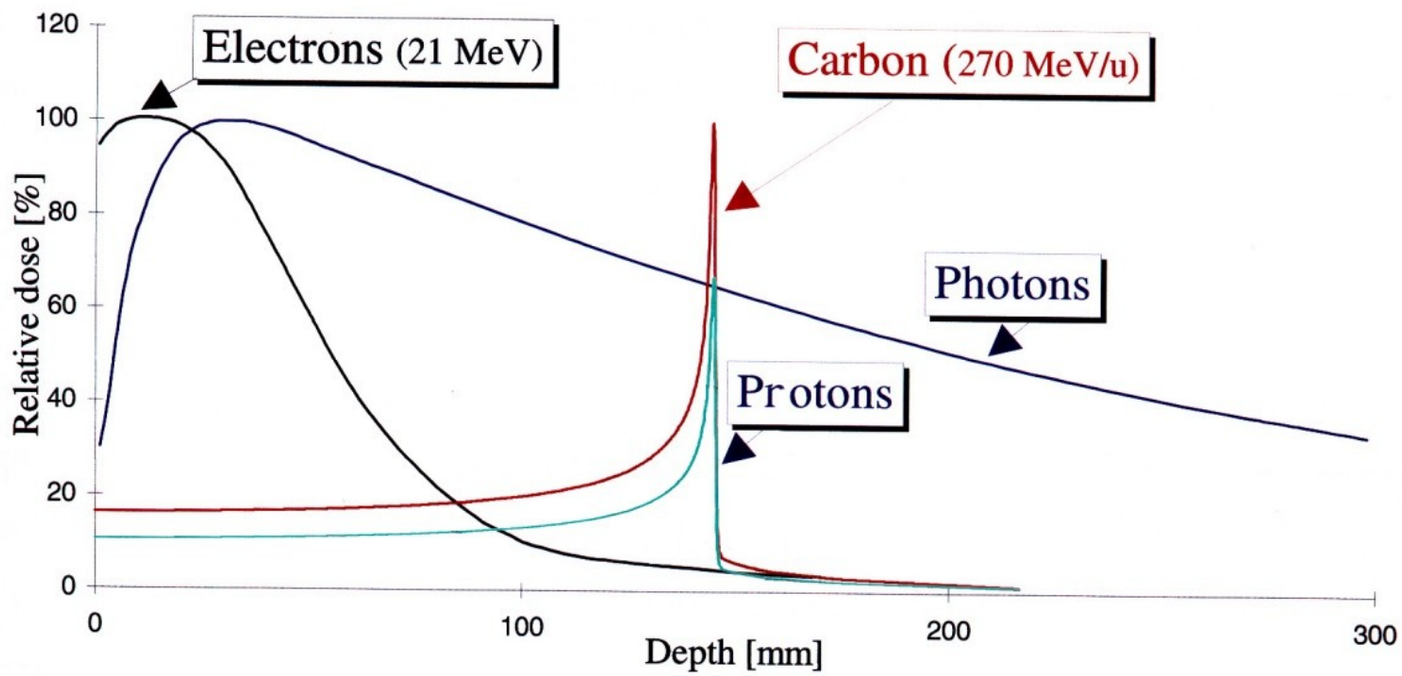
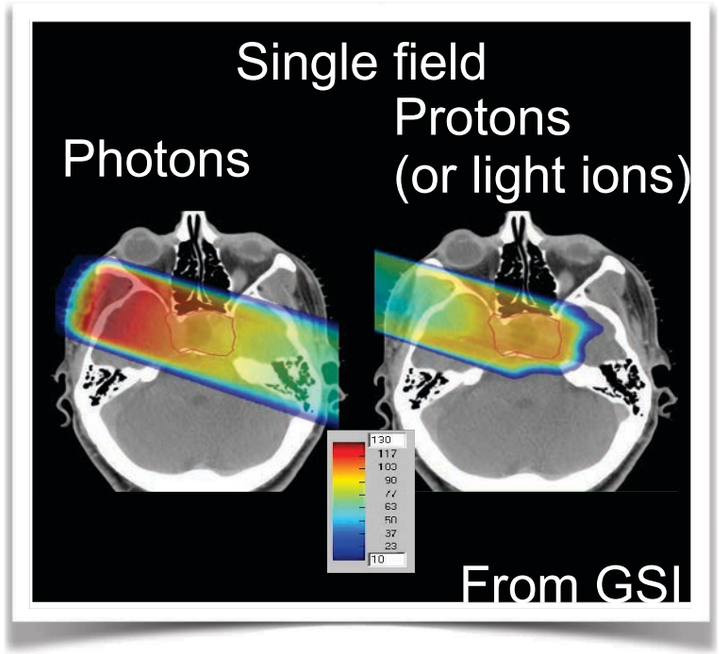
Deep Learning and Monte Carlo simulations, opportunities and challenges

carlo.mancini-terracciano@uniroma1.it

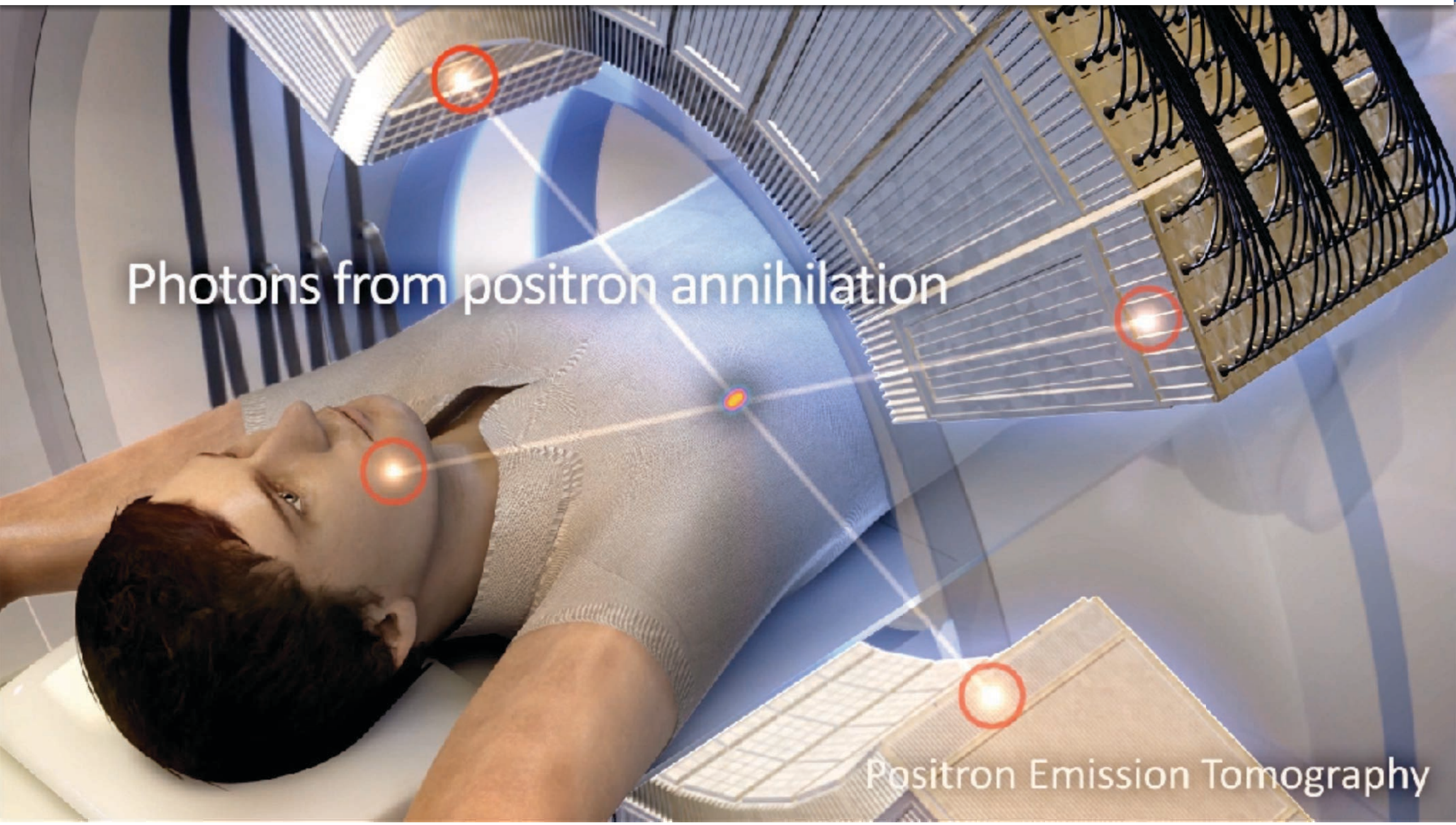
TECH-FPA PhD Retreat
LNGS - 18th February 2025

Radiotherapy





- Radiotherapy is, together with surgery, the most frequently used treatment for tumours



- The MC simulation is necessary to link the information
- The PCS is dispensable to link the information
- The PCS is necessary to link the information
- The MC simulation is dispensable to link the information

distribution with the dose distribution

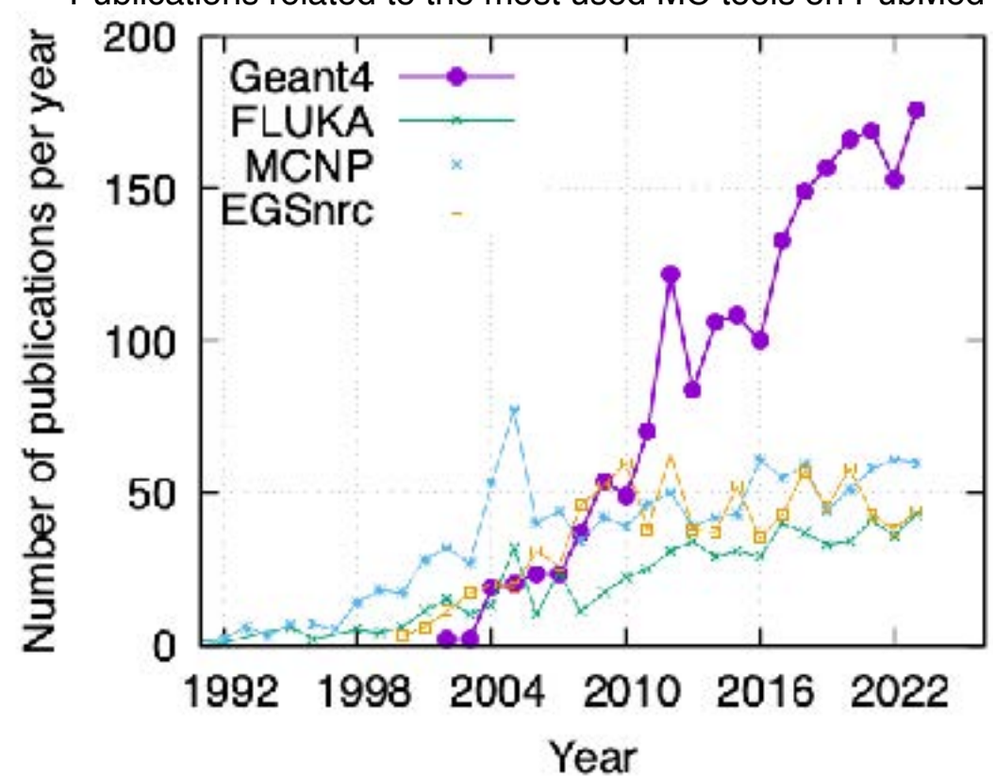
Geant4 (GEometry ANd Traking)

- Developed by an international collaboration
- Open source
- Written in C++ language
  - Takes advantage from the Object Oriented approach
  - It is multithread
- The most used MC tool for research in medical applications

[Geant4, a simulation toolkit Nucl. Inst. and Methods Phys. Res. A, 506 250-303

Geant4 developments and applications Transaction on Nuclear Science 53, 270-278]

Publications related to the most used MC tools on PubMed



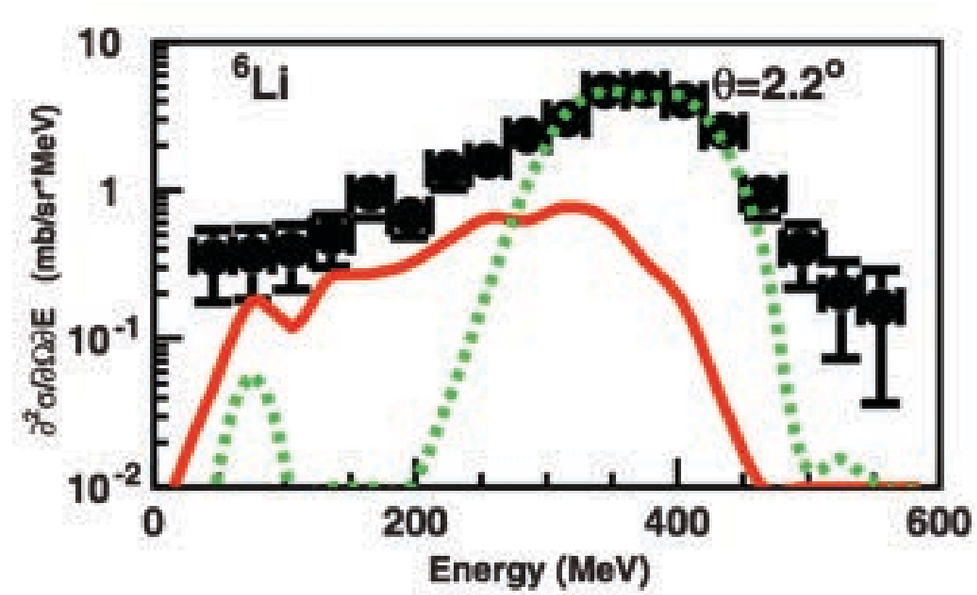
Problems in Geant4 below 100 MeV/u

- 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**

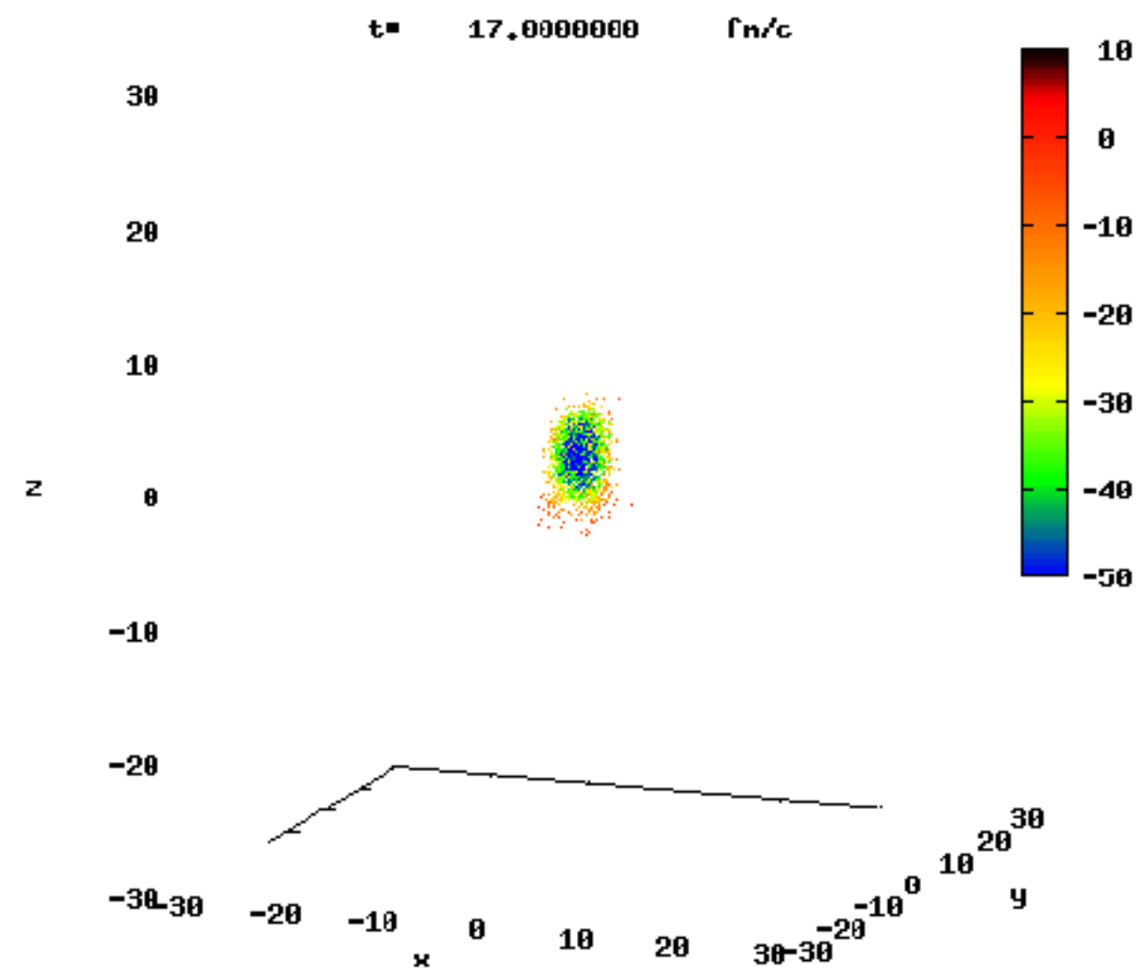
[Plot from De Napoli et al. Phys. Med. Biol., vol. 57, no. 22, pp. 7651–7671, Nov. 2012]



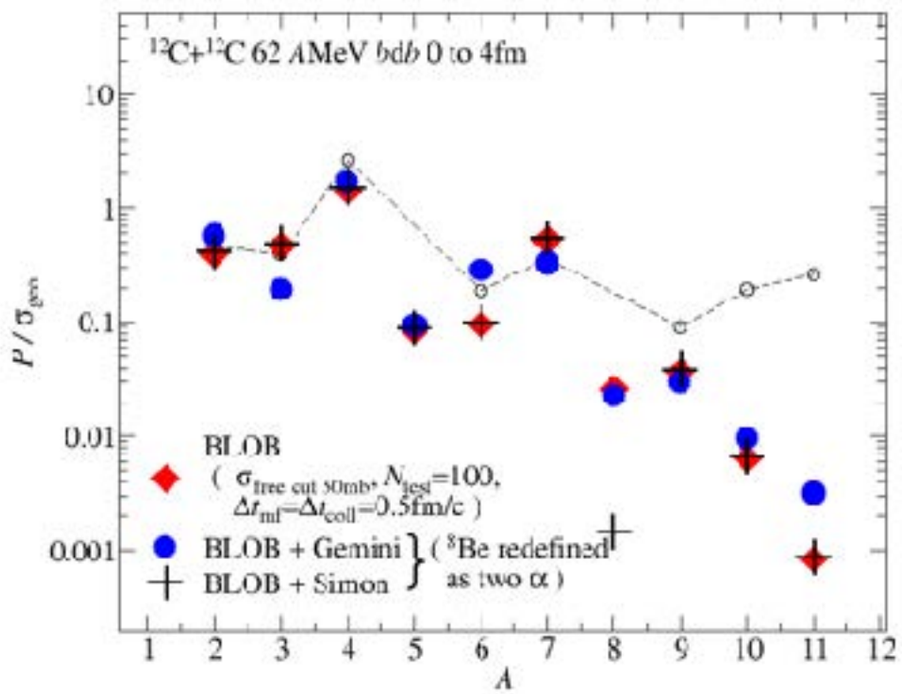
Cross section of the ^{6}Li production at 2.2 degree in a ^{12}C on ^{nat}C reaction at 62 MeV/u.

BLOB (Boltzmann-Lagevein One Body)

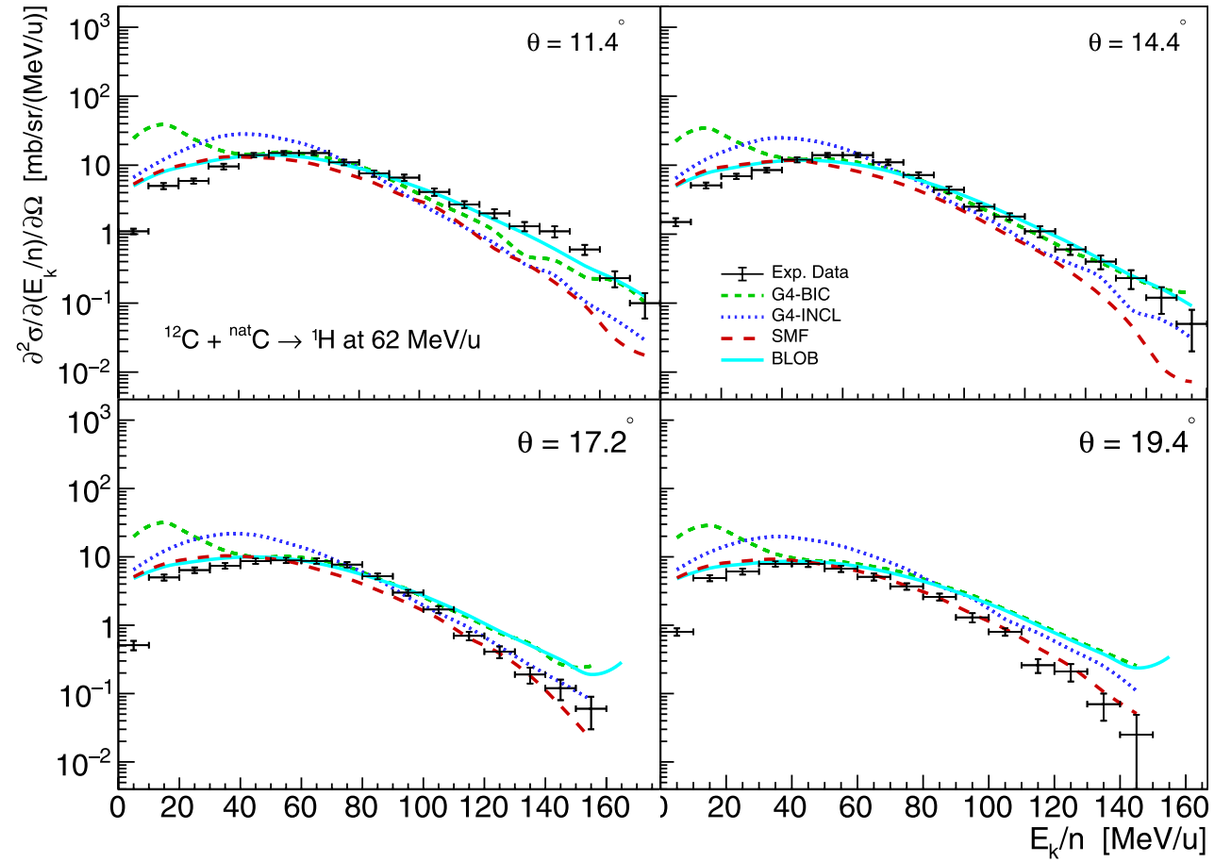
- Describes the time evolution of the density distribution
- Test-particle approach
- Self-consistent mean field + 2-body collisions
- Probability to find a nucleon in the phase space

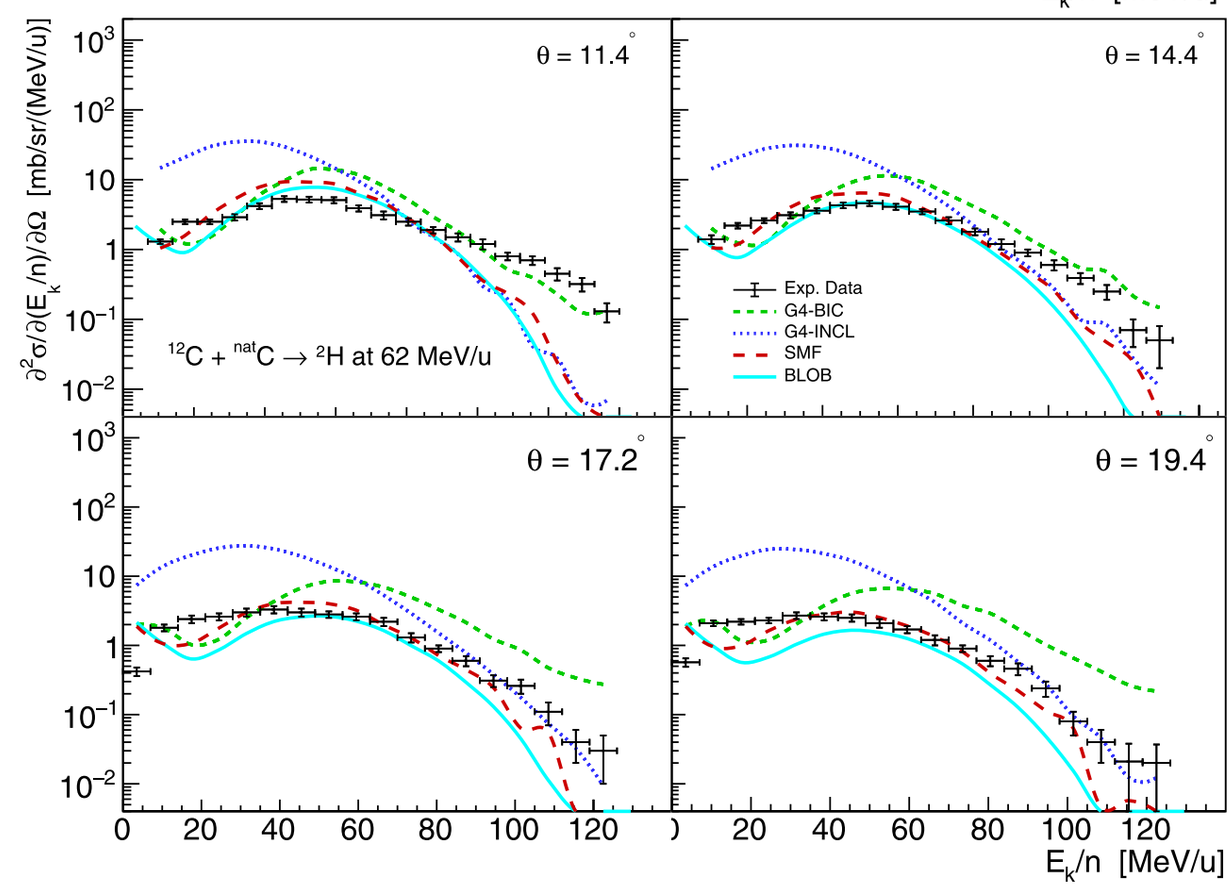


BLOB and Geant4



[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]





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BLOB Code optimisations

- We optimised BLOB without changing the code structure (52% speed-up overall)
- Not enough for practical applications

Elapsed Time: 231.966s

CPU Time:	231.930s
Total Thread Count:	1
Paused Time:	0s

Top Hotspots

This section lists the most active functions in your application. Optimizing these hotspot functions typically results in improving overall application performance.

Function	Module	CPU Time
lapla	run-orig	176.281s
erff	libm.so.6	17.201s
define_two_clouds_rp	run-orig	9.658s
sortrx	run-orig	7.018s
powf	libm.so.6	5.377s
[Others]		16.403s

Elapsed Time: 110.235s

CPU Time:	110.223s
Total Thread Count:	1
Paused Time:	0s

Top Hotspots

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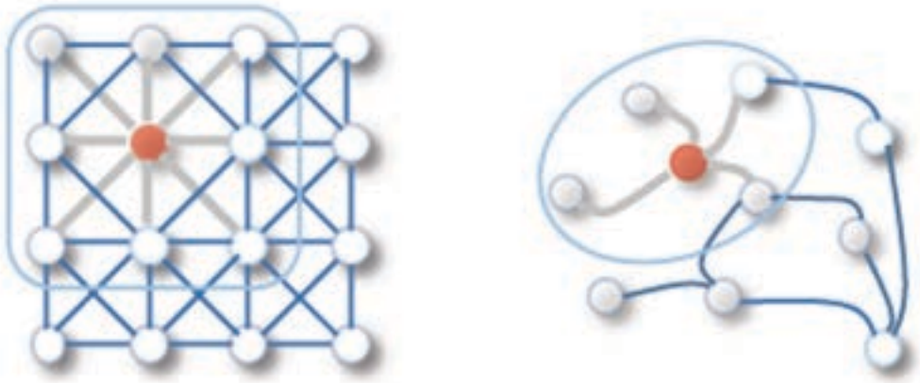
Function	Module	CPU Time
lapla	run	55.003s
erff	libm.so.6	17.038s
define_two_clouds_rp	run	9.051s
sortrx	run	7.450s
powf	libm.so.6	5.184s
[Others]		15.414s

Graph Network-based Simulators (GNS)

- We tested the possibility of emulating the whole interaction (i.e. producing the final state) using Graph CNN

- Encode graph-structured data

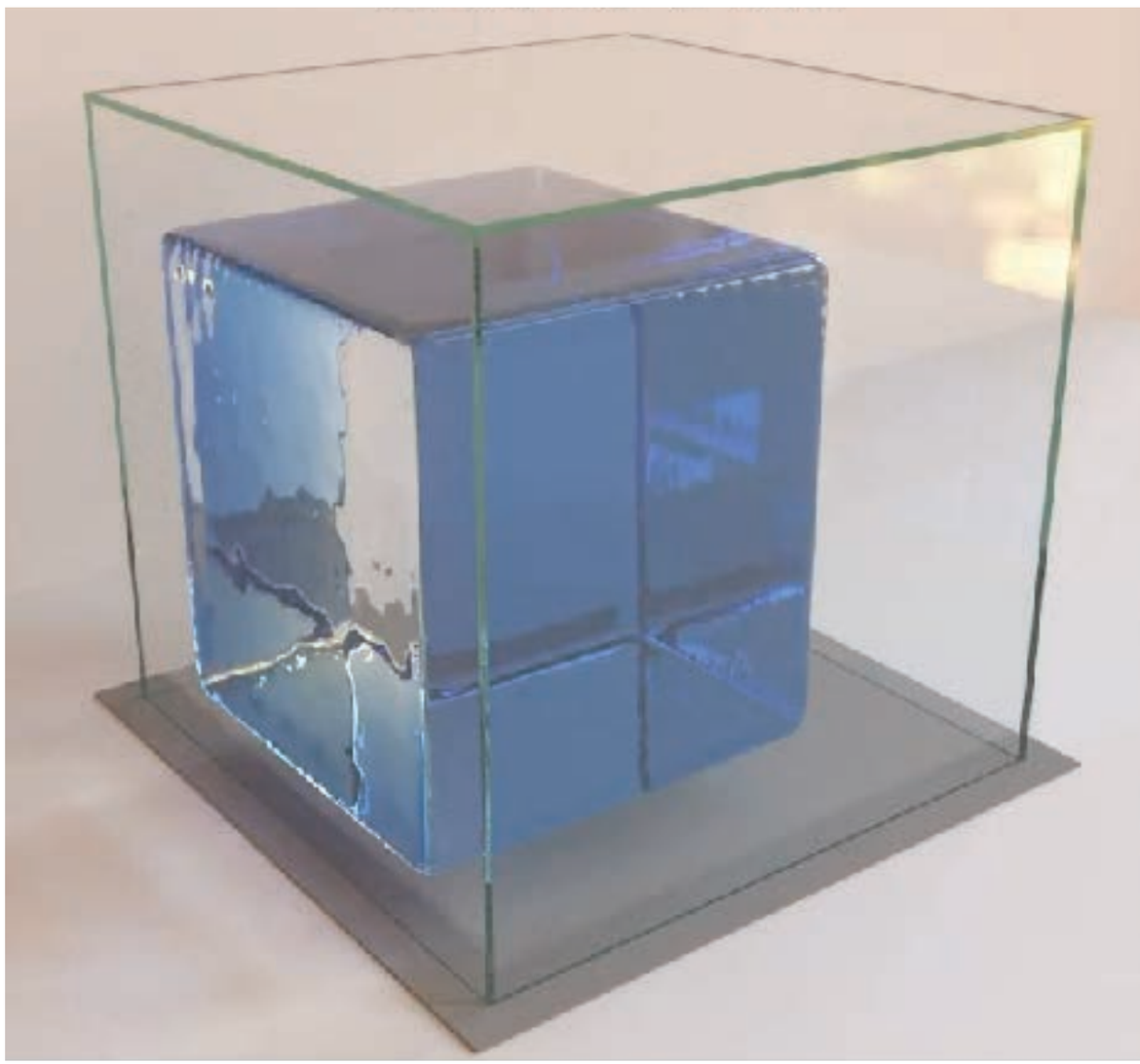


- Use of topological relationships among nodes

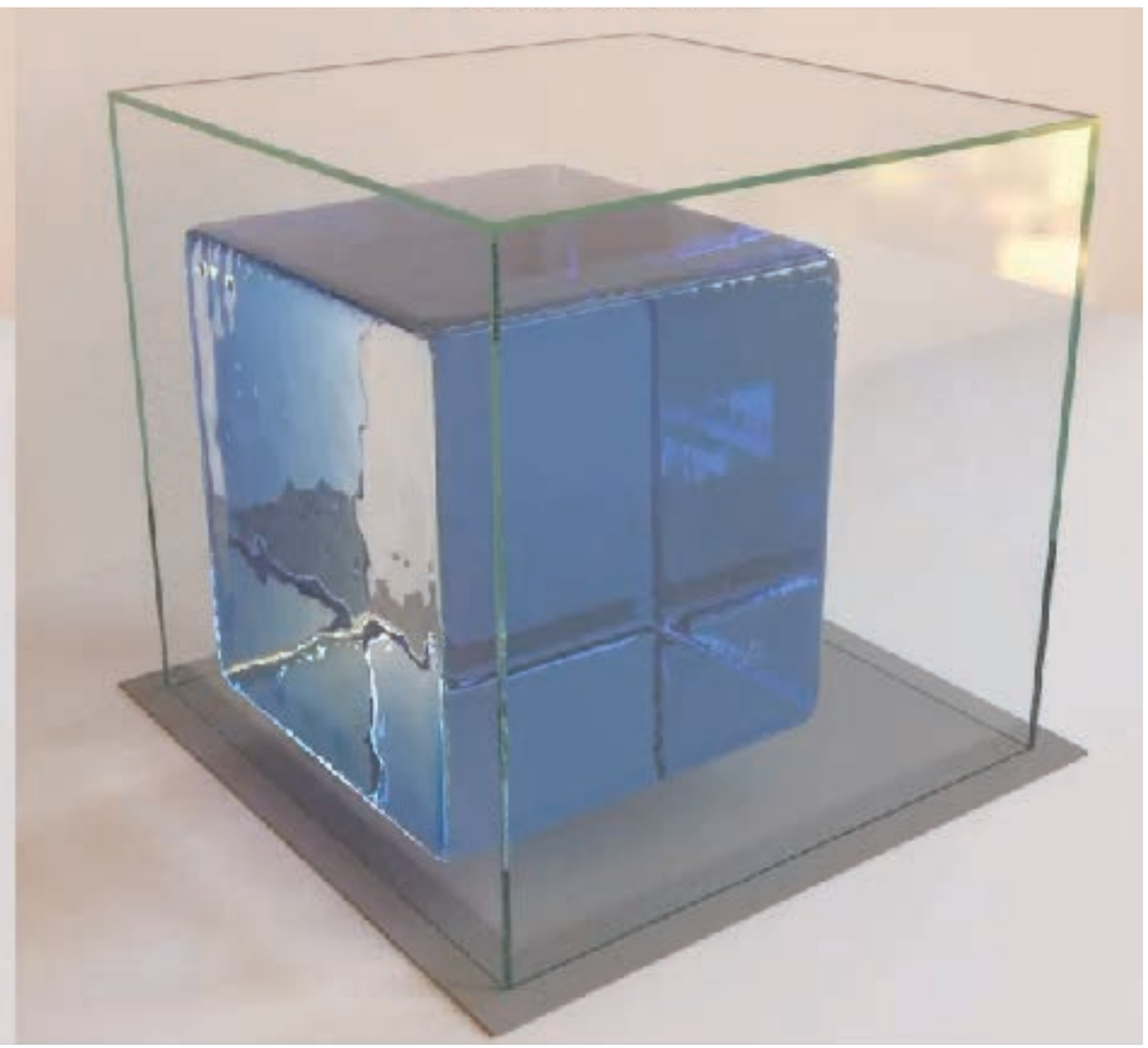
- Convolve the central node's representation with its neighbours' representations

Graph Network-based Simulators (GNS)

Ground truth



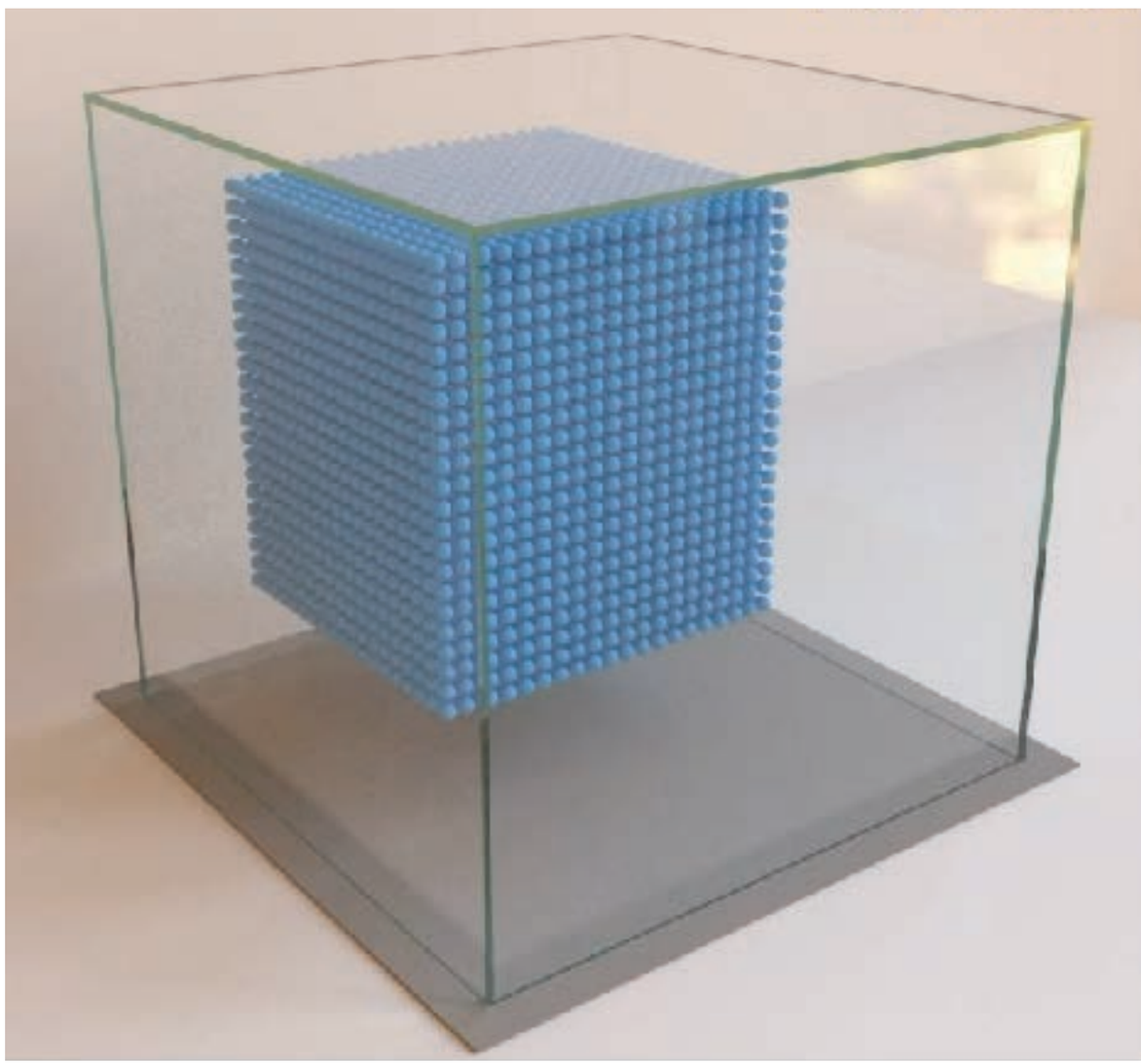
GNS



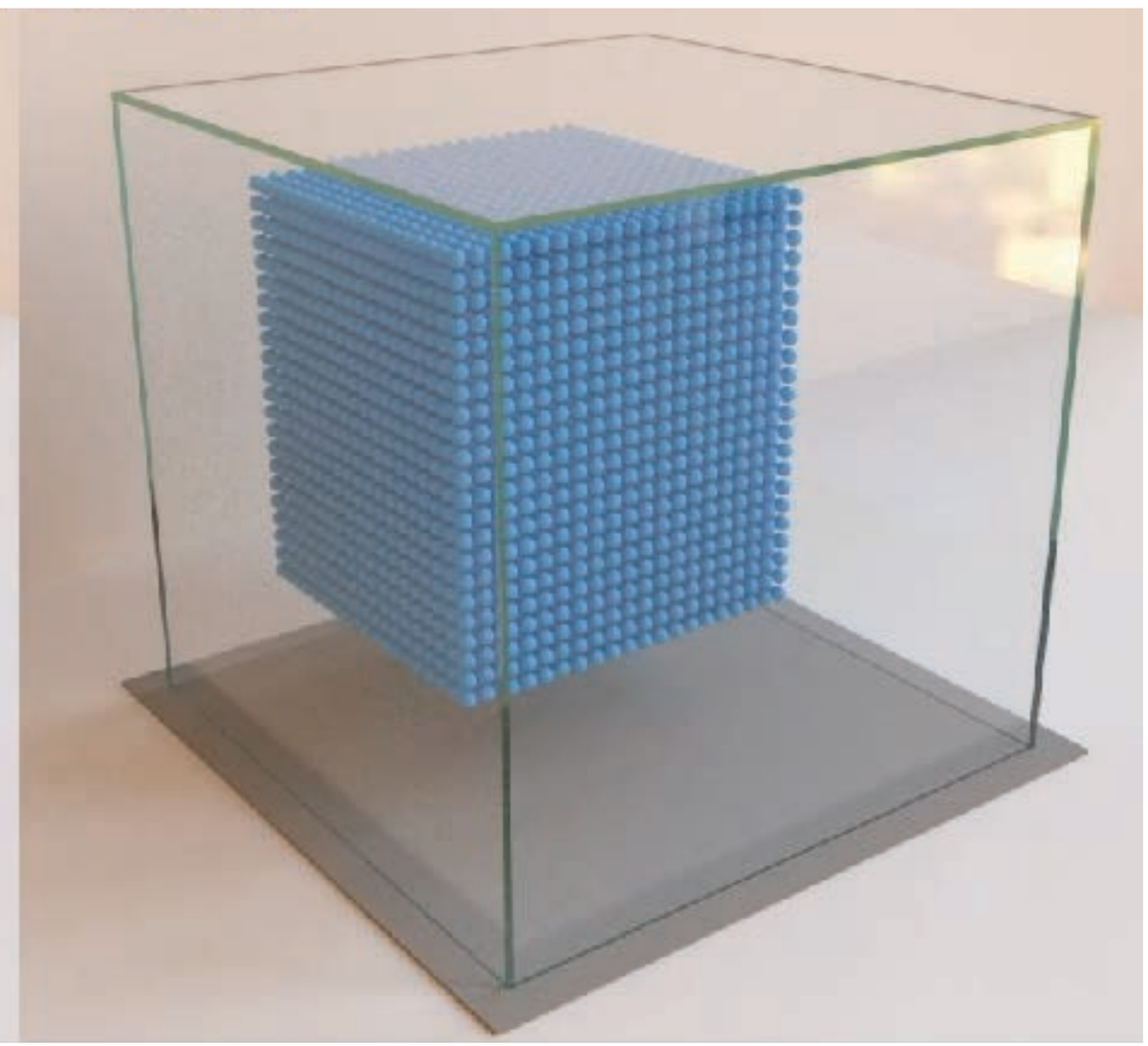
[A. Sanchez-Gonzalez et al. "Learning to simulate complex physics with graph networks." International Conference on Machine Learning. PMLR, 2020.]

Graph Network-based Simulators (GNS)

Ground truth



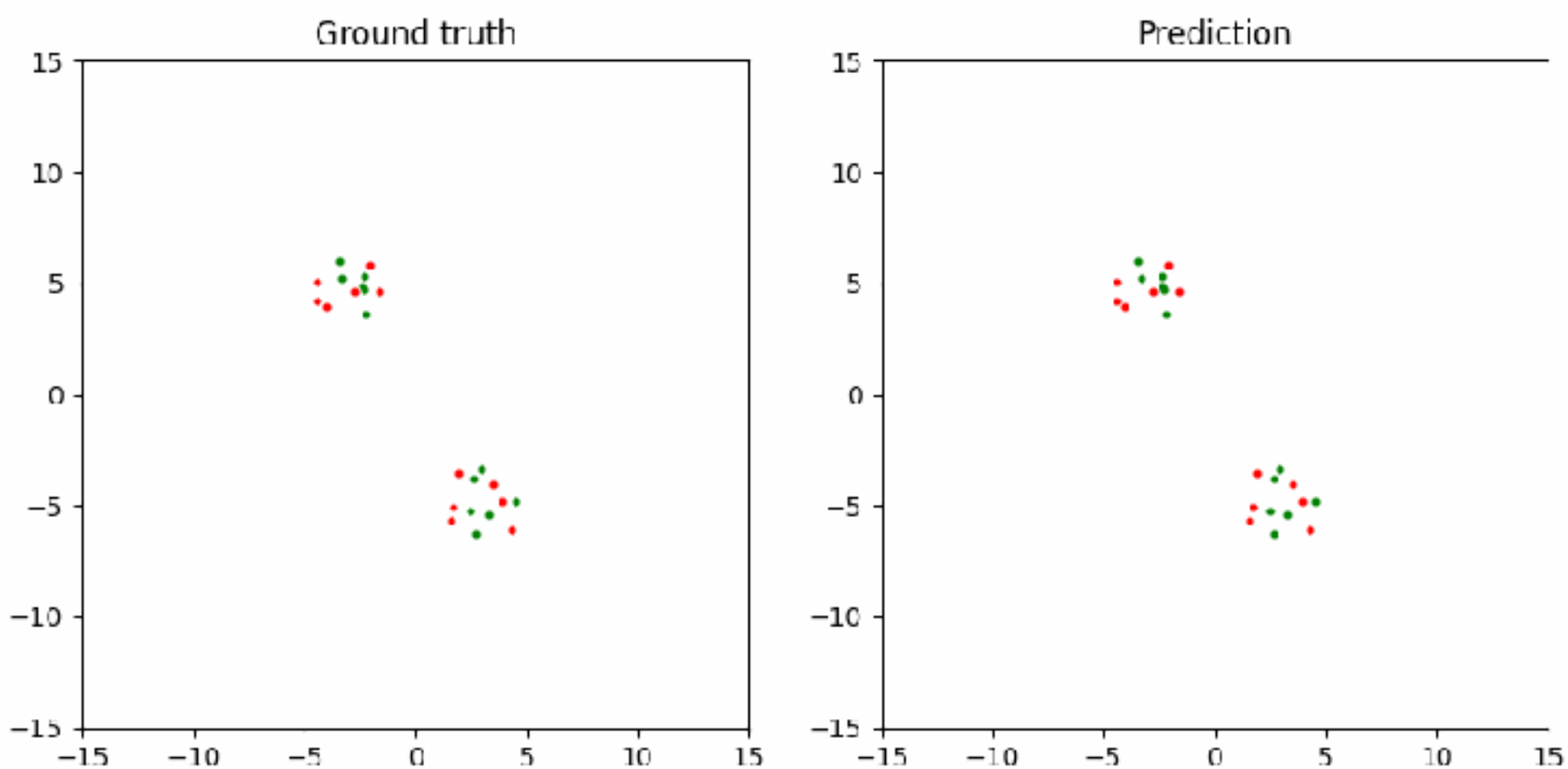
GNS



[A. Sanchez-Gonzalez et al. "Learning to simulate complex physics with graph networks." International Conference on Machine Learning. PMLR, 2020.]

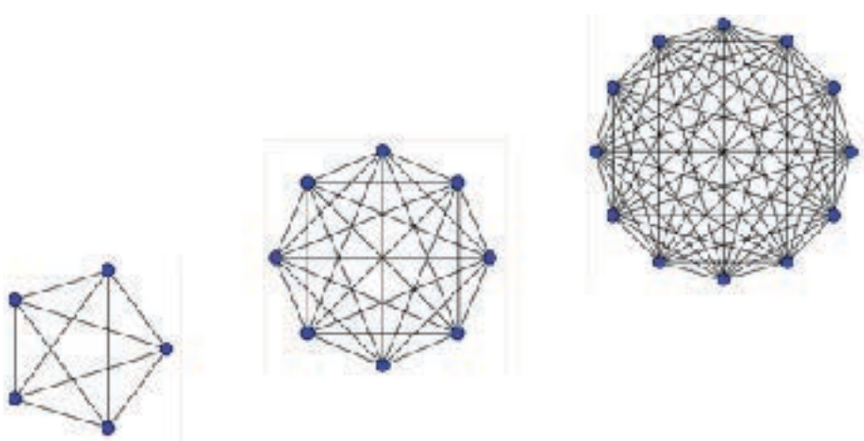
Emulating QMD with GNS

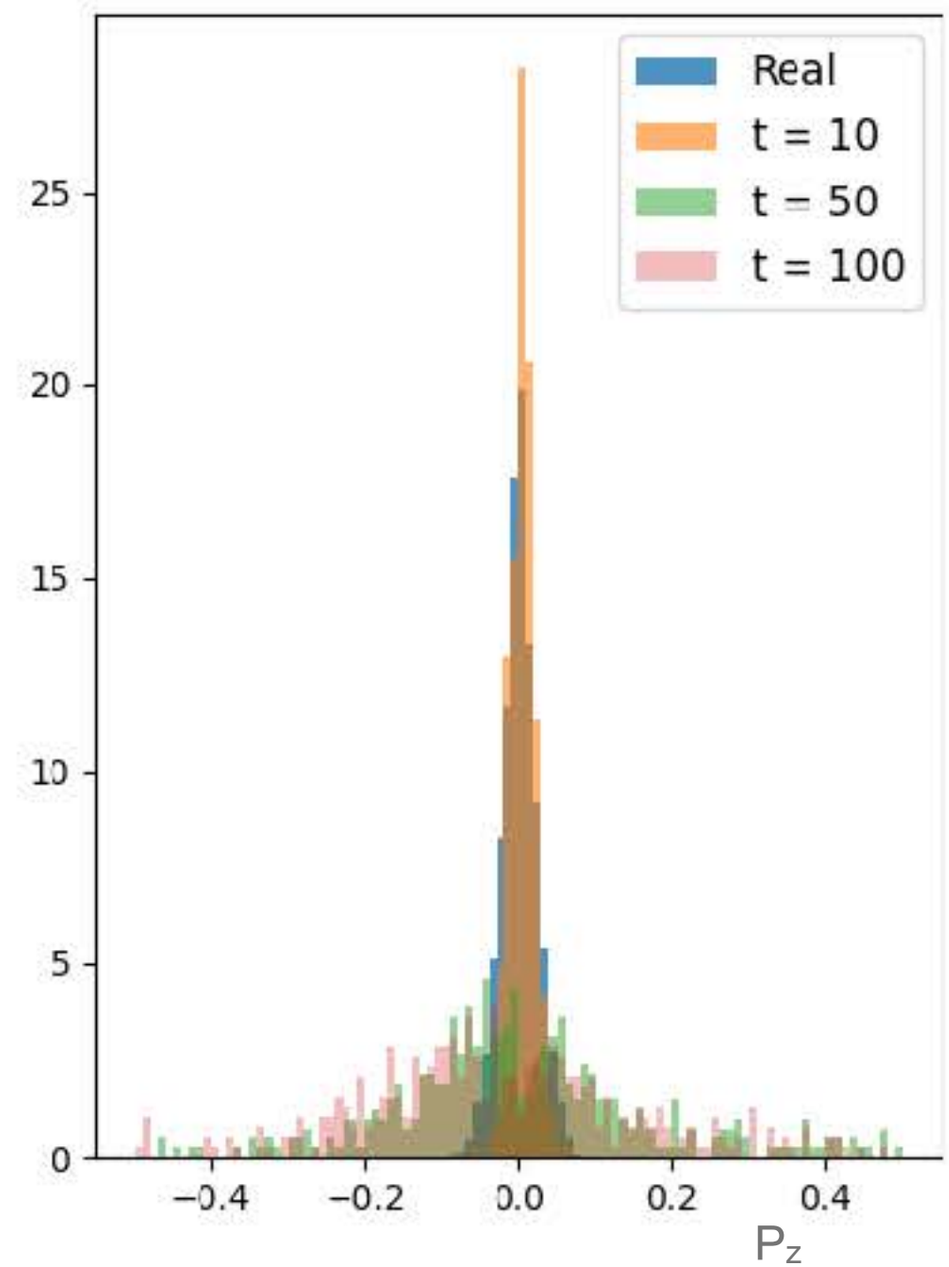
- G4-QMD to develop a demonstrator
- We trained a full connected GNN to reproduce the nuclear reaction dynamic
- Each nucleon is a node of the graph



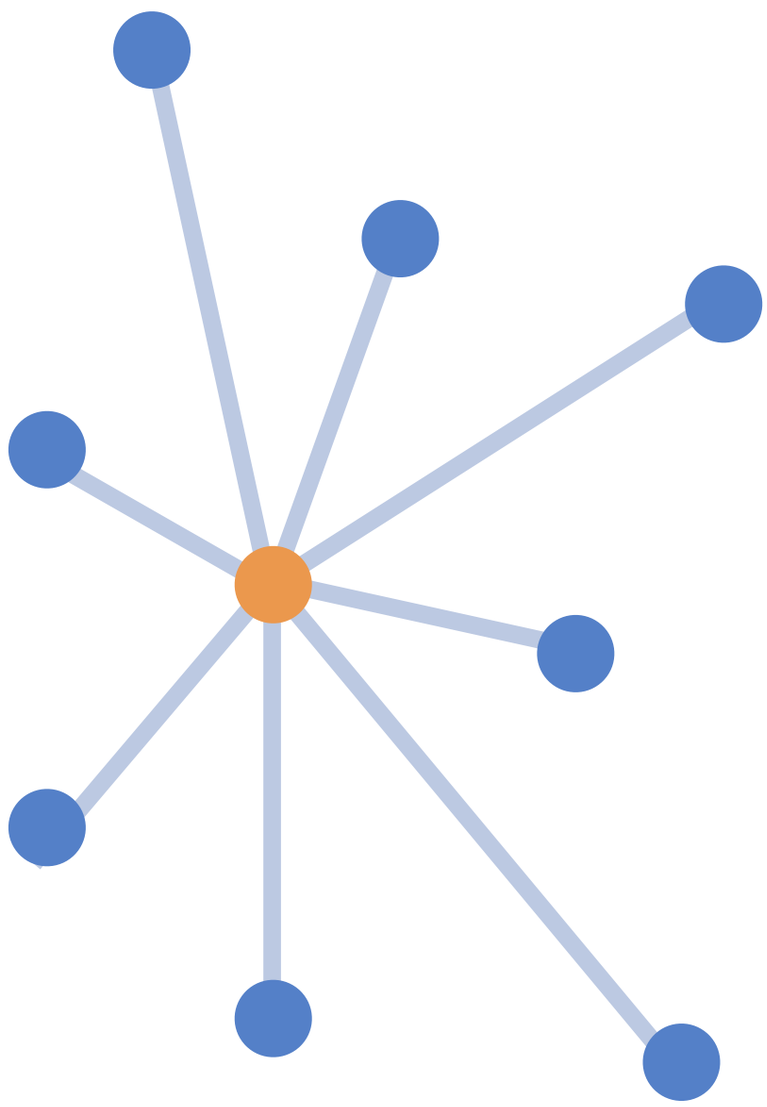
Emulating QMD with GNS

- Quantities are conserved on average
- Variance explodes increasing time steps
- $N_{edges} \propto N^2$



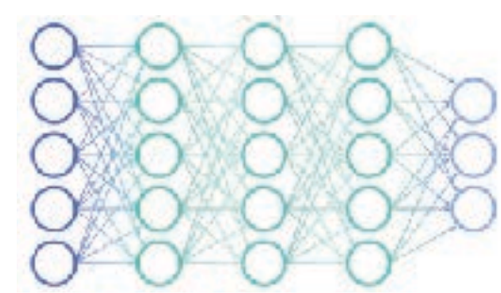


Emulating the Mean Field: DL model



$$V_i = \sum A_{ij} + \left(\sum B_{ij} \right)^{\gamma}$$

$$f\left(q_i, q_j, p_i, p_j, c_i, c_j\right) =$$



Hybrid model

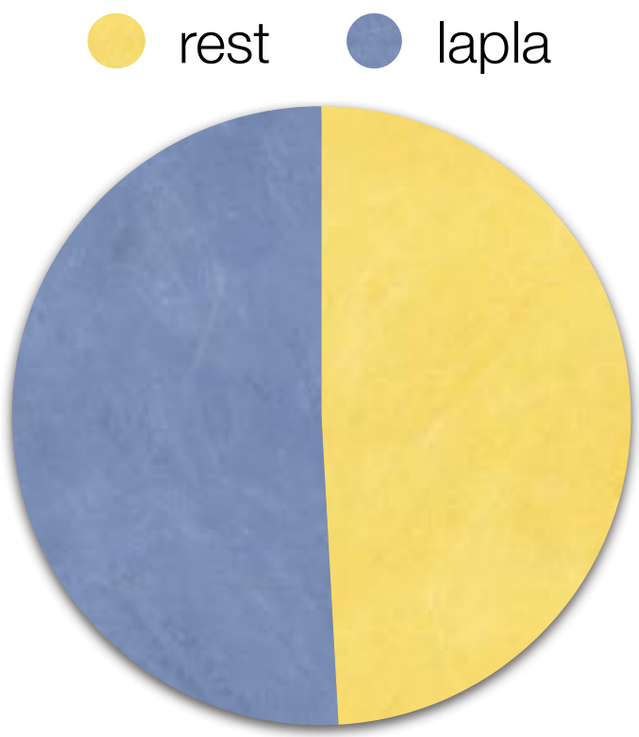
- Emulating the mean field calculation
- Keeping the model structure
- Enforcing physical conservation laws in the model
- Independent from the number of nucleons involved in the reaction

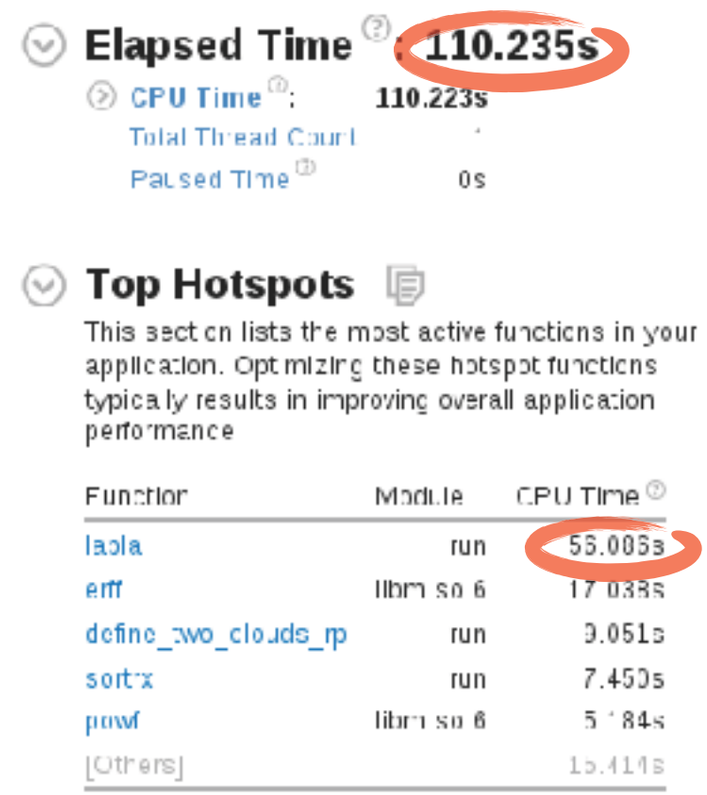
$$\{q_i, p_i, q_j, p_j\} \rightarrow$$

$$\rightarrow V_{ij}$$

Why the mean field

- It is the bottleneck of the BLOB computation





Elapsed Time 110.235s

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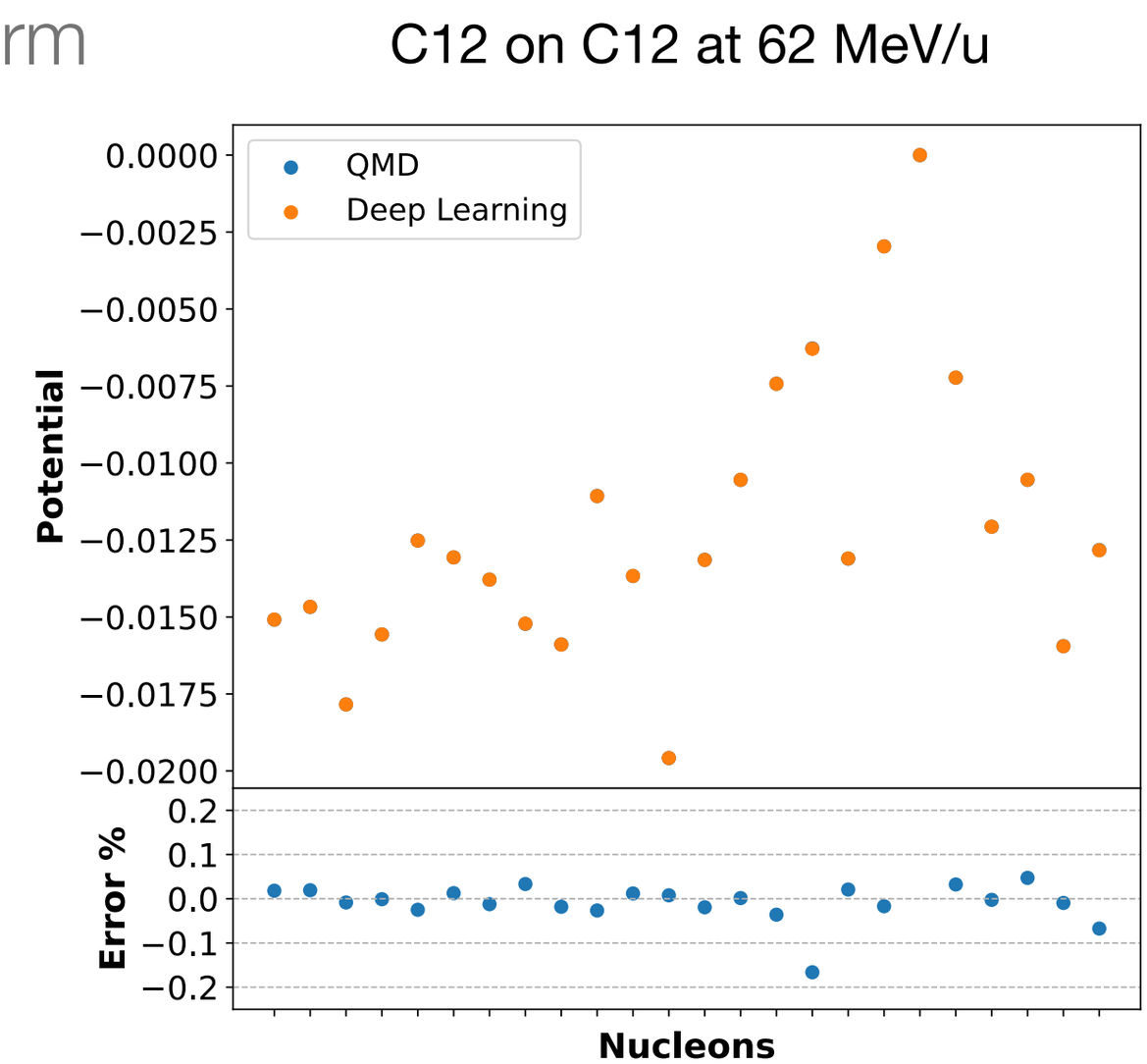
[Others]		15.414s

- It also would be possible to improve the mean field approximations

Preliminary results with QMD mean field

- Model:
  5 layers MLP + ReLu + LayerNorm
- Data:
  - 23k stories
  - 10 events
  - 24 particles : ~5 M examples
- Training:
  ~3d training on Nvidia V100



Geant4 implementation

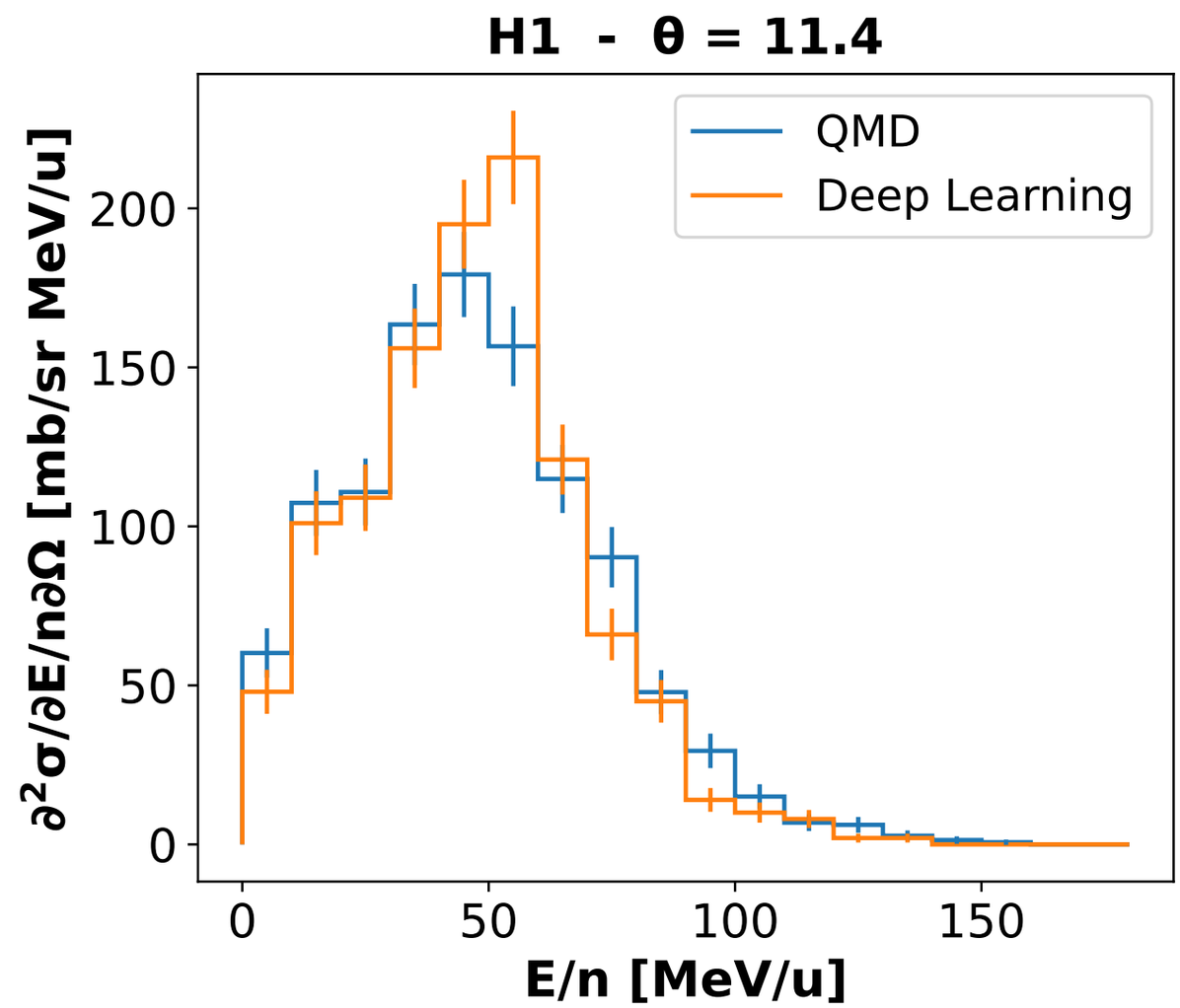
- We exported the DL models from pytorch to ONNX
- Substituting GetPotential() Method in QMD
- Using ONNX C++ API

```
G4double MyQMDMeanField::GetPotential_dl( G4int i )
{
    // ------------------------PREDICT WITH DEEP LEARNING ---------------------------
   return static_cast<G4double>( ONNXInterface::GetInstance()->Generate(i, system)[0]);
    // ------------------------------------------------------------------------------
}
```

- Thread-safe implementation

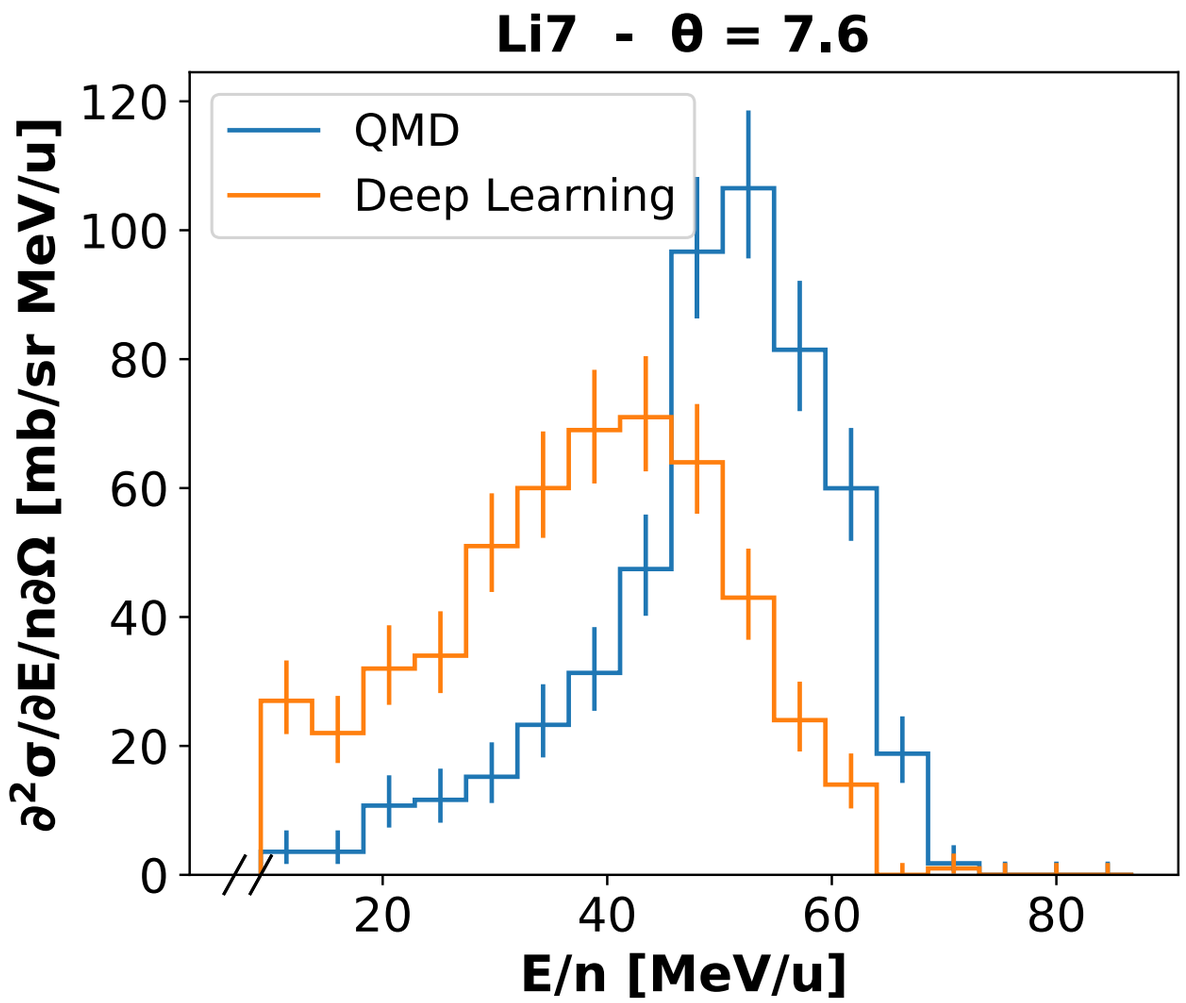
Results with mean field emulation

- C12 on C_nat at 62 MeV/u
- Reasonable accuracy on double differential cross section of lighter fragments



Results with mean field emulation

- On heavier fragments
- Even small errors on the potential propagate badly to the double differential cross sections



Emulating the Hamiltonian derivatives

- $\frac{\partial H}{\partial q}, \frac{\partial H}{\partial p}$

- It is the bottleneck of QMD

Callees	CPU Time: Total ▼
▼ MyQMDReaction::ApplyYourself	100.0%
▼ G4QMDMeanField::DoPropagation	88.7%
▶ G4QMDMeanField::CalGraduate	47.5%
▶ G4QMDMeanField::Cal2BodyQuantities	40.5%

- $$\frac{\partial H}{\partial q, p} \approx \sum A_{ij} + \sum_{\alpha^{(k)}} \left(\sum B_{ij}^{(k)} \right)^{\alpha^{(k)}}$$

- Hyper-parameter optimisation on the number of terms K

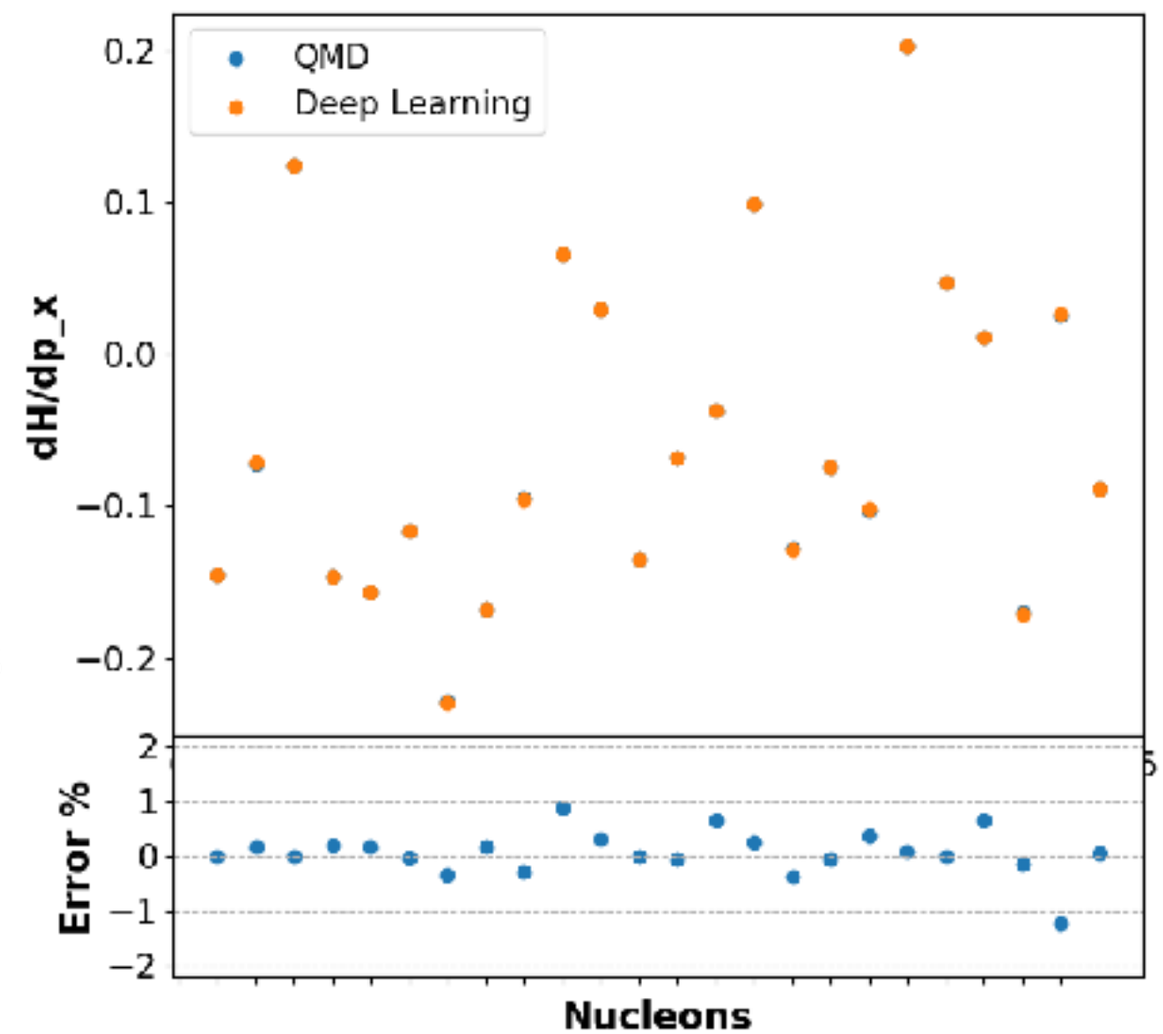
Preliminary results with QMD H derivatives

- Model:
  2 $\alpha^{(k)}$ terms + 5 layers MLP + ReLu + LayerNorm

- Data:
  - 12k stories
  - 1 event
  - 24 particles : ~300 k examples

- Training:
  ~3h training on Nvidia V100

C12 on C12 at 62 MeV/u



Geant4 implementation

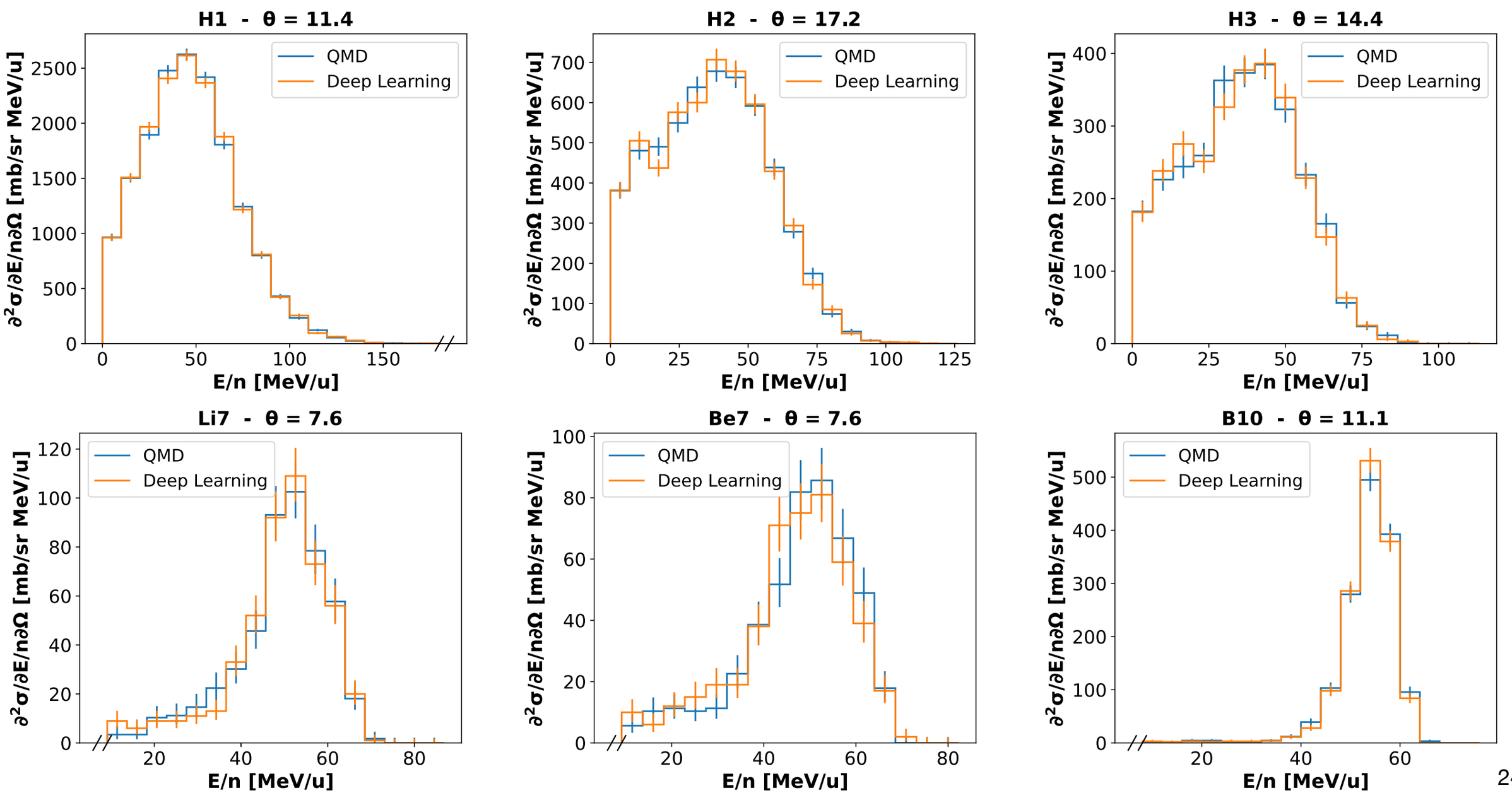
- We exported the DL models from pytorch to ONNX
- Substituting GetPotential() Method in QMD
- Using ONNX C++ API

```
void MyQMDMeanField::CalGraduate_dl()
{
   ffr.resize( system->GetTotalNumberOfParticipant() );
   ffp.resize( system->GetTotalNumberOfParticipant() );

  // ----------------- PREDICT WITH DEEP LEARNING -----------------
  auto gradients = ( ONNXInterface::GetInstance()->Generate(system));
  ffr = gradients[0];
  ffp = gradients[1];

}
```

- Thread-safe implementation

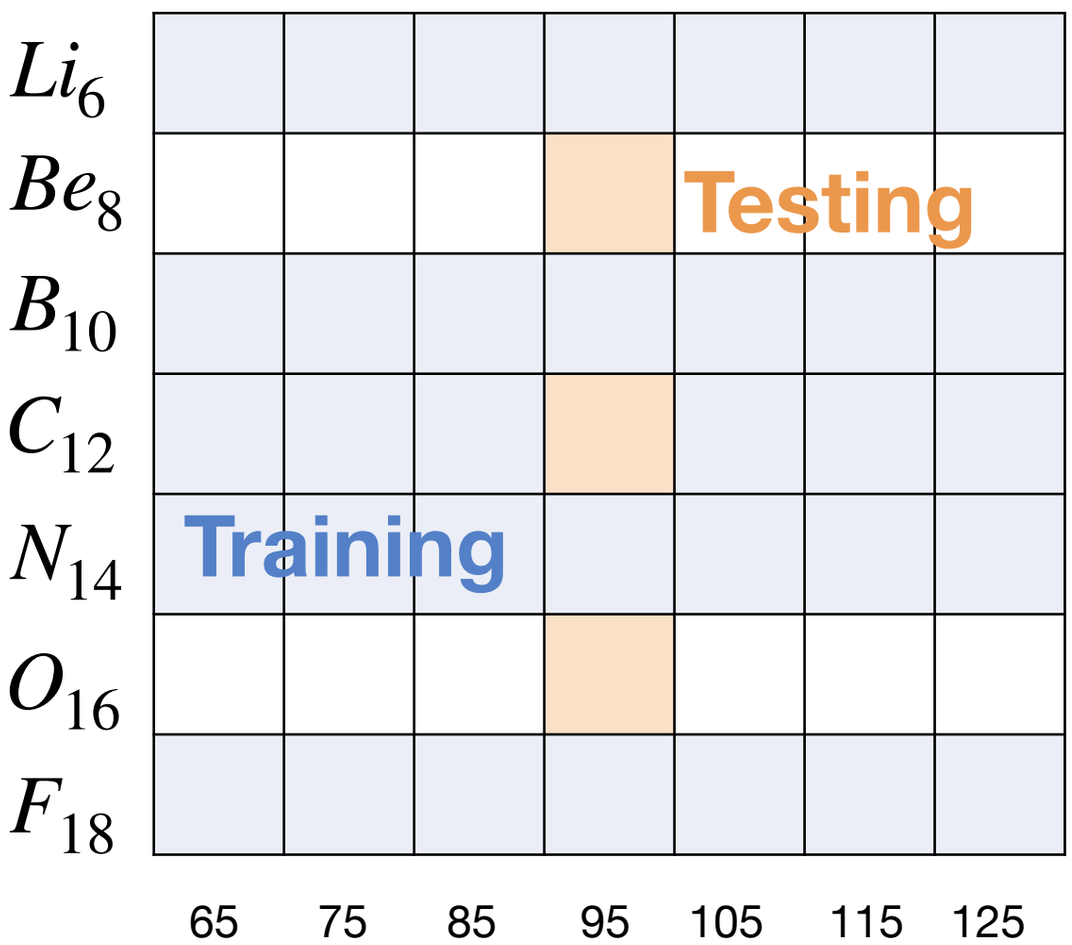
Results with H derivatives emulation

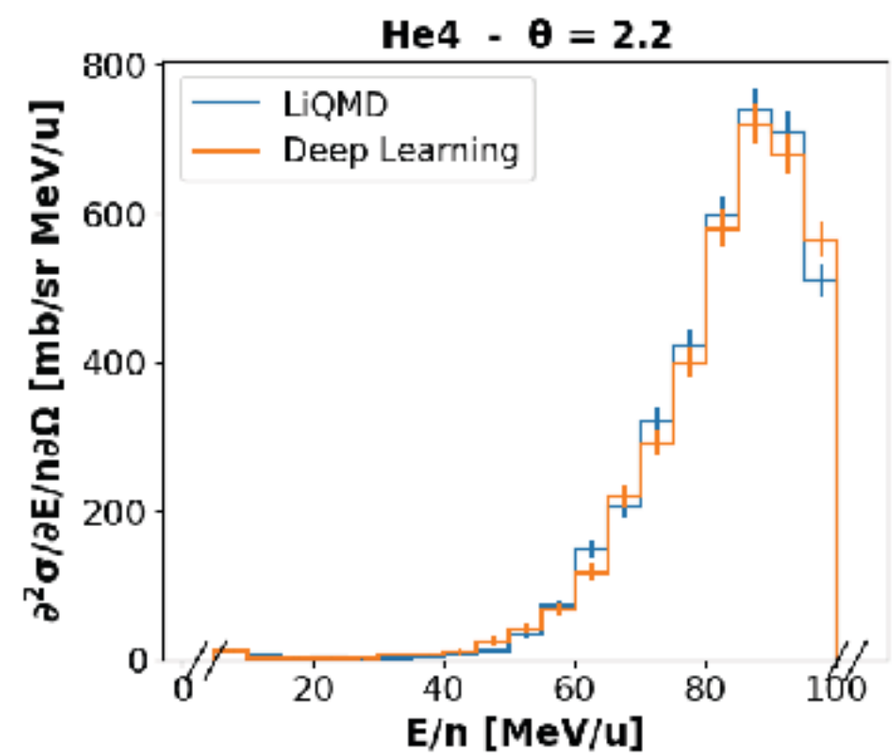
- Excellent agreement also on large fragments



Extending the training

- Training done on a subset of ions, with relatively few example each (~1k runs)





Next steps

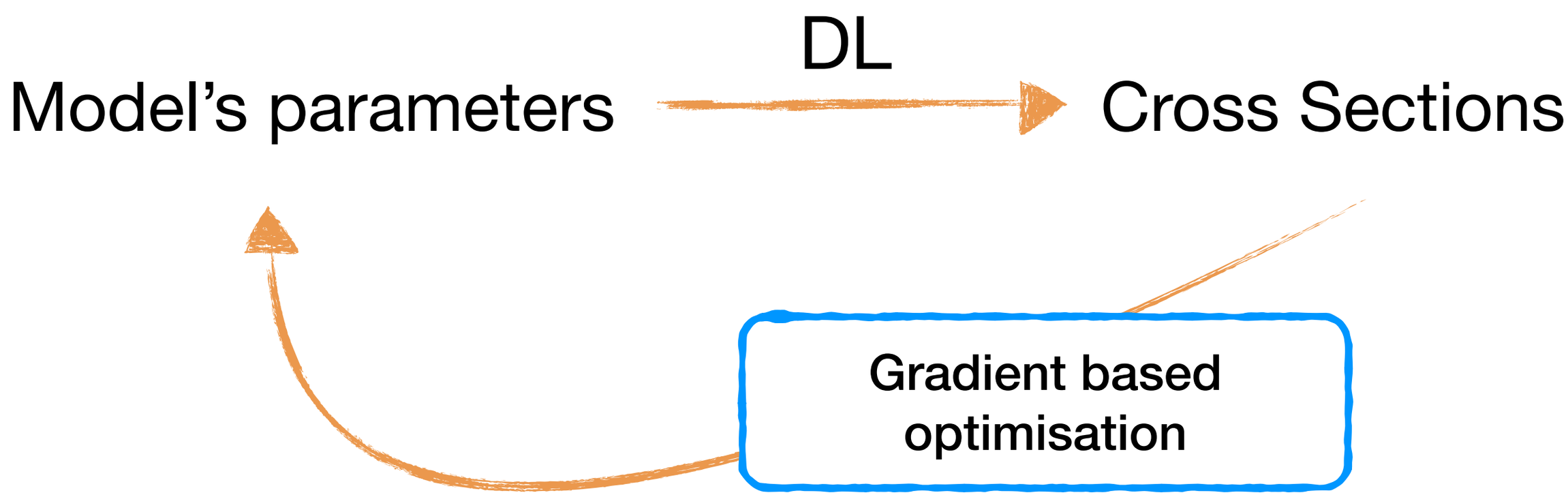
- Current implementation (on CPU) is slower than the original QMD

  "NVIDIA TensorRT-based applications perform up to 36X faster than CPU-only platforms during inference"

- Using NVIDIA TensorRT it could be possible a 4x-7x speed-up

Next steps

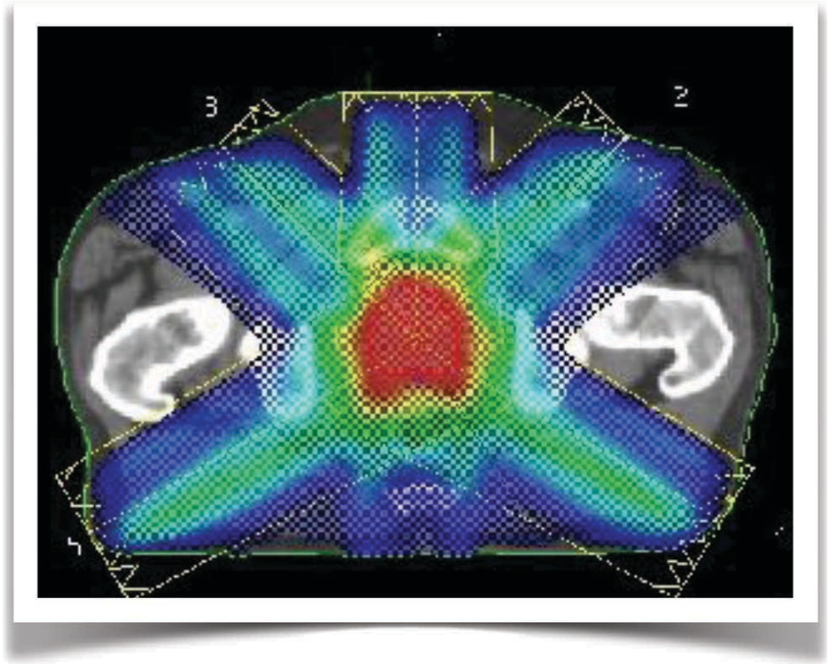
- Develop a fully differentiable pipeline to optimise the model free parameters

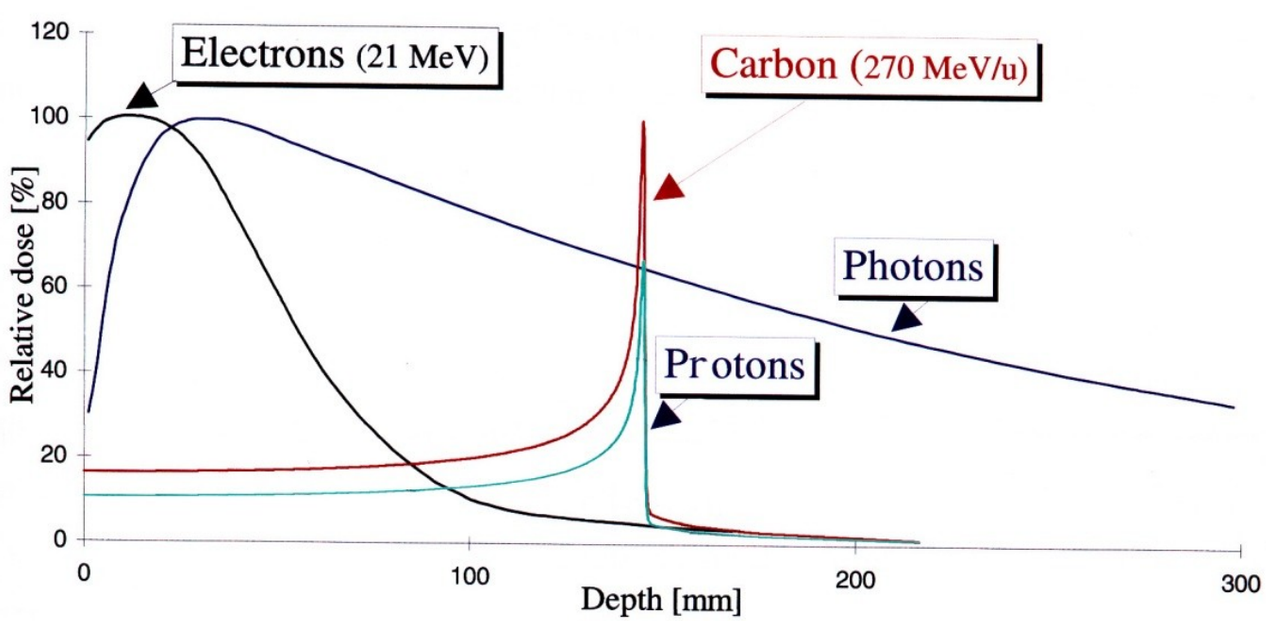


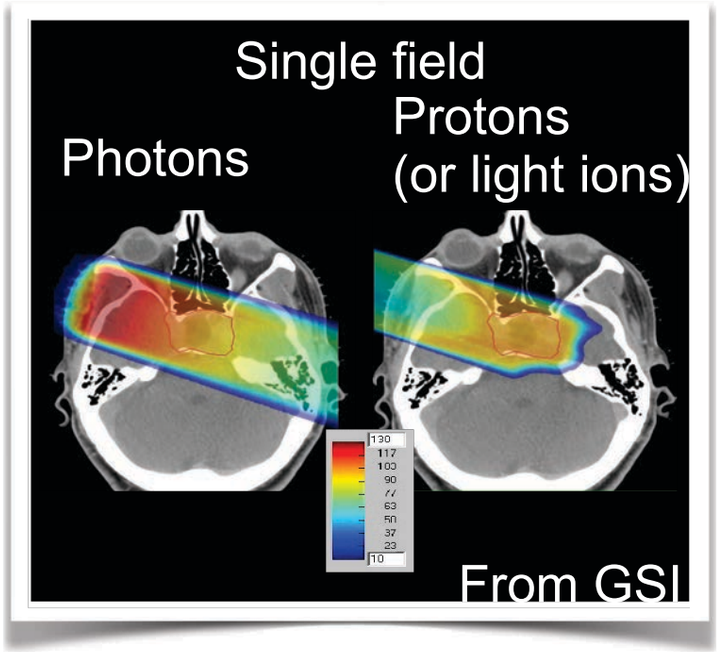
Emulating de-excitation model

Treatment plan optimisation

- The goal is to maximise tumour dose while minimising exposure to healthy tissues

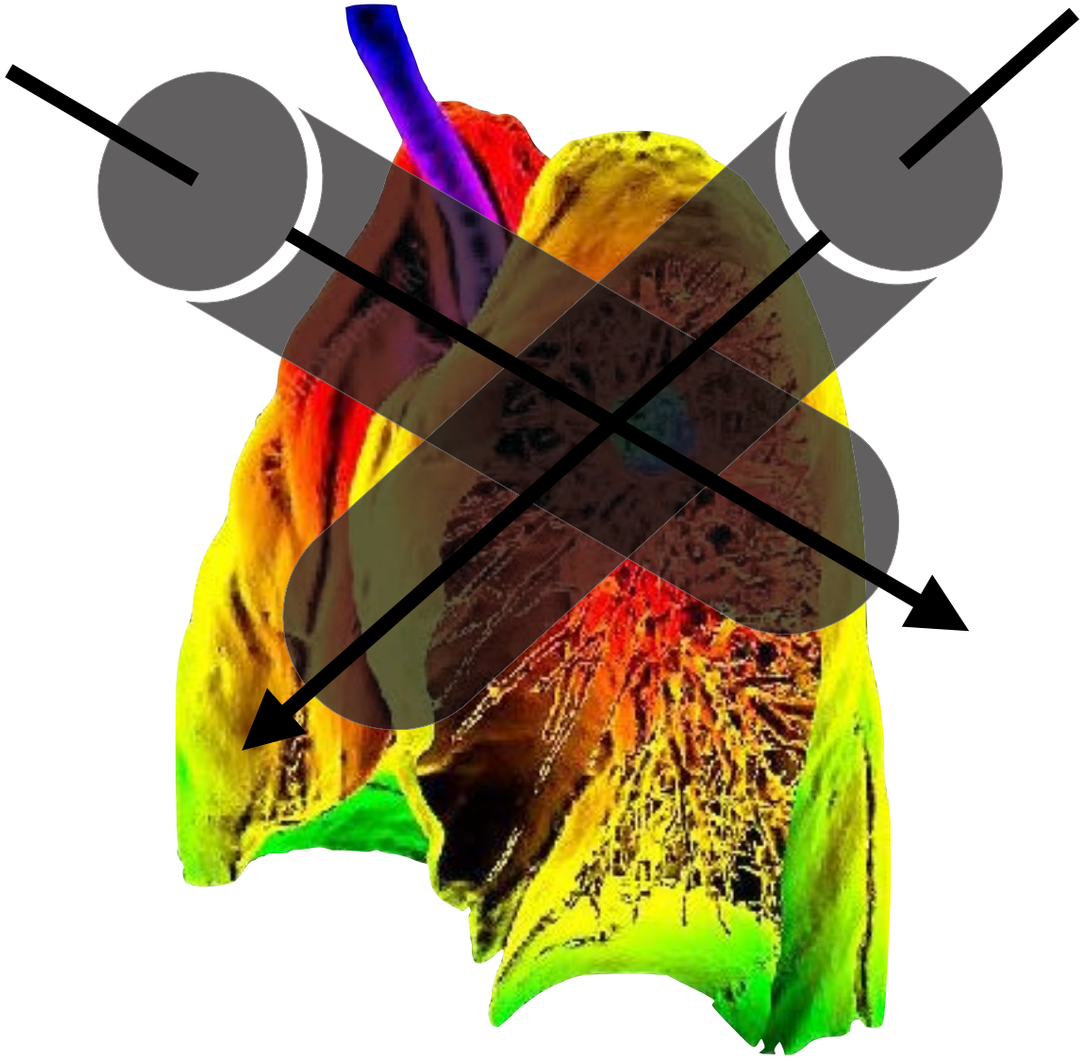




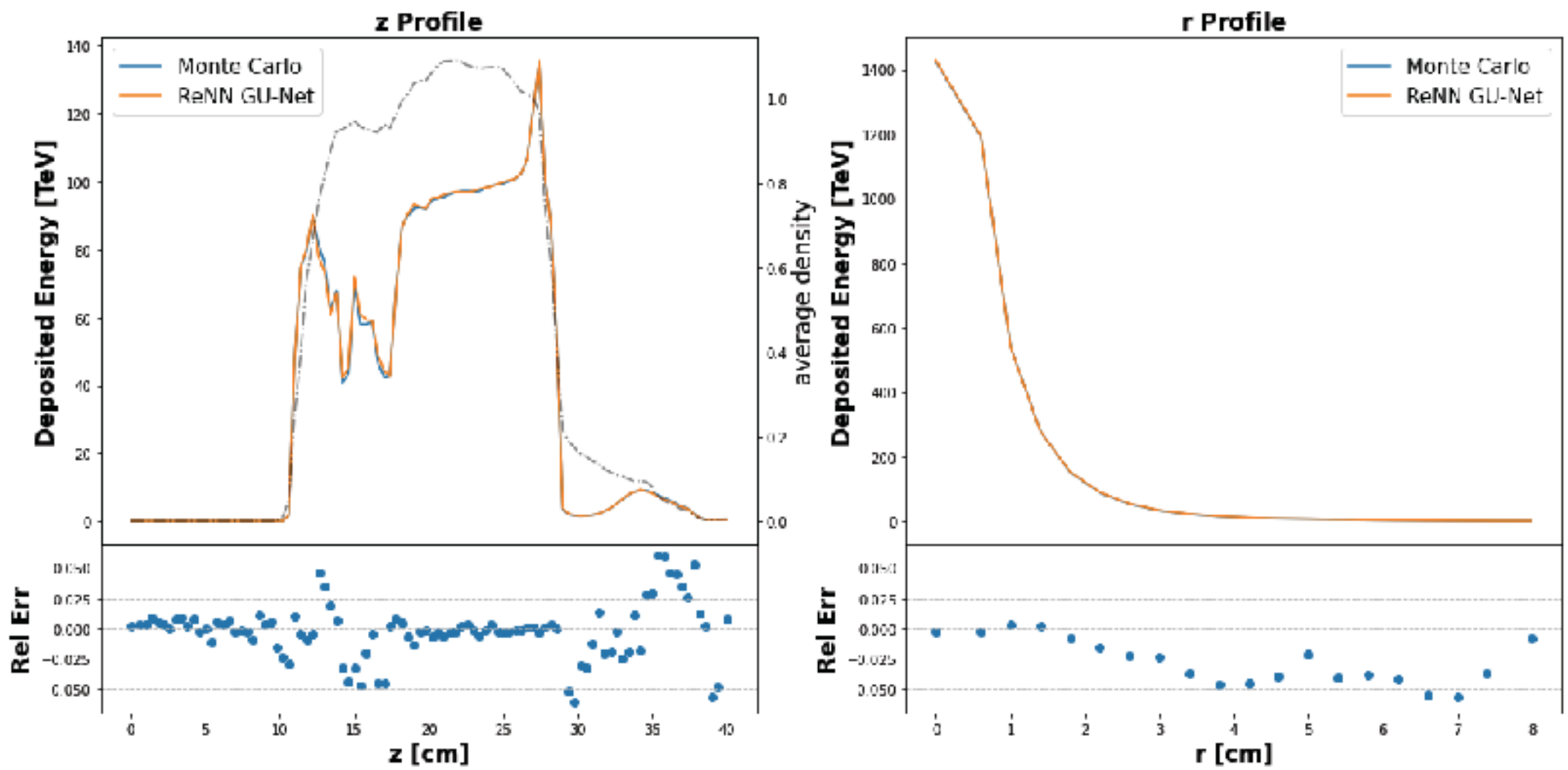


Cylindrical scorers

- We used cylinders around the beam
- Two main advantages:
  - Reduce complexity without loss of generalisation: the cylinder follows the beam
  - More resolution near the beam-line

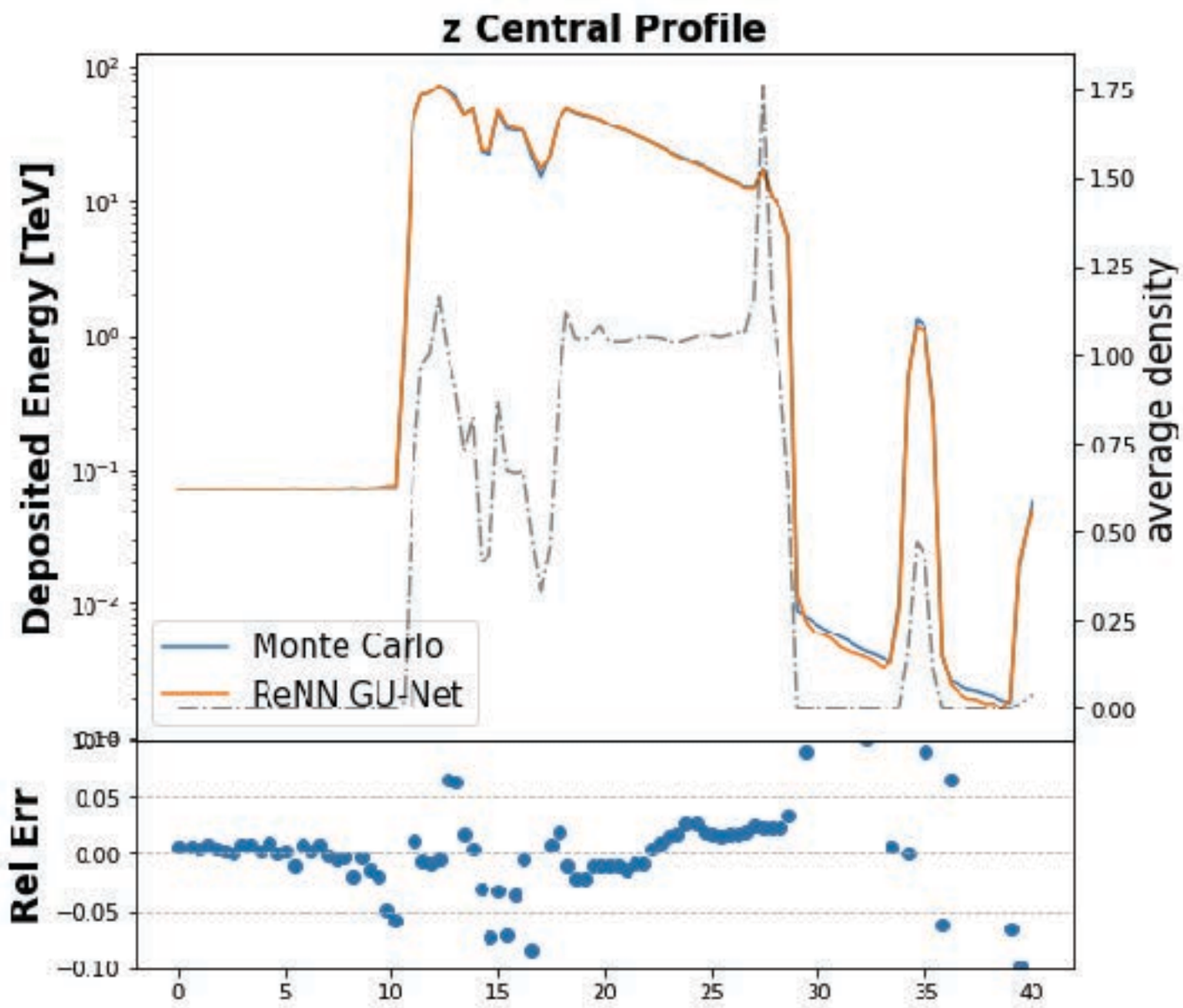


Integrated Energy Profiles on CT scan



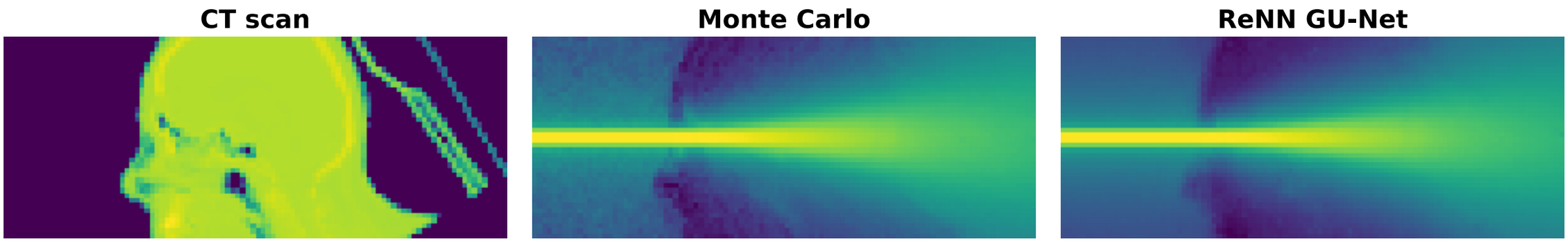
- Excellent agreement with MC

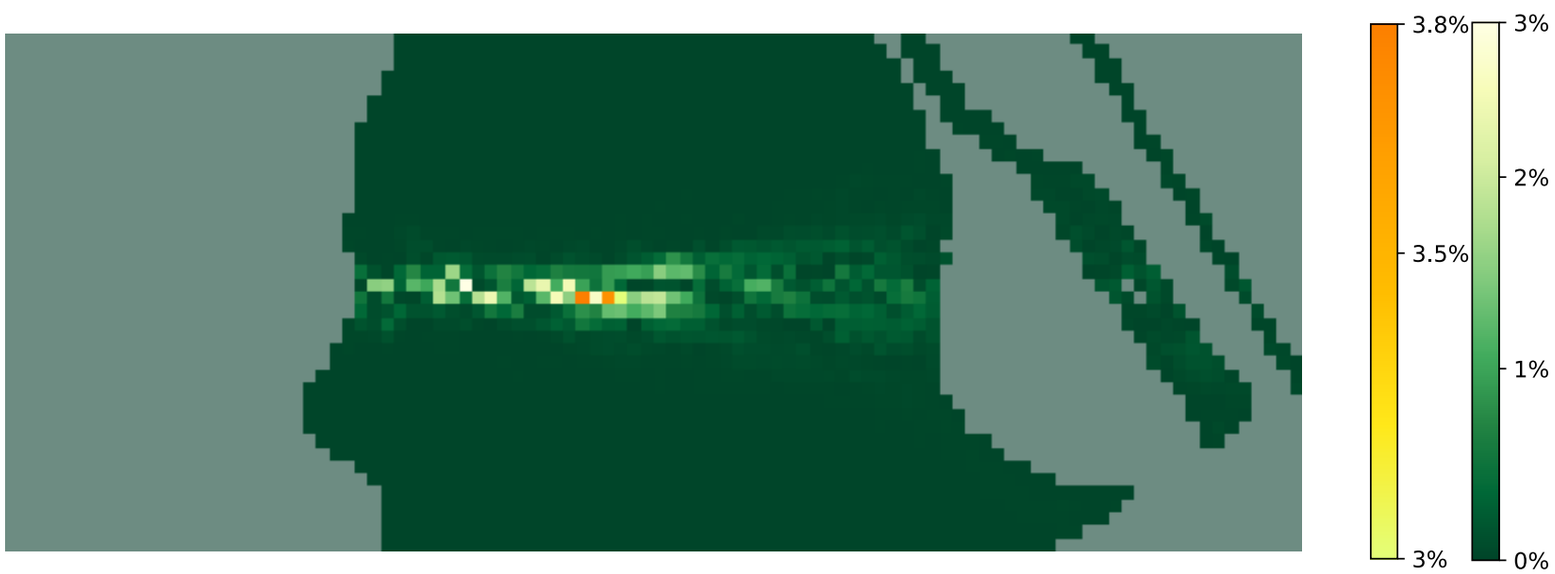
Precise also locally… …and fast!



	Generation time
Deep Learning	~ 0.01 - 0.1 s
Monte Carlo (48 cores) 1M primaries	~ 15 - 20 min

Dose prediction



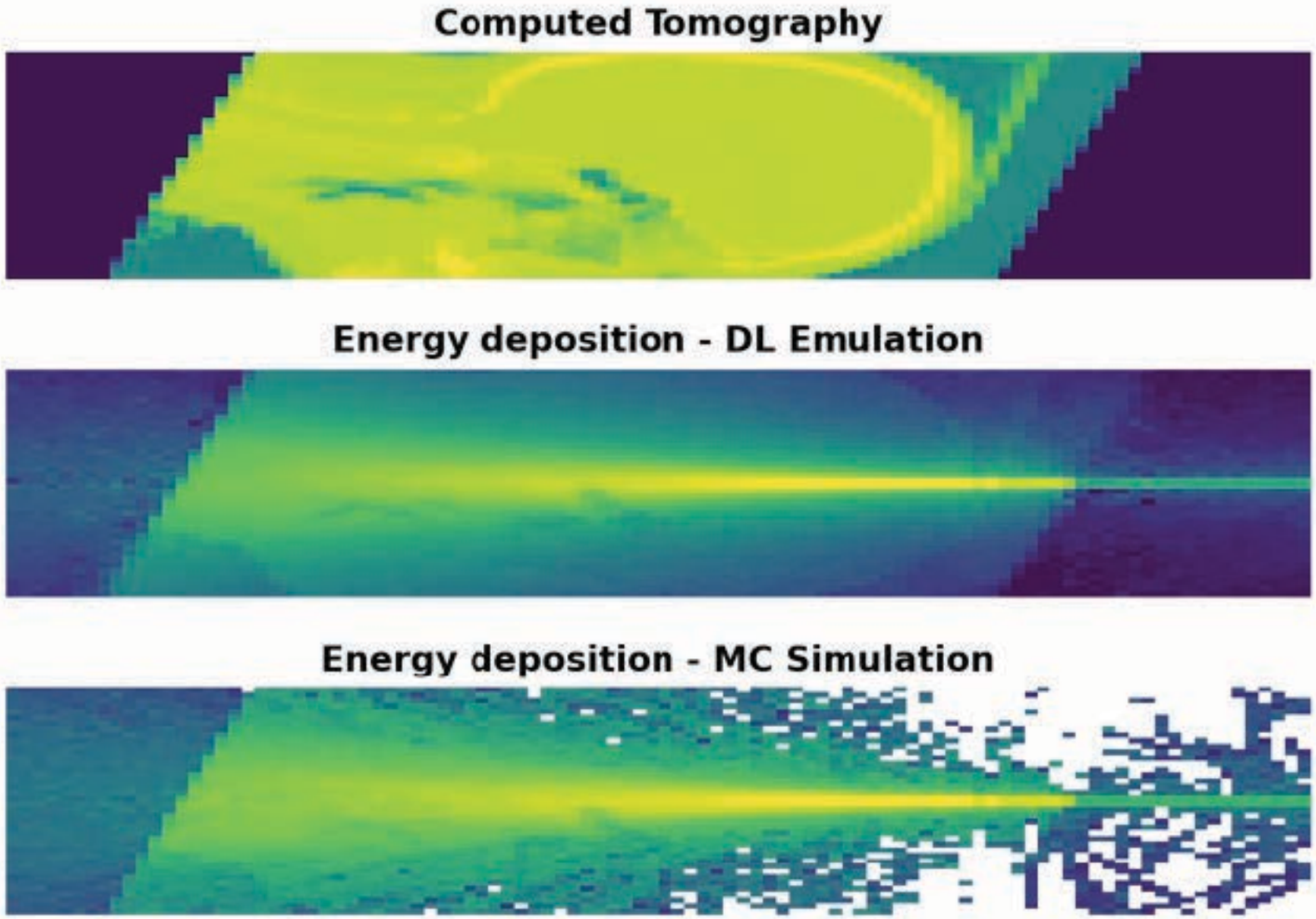


99.8 ± 0.2 %

of the voxels have

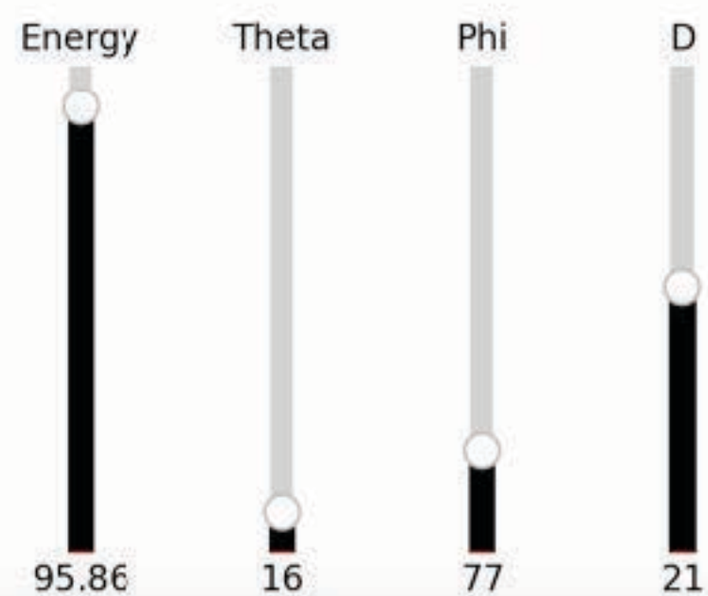
$$\delta = \frac{|D_{MC} - D_{DL}|}{max(D_{MC})} < 3\,\%$$

Generating dose distributions from beam's energy and density map

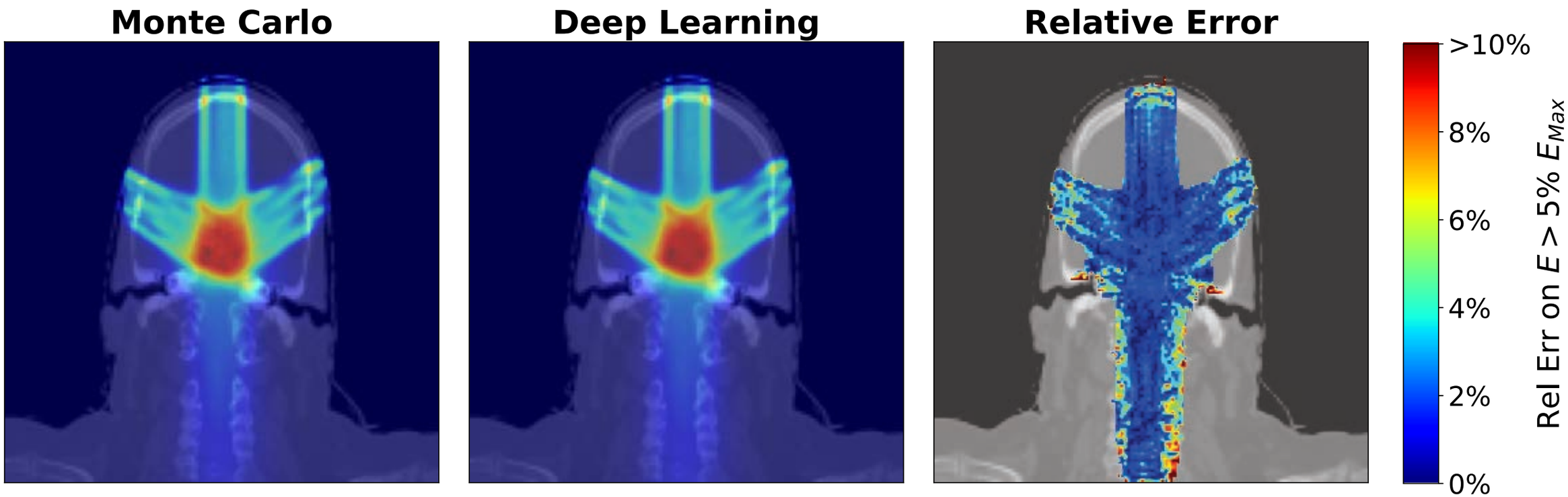


	Energy	Dose
γ-index(1%) :	90.70 %	99.01 %
γ-index(3%) :	98.49 %	99.60 %
γ-index(5%) :	99.63 %	99.81 %

Next Datapoint



Full Treatment Plan



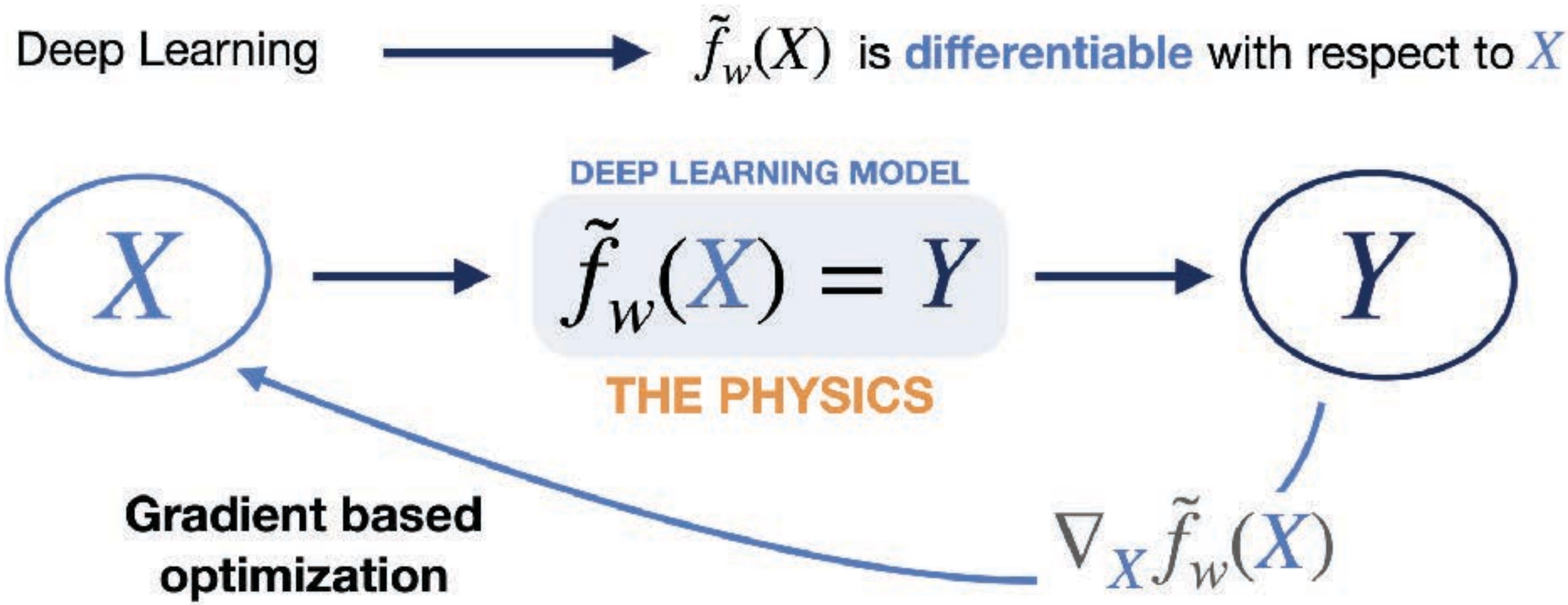
350 pencil beams in 6 seconds

On a single Nvidia Tesla V100 GPU

Local γ-index 3%/3mm: 98.4%

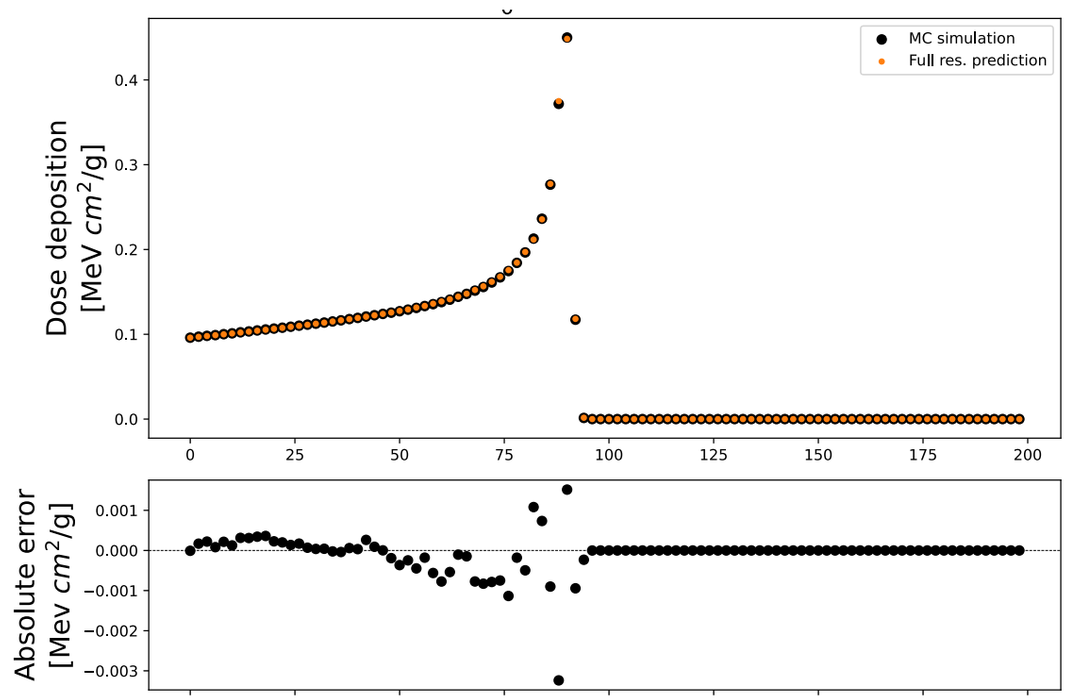
Gradient based optimisation

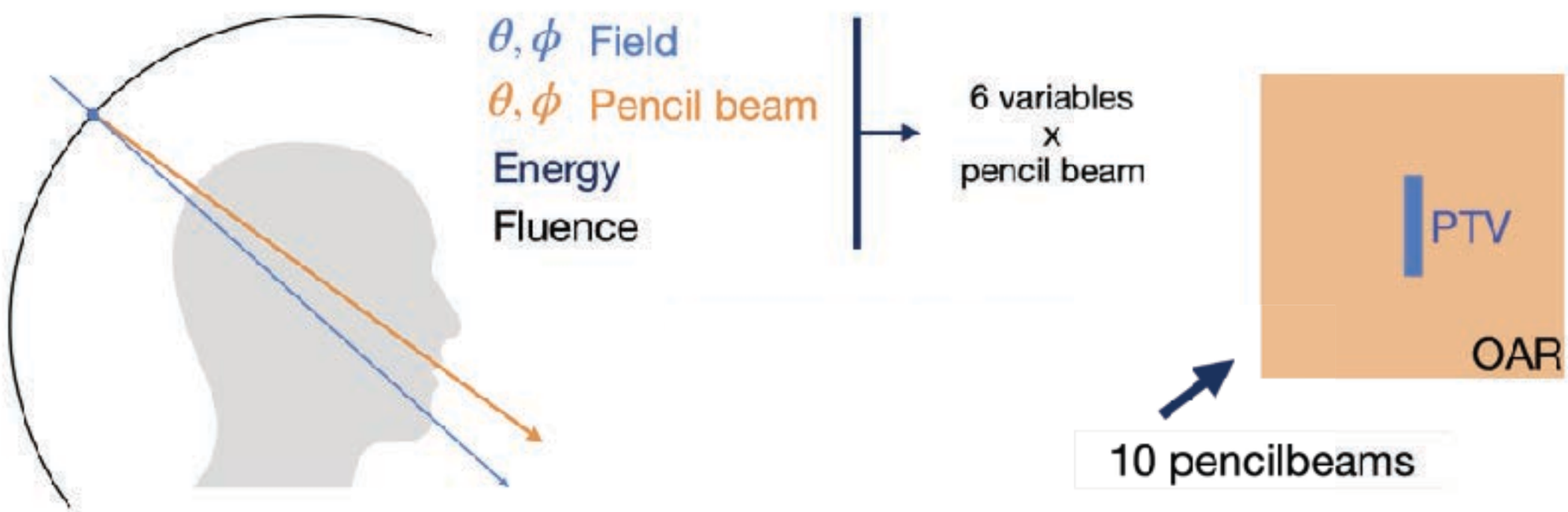
- It is possible to optimise the treatment plan with a differentiable programming approach



Test on proton therapy optimisation

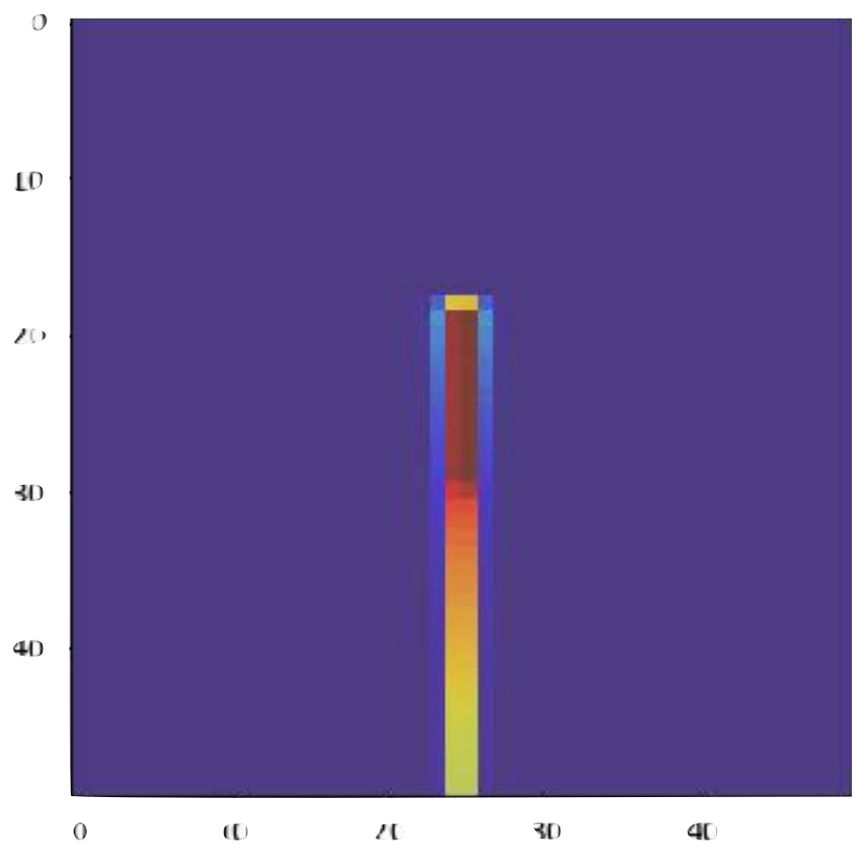
- Optimising:
  - Field Orientation
  - Pencil-beam Energy
  - Pencil-beam Fluence

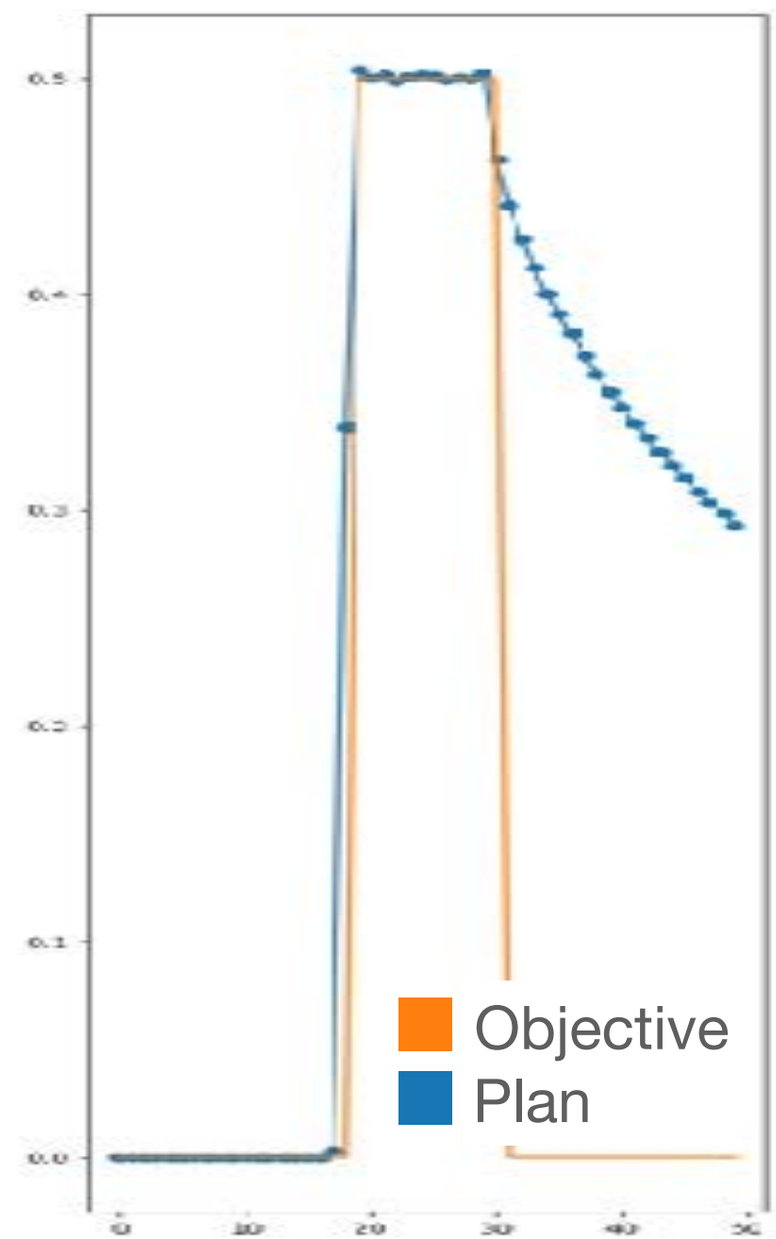




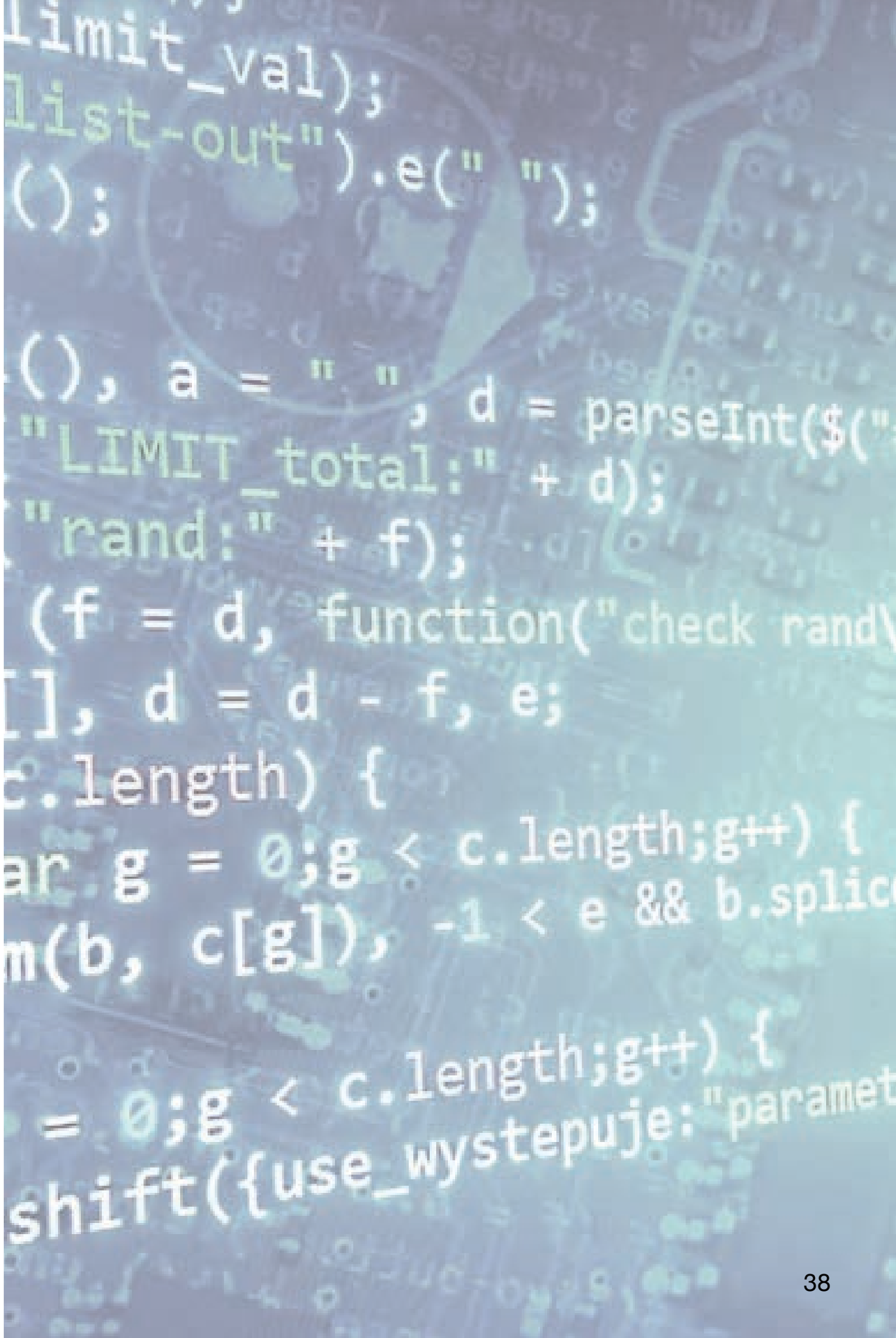
Optimisation results

- A gradient descent algorithm found the configuration to obtain a Spread Out Bragg Peak
- Optimising also the entrance direction





Technical details



Virtualisation!

- If you create a virtual machine with Geant4 and ONNX compiled in the way needed by our code it would work everywhere
- It’s heavy and slow!
- Containers overcome all the shortcomings of Virtual Machines

Virtualisation!

- Containers don’t require the installation of a separate guest operating system.
- They directly run and use the host operating system
- Containers only need the dependent file system and binaries for their functioning
- lightweight than Virtual Machines

What is a container?

- Containers (such as Docker) are
  - a standard for cloud computing and clusters
  - a good way to run an application in the same environment on different machines
  - a fast way to distribute code for multiple architectures
  - integrated in all the CI/CD platforms
  - light and efficient

Security issue and Apptainer

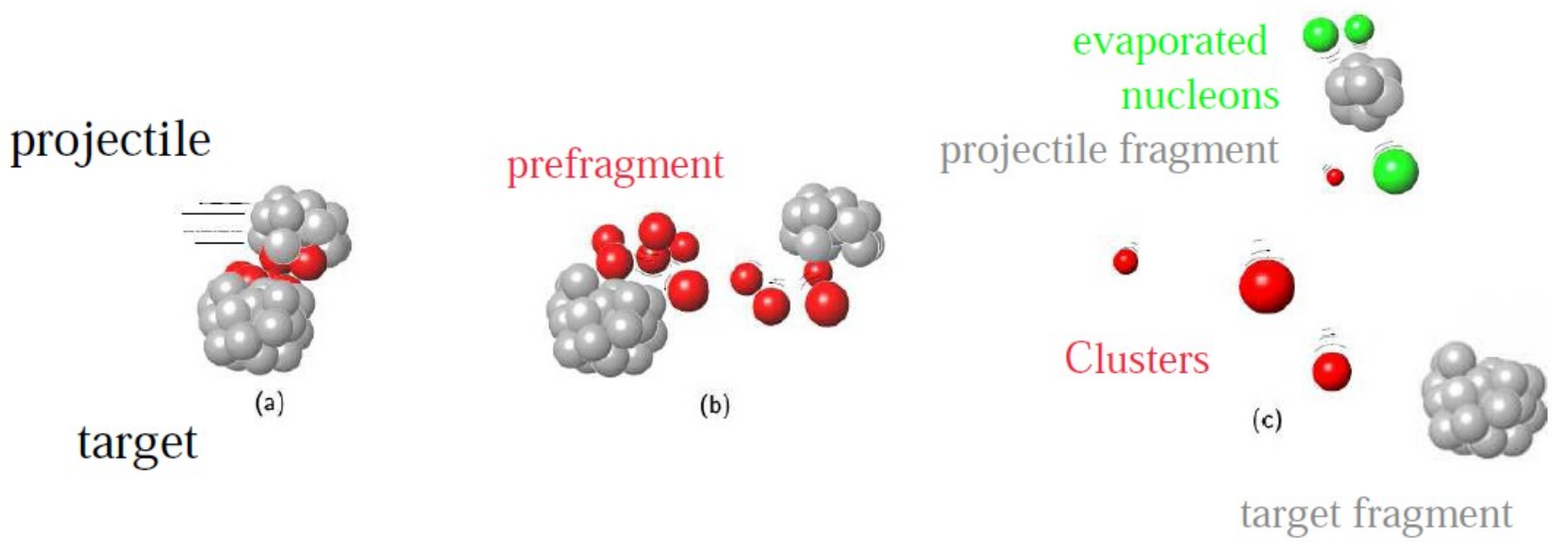
- Depending on how the Docker demon is installed, you could be root of the container (and if the host is Linux on the volumes mounted)

- Apptainer (formerly Singularity) is a container system (compatible with Docker images) which doesn't have this security issue

- https://apptainer.org/

- Largely available on scientific computing clusters
  eg: https://confluence.infn.it/display/TD/Singularity+in+batch+jobs

Nuclear interactions



- Hadronic interactions are simulated in two different stages:
  - The first one describes the interaction from the collision until the excited nuclear species produced in the collision are in equilibrium
  - The second one, such as the Fermi break-up, models the emission of such excited, but equilibrated, nuclei

Nuclear interactions

- **The entrance channel model characteristics have a larger effect** on particles and fragments production as compared to the choice of the exit channel

[Conclusions from: J. Dudouet et al. Phys. Rev. C, vol. 89, no. 5, p. 054616, May 2014]

- Hadronic interactions are simulated in two different stages:
  - The first one describes the interaction from the collision until the excited nuclear species produced in the collision are in equilibrium
  - BLOB is one of the entrance channel models

Geant4 interface to SMF and BLOB

- Dummy G4-model, loads the output from SMF/BLOB
- Sample the final state
  - Fragments mass and charge
  - Gas particles emitted
- Applies Geant4 de-excitation to excited fragments