Accelerating low-energy ion-ion models meeting

Outcomes of the GeNIALE project

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1st April 2020

About GeNIALE

- Geant4 Nuclear Interaction At Low Energy

- Granted by the INFN
  National Scientific Committee 5 (CSN5)
  for two years

- CSN5 is devoted to technological and
  inter-disciplinary research
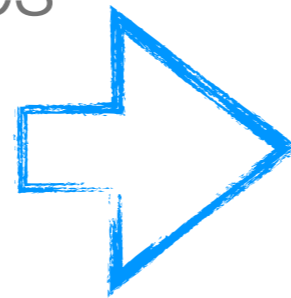
- and by Sapienza for 1 year

BLOB and Geant4

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

- obtaining promising results

- the BLOB computation time is too large for any medical application
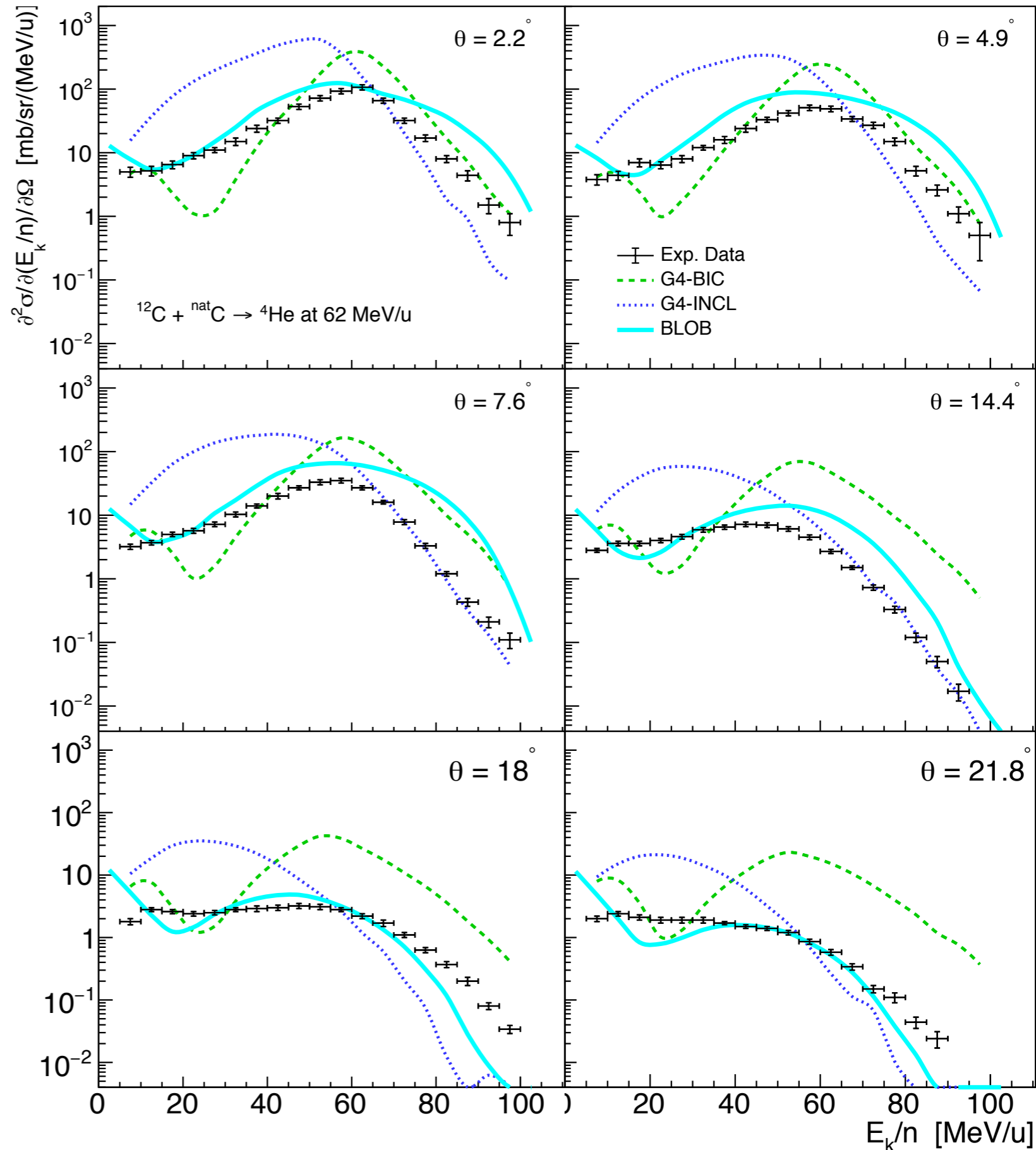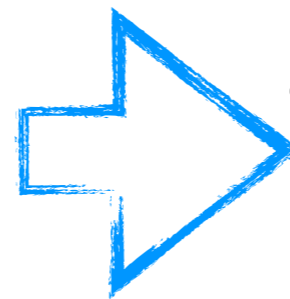
Embarrassing parallelizable?

- BUU and BL explore the time evolution of the density distribution with test particles
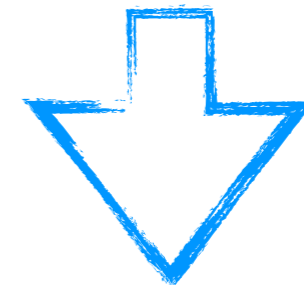
- 100 test particles per nucleon

- At each step the mean field potential is calculated

- The test particle can interact only with elastic scattering

- Many test particles

- All the same

- Only one possible interaction

Low thread divergency

ANIMA

- Accelerate the computation of a Nuclear Interaction model for Medical Applications

- Proposed as a Marie-Curie Global Fellow in 2018

- 2 years at SLAC and 1 at INFN

- To port BLOB on GPU

ANIMA

- Accelerate the computa[tion]
  model for Medical Applic[ations]

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- To port BLOB on GPU

- Support by NVIDIA

Letter of support for Dr. Carlo Mancini Terracciano for the MSCA-IF Global Fellowship project ANIMA

Santa Clara, May 9 2018

To whom it may concern:

It is my pleasure to support Dr. Carlo Mancini Terracciano for the MSCA-IF Global Fellowship proposal ANIMA (Accelerating Nuclear Interaction model for Medical Applications).
I am the Director of the High Performance Benchmarking group at NVIDIA where I work in the area of GPU computing. Prior to joining NVIDIA, I was a research staff member at Stanford University where I worked on applications for the Stanford Streaming Supercomputer. I hold a Laurea in Aeronautical Engineering and a PhD in Theoretical and Applied Mechanics from the University of Rome "La Sapienza".
My publication history includes more than 35 papers published in peer reviewed journals with a h-index of 35. I am also co-author of the book "CUDA Fortran for Scientists and Engineers: Best Practices for Efficient CUDA Fortran Programming".

My group frequently collaborates with scientific research groups pursuing projects involving the development and benchmarking of codes on GPU systems. For instance, we recently participated in the porting of the code "Quantum ESPRESSO", a popular quantum chemistry simulation tool, to GPUs.

My team and I will support Dr. Carlo Mancini Terracciano in the porting of the BLOB (Boltzmann Langevin One Body) code to GPUs using CUDA, by providing training in CUDA programming and assistance in benchmarking the ported code on machines at NVIDIA Corporation. Taking advantage of the proximity of SLAC National Accelerator Laboratory / Stanford University to our office at the NVIDIA headquarters in Santa Clara, we will have regular meetings to discuss the implementation of the code and provide feedback and suggestions for further development.

With my best regards,

Massimiliano Fatica

Dr. Massimiliano Fatica
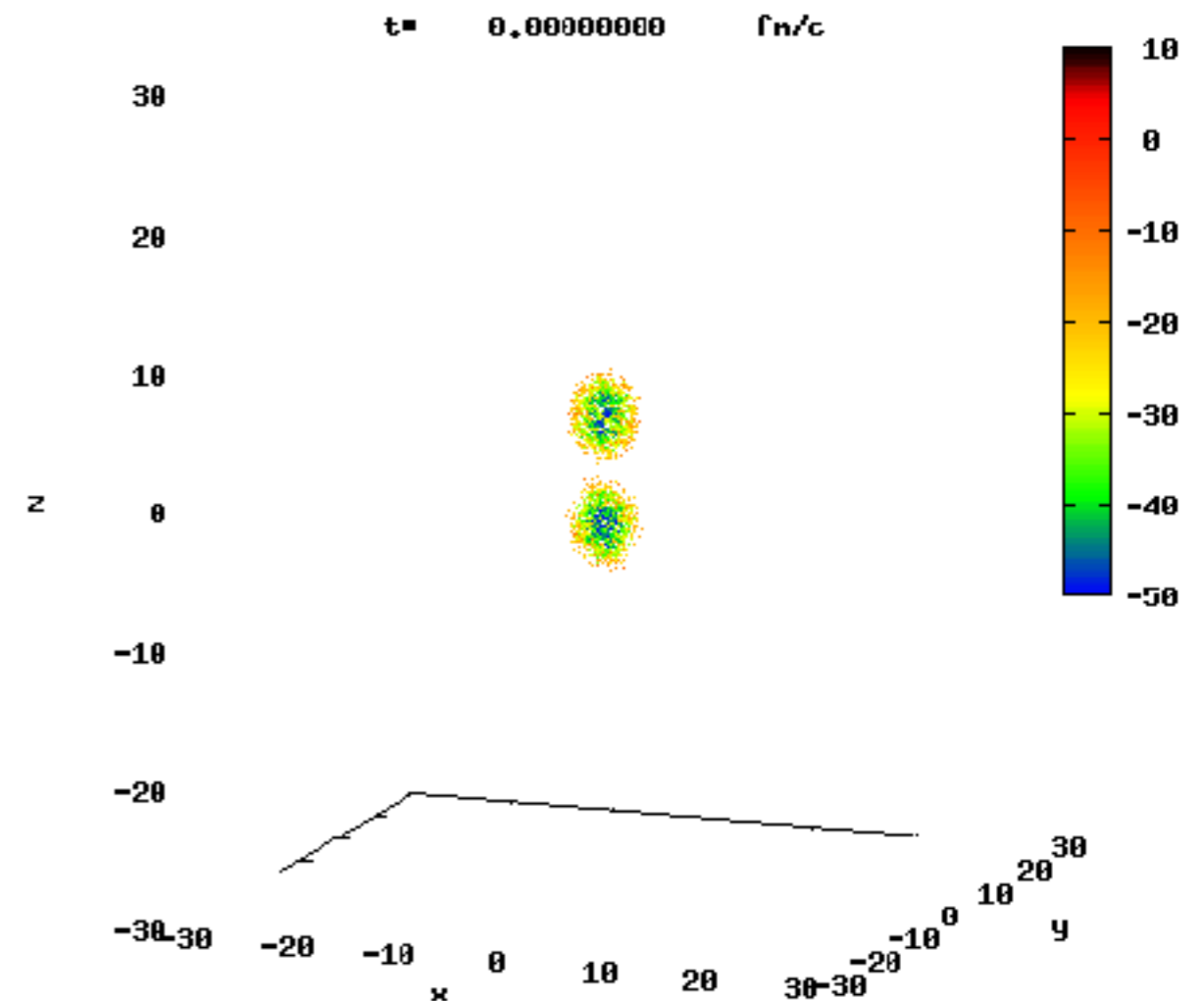Director High Performance Benchmarking group,
NVIDIA Corporation

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ANIMA

- Accelerate the computation o~~f~~
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- Not granted but obtained the "Seal of Excellence"

Certificate delivered by the European Commission,
as the institution managing Horizon 2020,
the EU Framework Programme for Research and Innovation 2014-2020

The project proposal 840121, ANIMA

Accelerate the computation of a Nuclear Interaction model for Medical Applications

Submitted under the Horizon 2020's Marie Skłodowska-Curie actions
call H2020-MSCA-IF-2018 of 12 September 2018
by
Carlo MANCINI TERRACCIANO
and
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00044 FRASCATI
Italy

following evaluation by an international panel of independent experts

WAS SCORED AS A HIGH-QUALITY PROJECT PROPOSAL
IN A HIGHLY COMPETITIVE EVALUATION PROCESS*

This proposal is recommended for funding by other sources since Horizon 2020 resources
available for this specific Call were already allocated following a competitive ranking.

* This means passing, with a score of 85% or more, all stringent Horizon 2020 assessment thresholds for the 3 award criteria
(excellence, impact, quality and efficiency of implementation) required to receive funding from Horizon 2020.

Carlos Moedas
Commissioner for Research
Science and Innovation

Tibor Navracsics
Commissioner for Education, Culture
Youth and Sport

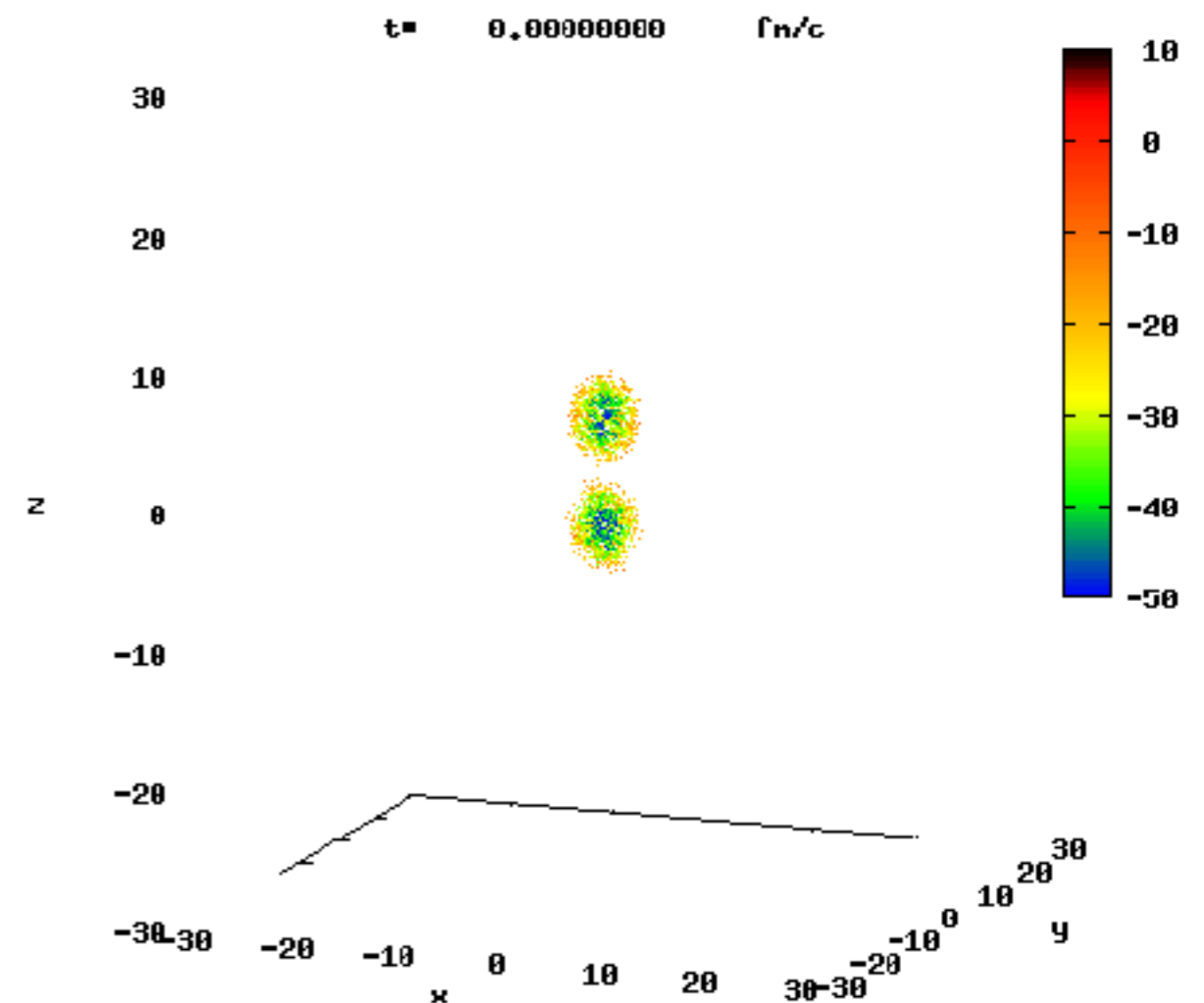Brussels, 19/03/2019

BLOB (Boltzmann-Lagevein One Body)

- describes the time evolution of the density distribution

- involves the implementation of an effective attractive mean-field nuclear interaction

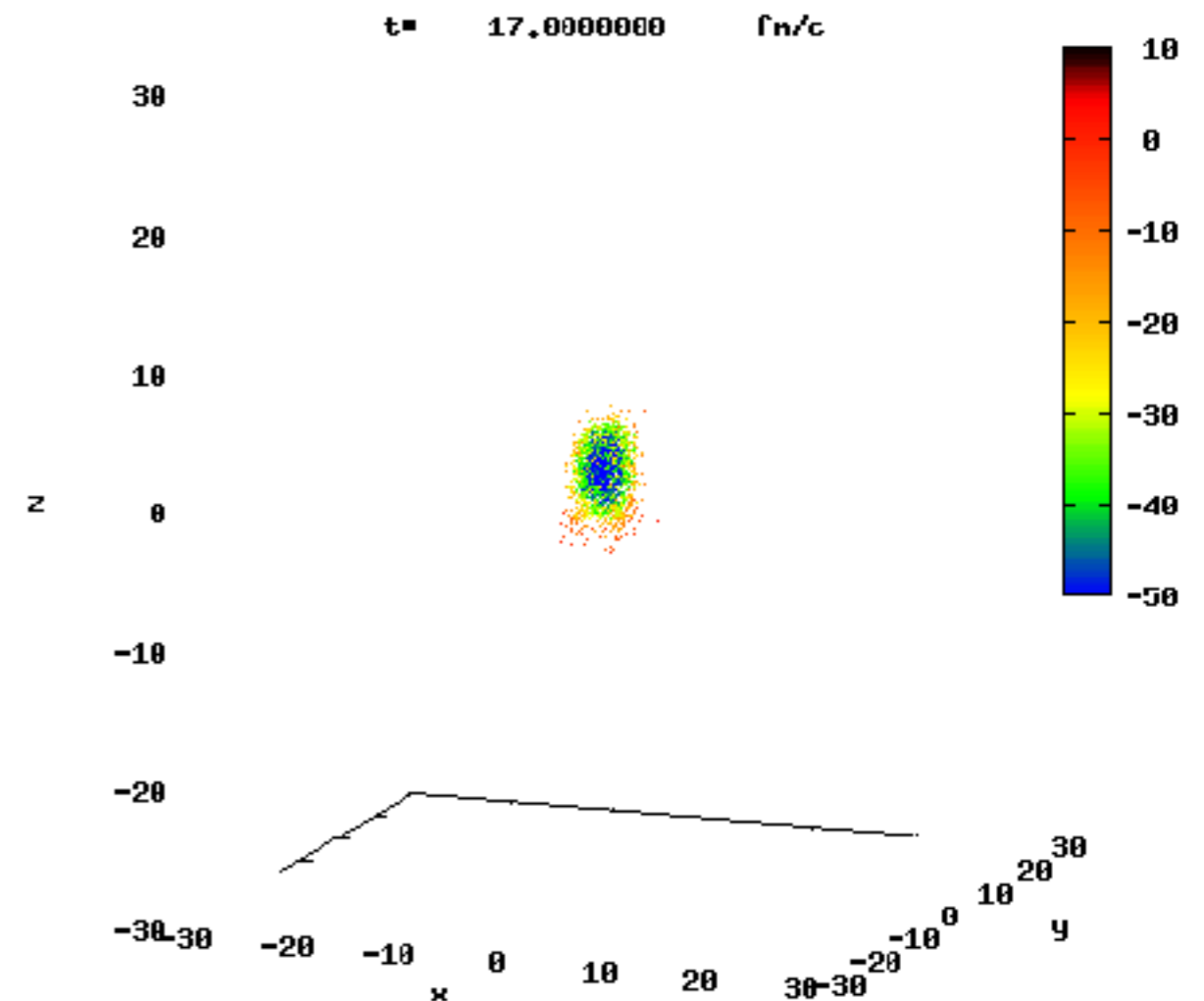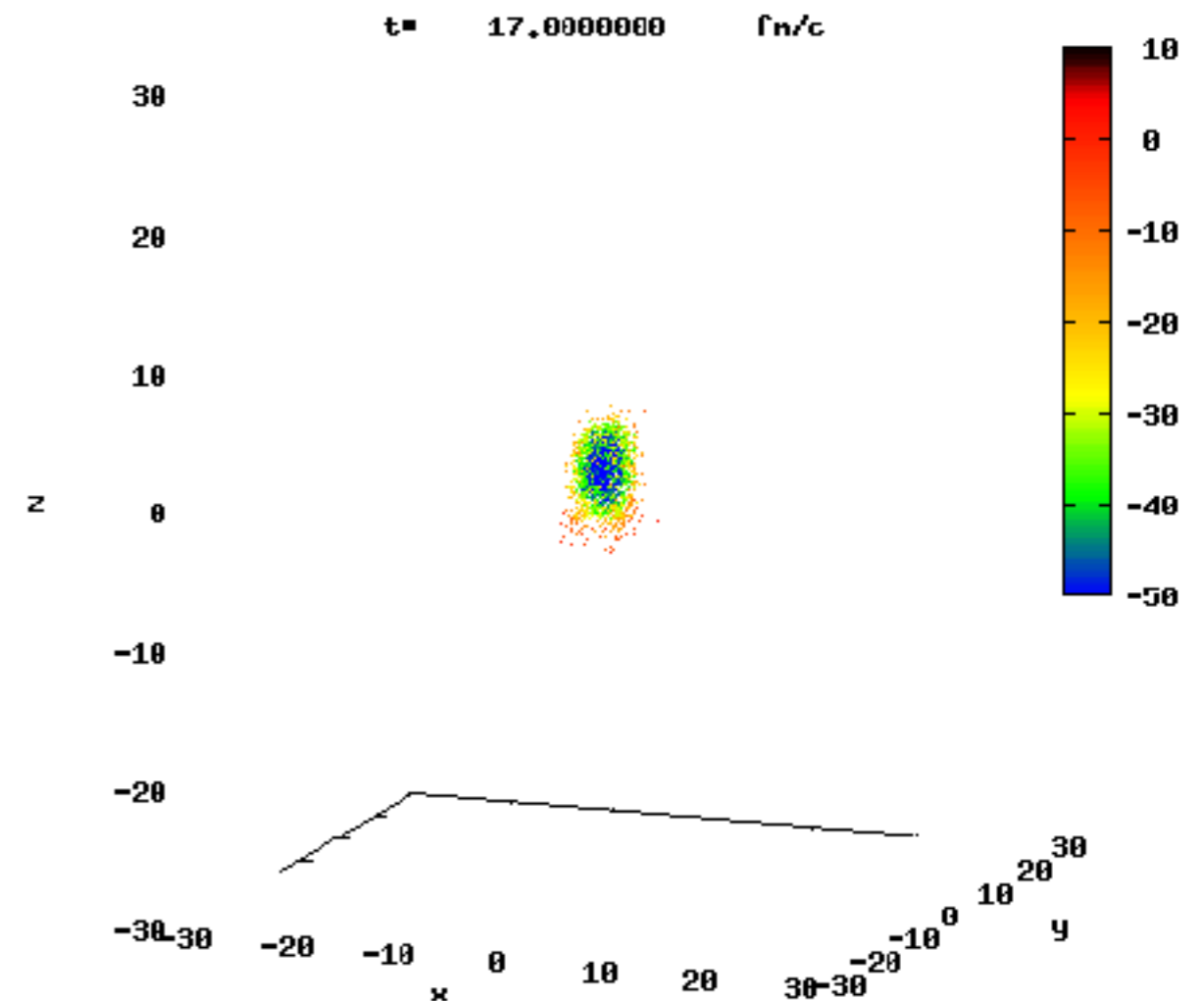- mean-field is self-consistent, depends on the density

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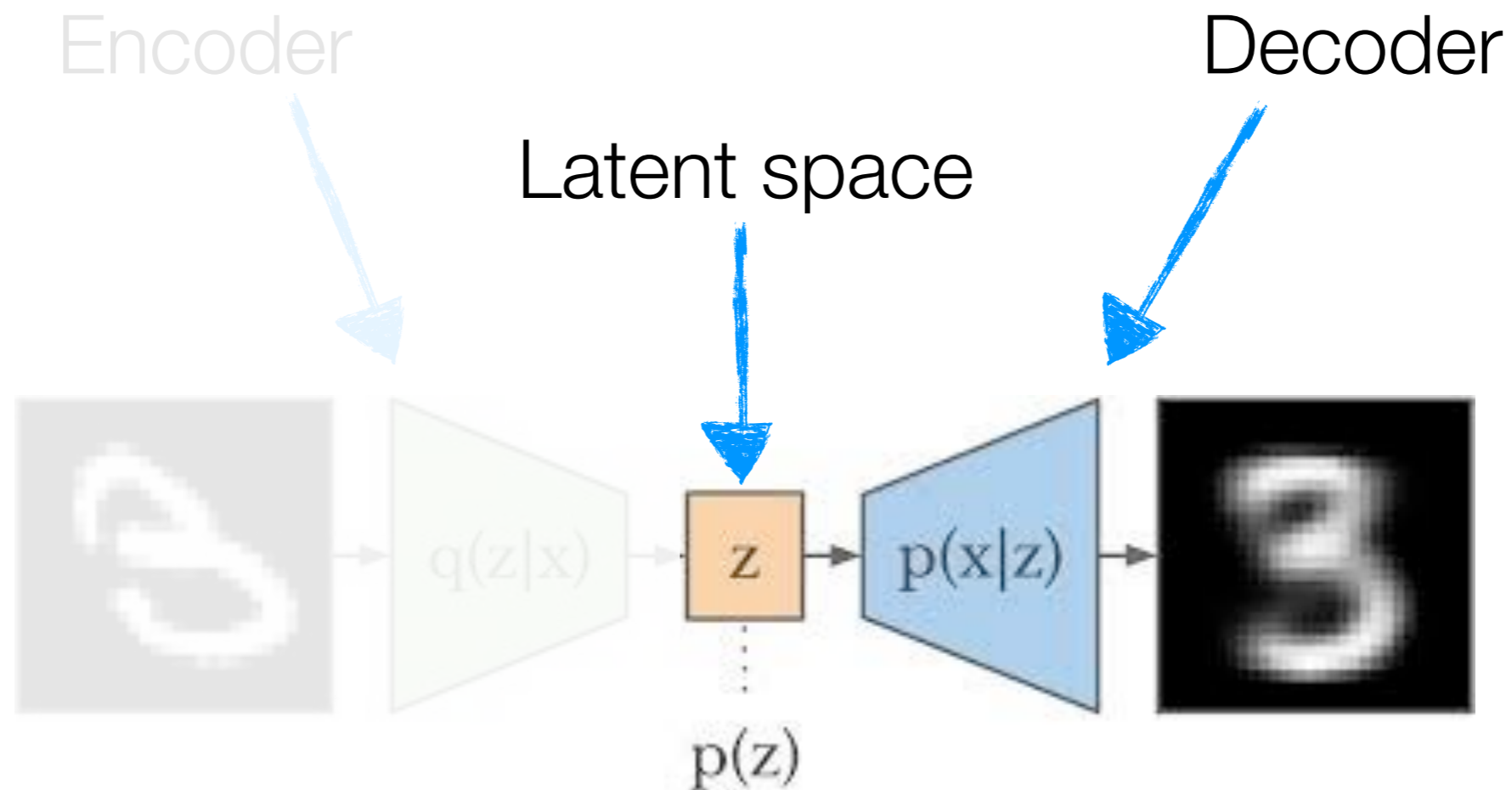- from which the physical state has to be sampled

Variational Auto Encoders

Encoder

Latent space

Decoder

$$q(z|x) \quad z \quad p(x|z)$$

$$p(z)$$
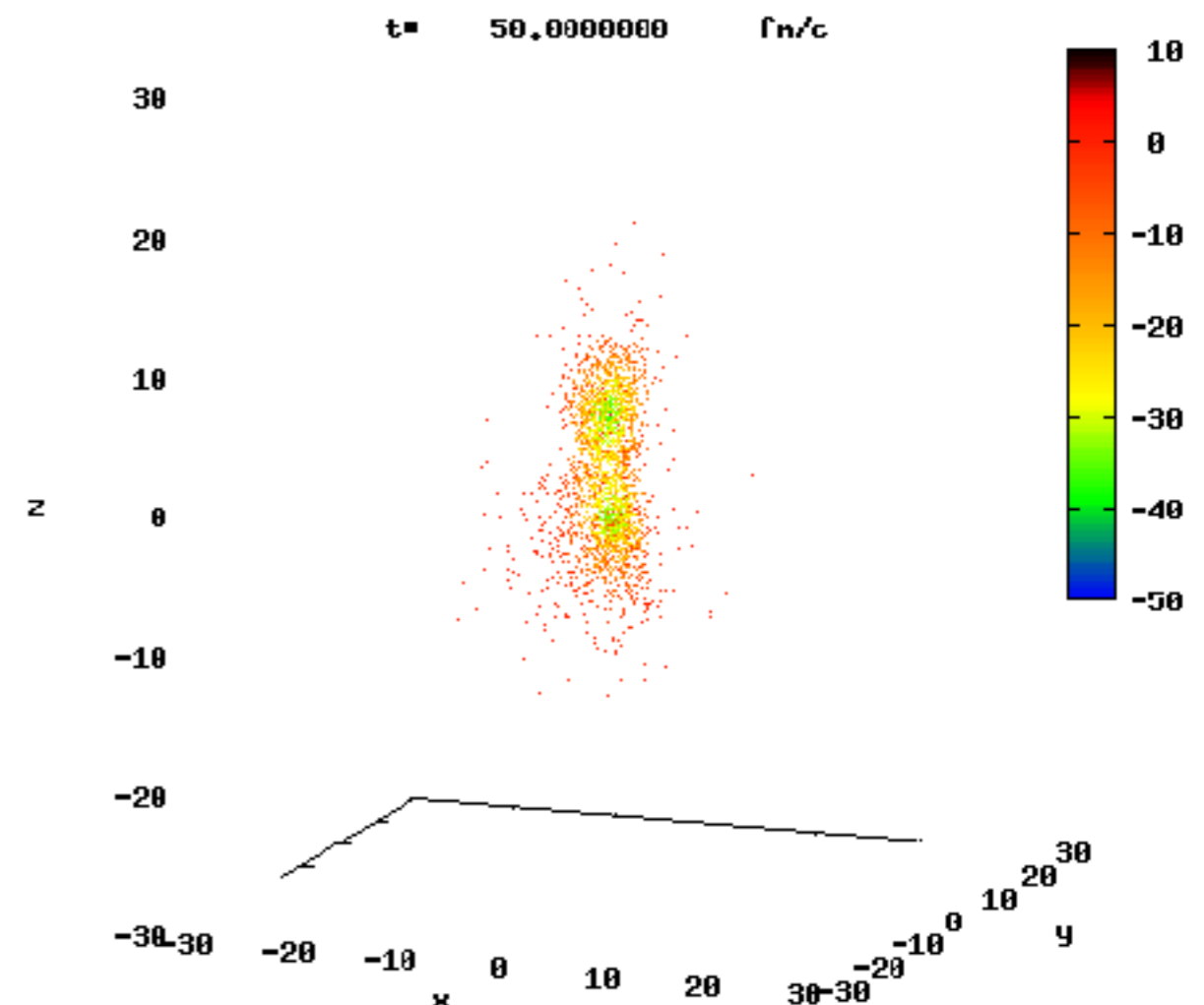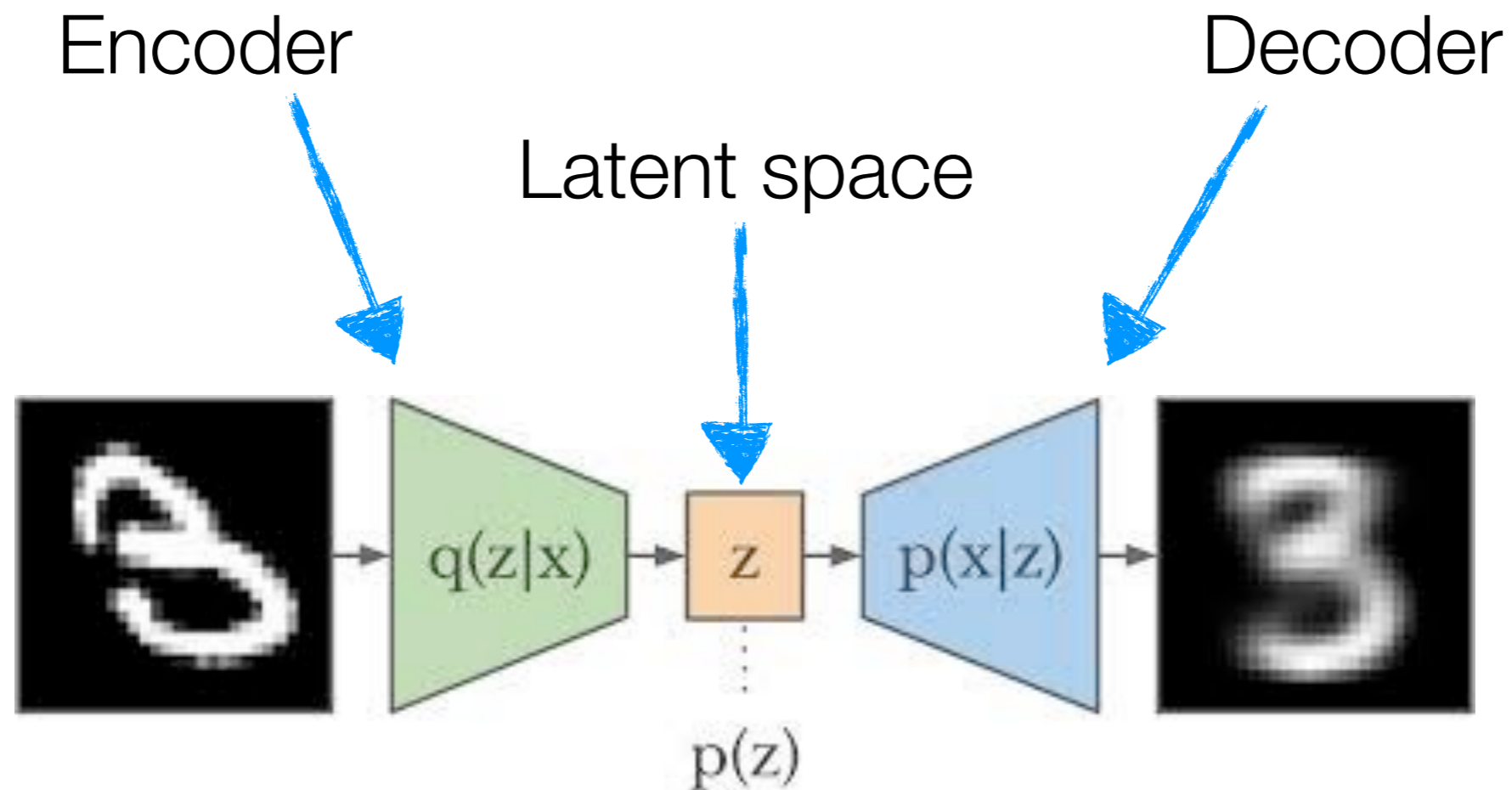
- Train an identity function

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
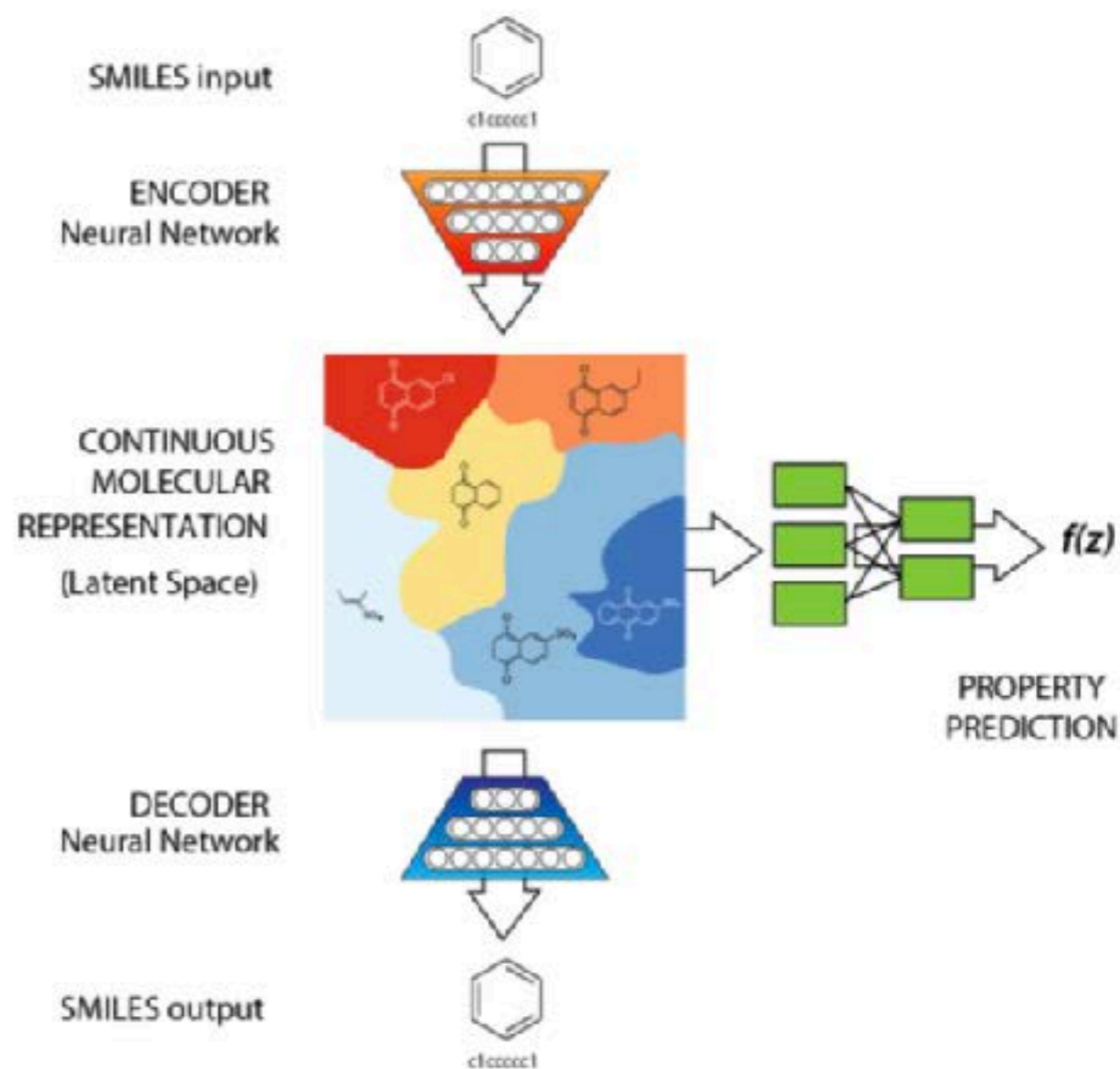
Conditional VAE

- Convolutional 3D encoding

- Conditioned latent space

- Symmetric decoding
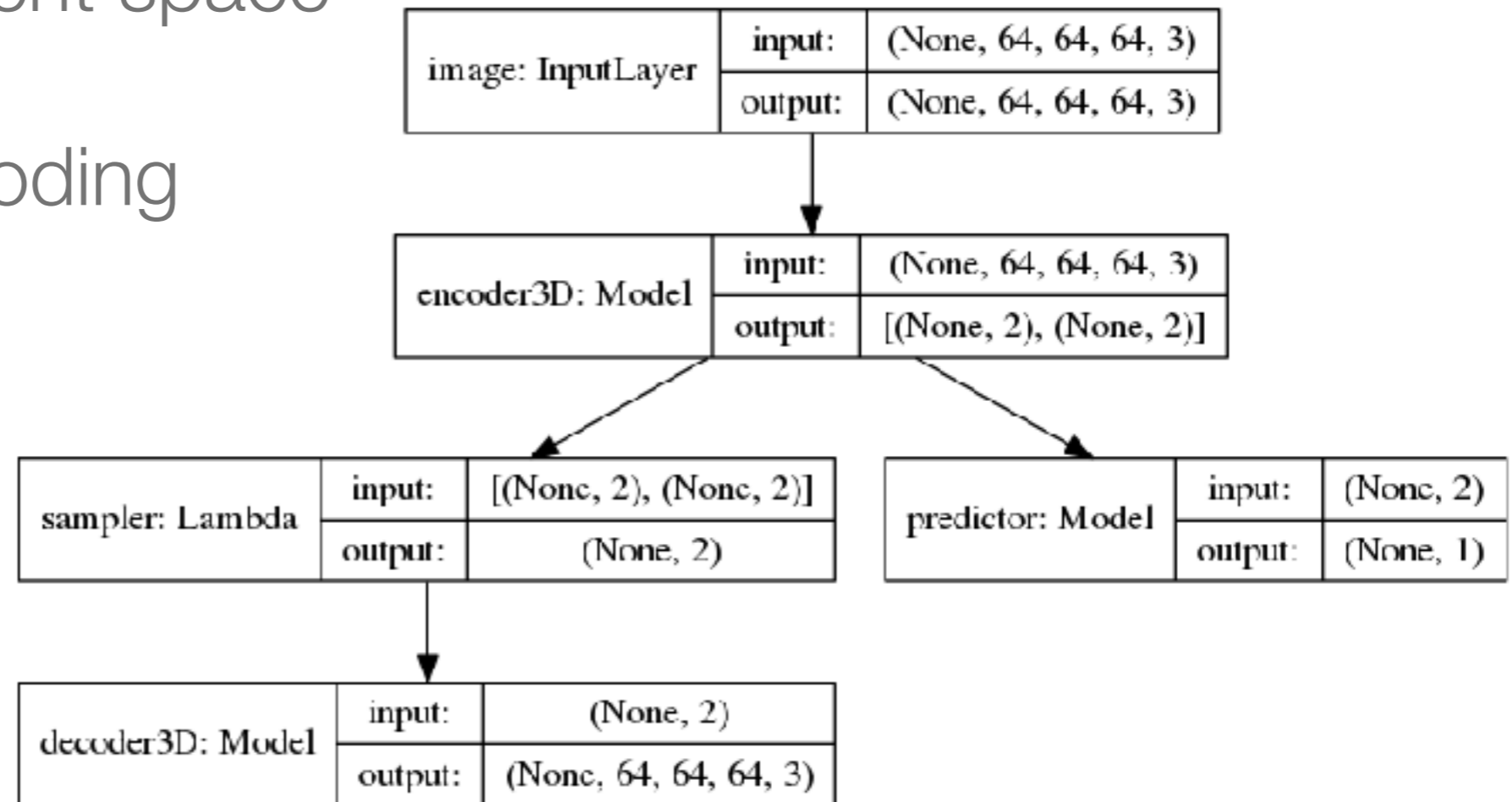
Training dataset

- 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

- 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):
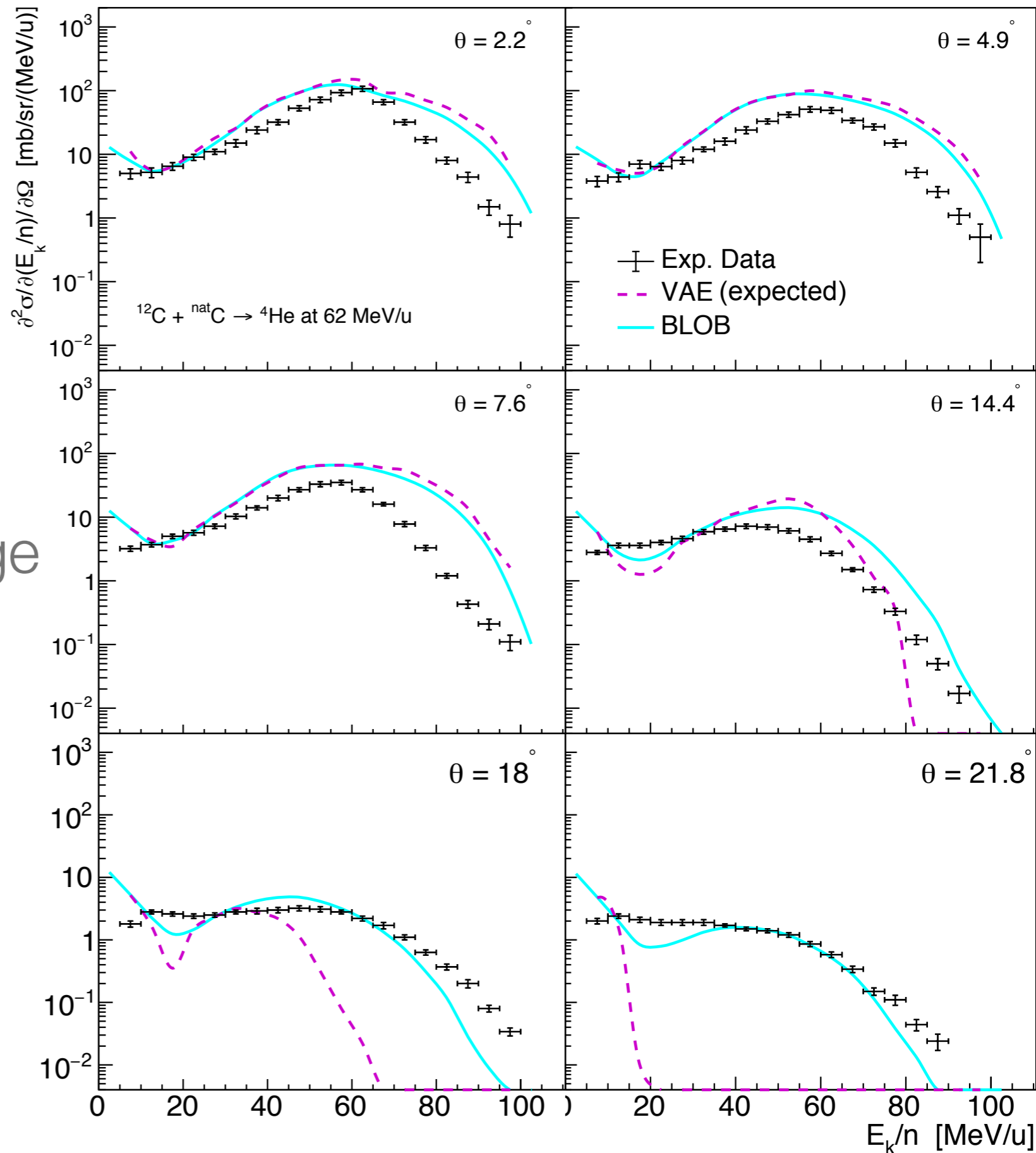
  - To use the color channels

16
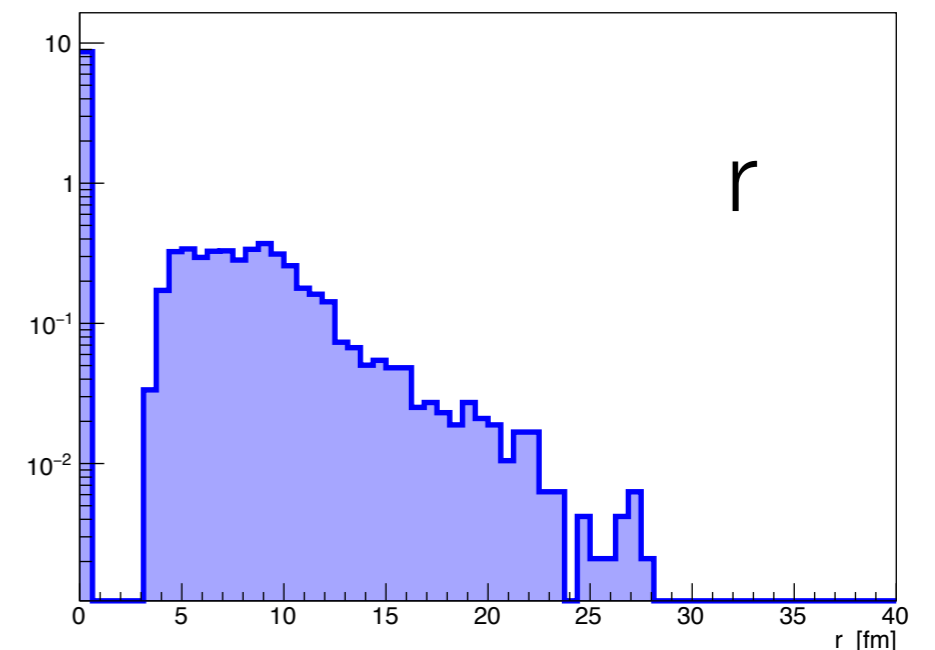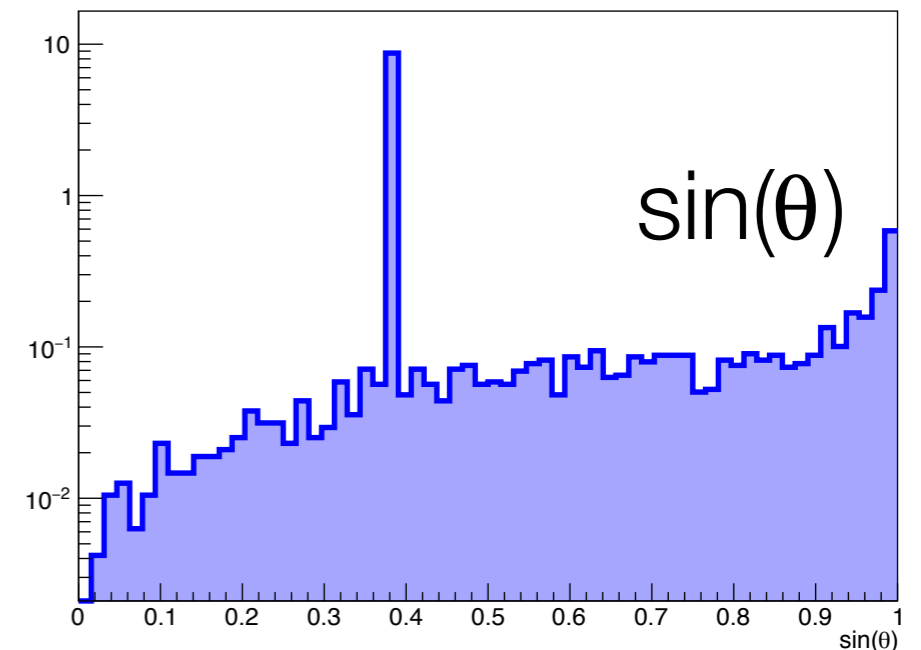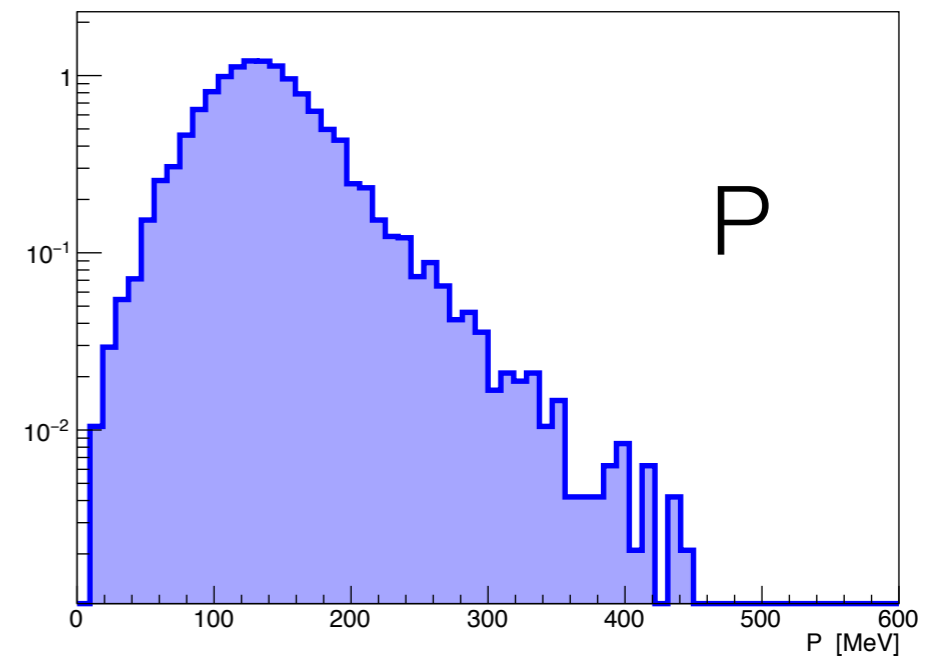
Reducing dimensionality

- Fragments are represented by 500*A particles

- P is sampled with gaussian distribution:

  - mean = P_{frag}

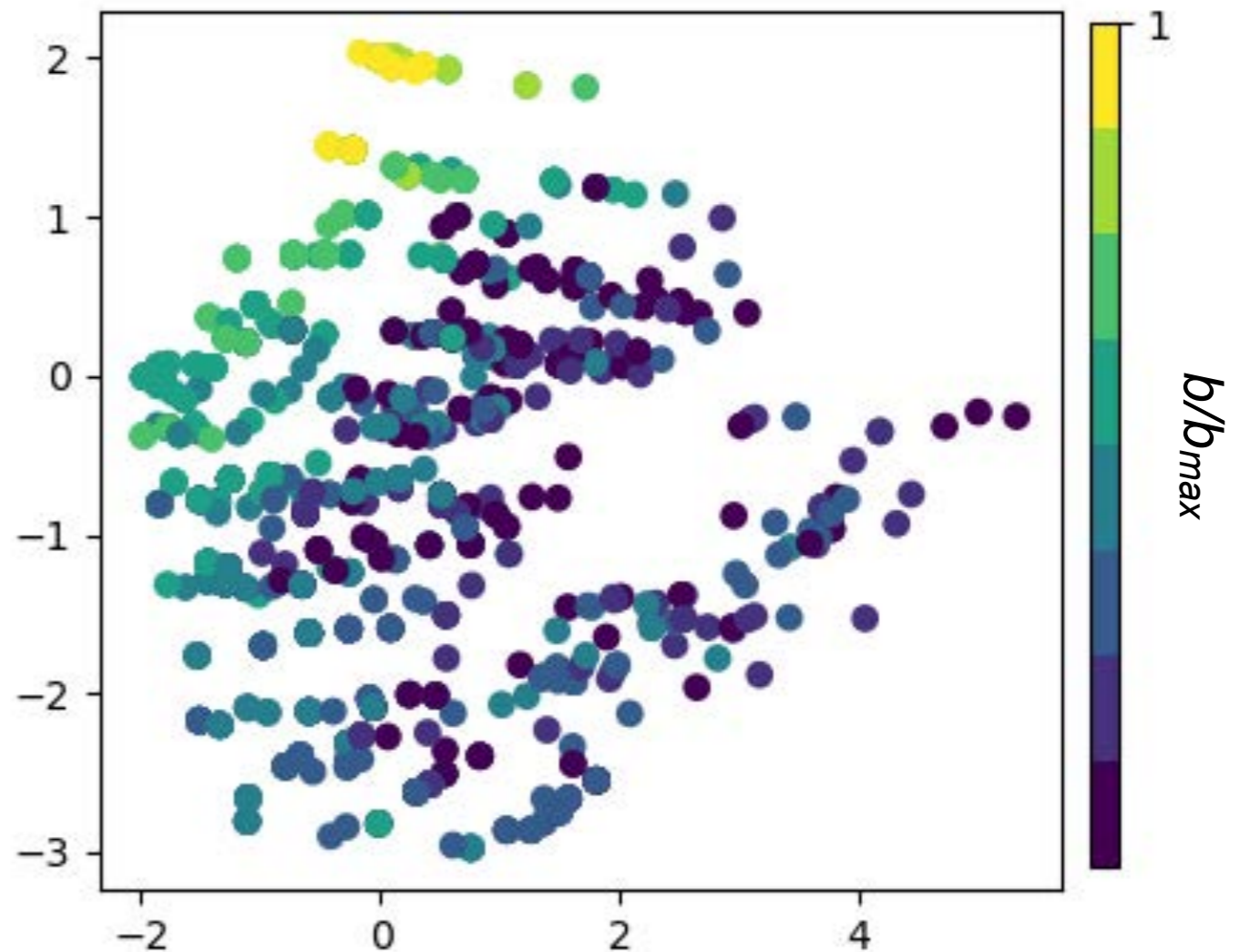 - sigma = Excitation energy

- All with the same θ

- r = 0
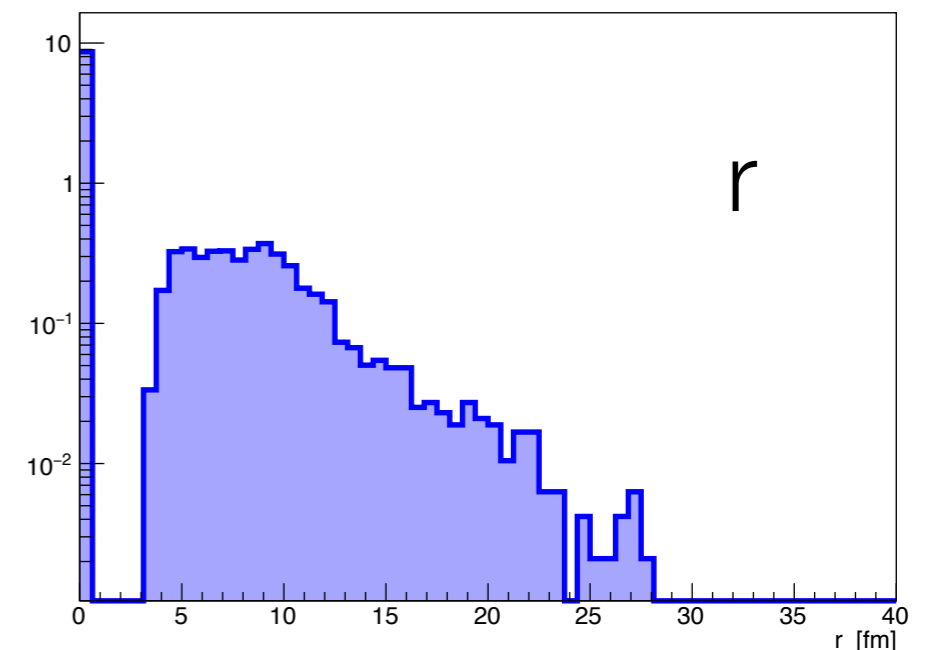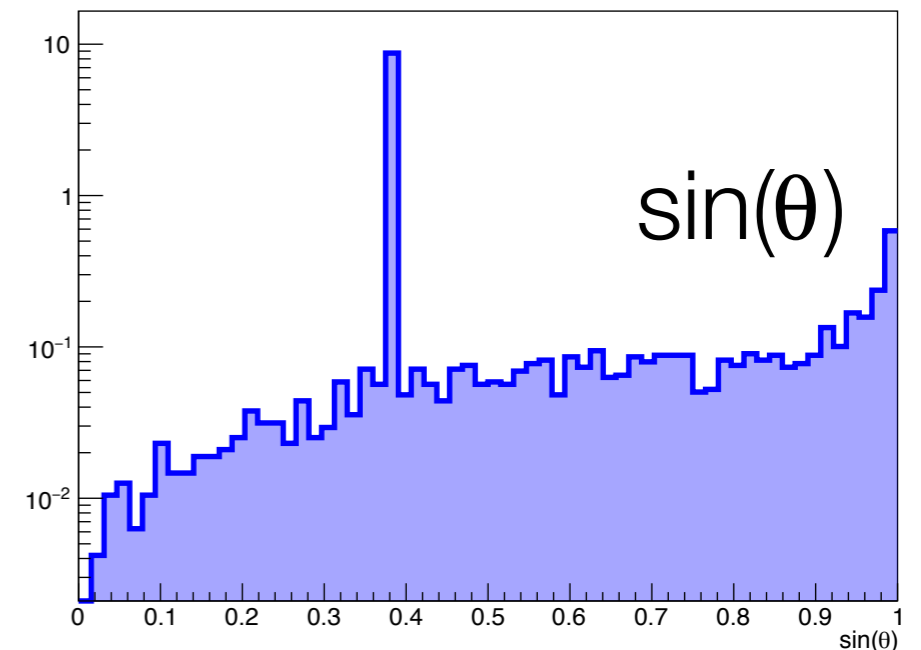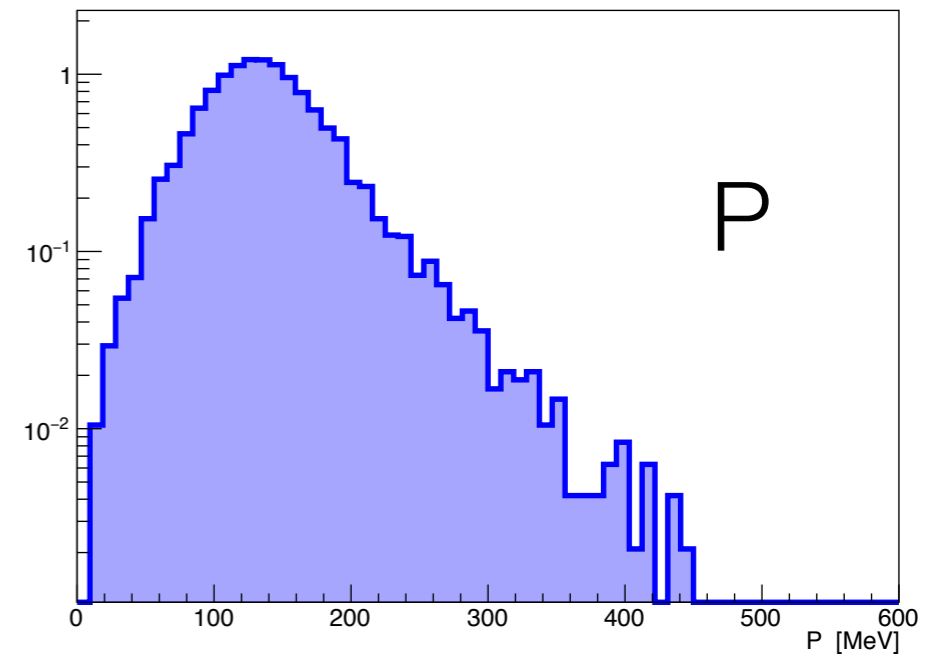
Testing reconstruction

- Fragments are identified selecting r<1 fm

- Momentum = average

- Excitation energy = variance

- θ = average


18

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
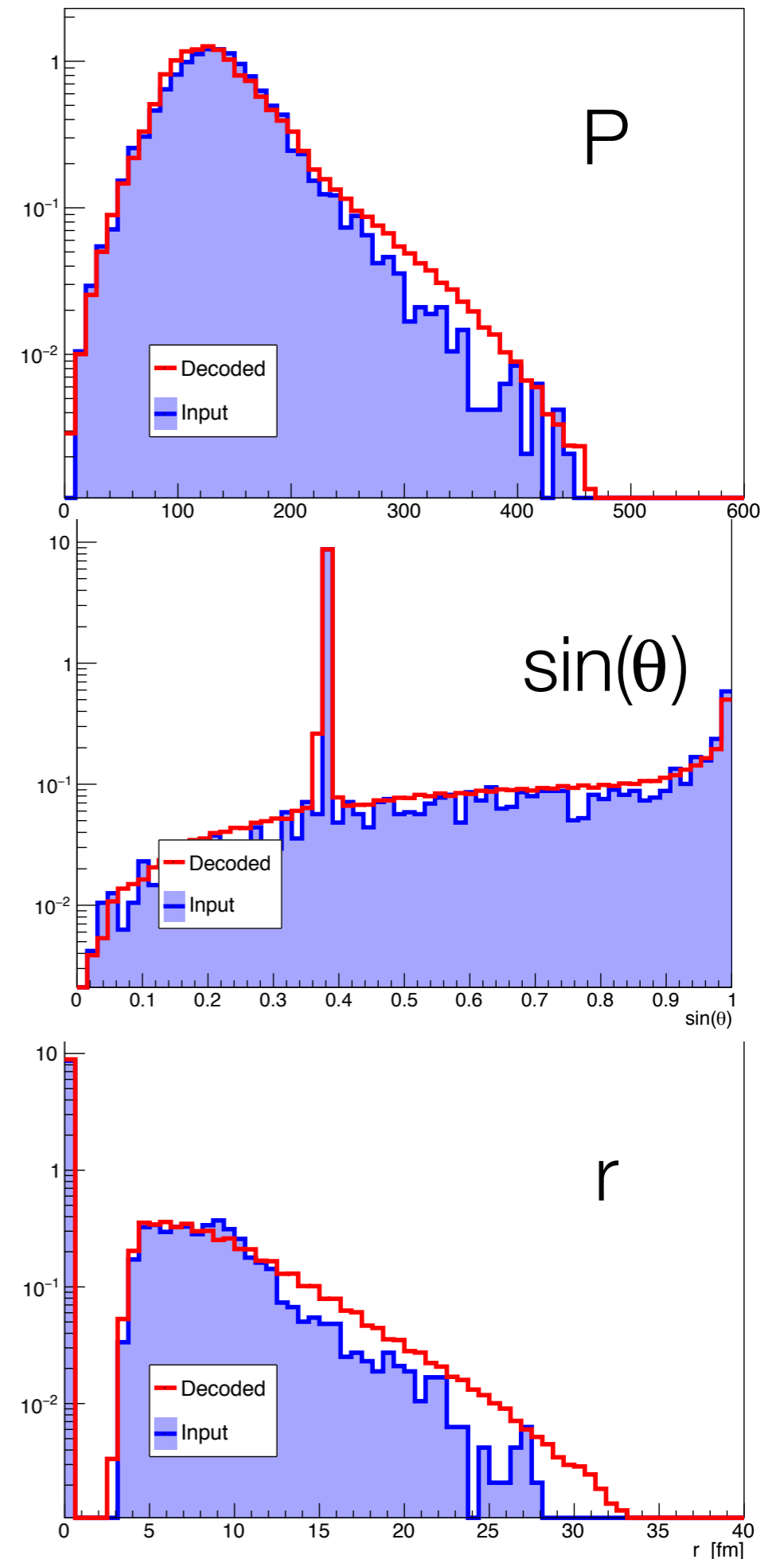
Preliminary results

- A paper with preliminary results has been submitted to Physica Medica

- *"Preliminary results in using Deep Learning to emulate BLOB, a nuclear interaction model"*

- We just submitted the revised version

Preliminary results in using Deep Learning to emulate BLOB, a nuclear interaction model

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[c]SLAC National Accelerator Laboratory, Menlo Park, United States
[d]National Center for Radiation Protection and Computational Physics,
Istituto Superiore di Sanità, Italy
[e]INFN, Laboratori Nazionali del Sud, Catania, Italy
[f]IPN, CNRS/IN2P3, Université Paris-Sud 11, Université Paris-Saclay, 91406 Orsay Cedex, France

Abstract

Purpose: A reliable model to simulate nuclear interactions is fundamental for Ion-therapy. We already showed how BLOB ("Boltzmann-Langevin One Body"), a model developed to simulate heavy ion interactions up to few hundreds of MeV/u, could simulate also ^{12}C reactions in the same energy domain. However, its computation time is too long for any medical application. For this reason we present the possibility of emulating it with a Deep Learning algorithm.

Methods: The BLOB final state is a Probability Density Function (PDF) of finding a nucleon in a position of the phase space. We discretised this PDF and trained a Variational Auto-Encoder (VAE) to reproduce such a discrete PDF. As a proof of concept, we developed and trained a VAE to emulate BLOB in simulating the interactions of ^{12}C with ^{12}C at 62 MeV/u. To have more control on the generation, we forced the VAE latent space to be organised with respect to the impact parameter (b) training a classifier of b jointly with the VAE.

Results: The distributions obtained from the VAE are similar to the input ones and the computation time needed to use the VAE as a generator is negligible.

Conclusions: We show that it is possible to use a Deep Learning approach to emulate a model developed to simulate nuclear reactions in the energy range of interest for Ion-therapy. We foresee the implementation of the generation part in C++ and to interface it with the most used Monte Carlo toolkit: Geant4.

Keywords: Monte Carlo simulations, Deep Learning, Nuclear reactions, Ion-therapy, Hadron-therapy,

1. Introduction

Ion-therapy is a technique that aims at treating tumour deeply located in the patient body exploiting the ions characteristic dose deposition shape, with the peak at the end of their range, the so-called Bragg peak. It is performed mainly with protons but also with heavier ions, like ^{12}C.

Having reliable nuclear fragmentation models in MC simulation toolkits is of utmost importance for Ion-therapy [1] as they are considered the gold standard for dosimetric calculations [2]; they are used to generate the input parameters of the treatment planning algorithms [3] and to validate the dose calculation of such algorithms, especially in cases with large tissue heterogeneities [4]. Finally, a large effort is ongoing to develop detectors to measure the radiation emitted during the treatment to allow a non-invasive on-line monitoring of the treatment itself, see for instance [5–8], and MC calculations are needed to infer the delivered dose from the observed spectra [9, 10]

Geant4 [11] is one of the most widely used MC toolkits, also for medical applications. It is written in C++ and takes ad-

vantage of its object-oriented coding paradigm. Geant4 also exploits the multithread capabilities of C++11, allowing an efficient use of modern CPUs. It is developed by a large international collaboration and distributed with an open source licence, which allows also to develop wrappers around it. In the last years many programs dedicated to MC medical simulations have been developed wrapping Geant4, and then using its Physics models, such as GATE [12], GAMOS [13], and TOPAS [14]. The latter in particular is dedicated to Ion-therapy simulations.

Finally, Geant4 has the capability to simulate the body of a specific patient importing his Computed Tomography (CT) scan in DICOM format [15].

Many critical aspects must be taken into account when modelling the therapeutic ion beams, e.g. although elastic and multiple Coulomb scattering events are negligible for charged particles, they contribute to dosimetric uncertainty especially in oncological applications, because they cause beam widening [16]. However, one of the main uncertainties comes from nuclear interaction models. Moreover, while there are several models for electromagnetic interactions in the Geant4 package [17–19], there is no dedicated model to describe inelastic nuclear reac-