Development and implementation of new Geant4 QMD model and its validation

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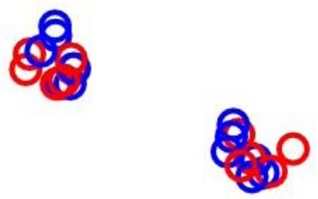
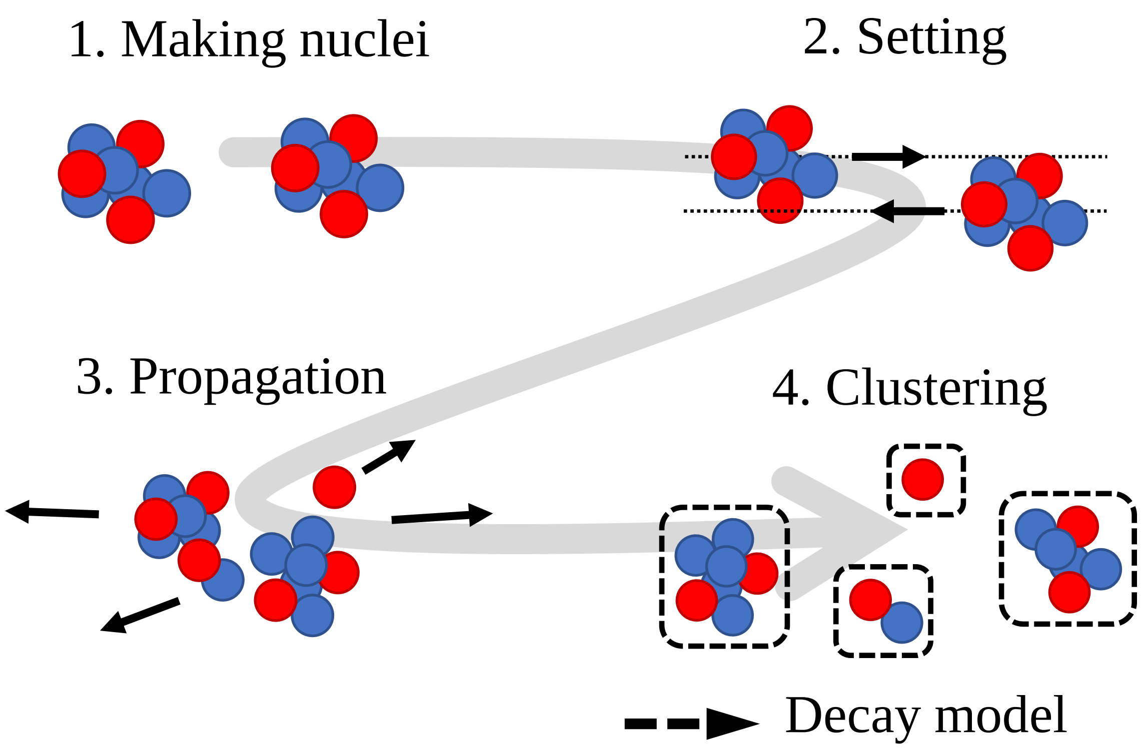
Quantum Molecular Dynamics (QMD)

Introduction

The QMD model is a quantum extension of the classical molecular-dynamics model and can describe hadronic processes, especially inelastic processes, in Geant4.

Collision between ^{12}C





Development of more accurate QMD model for hadron therapy

Introduction

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Physics in Medicine & Biology

IPEM Institute of Physics and Engineering in Medicine

CrossMark

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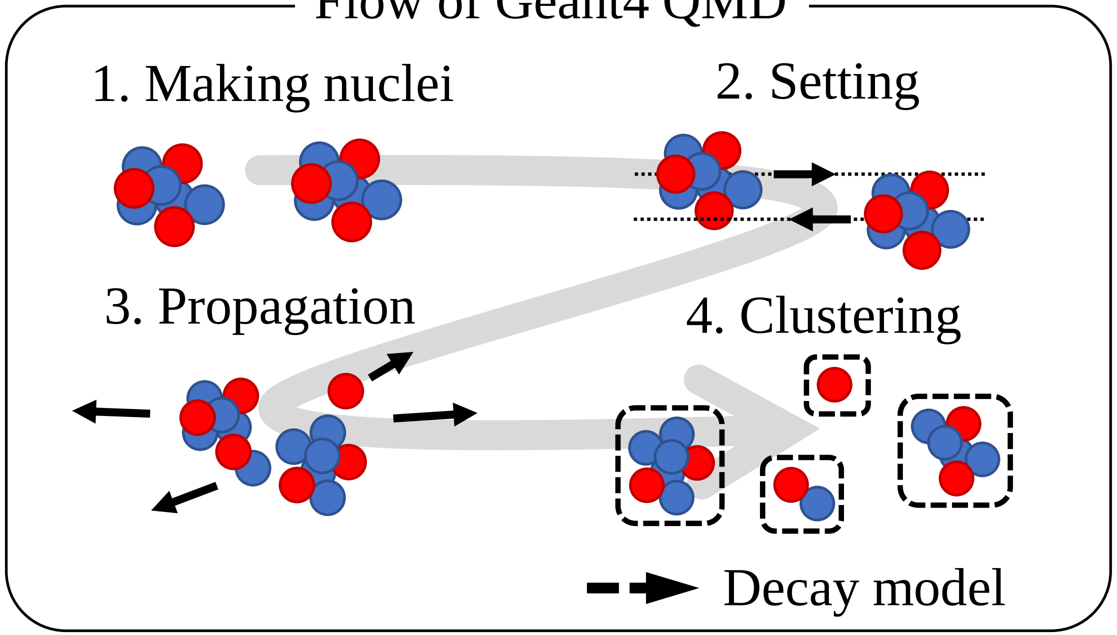
PAPER

Development of a more accurate Geant4 quantum molecular dynamics model for hadron therapy

Yoshi-hide Sato[1], Dousatsu Sakata[2,3,*], David Bolst[4], Edward C Simpson[5], Susanna Guatelli[4] and Akihiro Haga[1,*]

Sato, Y.-H. *et al*. Development of a more accurate Geant4 quantum molecular dynamics model for hadron therapy. *Phys. Med. Biol.* **67**, (2022)

Flow of Geant4 QMD

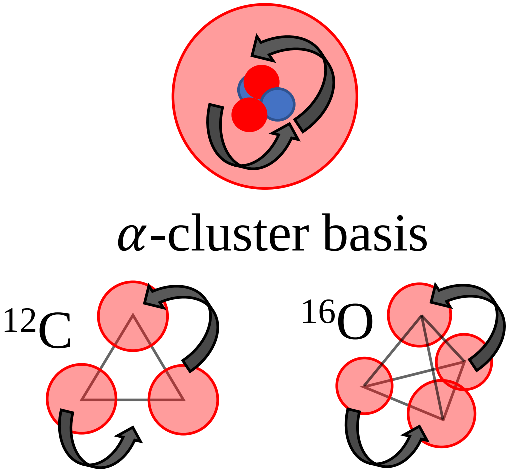


Three improvements

1. Modern interaction

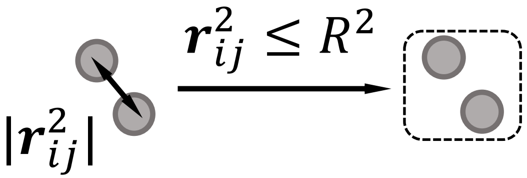
	JQMD[b] (G4QMD)	SLy4[c]	SkM*[c]	SIII[c]
A [MeV]	−219.4	−297.82	−318	−122.921
B [MeV]	165.3	219.21	249.5	55.343
g_0 [MeV fm^2]	—	24.569	21.86	18.286
g_τ [MeV]	—	9.70	5.9357	6.439
C_s [MeV]	25	32	32	32
κ_s [fm^2]	—	0.08	0.08	0.08
γ	4/3	7/6	7/6	2
η[a]	—	5/3	5/3	5/3
ρ_0 [fm^{-3}][a]	0.168	0.160	0.165	0.1452
BE [MeV][a]	−16.00	−15.97	−15.77	−15.83
K_0 [MeV][a]	237.8	230.2	216.8	355.9

2. α-cluster structure



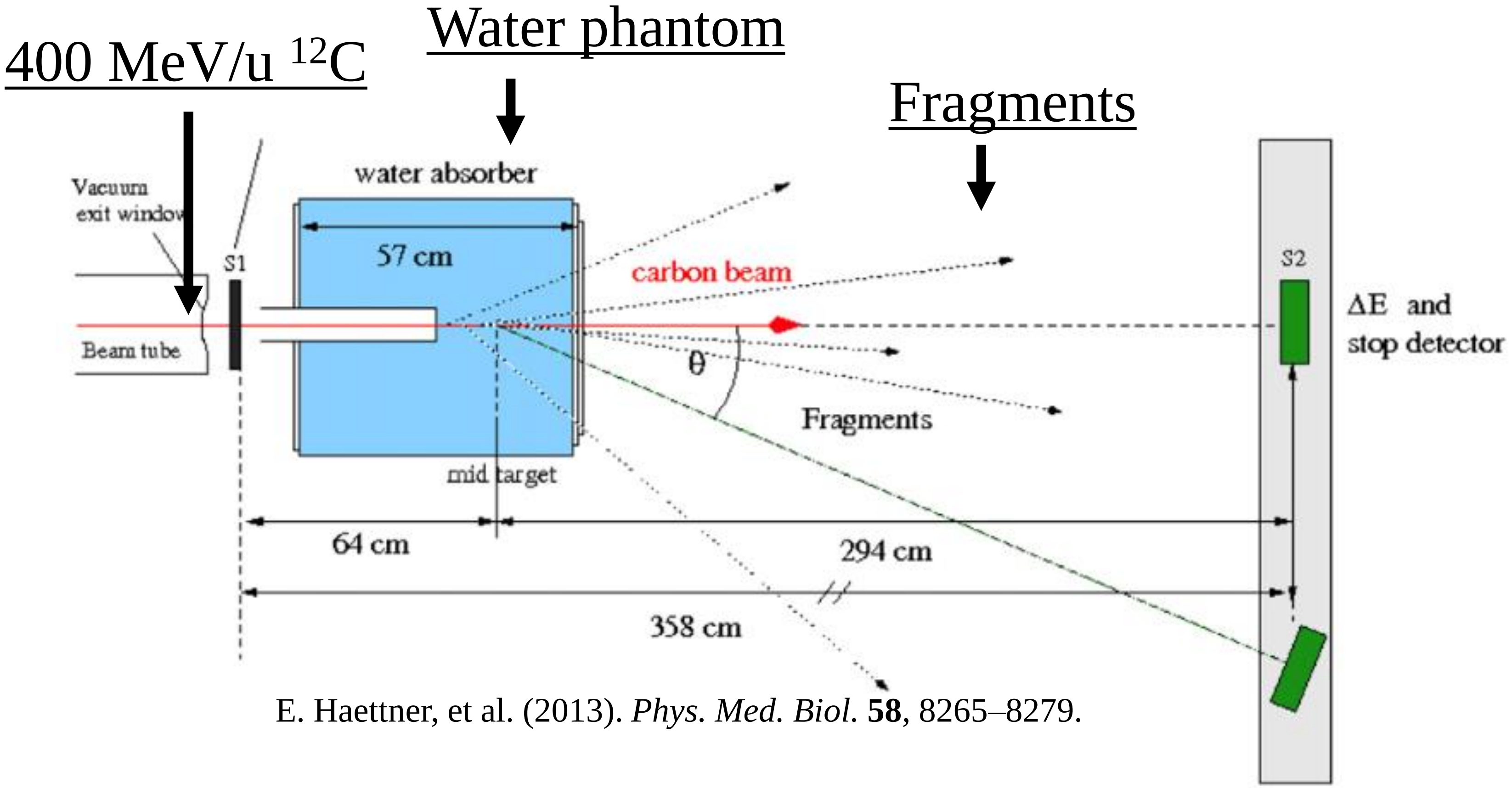
3. QMD model Parameter optimization

$$\varphi_i(\boldsymbol{r}) \equiv \frac{1}{(2\pi L)^{3/4}} \exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}_i)^2}{4L} + \frac{i}{\hbar}\boldsymbol{r}\cdot\boldsymbol{p}_i\right)$$



Water Phantom

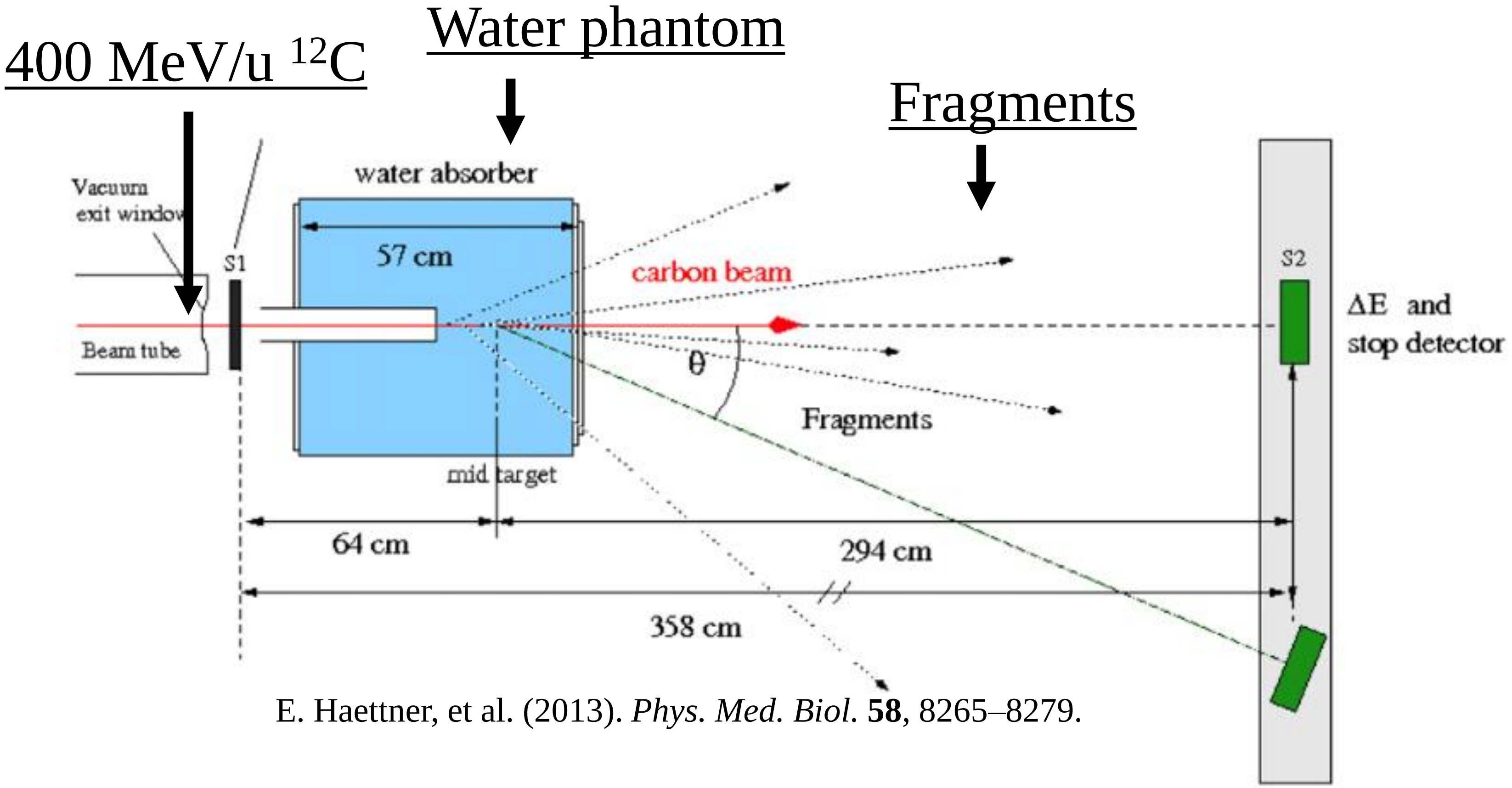
Materials and Methods



E. Haettner, et al. (2013). *Phys. Med. Biol.* **58**, 8265–8279.

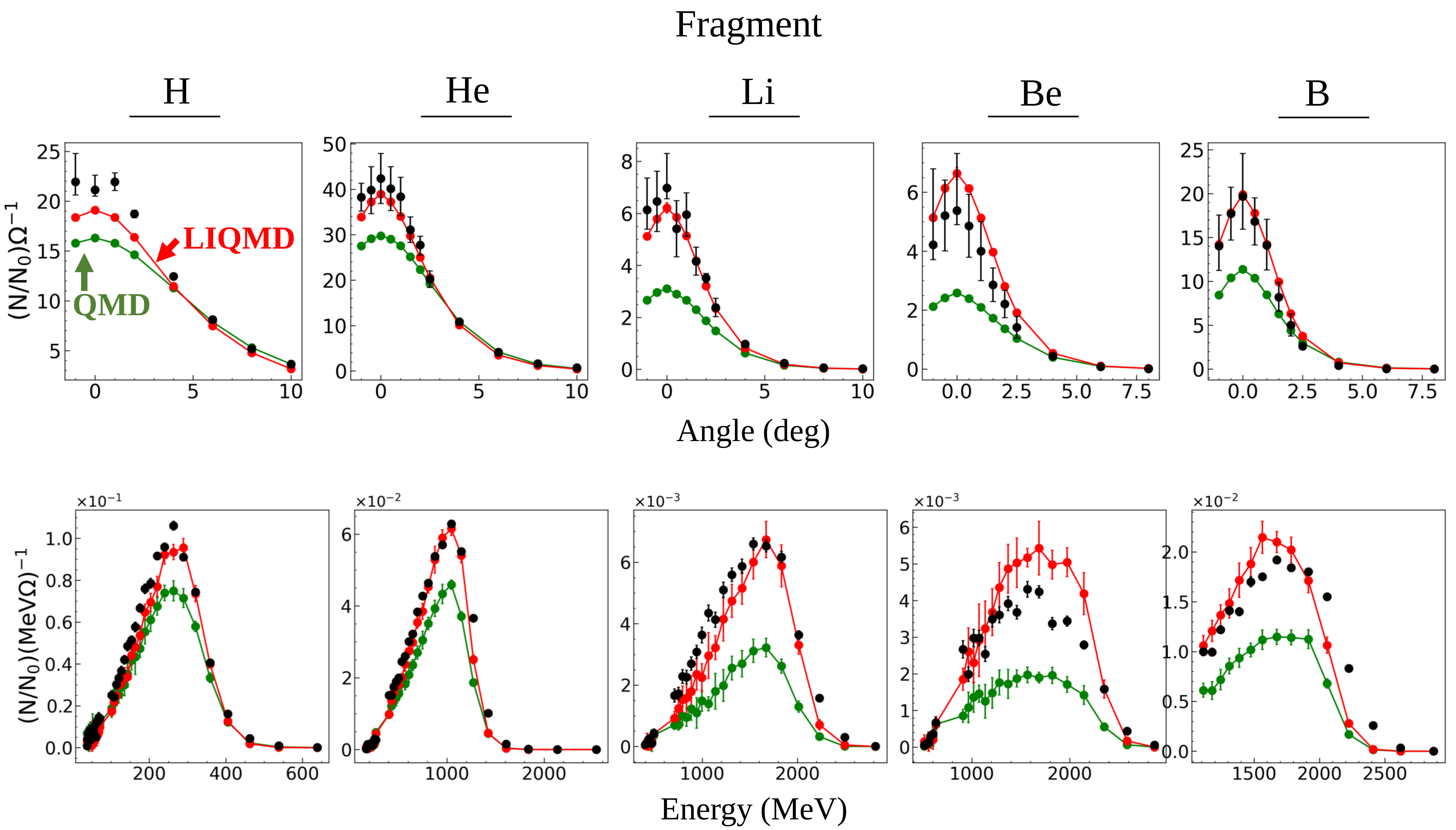
Water Phantom

Materials and Methods



E. Haettner, et al. (2013). *Phys. Med. Biol.* **58**, 8265–8279.

Light Ion QMD (LIQMD)



Fragment
H
He
Li
Be
B
LIQMD
QMD
$(N/N_0)\Omega^{-1}$
Angle (deg)
$(N/N_0)(\mathrm{MeV}\Omega)^{-1}$
Energy (MeV)

Validation

- Water phantom with 400 MeV/u ^{12}C beam [1]
- Thin target with 95 MeV/u ^{12}C beam [2]
- Dose-Depth curve of water phantom [3]
- Positron-emitting nucleus yield [3]

[1] E. Haettner, et al. (2013). *Phys. Med. Biol.* **58**, 8265–8279.

[2] Dudouet, J. et al. (2013). *Physical Review C*, *88*(2), 024606.

[3] A. Chacon, et. al.(2019), *Phys. Med. Biol*. **64**, 155014.

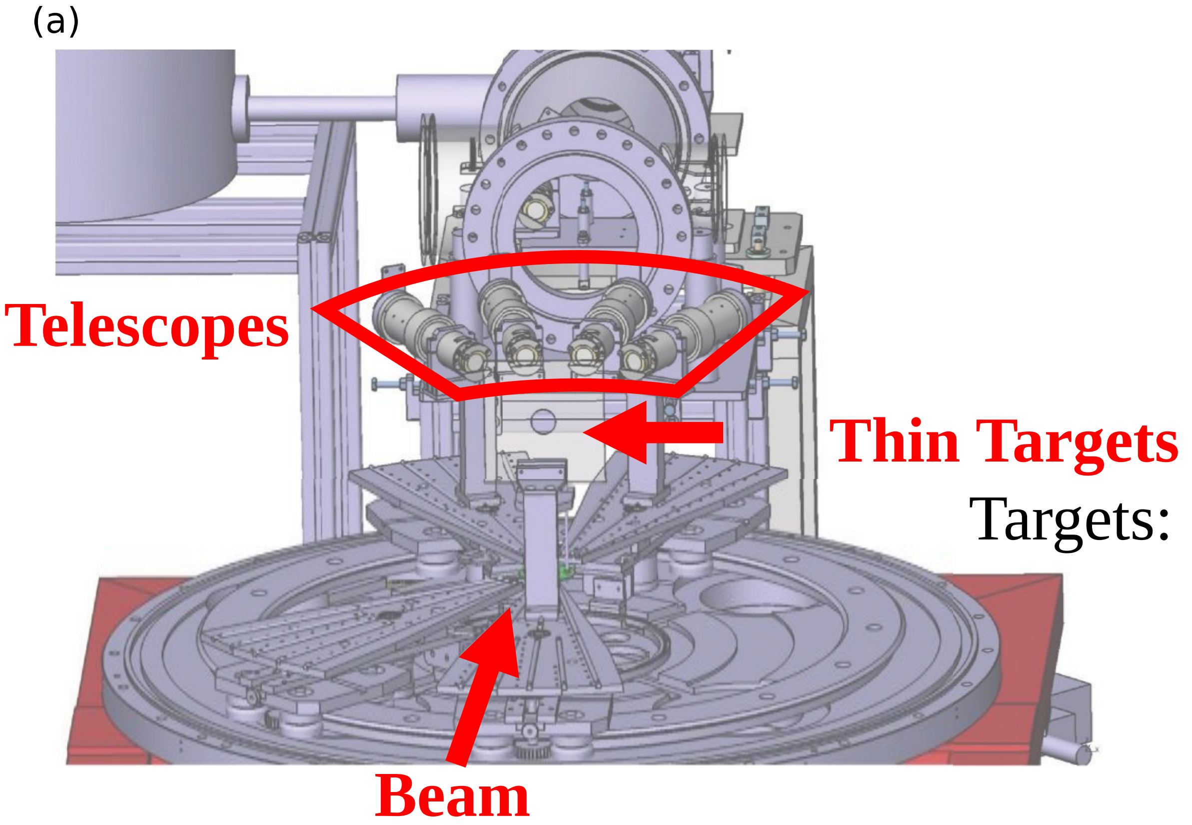
Validation

- Water phantom with 400 MeV/u ^{12}C beam
- Thin target with 95 MeV/u ^{12}C beam
- Dose-Depth curve of water phantom
- Positron-emitting nucleus yield

Thin Target

Materials and Methods

Fragments: $^{1,2,3}H$, $^{3,4,6}He$, $^{6,7}Li$, $^{7,9,10}Be$, $^{8,10,11}B$, $^{10,11,12}C$

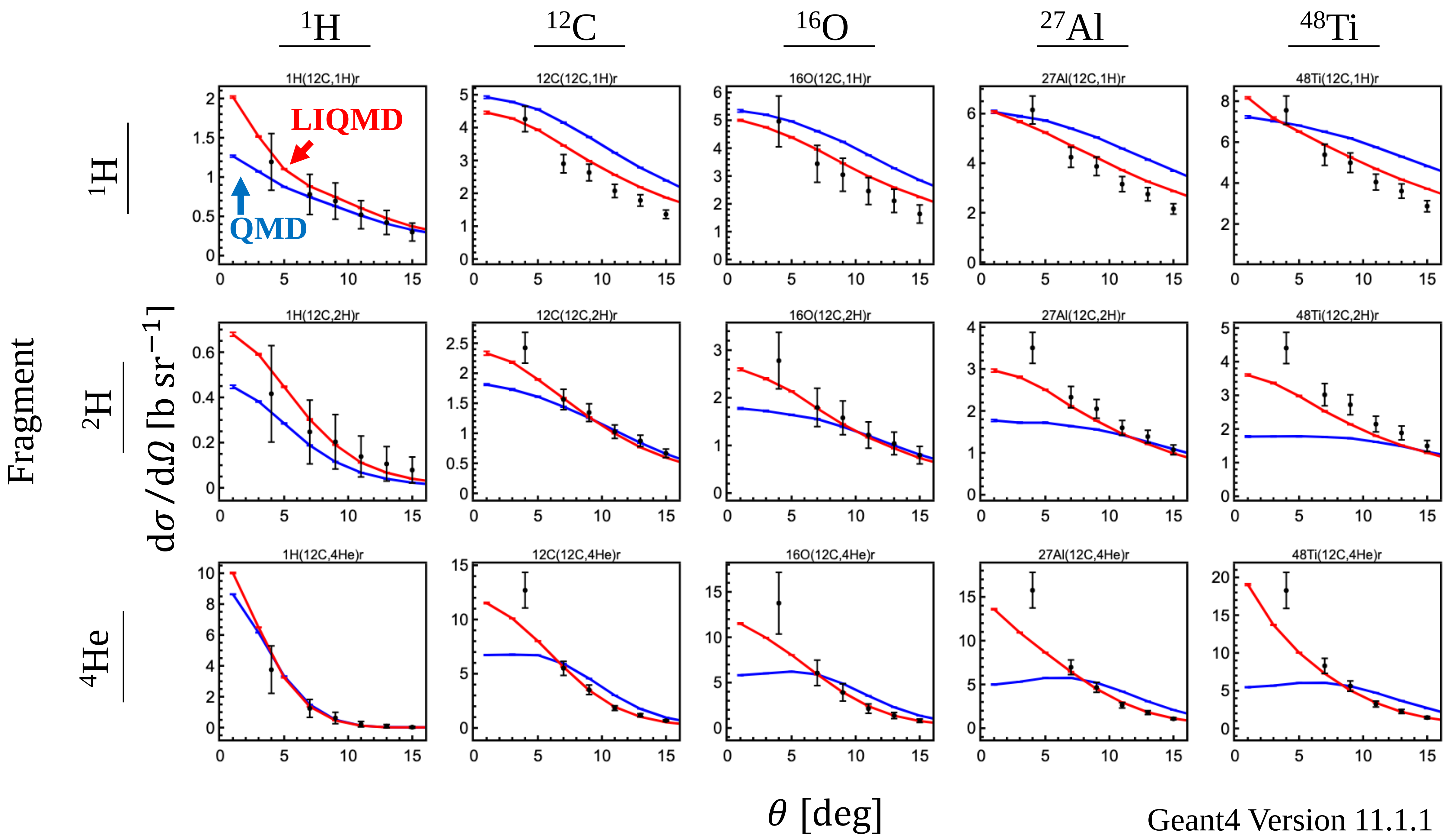


Targets: ^{1}H, ^{12}C, ^{16}O, ^{27}Al, ^{48}Ti

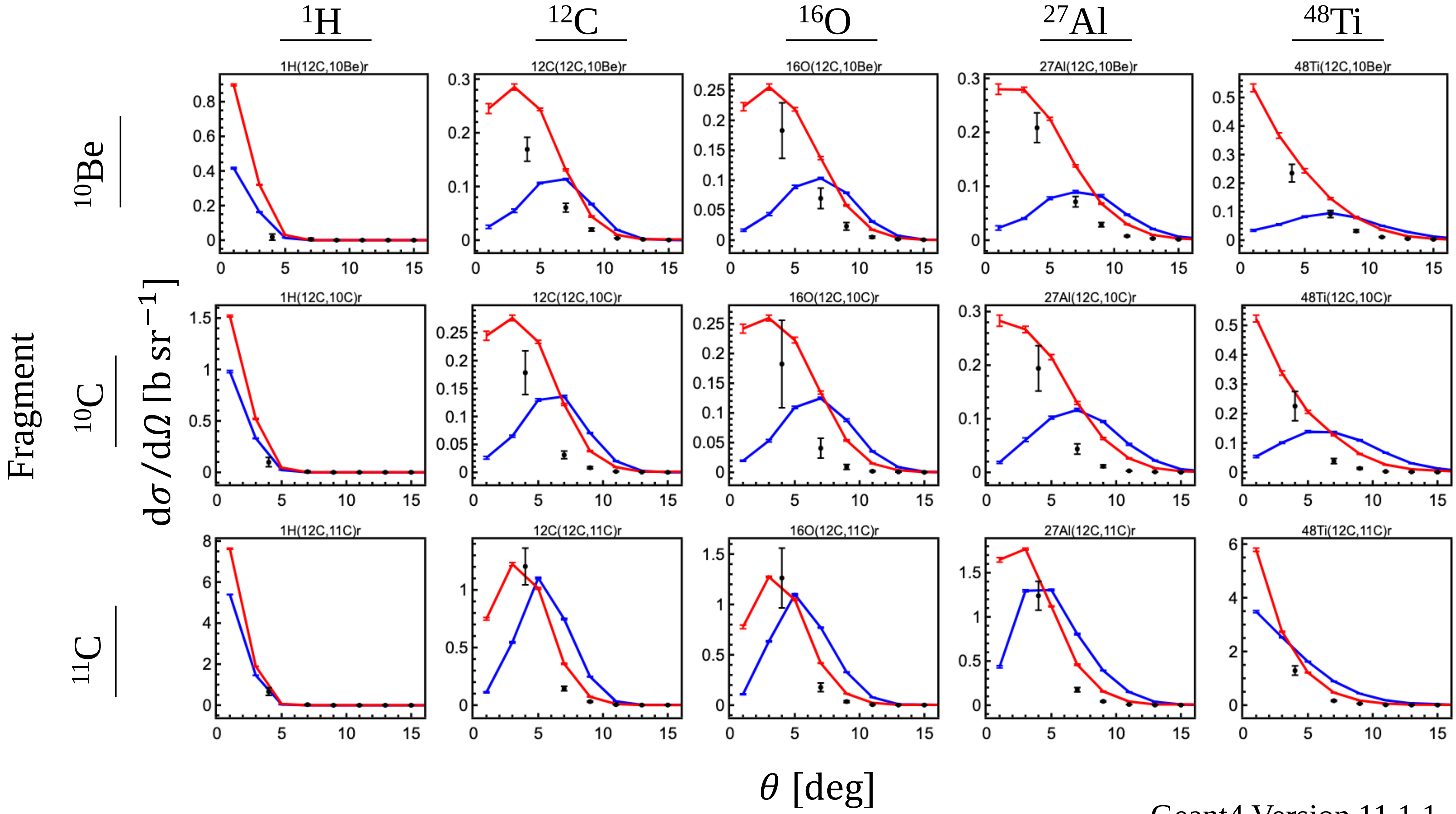
Beam: ^{12}C, 94.6±0.09 MeV/A

Dudouet, J. et al.. (2013). *Physical Review C*, *88*(2), 024606.

E600 experiment at the Grand Accelerateur National d'Ions Lourds (GANIL) facility.



Geant4 Version 11.1.1



Geant4 Version 11.1.1

Validation

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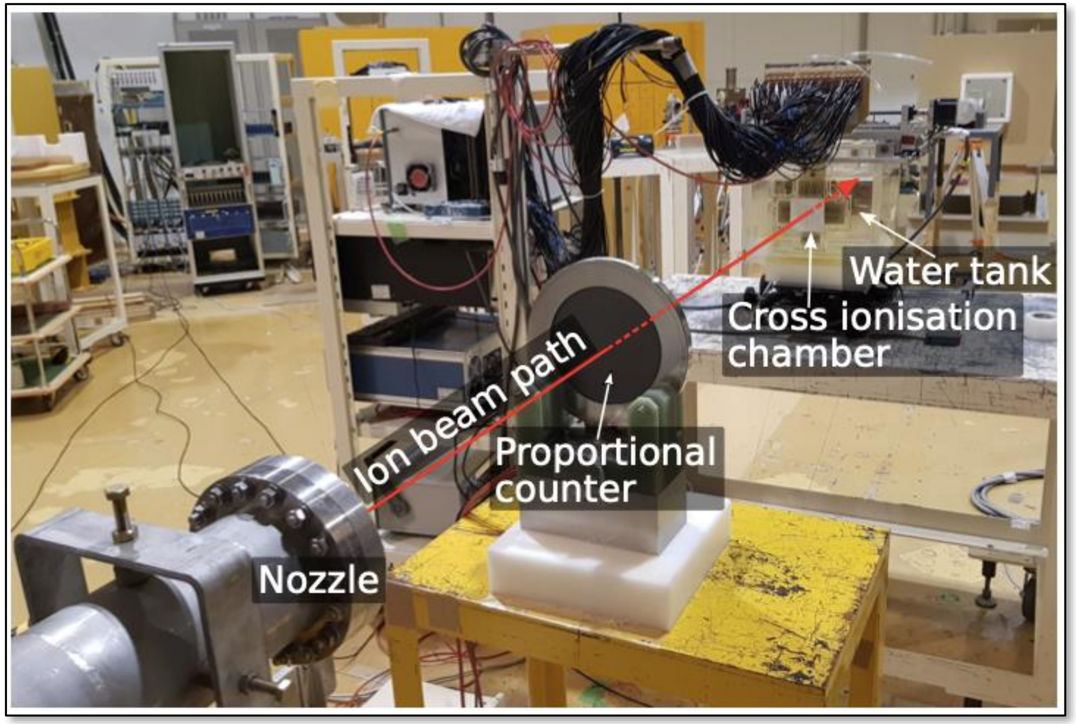
- Positron-emitting nucleus yield

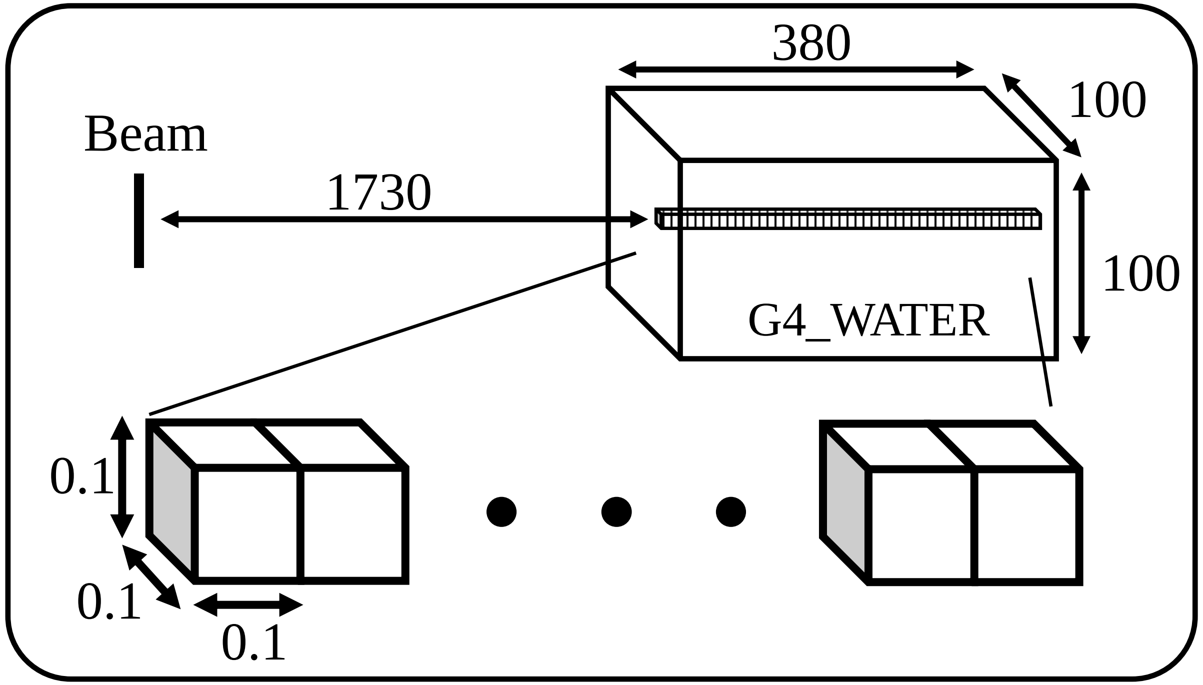
Depth-Dose Curve

Materials and Methods



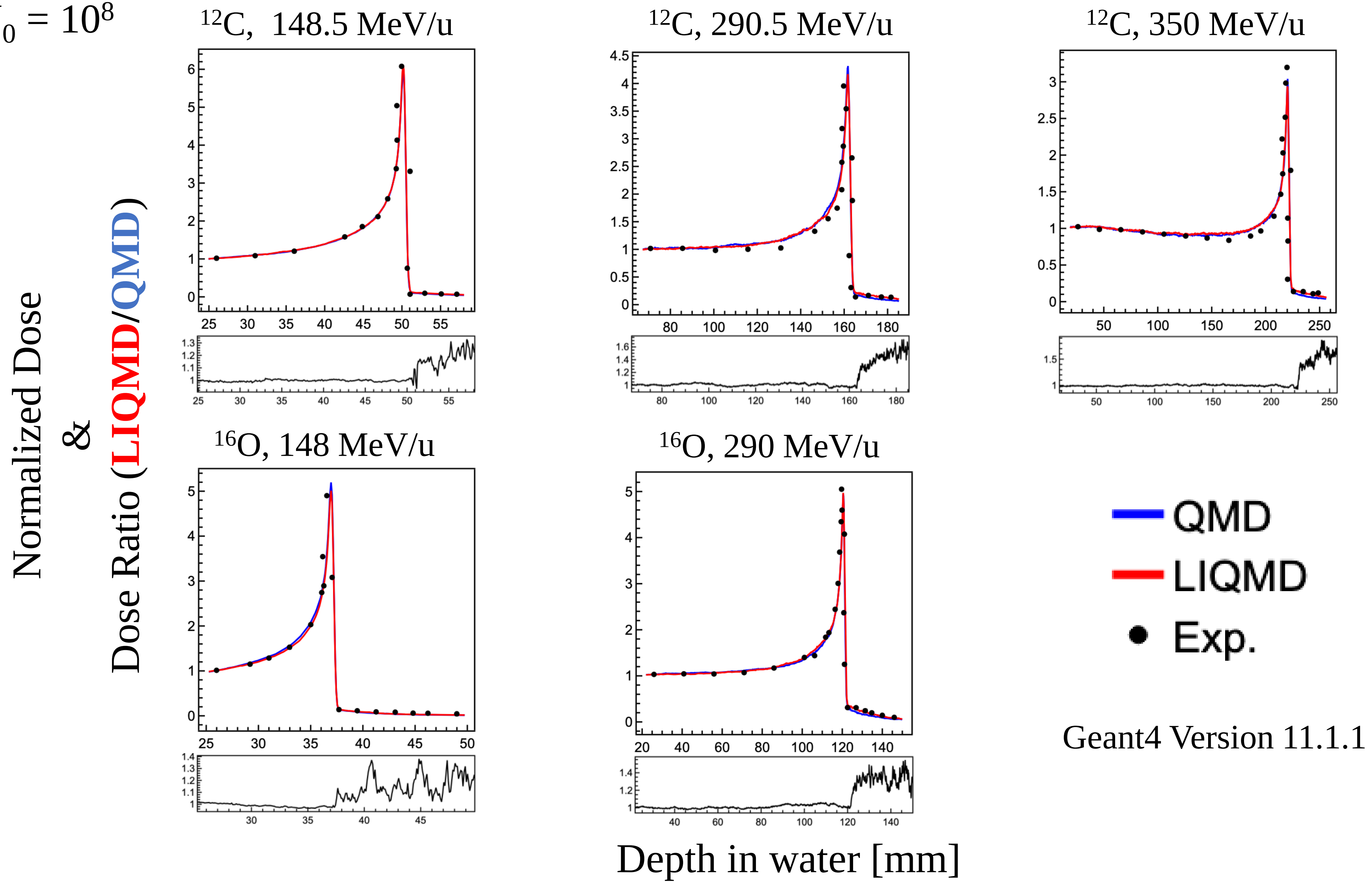
[1] A. Chacon, et. al., *Phys. Med. Biol.* **64**, 155014 (2019).

Simulation geometry (Unit : mm)



- ❑ Recording the energy deposition to each voxel on the beam axis by Command-based scoring.

$N_0 = 10^8$



Geant4 Version 11.1.1

Validation

- Water phantom with 400 MeV/u ^{12}C beam
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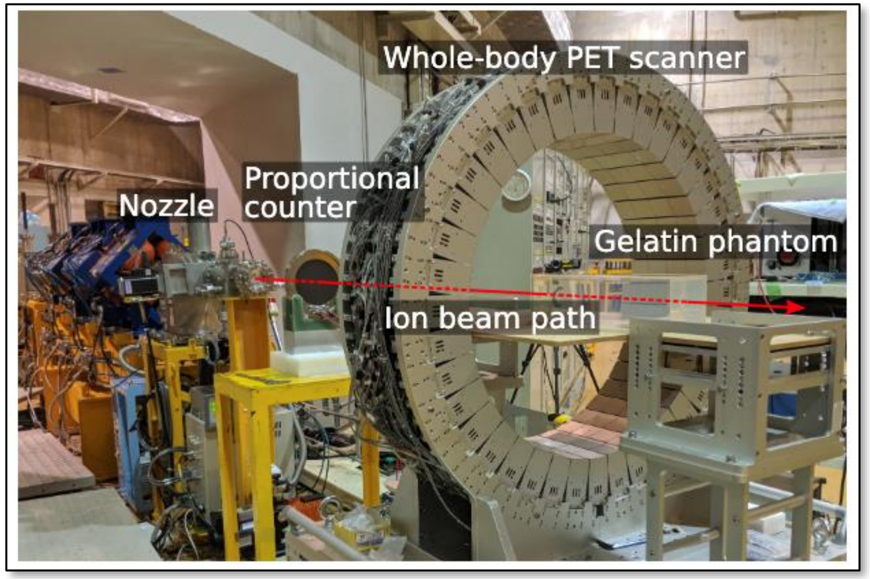
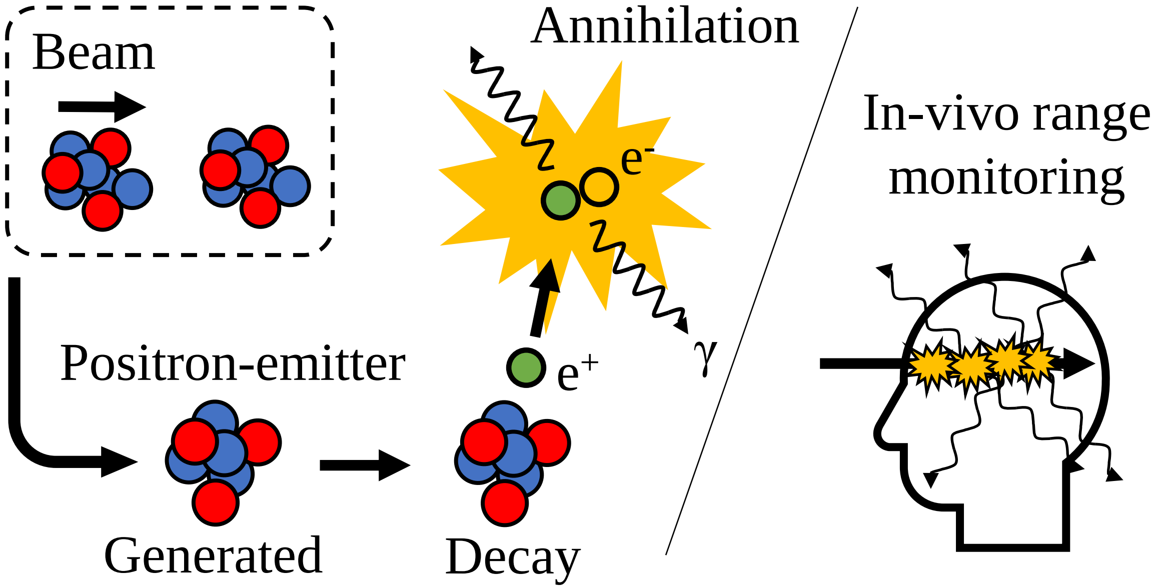
Positron-Emitting Nuclide Yield

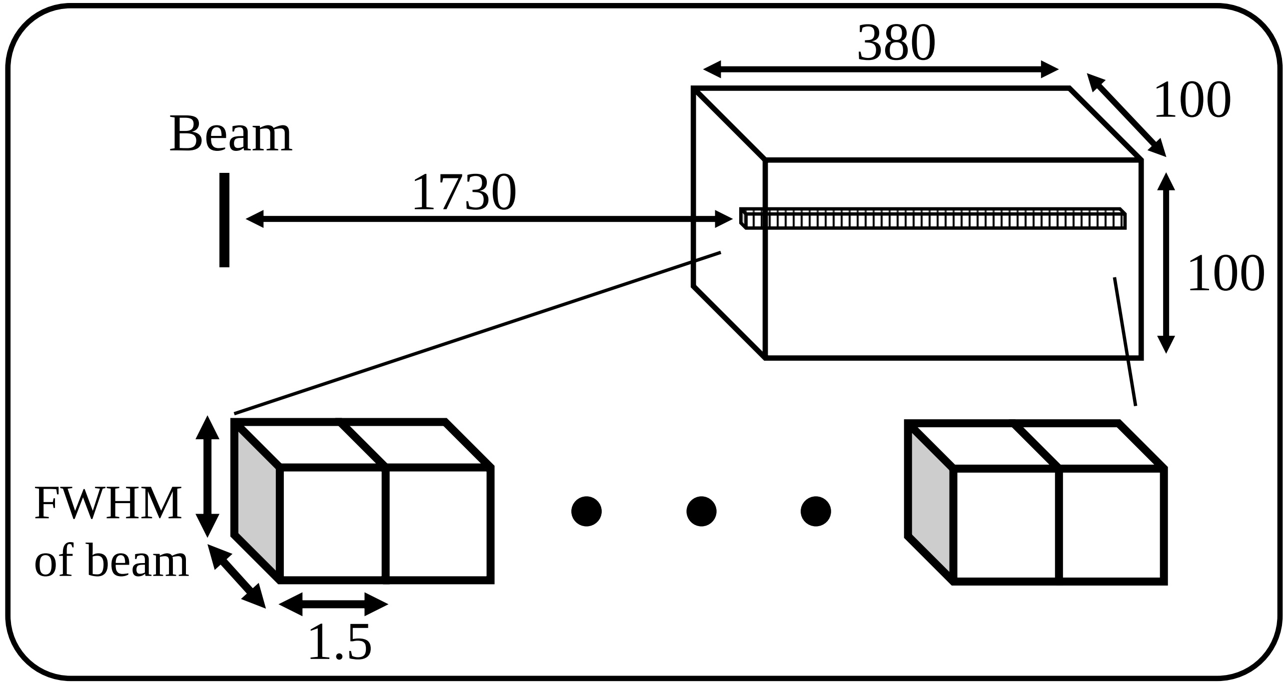
Materials and Methods



A. Chacon, et. al., *Phys. Med. Biol.* **64**, 155014 (2019).



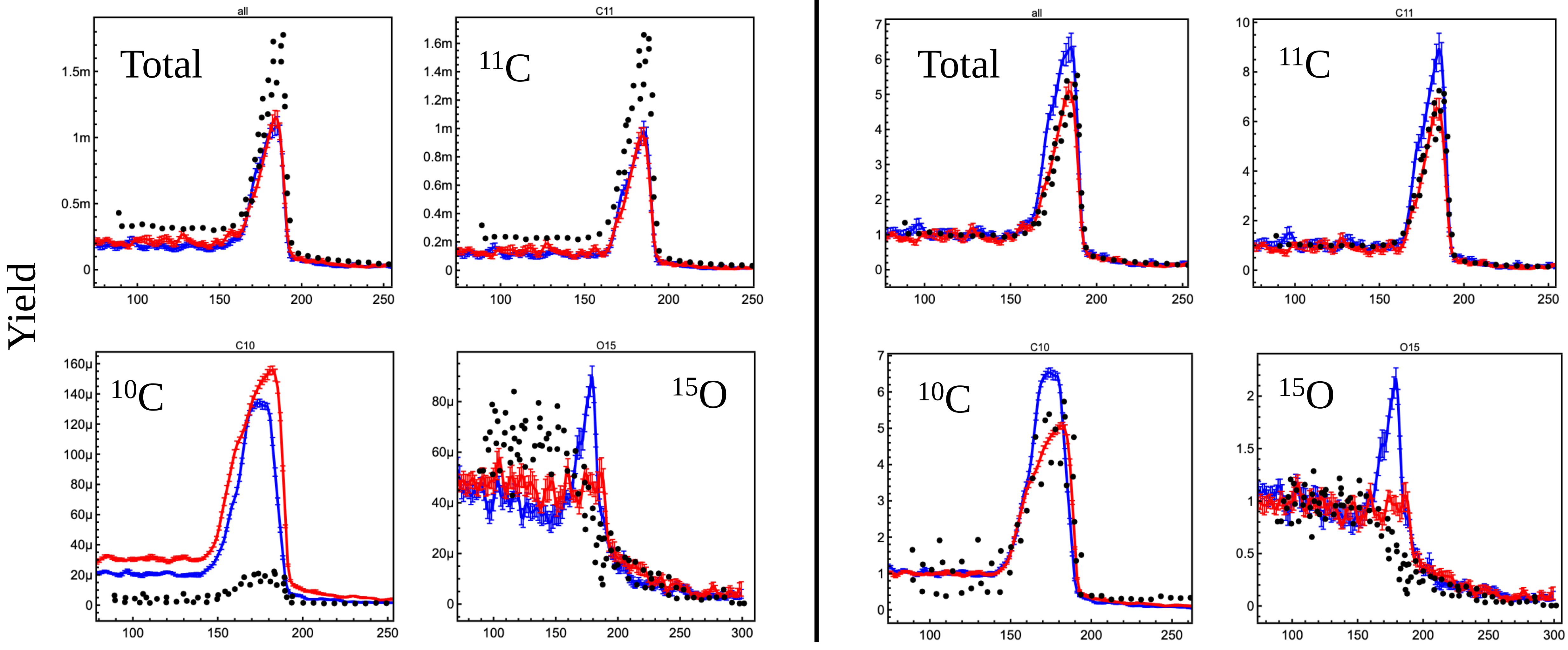
Simulation and analysis geometry (Unit : mm)



- ❑ Calculating the number of positron-emitting nuclide in each voxel on the beam axis at the initial.

QMD LIQMD ● Exp. ^{12}C, 350MeV/u, PMMA $N_0 = 10^8$ 10 repetitions

Normalized (Focus on shape)



Depth in water [mm]

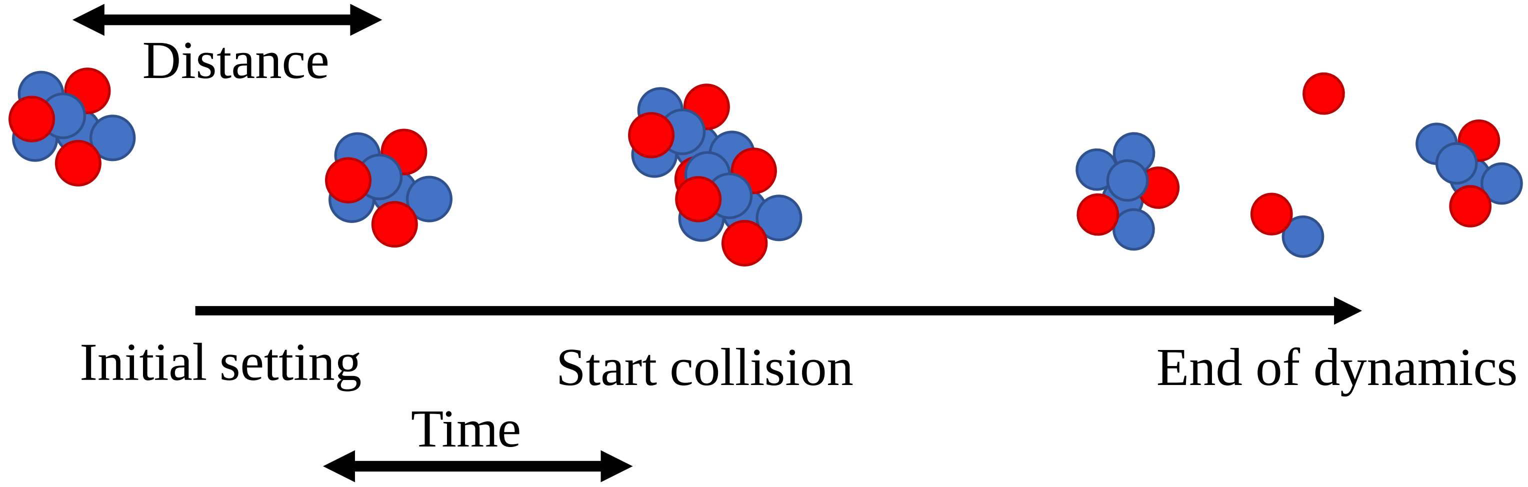
Geant4 Version 11.1.1

Limitation in LIQMD

- Energy range
- Mass range

Energy Range Recommended in LIQMD

Projectile and target should be separated by at least about b-value.



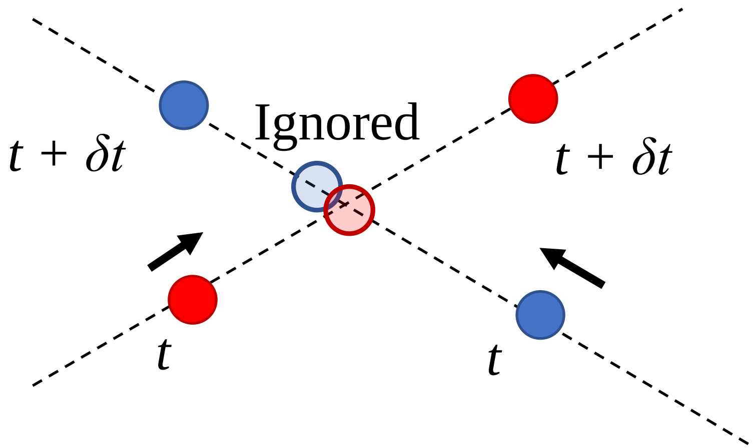
If the speed is slow (Low kinetic energy per nucleon), it will take a long time to collide, leaving not enough time for simulation after the collision.

It is better to have at least about 30 MeV/u.

Energy Range Recommended in LIQMD

Materials and Methods

Too high energy



500 MeV/u gives 1.5 fm gap in time step δt = 2 fm/c.
Due to this large gap, collisions that should occur may be ignored.

<u>Energies below about 500 MeV/u are recommended.</u>

Mass Range Recommended in LIQMD

Materials and Methods

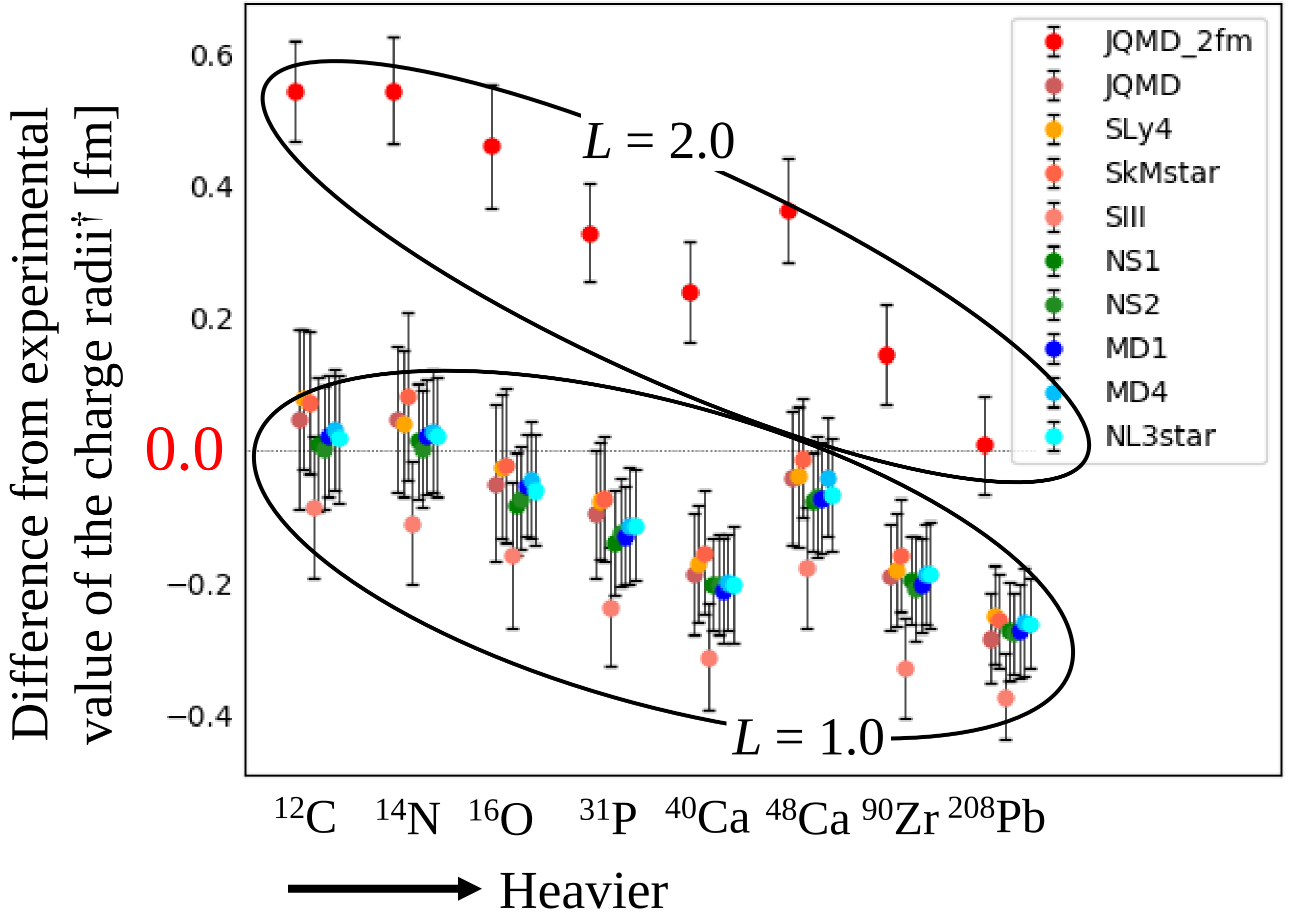
Wave function of nucleon

$$\varphi_i(\boldsymbol{r}) \equiv \frac{1}{(2\pi L)^{3/4}} \exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}_i)^2}{4L} + \frac{i}{\hbar}\boldsymbol{r}\cdot\boldsymbol{p}_i\right)$$

L = 2.0 [fm] for QMD

L = 1.26[fm] for LIQMD

Charge radii of nucleus



†: I. Angeli, K.P. Marinova, Atomic Data and Nuclear Data Tables, 99, 2013, 69-95.

Mass Range Recommended in LIQMD

Materials and Methods

Wave function of nucleon

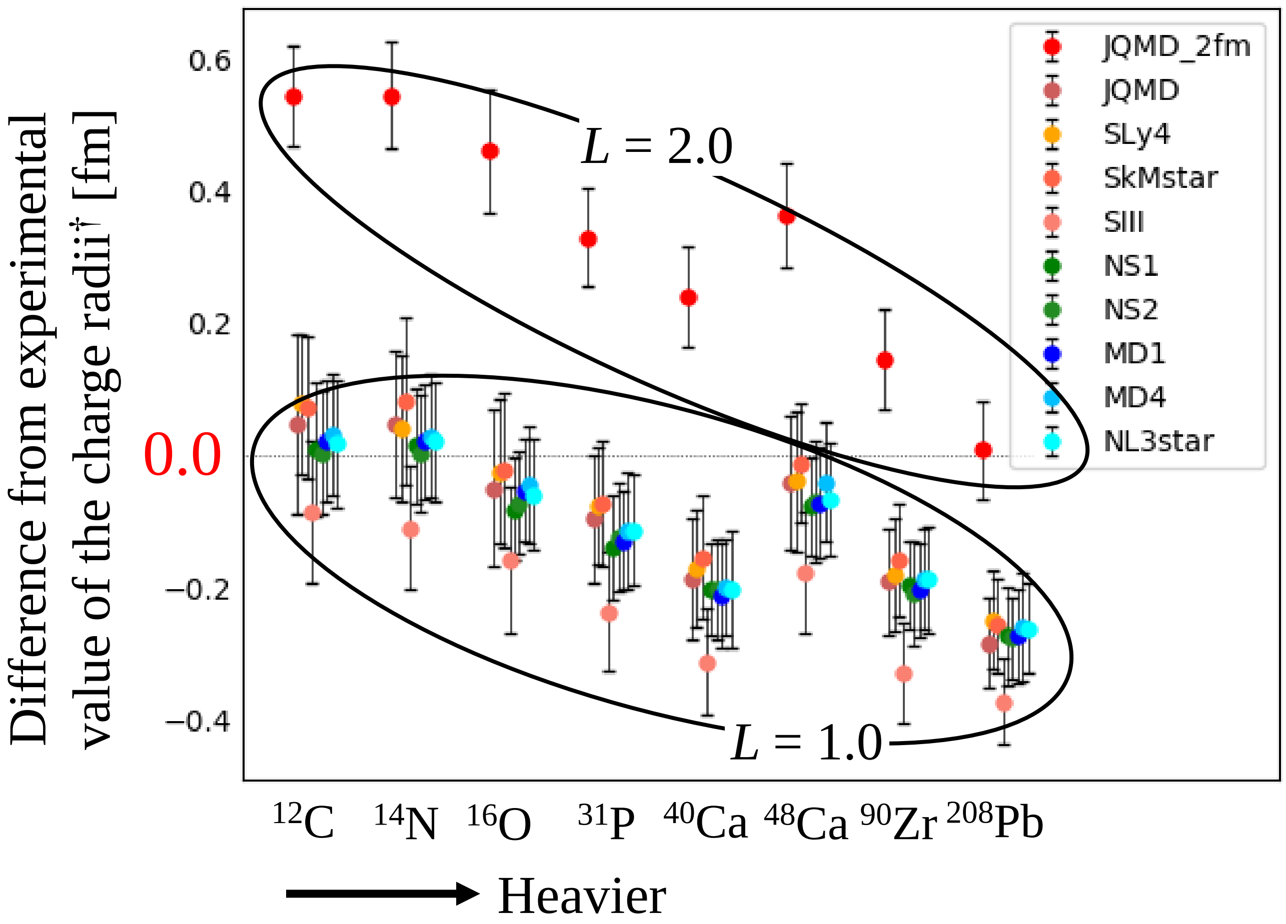
$$\varphi_i(\boldsymbol{r}) \equiv \frac{1}{(2\pi L)^{3/4}} \exp\left(-\frac{(\boldsymbol{r}-\boldsymbol{r}_i)^2}{4L} + \frac{i}{\hbar}\boldsymbol{r}\cdot\boldsymbol{p}_i\right)$$

L = 2.0 [fm] for QMD

L = 1.26[fm] for LIQMD

For heavier nuclei, the difference from the experimental values is larger with small L. For this reason, at best, mass number $A \leq 64$ is recommended.

Charge radii of nucleus



†: I. Angeli, K.P. Marinova, Atomic Data and Nuclear Data Tables, 99, 2013, 69-95.

Implementation

Implementation of LIQMD

Materials and Methods

qmd	Source code source/processes/hadronic/models/	light_ion_qmd

qmd	light_ion_qmd
G4QMDReaction	G4LightIonQMDReaction
G4QMDMeanField	G4LightIonQMDMeanField
G4QMDCollision	G4LightIonQMDCollision
G4QMDParameters	G4LightIonQMDParameters
G4QMDNucleus	G4LightIonQMDNucleus
G4QMDGroundStateNucleus	G4LightIonQMDGroundStateNucleus
G4QMDSystem	G4LightIonQMDSystem
G4QMDPaticipant	G4LightIonQMDPaticipant

I might put these files in the qmd folder.

Implementation of LIQMD

Materials and Methods

qmd

Source code

source/processes/hadronic/models/

light_ion_qmd

↑ use

G4IonQMDPhysics

Physics constuctor

source/physics_lists/constructors/ions/

G4LightIonQMDPhysics

Implementation of LIQMD

Materials and Methods

qmd	Source code source/processes/hadronic/models/	light_ion_qmd
	↑ use	
G4IonQMDPhysics	Physics constuctor source/physics_lists/constructors/ions/	G4LightIonQMDPhysics
	↑ use	
Shielding	Physics list source/physics_lists/lists/	Shielding, QGSP_BIC_AllHP Add an option (G4bool useLightIonQMD)

Implementation of LIQMD

Materials and Methods

qmd	Source code source/processes/hadronic/models/	light_ion_qmd
	↑ use	
G4IonQMDPhysics	Physics constuctor source/physics_lists/constructors/ions/	G4LightIonQMDPhysics
	↑ use	
Shielding	Physics list source/physics_lists/lists/	Shielding, QGSP_BIC_AllHP Add an option (G4bool useLightIonQMD)
	↑ use	
test61	Example or test examples/extended/medical/ geant4-dev/tests/	test61 LIQMD testing is also possible.

Summary and Future plan

- ❑ We have improved the QMD especially for hadron therapy using light ions and are considering to implement it as “Light Ion QMD” in Geant4.
- ❑ We have verified the performance of Light Ion QMD with various experimental data and confirmed that it is as good as or better than the conventional QMD model, at least in light ion beams and targes.
- ❑ Currently, the merge request is underway.

Thank you for listening