Emulating BLOB with Deep Learning

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BLOB-ML meeting
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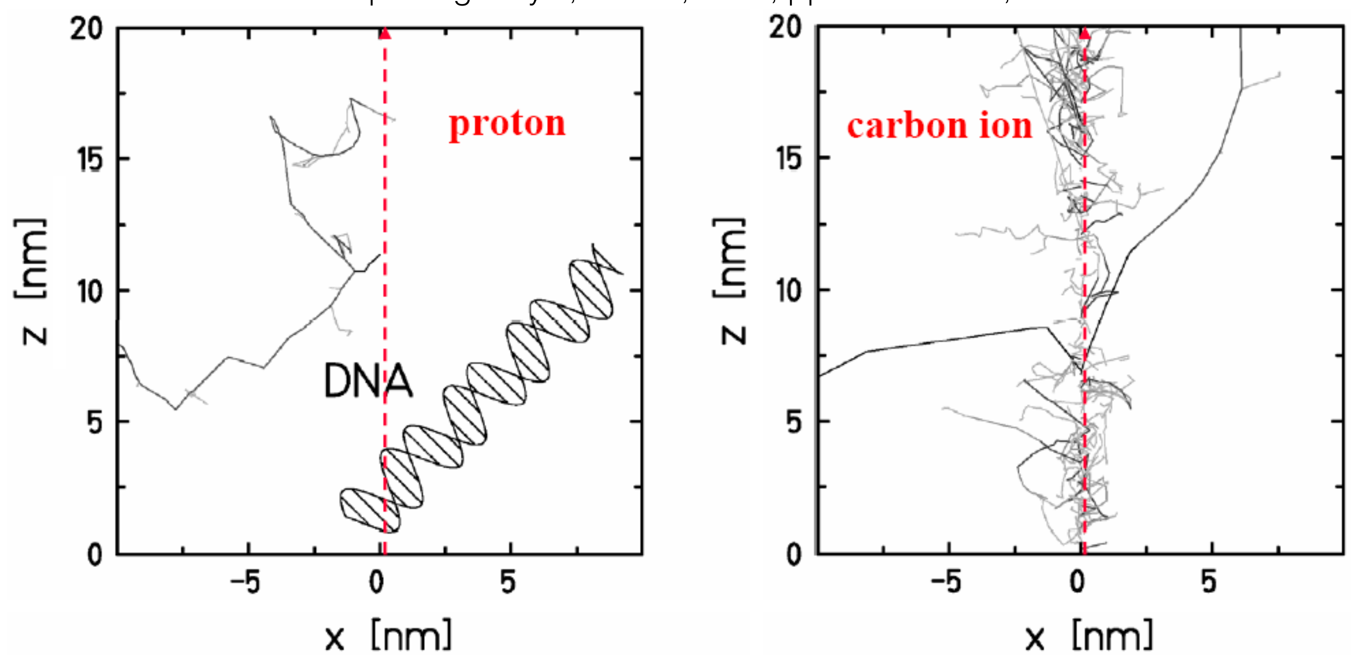
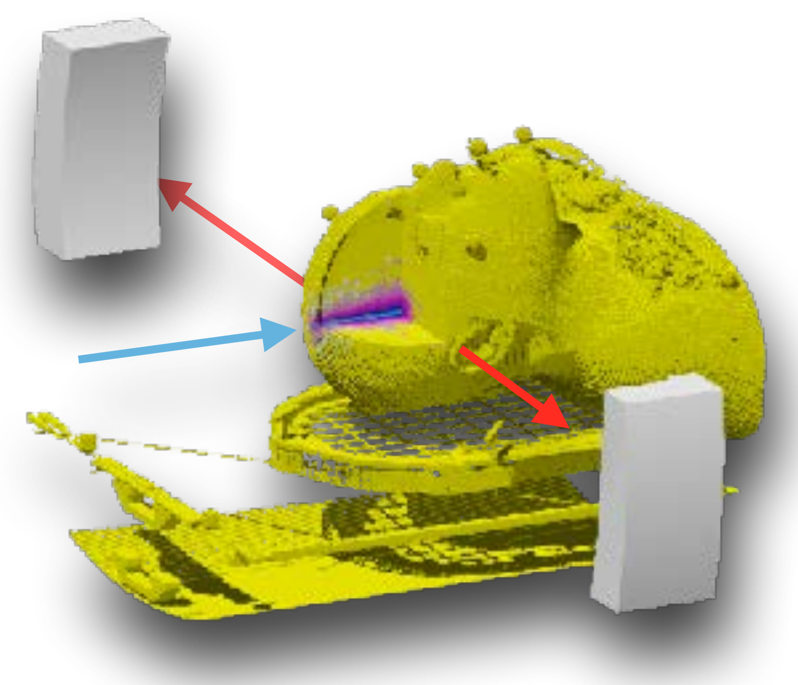
Nuclear fragmentation models are important for:

- Nuclear Physics experiments
- Hadrontherapy
- Radiobiology

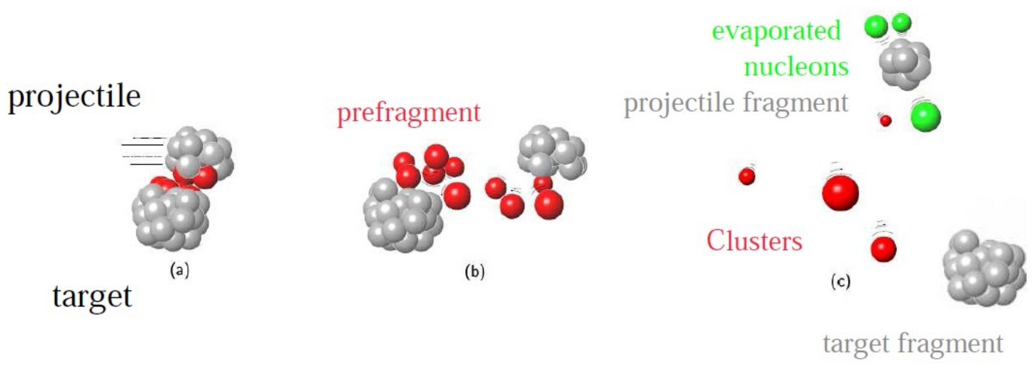
image from: U. Amaldi and G. Kraft,
Rep. Prog. Phys., vol. 68, no. 8, pp. 1861–1882, Jul. 2005.

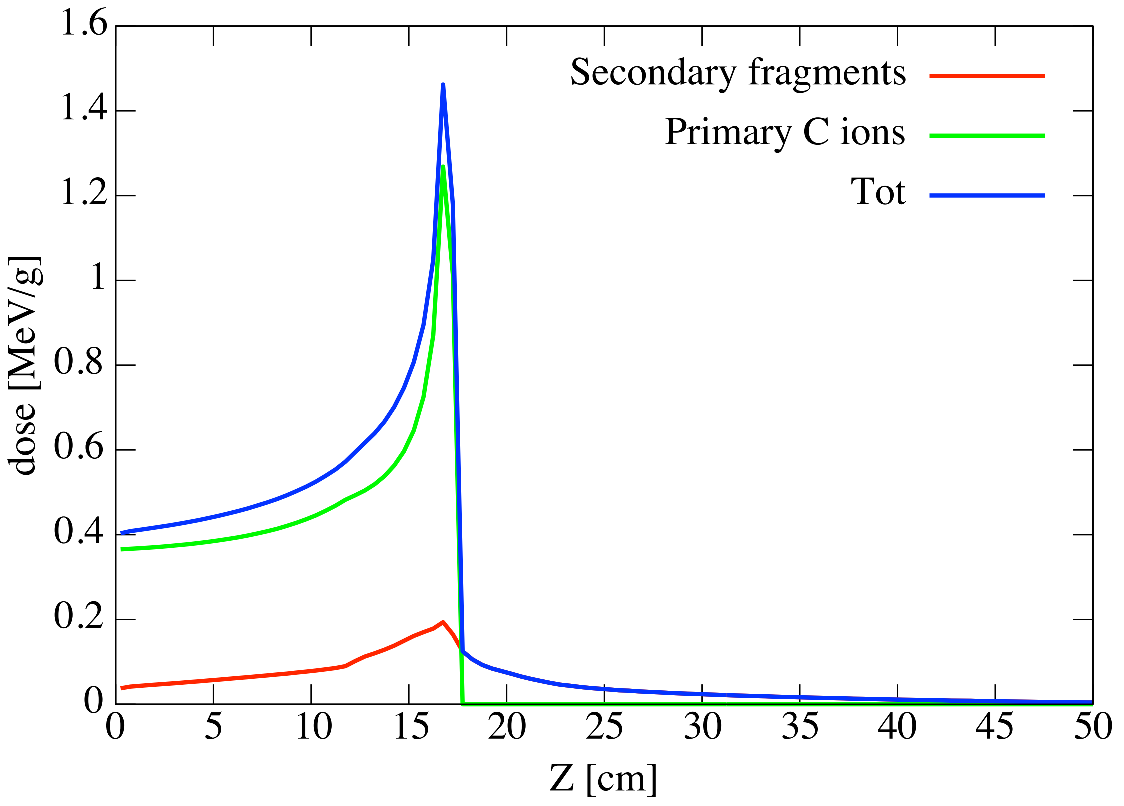




Carbon could breakup

- C ions could fragment in lighter particles
- The fragments contribute significantly to the total dose





About GeNIALE

- Geant4 Nuclear Interaction At Low Energy
- Aimed at improving Geant4 in simulating nuclear interaction below 100 MeV/u
- Granted by the INFN National Scientific Committee 5 (CSN5) for 2 years
- and by Sapienza for 1 year
- Nowadays included in the MC-INFN project (which contains all the INFN efforts to develop MC codes, such as Geant4)

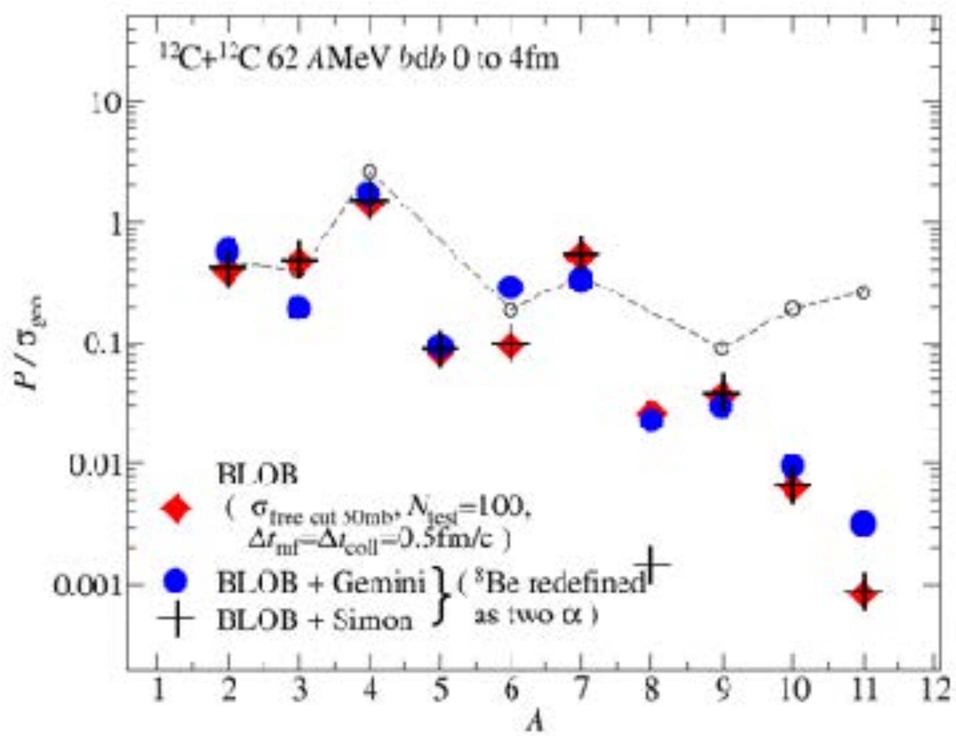
INFN
Istituto Nazionale di Fisica Nucleare

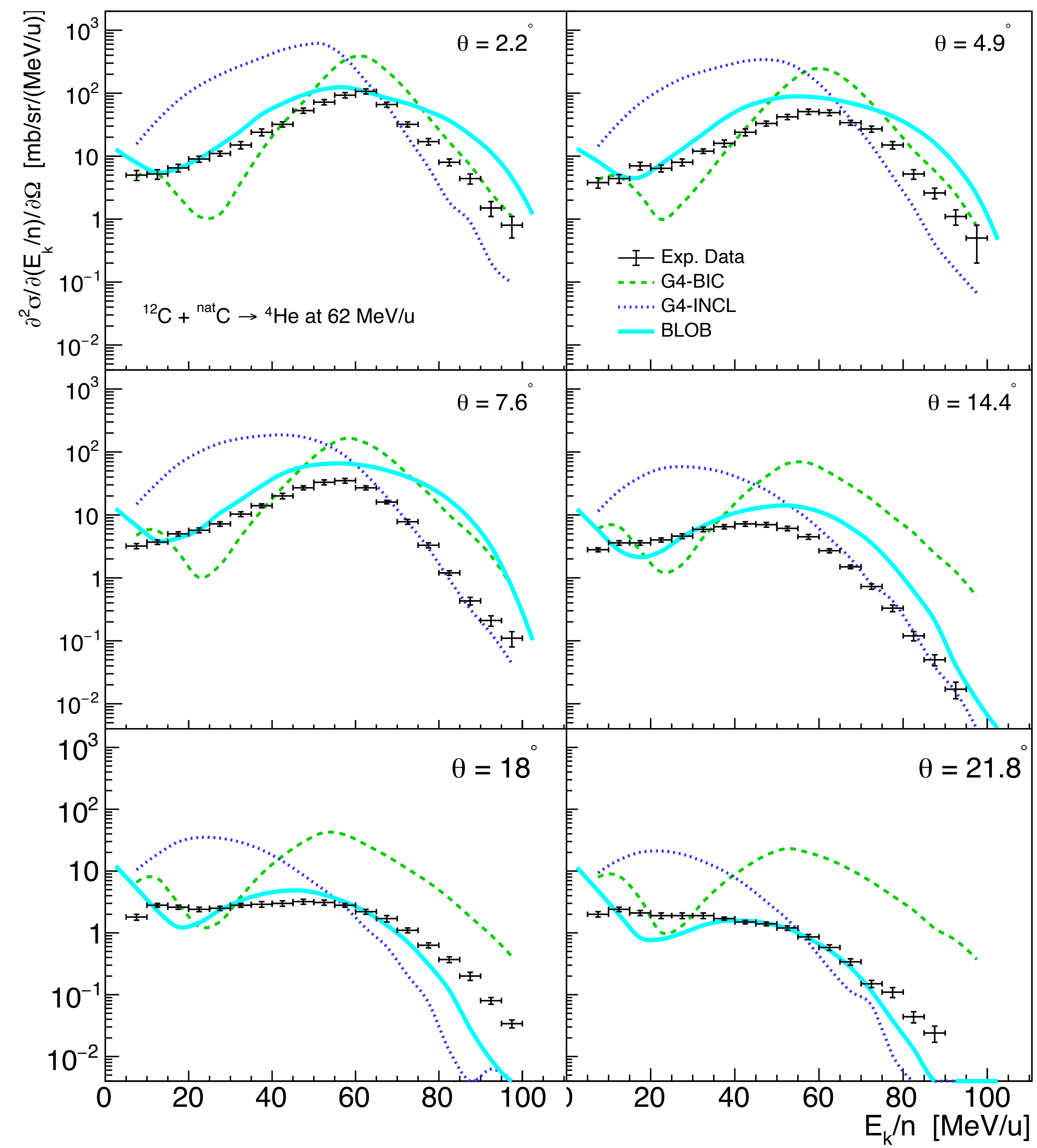
CSN5

SAPIENZA
UNIVERSITÀ DI ROMA

BLOB and Geant4

- We interfaced BLOB with Geant4 and its de-excitation model
- obtaining promising results

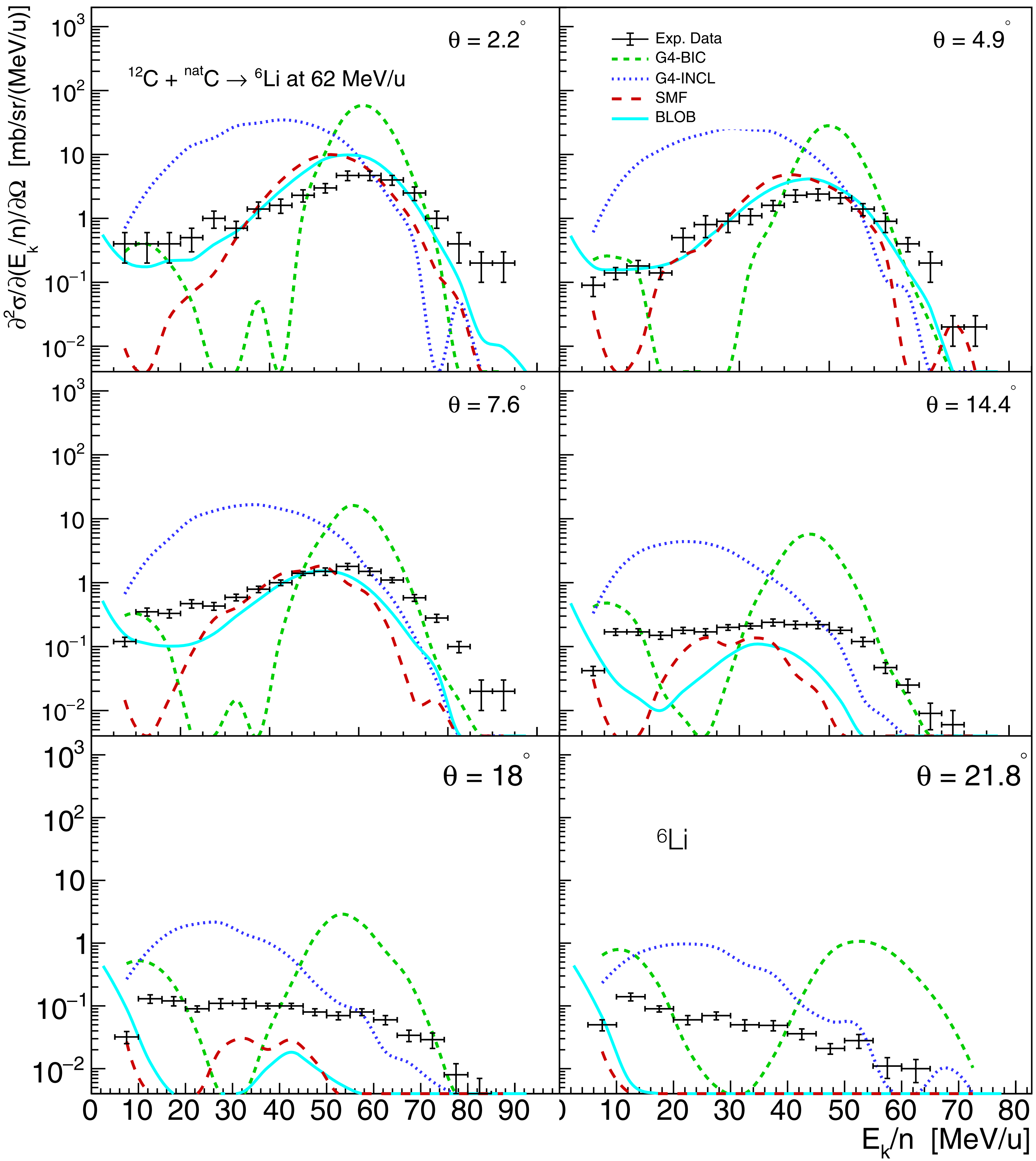




BLOB and Geant4

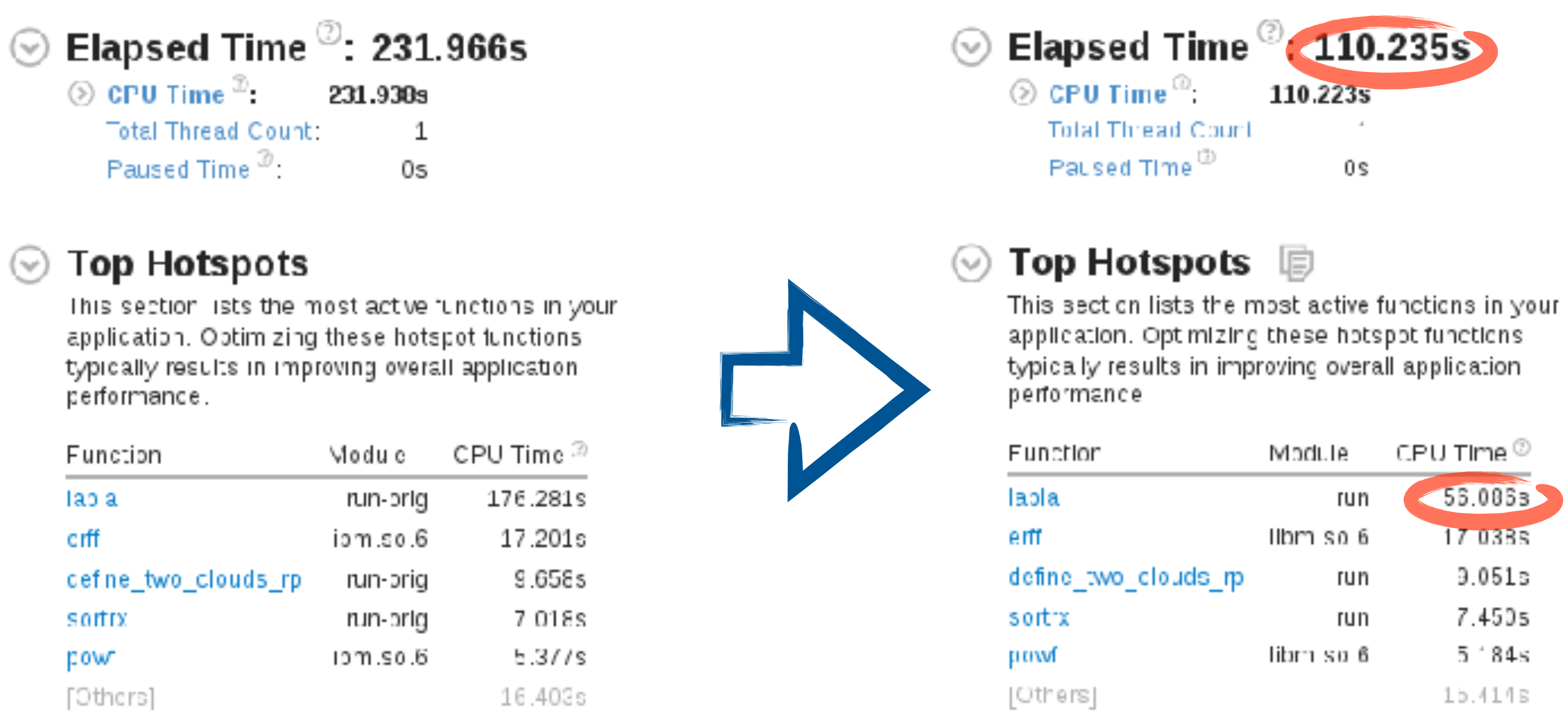
- The advantage of using BLOB instead of G4 models is clearer with heavier ejectiles (like ^{6}Li)

[C. Mancini-Terracciano et al. Preliminary results coupling “Stochastic Mean Field” and “Boltzmann-Langevin One Body” models with Geant4. Phys. Med. 67 (2019), pp. 116–122. https://doi.org/10.1016/j.ejmp.2019.10.026]

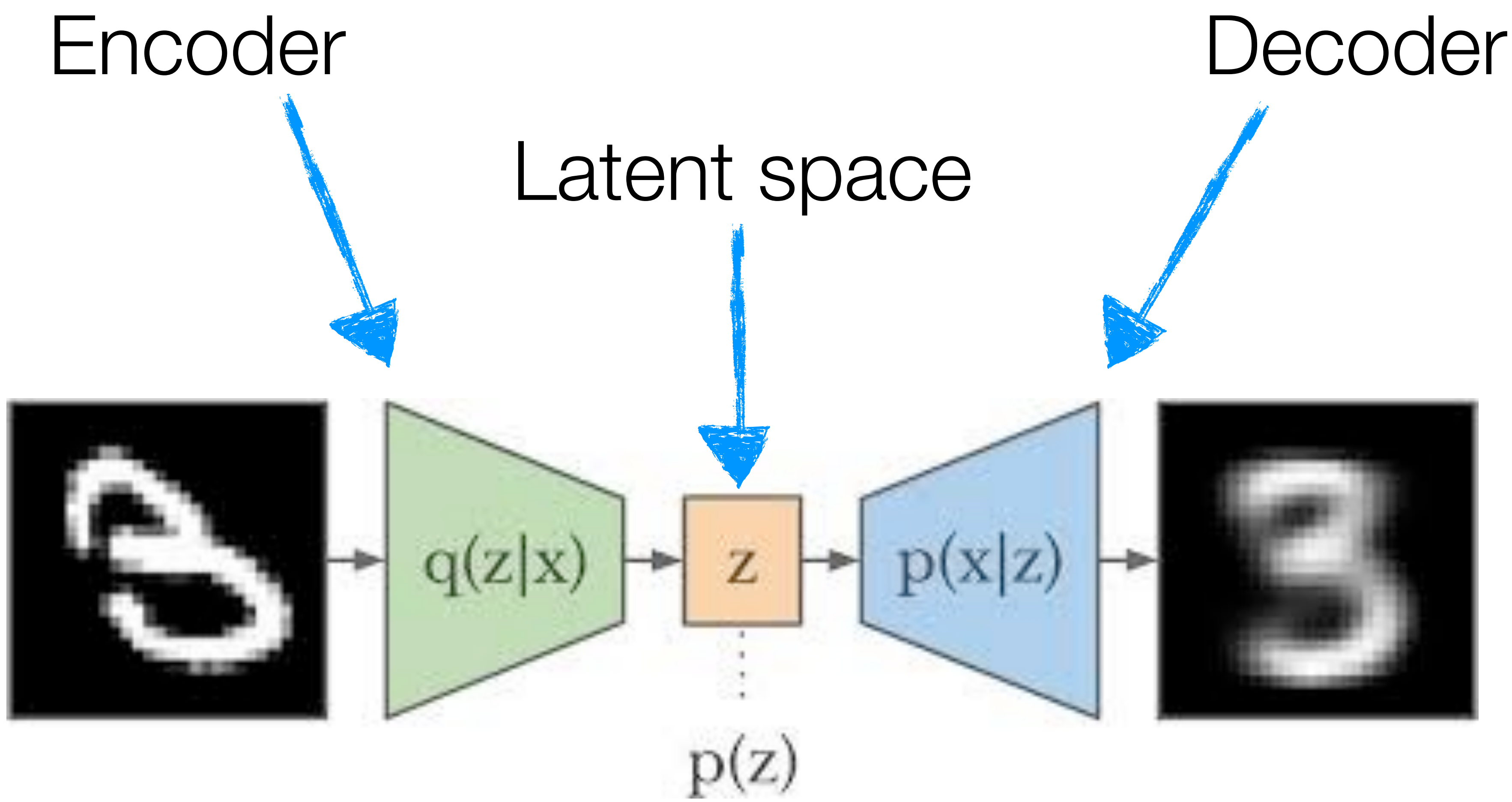


BLOB Code optimisations

- We optimised BLOB without changing the code structure (52% speed-up overall)
- Not enough for medical application
- Possibilities:
  - porting BLOB to GPU
  - emulating it with Deep Learning

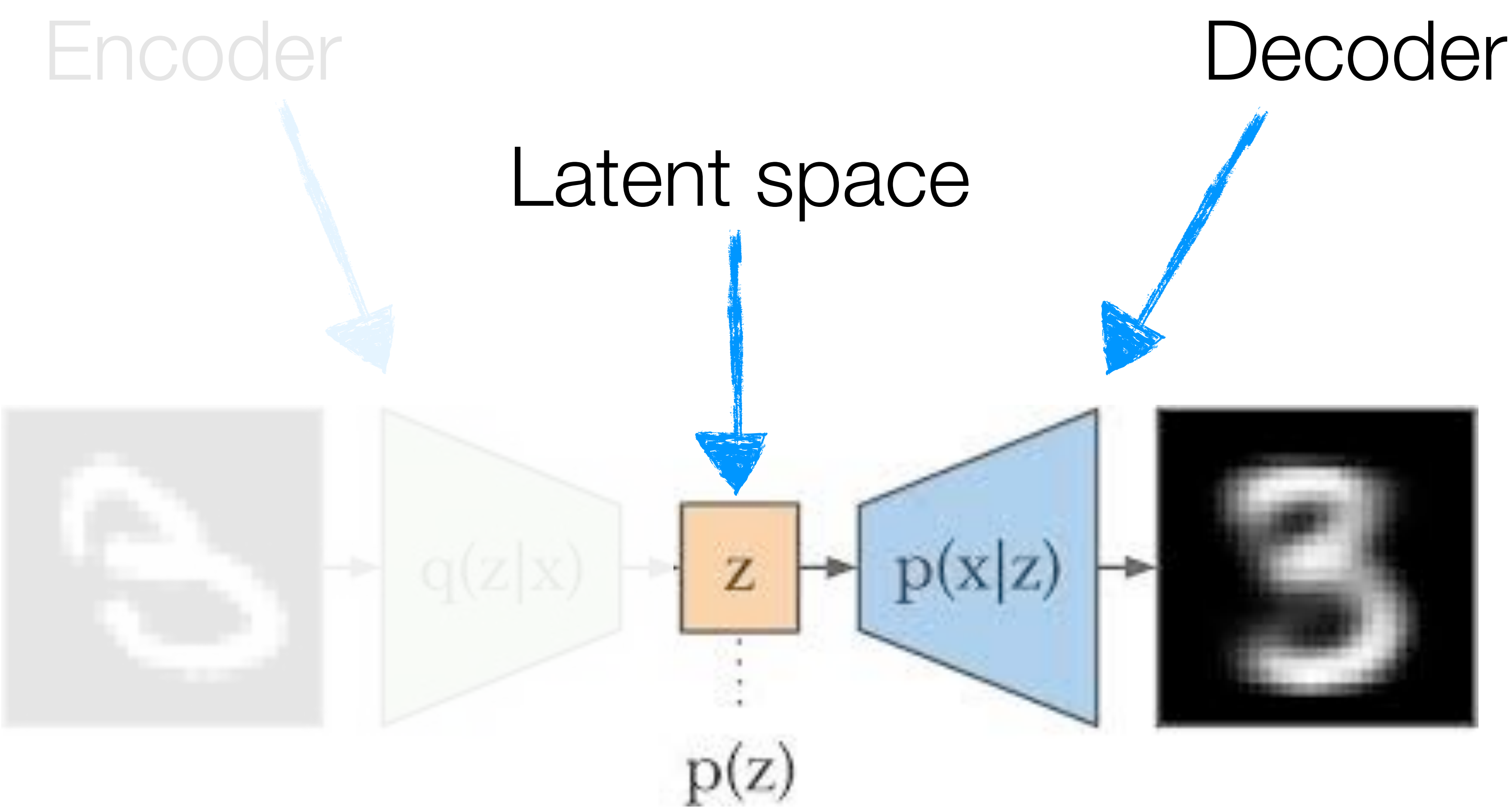


Variational Auto Encoders



- Train an identity function

Variational Auto Encoders



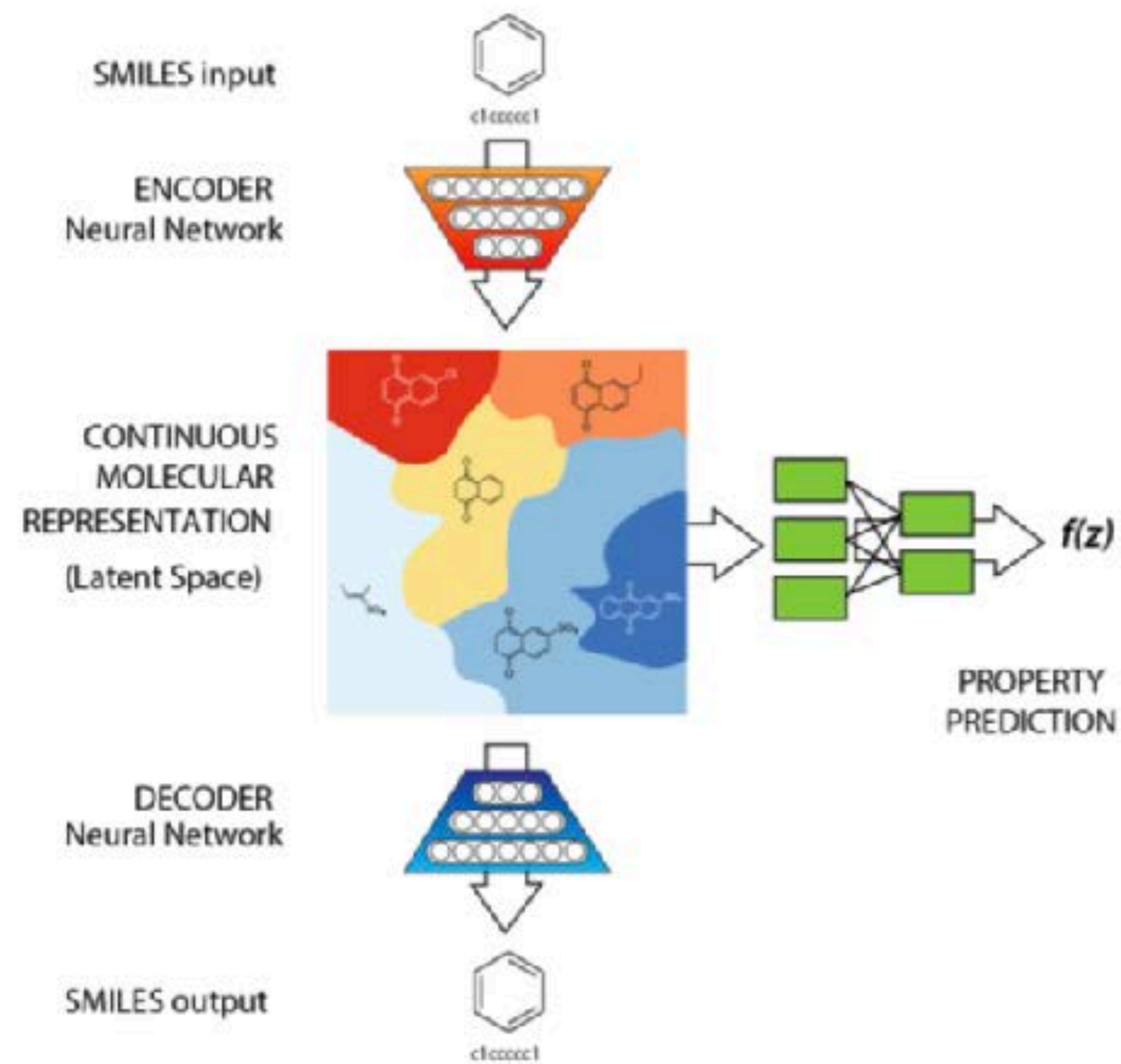
- Use the decoder to produce artificial images

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

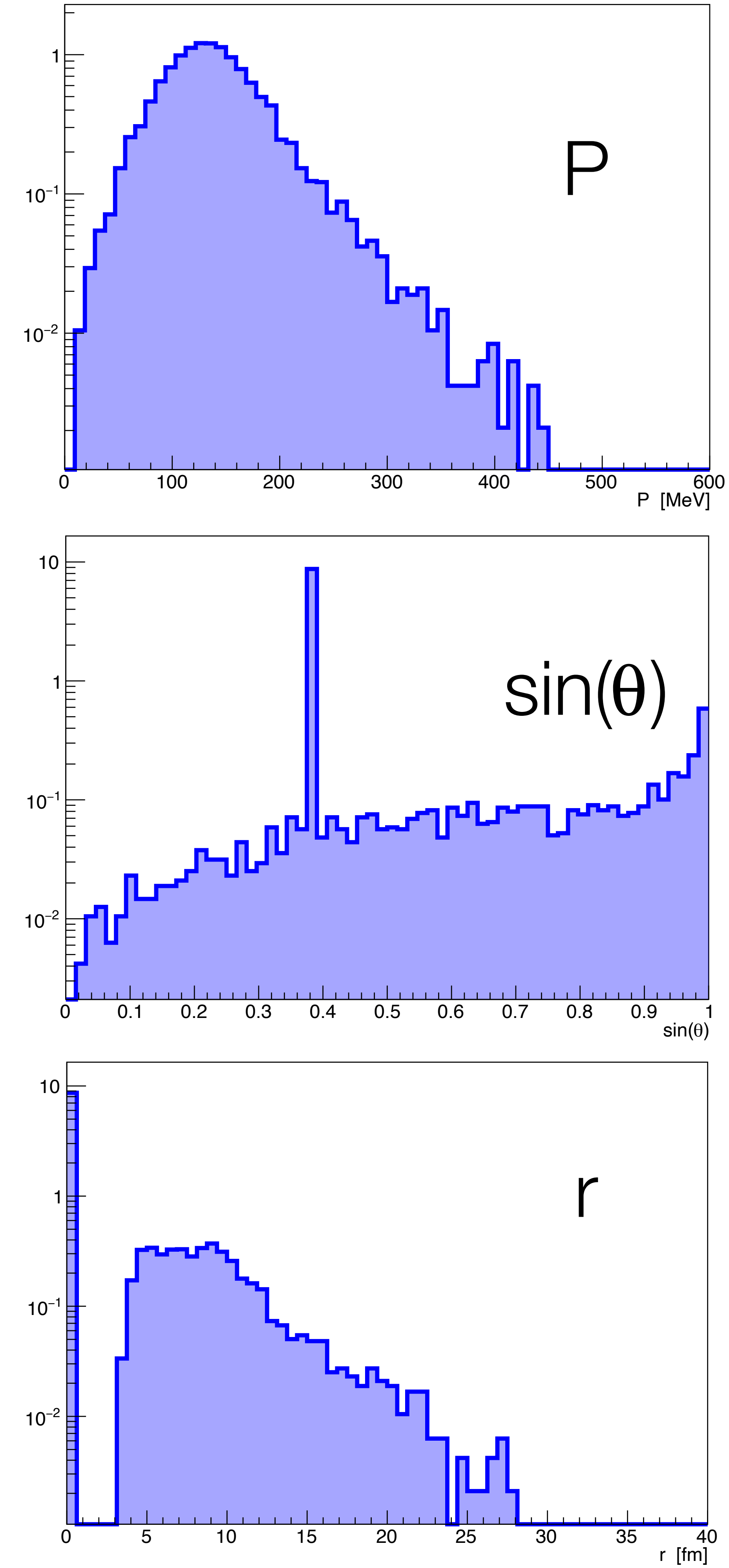


Training dataset

- The BLOB final state is a list with the position in the phase space of fragments and gas particles
- Fragments: A and Z (real), $\overrightarrow{P}$, $\overrightarrow{Q}$ and Excitation energy
- Gas particles: Z, $\overrightarrow{P}$ and $\overrightarrow{Q}$. Each representing a 1/500 probability of having a nucleon in that position of phase space
- 2’000 events
- Generated with uniform impact parameter (*b*)
- 1’500 of them for training and 500 for testing

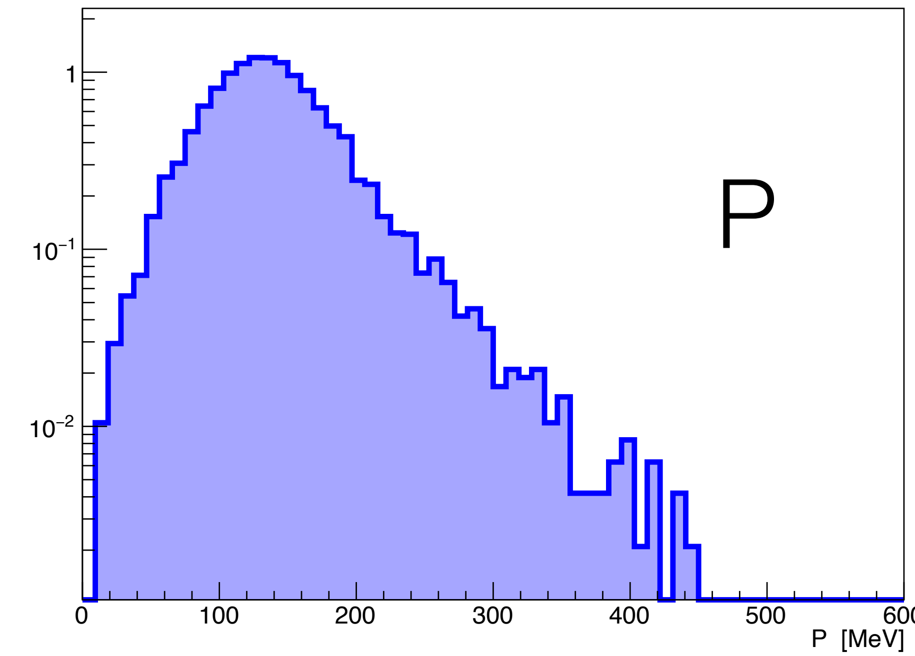
Reducing dimensionality

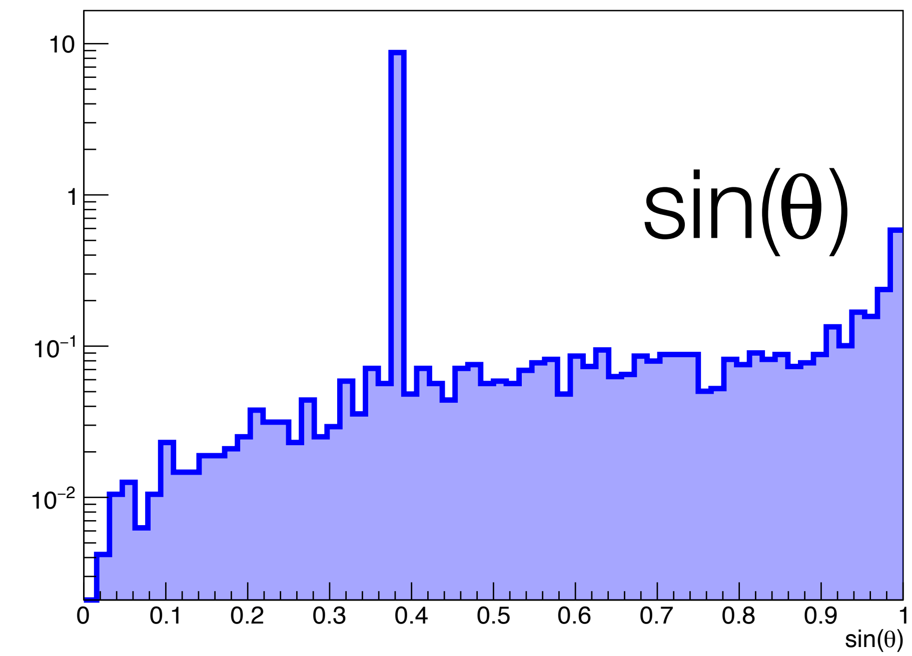
- To reduce the dimensionality and use the Keras 3D kernels
- We consider only:
  - The modulus of the momentum
  - its angle with the collision axis
  - The distance of each test particle with the fragment center
- We divided the test particles in three samples (one for each possible large fragment):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

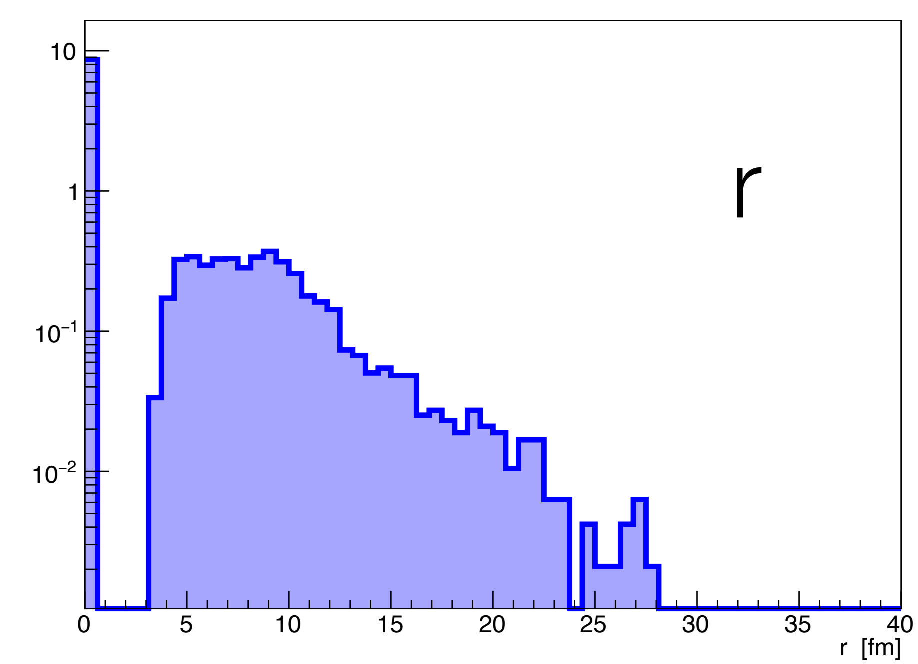


Reducing dimensionality

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

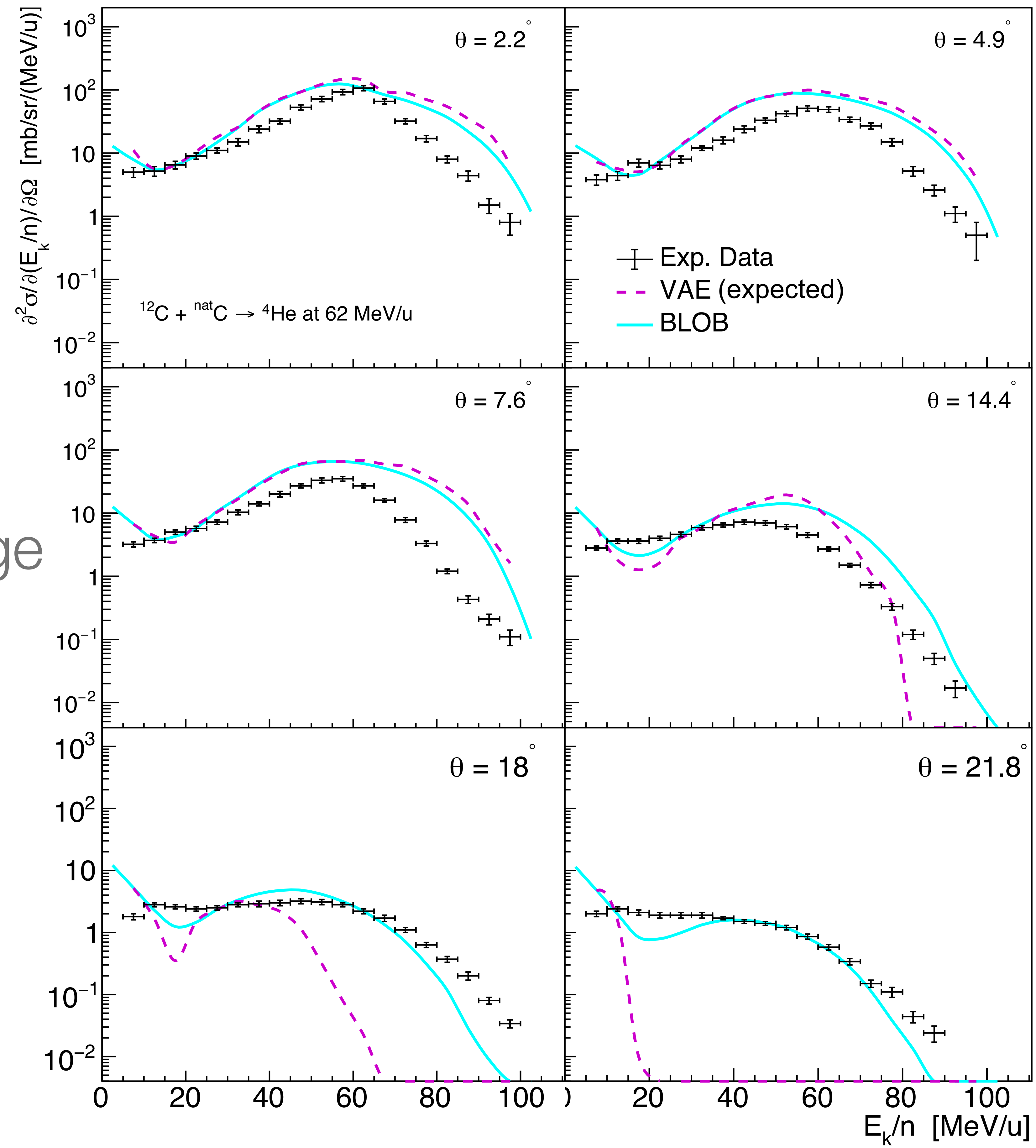






Testing reconstruction

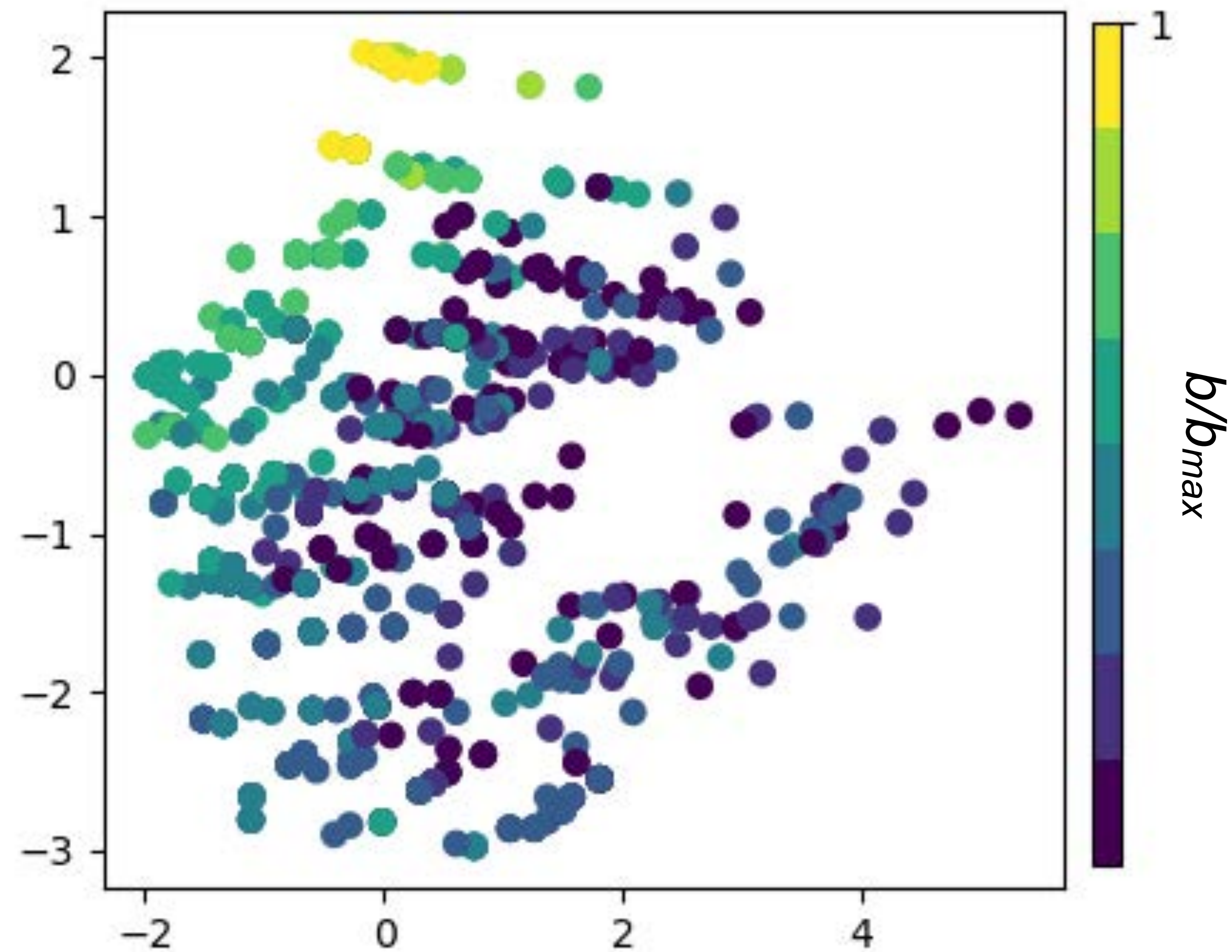
- Fragments are identified selecting r<1 fm
- Momentum = average
- Excitation energy = variance
- θ = average



Latent space

- Events with similar impact parameters are close in latent space

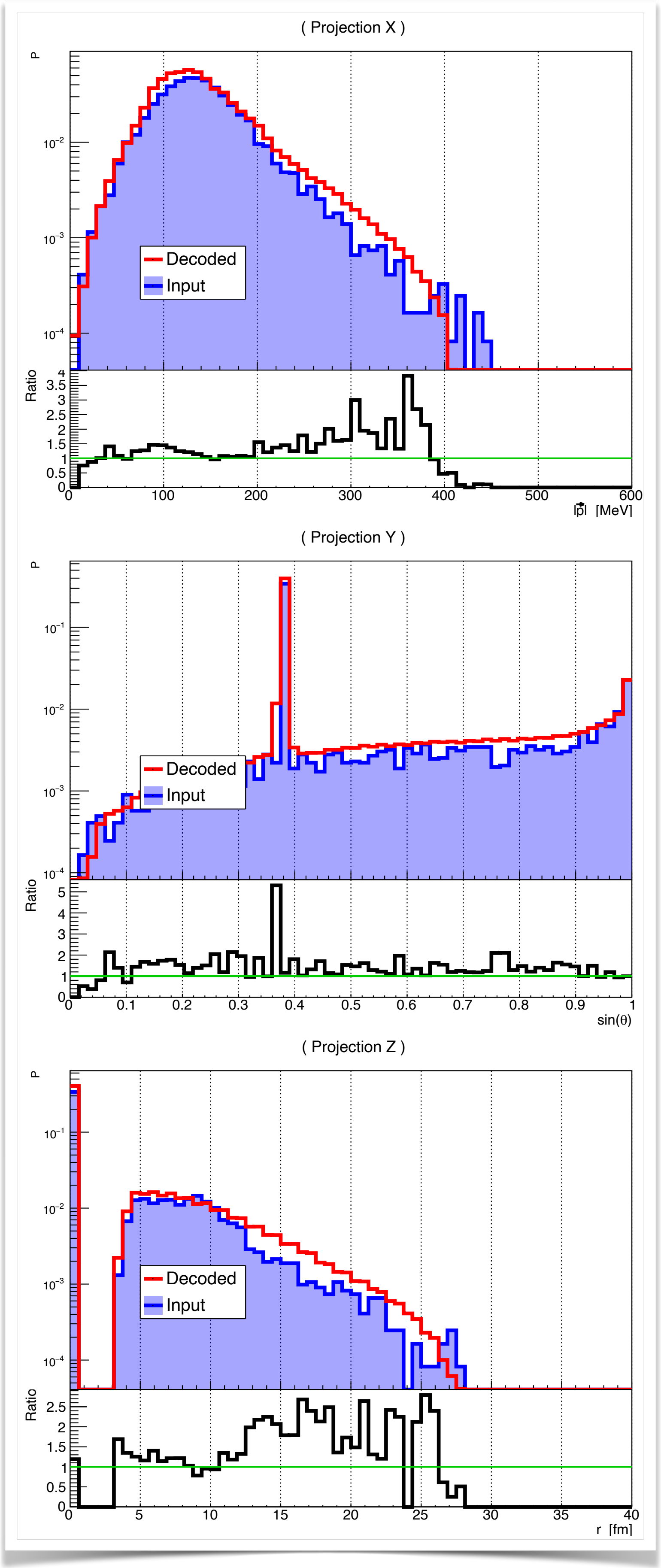
- Especially the events with very large impact parameters



Preliminary results are encouraging

- 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 test dataset (i.e. the VAE has not been trained with it)

[A. Ciardiello et al. *Preliminary results in using Deep Learning to emulate BLOB, a nuclear interaction model.* Phys. Med. 73, 2020. https://doi.org/10.1016/j.ejmp.2020.04.005]

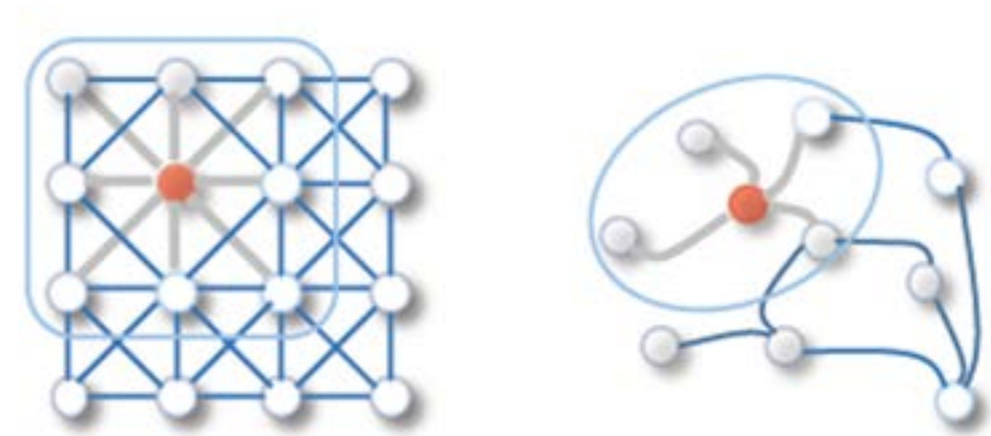


Dynamic Graph Convolutional Neural Networks

- We are testing also the possibility of emulating the whole interaction using Graph CNN

- Encode graph-structured data

- Use of topological relationships among nodes

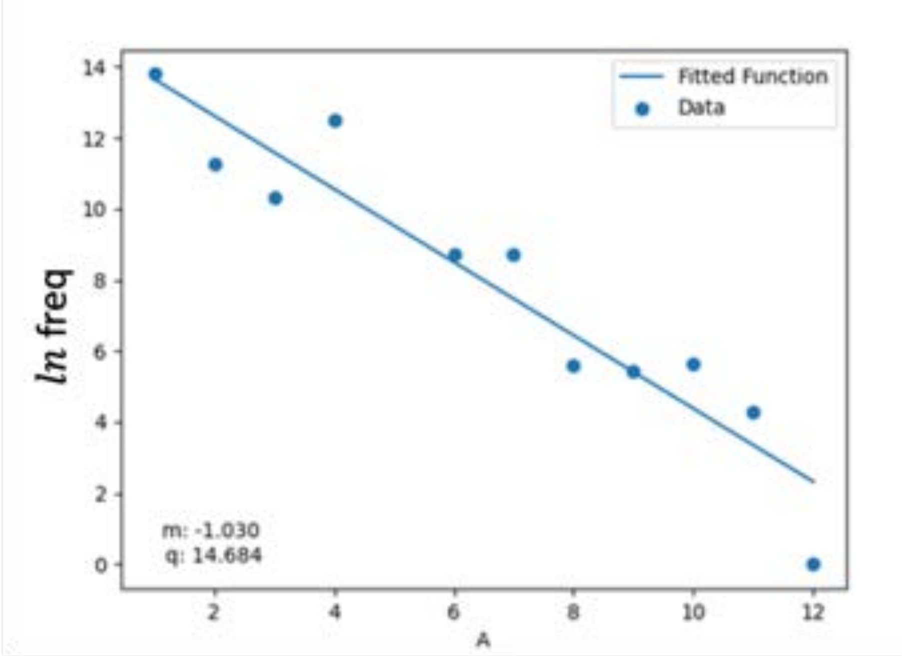


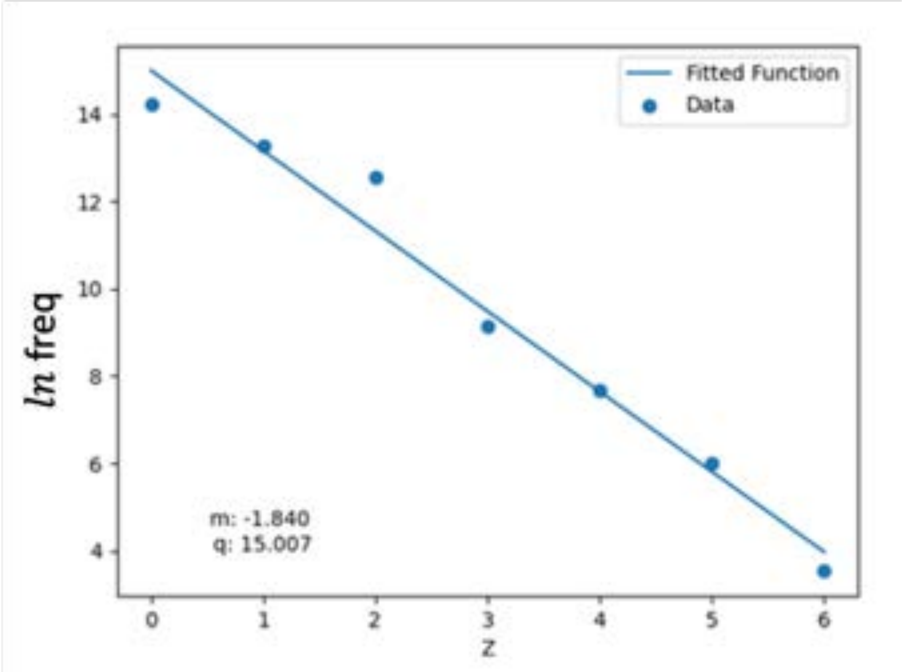
- Convolve the central node's representation with its neighbours' representations

- The model learns how to construct the graph

Merit (loss) function

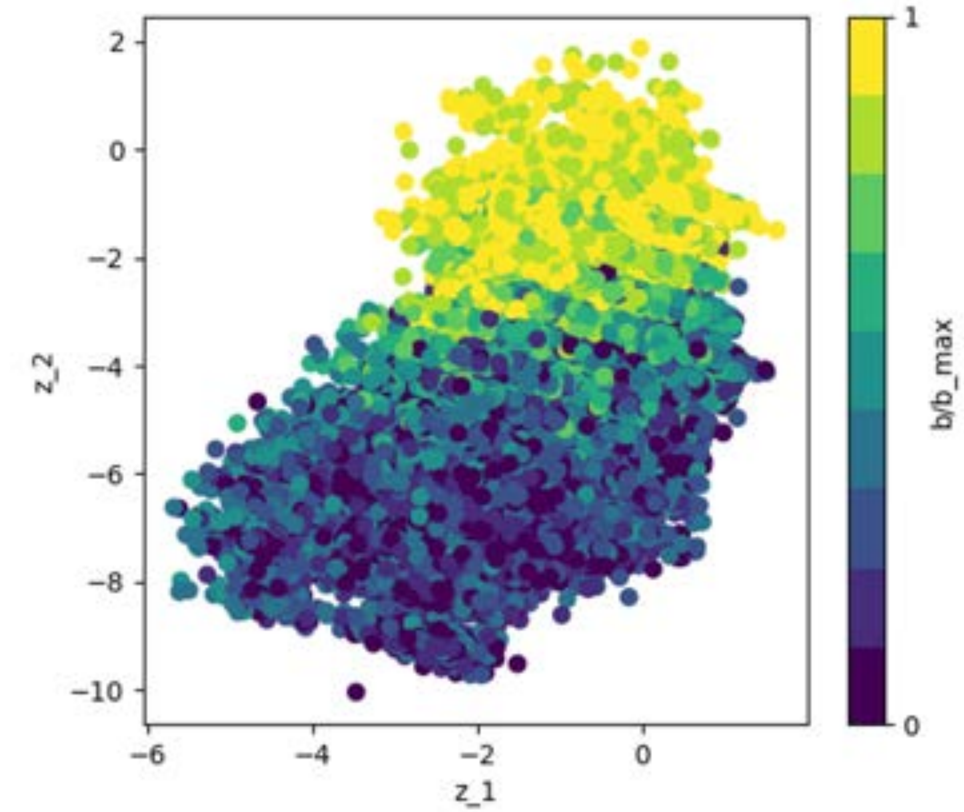
- The loss function is made of 4 terms
  - Reconstruction loss
  - Kullback-Leibler divergence
  - Predictor loss
  - **Penalty loss** (to force the VAE to learn the heavier fragments production)

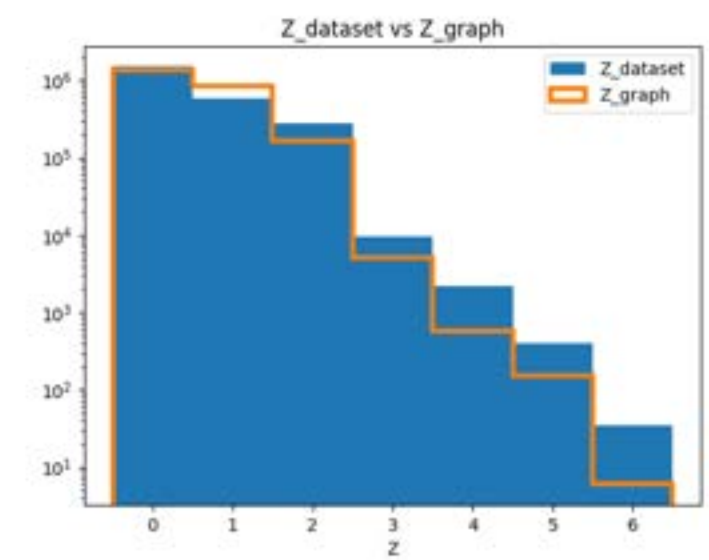


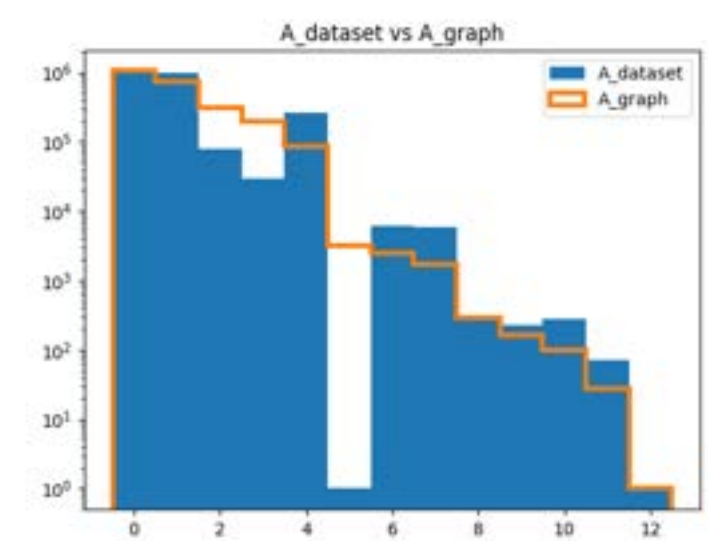


Graph CNN - First results

- Up to now we only tested A and Z multiplicities
- The organisation of the latent space and these first results are encouraging
- We will further test this possibility







Short term plan

- Interfacing the generative part of the VAE with Geant4 (on going)
- Preparate a Docker container with TF C++ API and Geant4 (almost done)
- Validate the VAE with experimental data
- Add the interaction energy as a parameter (as done for *b*)
- Train the VAE with energy below and over 62 MeV/u and test it in generation at that energy

Not so long therm plan

- Add *A* and *Z* of projectile and target as parameters

Long therm plan

- Develop 6D convolutional layers
- Explore VAE with both, encoder and decoder, with graph

thank you for your attention!