Graph Neural Networks for fast emulation of Monte Carlo and nuclear interaction models

XX Seminar on Software for Nuclear, Subnuclear and Applied Physics

L. Arsini[1,2], B. Caccia[3], A. Ciardiello[1], S. Giagu[1,2], C. Mancini Terracciano[1,2]

Department of Physics, University of Rome “La Sapienza”, Rome, Italy. 2INFN, Section of Rome, Rome, Italy. 3Istituto Superiore di Sanità, Rome, Italy

08/05/2023

Outline

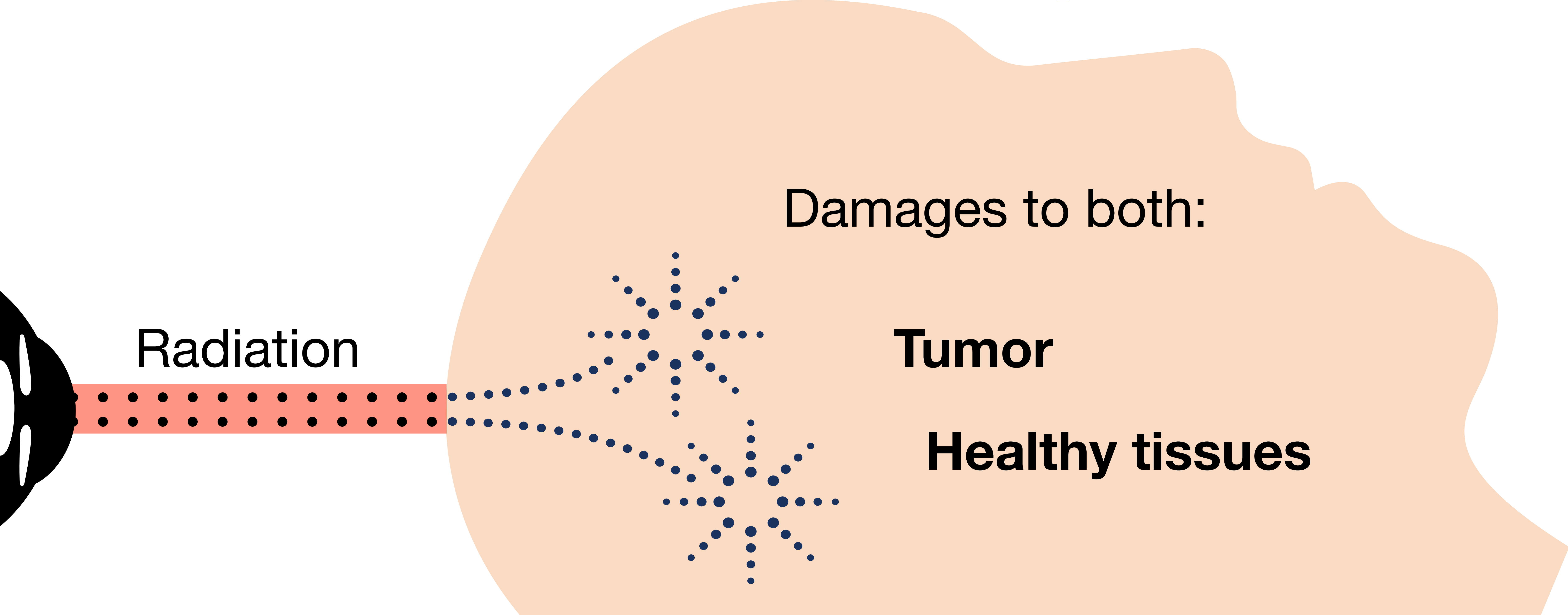
- Dose distribution emulation for novel **Radiotherapy** Treatment Plan Optimization:
  - Emulating Geant4
  - Preliminary results
- Towards the emulation of BLOB, a **nuclear interaction model**:
  - Graphs for physical system emulation
  - Approach to QMD

Radiotherapy

Deposited energy / mass

Goal → deliver

- Right **dose** to the tumor
- Minimal dose to healthy tissues



50% of cancer treatments

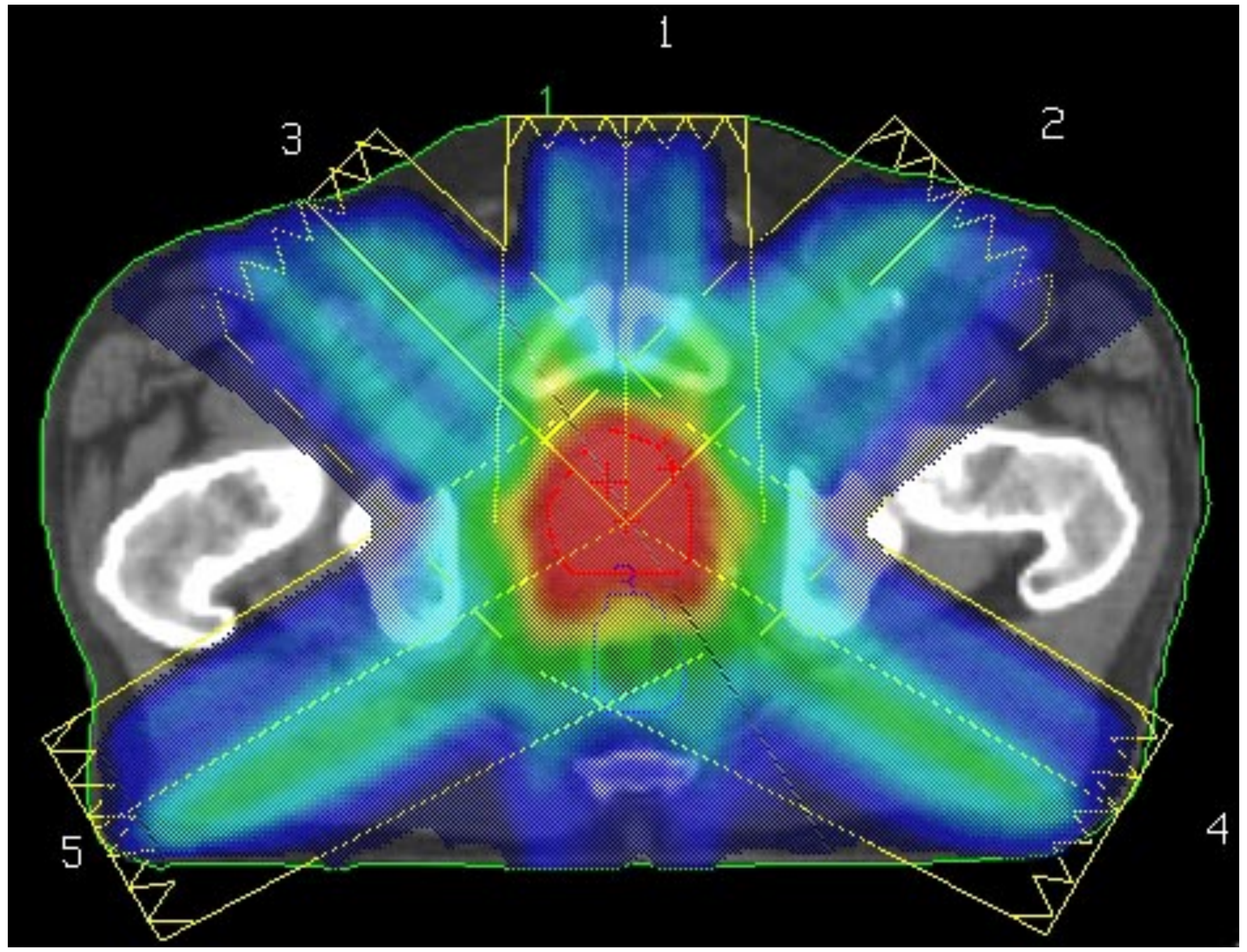
10 million people/year

Treatment Planning Optimization

Choice of directions, energies and intensities of the beamlets

to

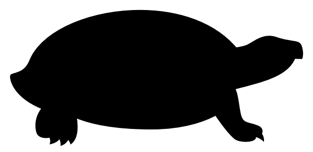
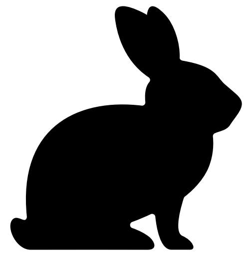
Fit dose medical prescription



2 steps → **Dose deposition estimation**

Plan Optimisation

Current methods

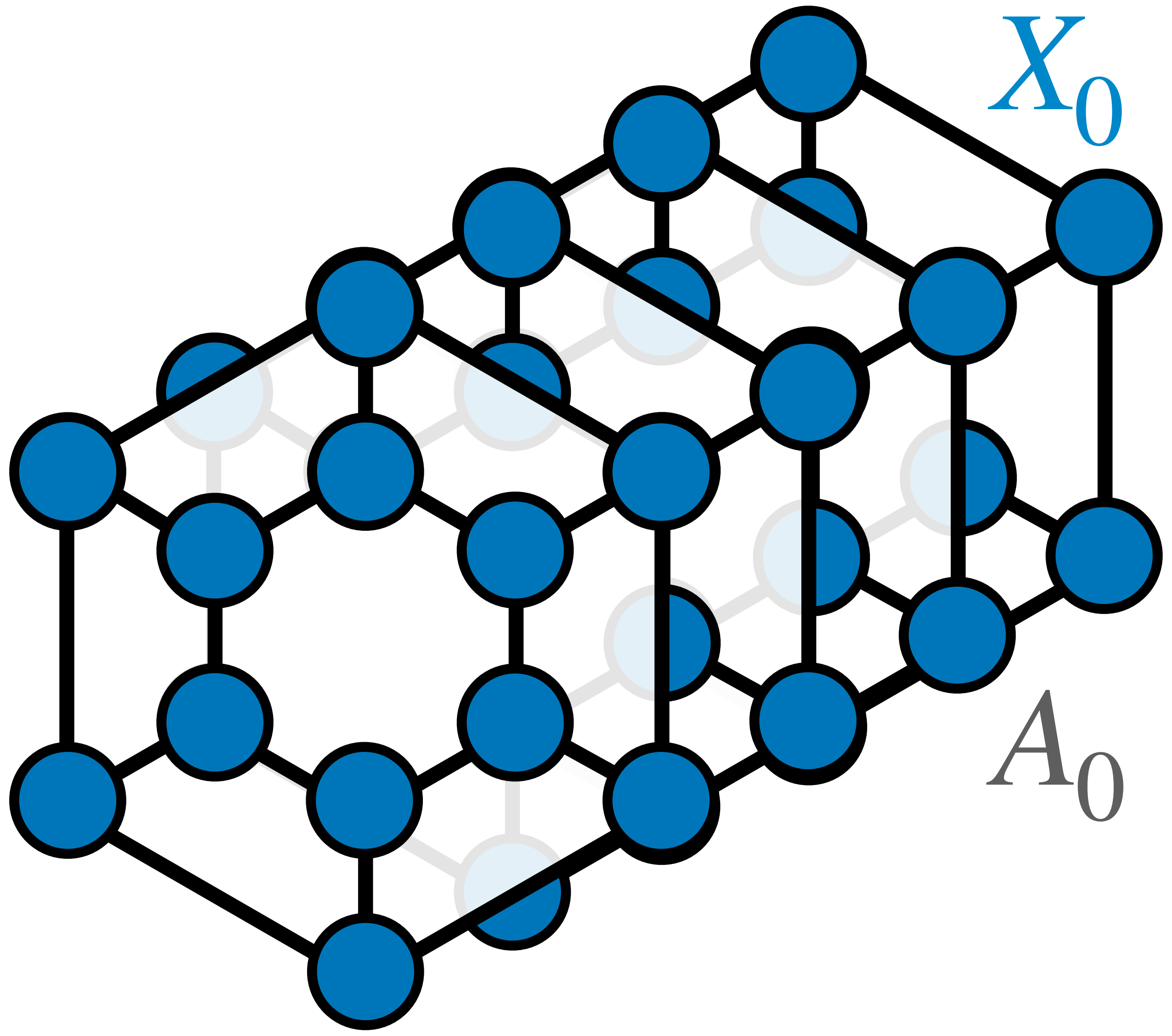
Dose deposition estimation		Speed	Precision
	Monte Carlo simulations		✓
	Deterministic algorithms		✗

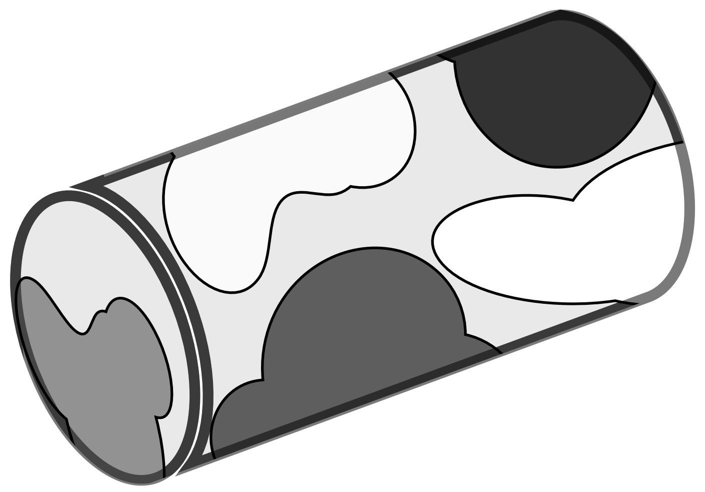
Goal → Train a Deep Learning model to **emulate** Monte Carlo

- Both fast and precise → Runs on GPU
- Relevant for novel therapies: e- FLASH RT, MRT etc.

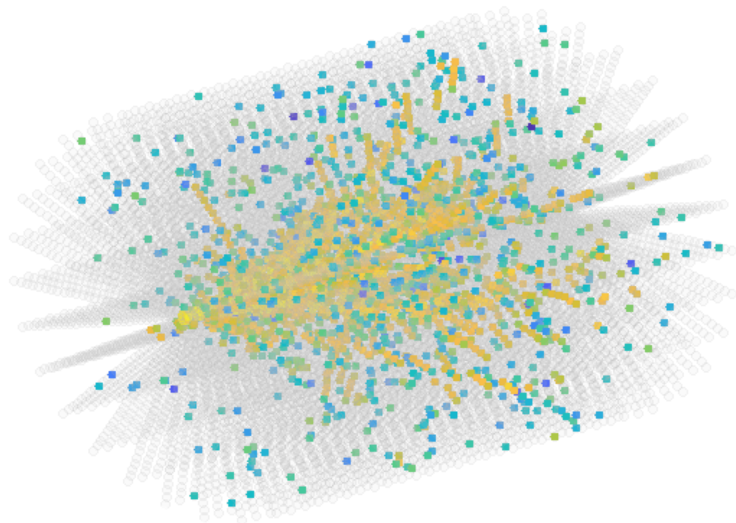
Dose deposition estimation

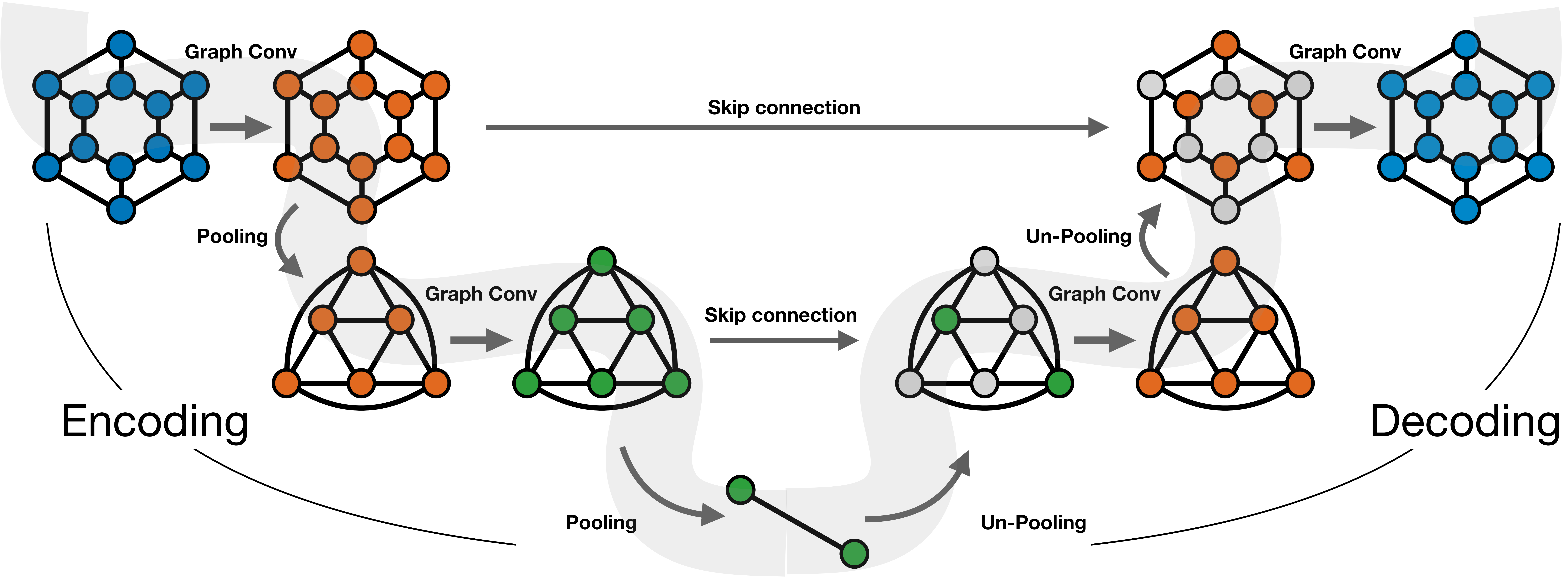
Our Cylindrical Graphs





Graph U-Net





Original pooling technique: ReNN-Pool *Algorithms* **2023**, *16*(3), 143; **https://doi.org/10.3390/a16030143**

Differentiable optimization

Trained Neural Network → $\tilde{f}_w(X)$ is **differentiable** with respect to X

X → $\tilde{f}_w(X) = Y$ → Y

THE PHYSICS

Differentiable optimization

Trained Neural Network → $\tilde{f}_w(X)$ is **differentiable** with respect to X

X → $\tilde{f}_w(X) = Y$ → Y

THE PHYSICS

$\nabla_X \tilde{f}_w(X)$

Gradient based optimization

Plan Optimisation

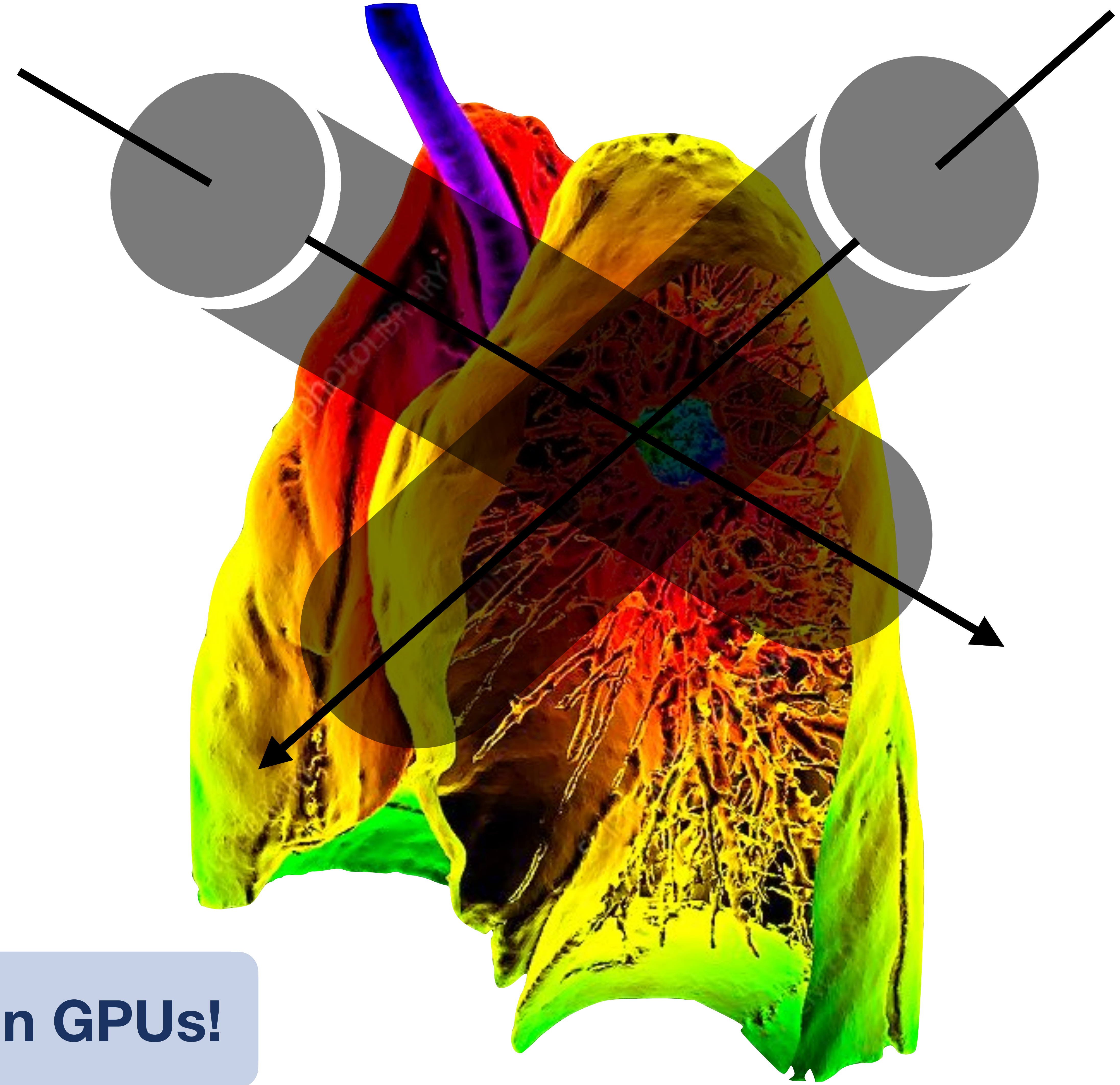
$\tilde{D}_w(\rho, \{B\})$ is **differentiable** with respect to $\{B\}$

$$\nabla_{\{B\}} \tilde{D}_w(\rho, \{B\})$$

Optimize the dose to each organ with **gradient descent**

Fit with medical prescriptions

on GPUs!



Preliminary results

Fast:

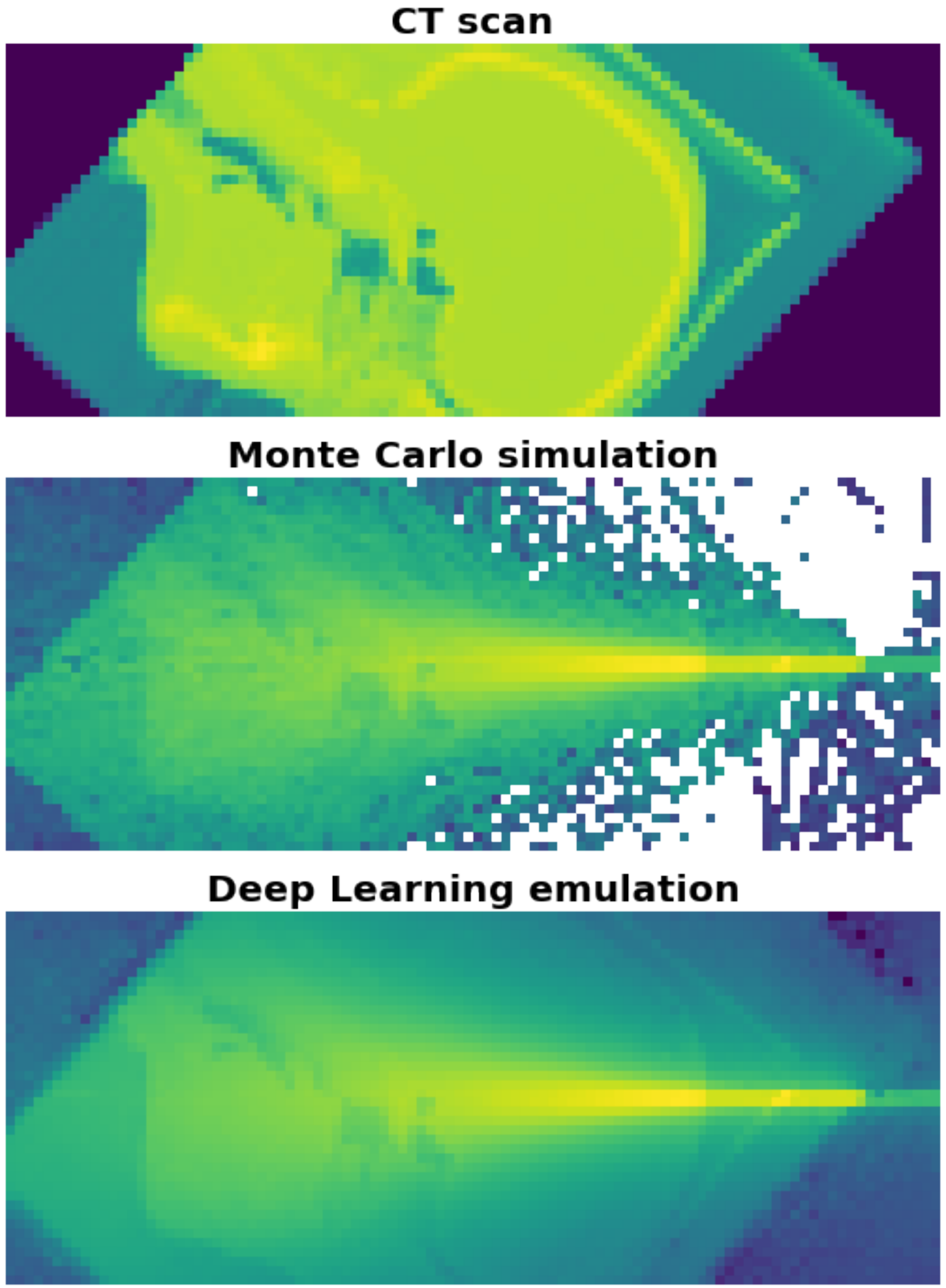
Batched generation: up to **0.001 s** per beam

Precise:

Voxelized Global γ index

$$\gamma = \left\langle \frac{|D_{real} - D_{reco}|}{max(D_{real})} \right\rangle$$

	% of voxels
$\gamma < 1\%$	98.52 %
$\gamma < 3\%$	99.04 %
$\gamma < 5\%$	99.21 %



Towards the emulation of BLOB, a nuclear interaction model

Problems in Geant4 below 100 MeV/u

No dedicated model to nuclear interaction **below 100 MeV/u** in Geant4

Many papers showed discrepancies:

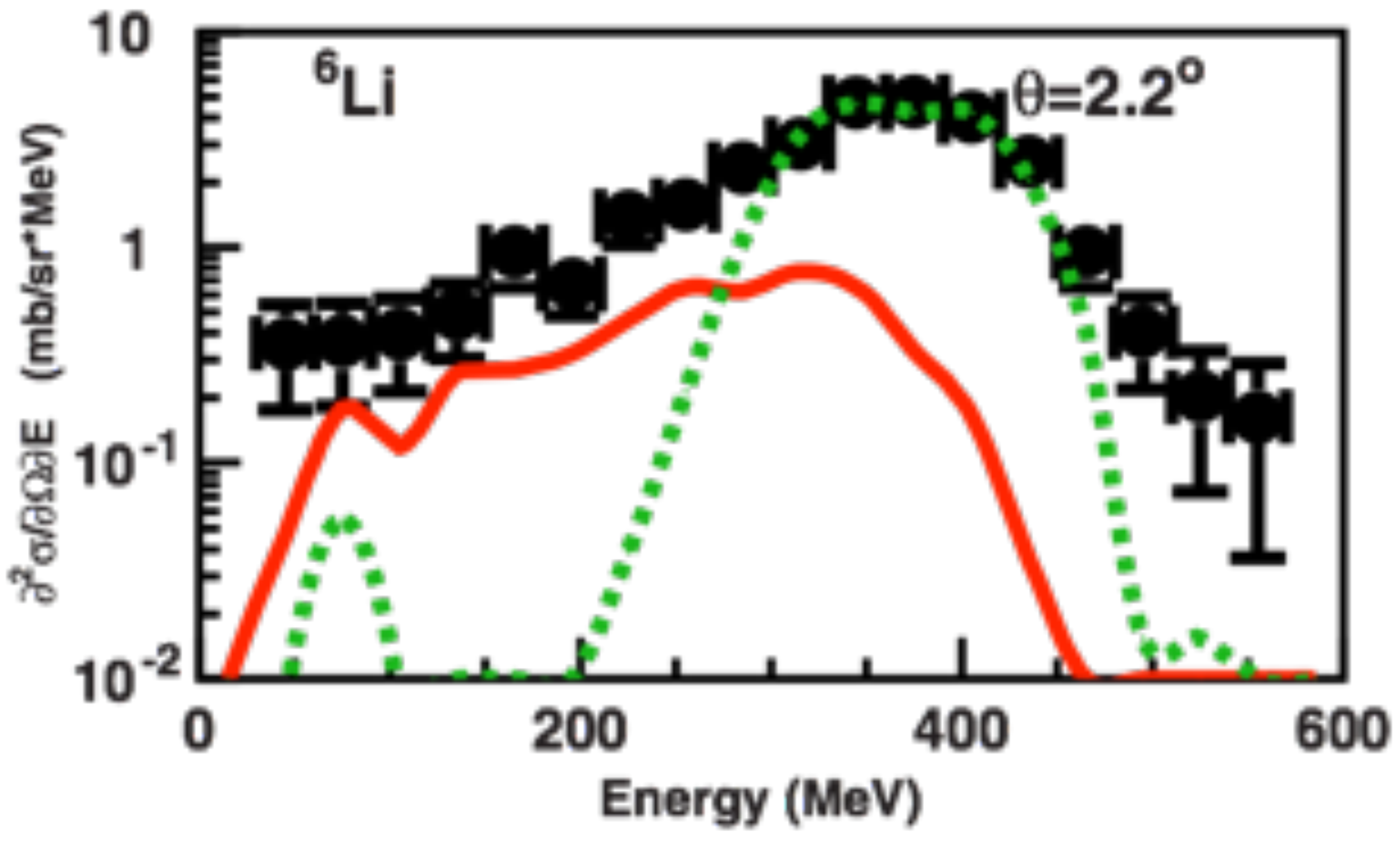
Braunn et al. : one order of magnitude in 12C fragmentation at 95 MeV/u on thick PMMA target

De Napoli et al. : angular distribution of the secondaries emitted in the interaction of 62 MeV/u 12C on thin carbon target

Dudouet et al. : similar results with a 95 MeV/u 12C 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]

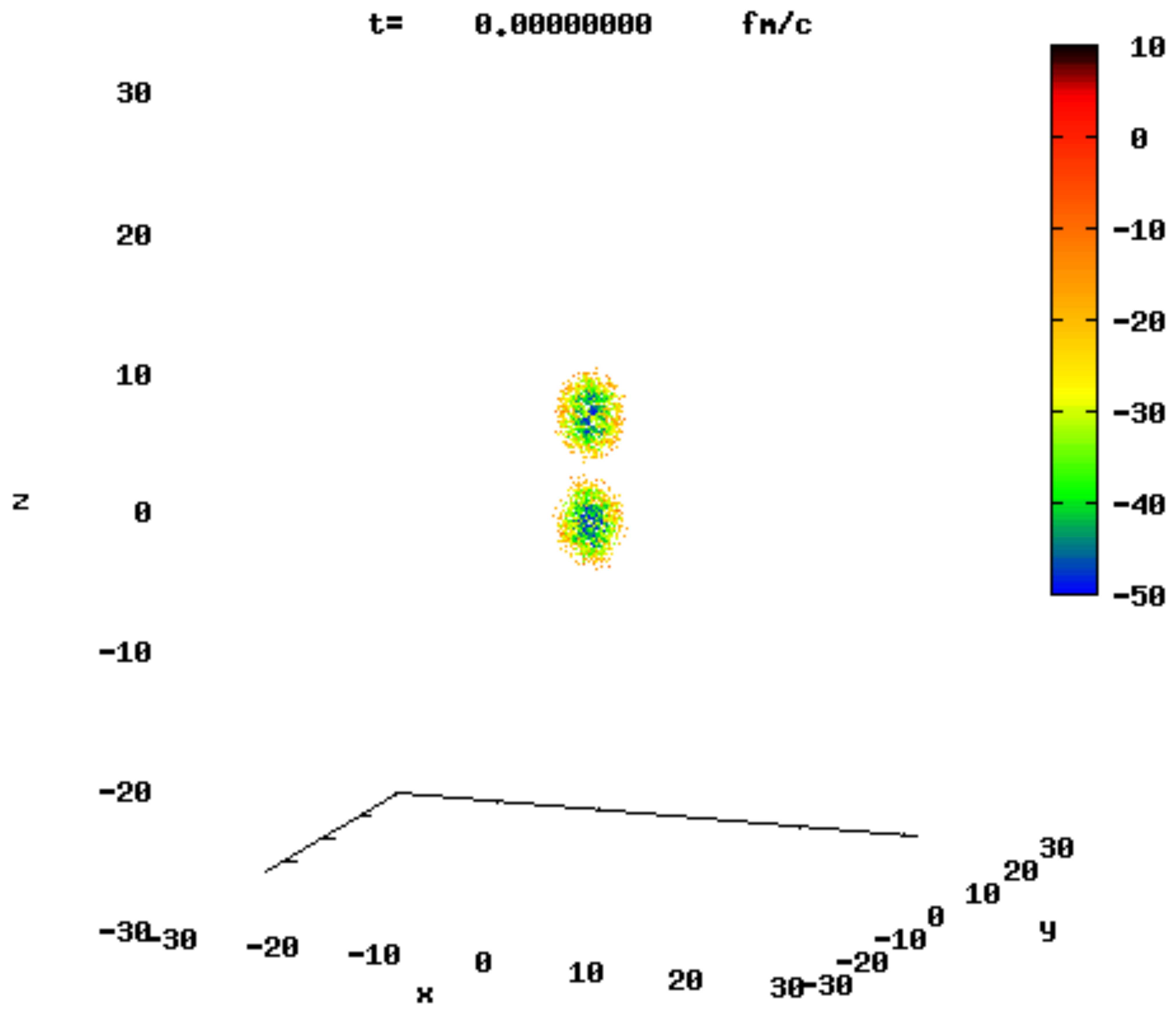


Cross section of the ^{6}Li production at 2.2 degree in a ^{12}C on ^{nat}C reaction at 62 MeV/u.

BLOB (Boltzmann-Lagevein One Body)

- Test-particle approach
- Self-consistent **mean field** + collisions
- Probability to find a nucleon in the phase space

Accurate



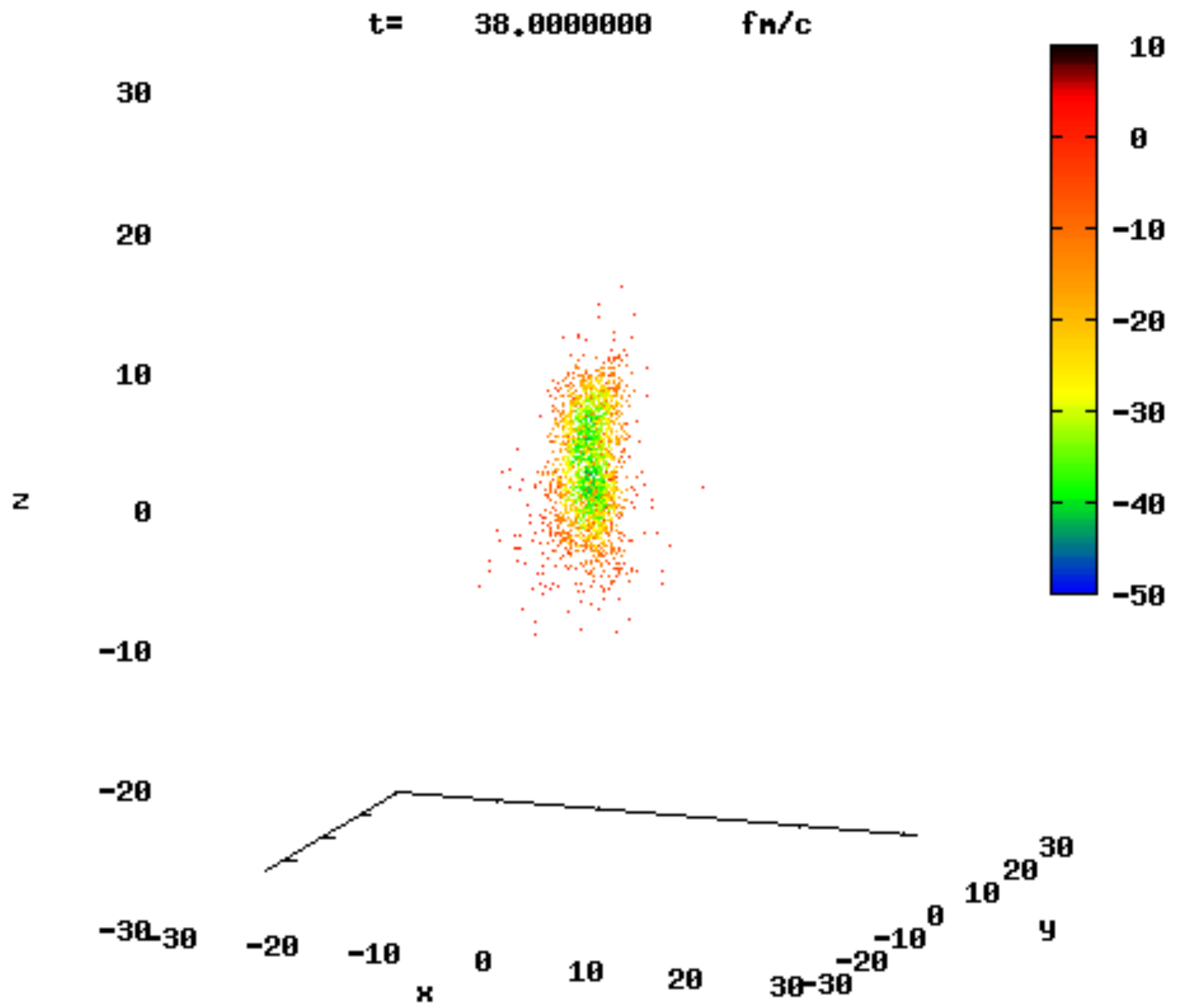
BLOB (Boltzmann-Lagevein One Body)

- Test-particle approach
- Self-consistent **mean field** + collisions
- Probability to find a nucleon in the phase space

Accurate

Slow

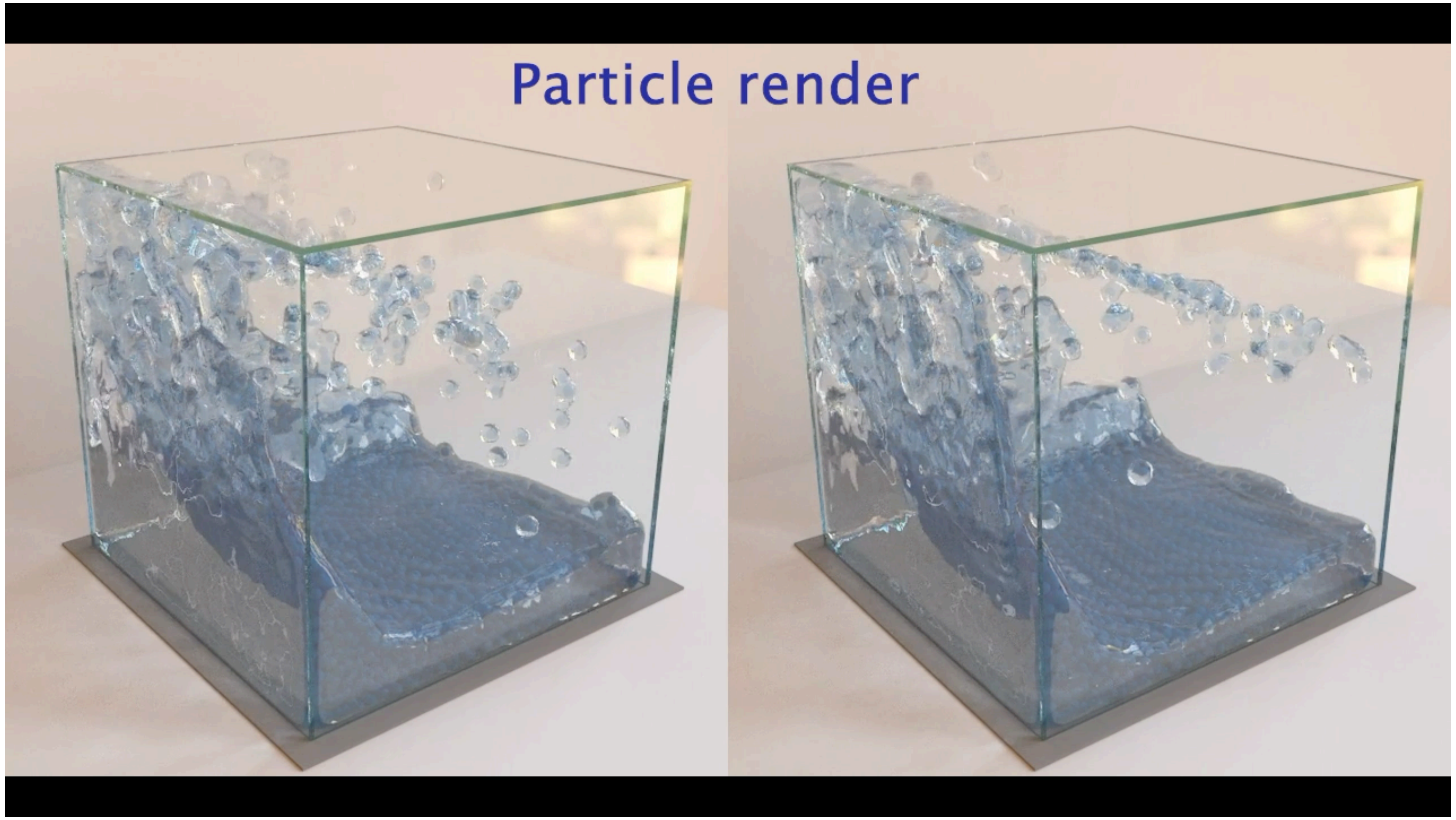
Up to 10 min per interaction!



Complex Physics Simulations

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

https://arxiv.org/abs/2002.09405



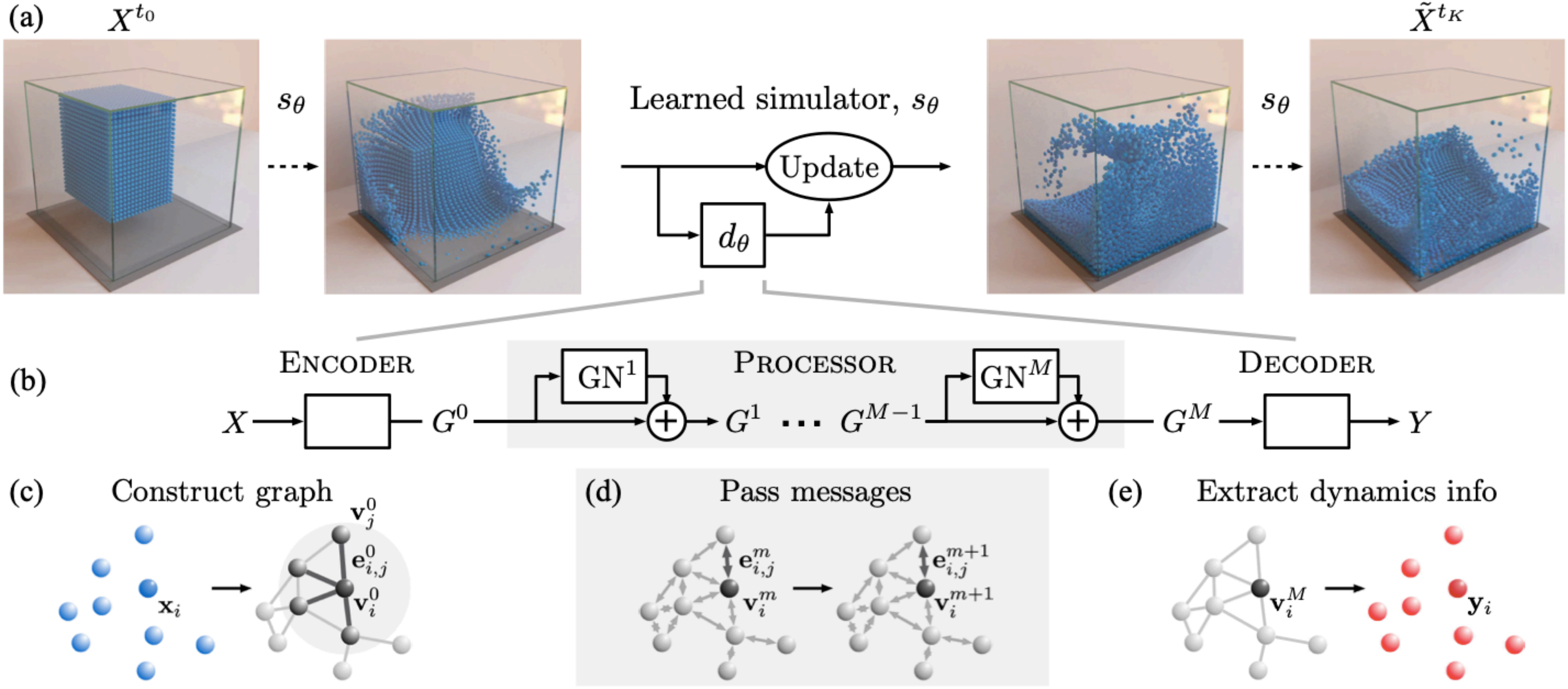
Github

github.com/deepmind/deepmind-research/tree/master/learning to simulate.

Videos

https://sites.google.com/view/learning-to-simulate

Graph Network-based Simulators (GNS)



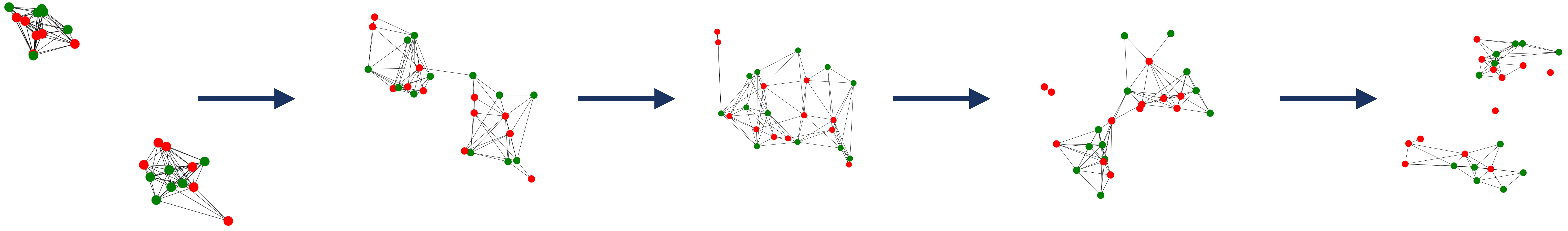
Starting simple: emulating QMD

Starting from: → a simpler model → **QMD**

→ a specific case → **^{12}C on ^{12}C**

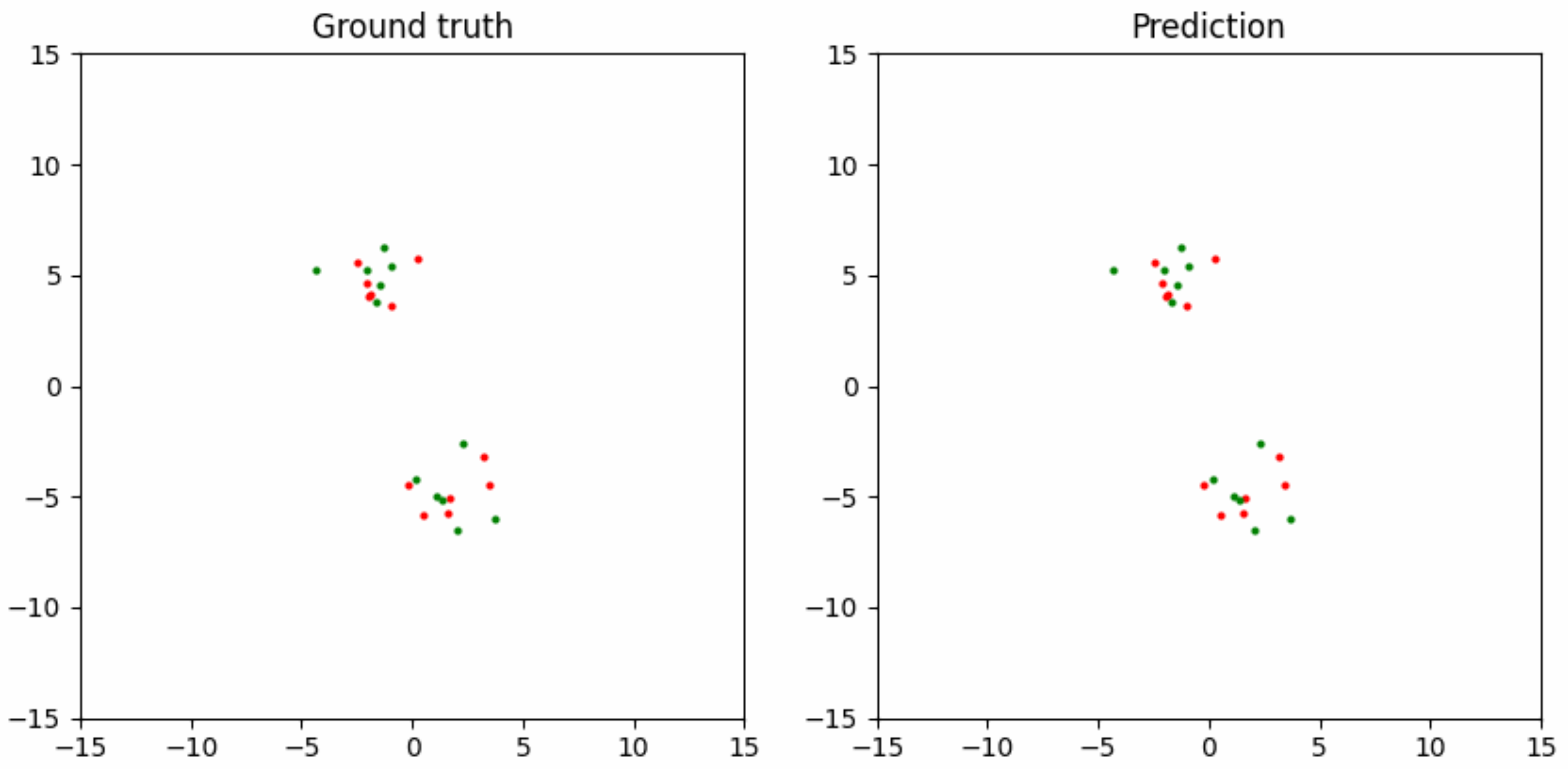
12 MeV/u

Each nucleon is a node of the graph



Emulating BLOB

- **Train** a Graph Neural Network to emulate the dynamics
- **Export** the model in **ONNX**
- **Integrate** into **Geant4**



Thank you for your attention!

- Deep-Learning-based dose deposition emulation:
  - Both fast and accurate dose estimation
  - Cylindrical Graph Neural Network model:
    From CT scan to dose deposition
  - Gradient based plan optimization on GPUs
- GNNs for nuclear interaction model emulation:
  - Emulation of the dynamics
  - Possible Geant4 integration