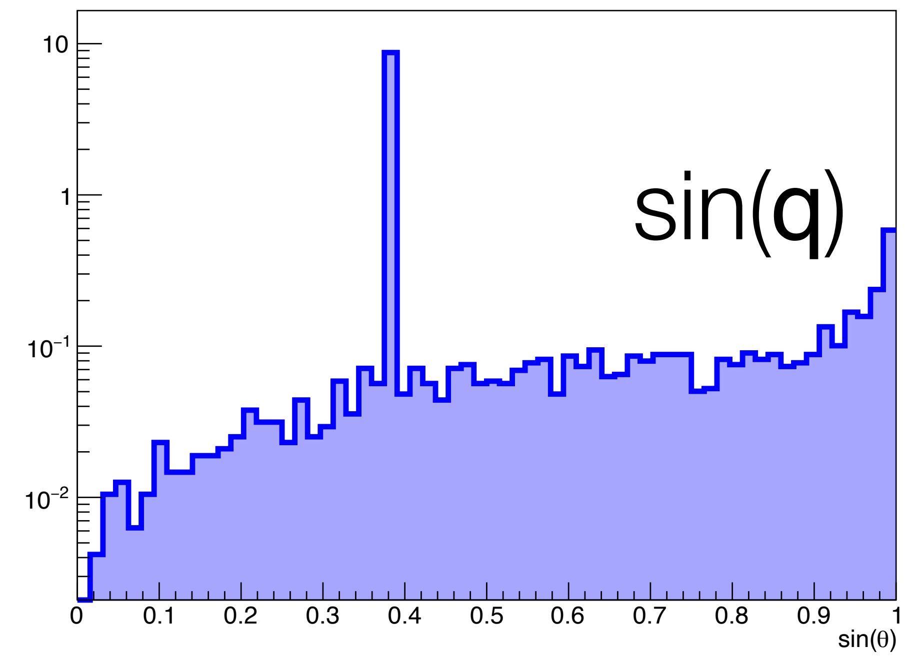



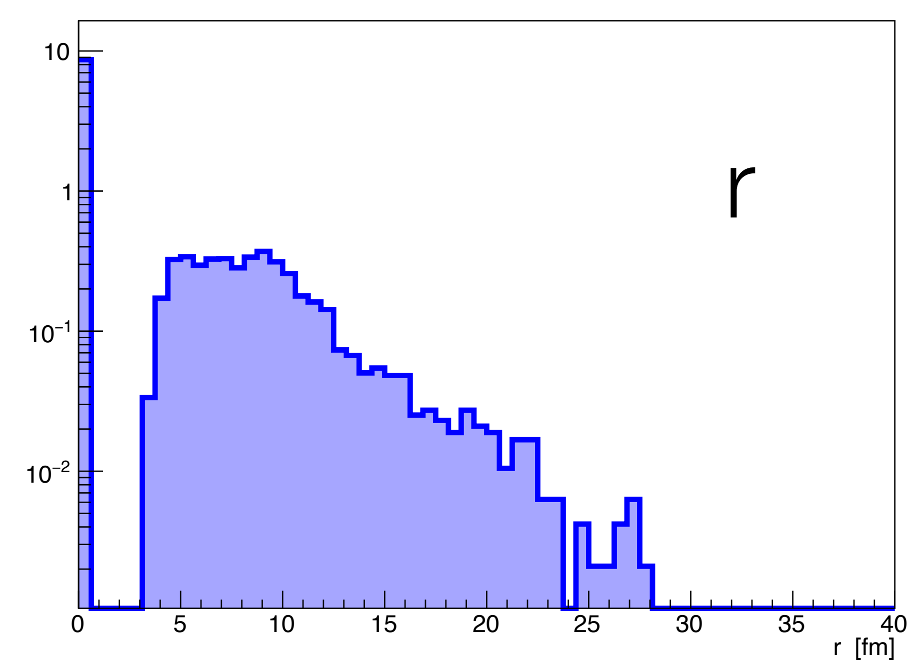



# Reducing dimensionality

- Fragments are represented by 500*A particles
- P is sampled with gaussian distribution:
  - mean = $P_{frag}$
  - sigma = Excitation energy
- All with the same **q**
- r = 0



# Challenges

- Sparse
- Large input ($128^3$ numbers)
- Small dataset (for the moment)
- Impact parameter distribution non uniform (for the moment)