From particle to medical physics: Update on (physics) developments in the Geant4 Monte Carlo toolkit

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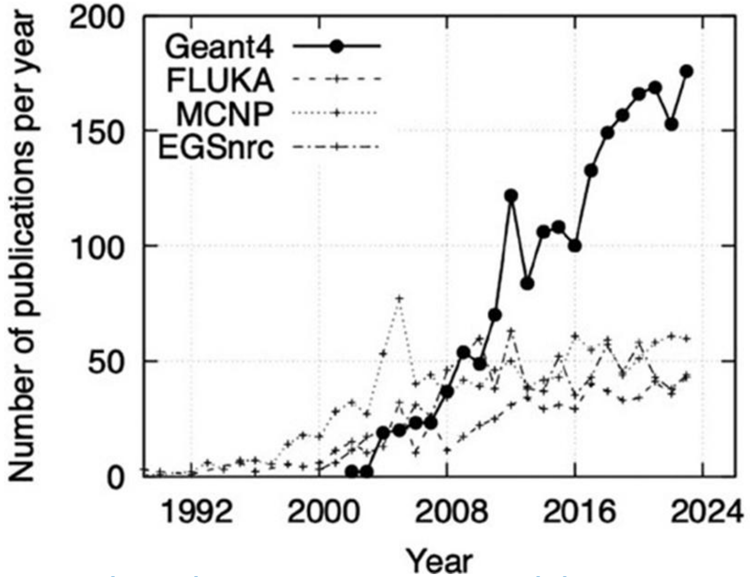
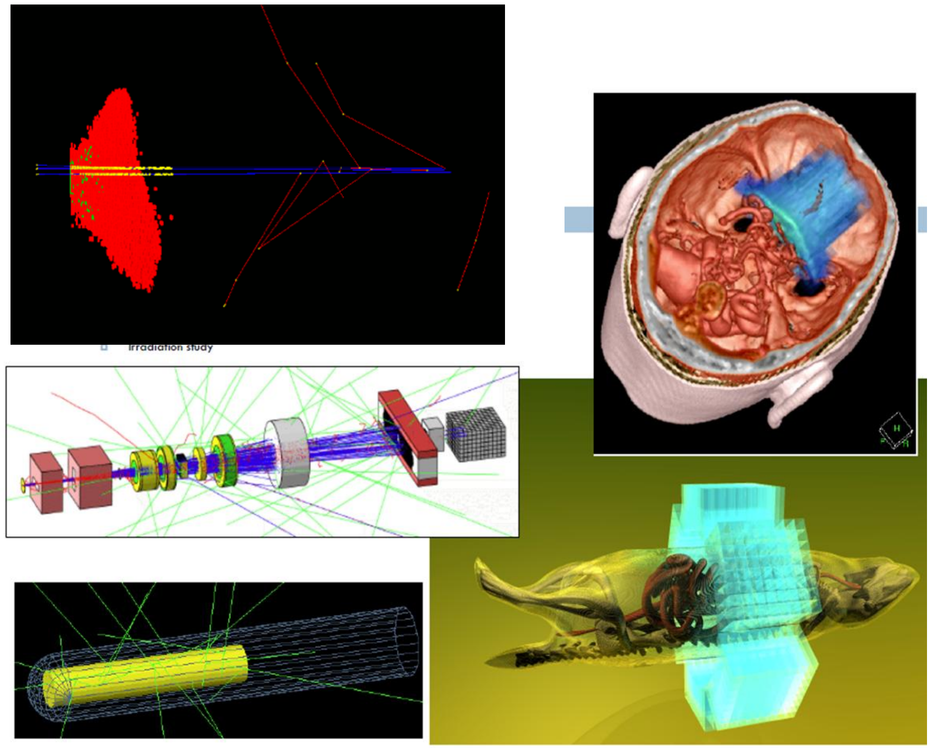
Mini Symposium on Monte Carlo Simulation of Particles and Radiation, February 3rd, 2026,
Holland Proton Therapy Center, Delft, Netherlands

Geant4 www.geant4.org



Arce et al (2025), Medical Physics, 52 (5), pp:2707-2761

- Applications in medical physics, including:
  - Verification of clinical TPS
  - Development of detectors
  - Dosimetry
  - Imaging (e.g PET, SPECT, CT)
  - Radiopharmaceutical production
  - Radiation protection
- Dosimetry, micro-dosimetry to DNA damage
- Beta release in July, public release per year (December), eventual patches
- Most recent release: 11.4 (December 2025)



Geant4 processes

From V. Ivantchenko, Geant4 Advanced course 2020, CERN, Geneva, Switzerland

- **Electromagnetic physics**
  - provides a complete set of EM interactions (processes) of charged particles and photons from low energy to ~PeV
- **Optical photons**
  - reflection/refraction, absorption, wavelength shifting, Rayleigh scattering
- **Hadronic**
  - Pure hadronic interactions for 0 to 100 TeV (elastic, inelastic, capture, fission)
  - Radioactive decay: – both at-rest and in-flight
  - Photo-nuclear interaction from ~1 MeV up to 100 TeV
  - Lepto-nuclear interaction from ~100 MeV up to 100 TeV – e+ and e-, neutrino and muon induced nuclear reactions.
- **Radioactive decay**
- **Decay**
  - leptonic, semi-leptonic decay, electromagnetic decay (π^0 , Σ^0 , etc.)
- **Phonon physics**
  - Creation, propagation, scattering and absorption
- **Parameterized**
  - Skips detailed tracking and provides hits in the logical volume and list of particles living the volume – for example, EM shower generation in a calorimeter
- **Transportation**
  - responsible for propagating a particle through the geometry

Geant4 developments

- Regular collection of User Requirements (URs)
- URs implemented depending on resources within the Geant4 Collaboration
- User Requirements doc:
  - https://jira-geant4.kek.jp/projects/UR/issues/UR-89?filter=allopenissues
- UR Collection managed by a Geant4 team coordinated by Krzysztof Genser (Fermilab, US)
  - Makoto Asai - nuclear physics, space applications
  - Krzysztof Genser - HEP Intensity Frontier
  - Susanna Guatelli - Medical Physics
  - Mike Kelsey - Material Science/Cosmic/Dark Matter Physics
  - Alberto Ribon - HEP Energy Frontier
  - Giovanni Santin - Space Physics
- S. Guatelli, "Open and new requirements - Medical applications", 2025 Geant4 Collaboration Meeting

Note

- Show major physics developments of interest for medical physics released since 11.1 (past four years)
    - EM physics, hadronic physics, Geant4-DNA
- Illustrate some work in progress
- For more information, please, refer to the Geant4 physics reference manual and presentations in Geant4 Collaboration meetings and Technical Forums

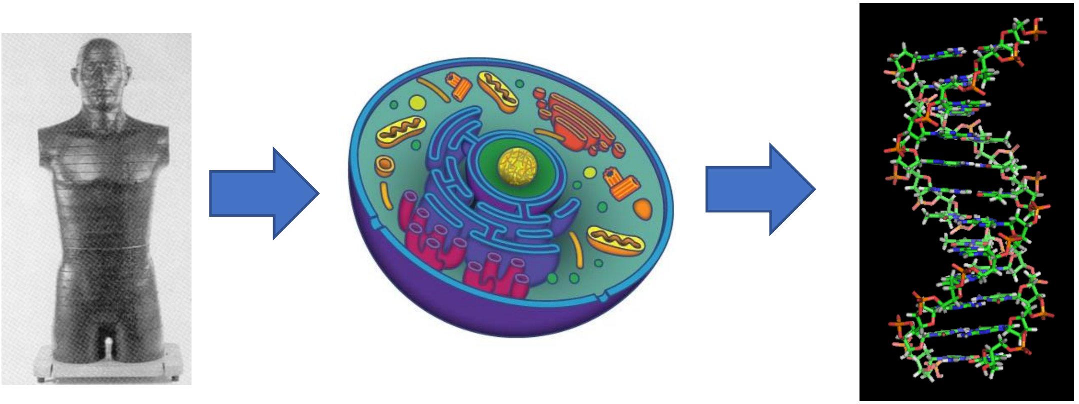
G4 EM Physics

Condensed History approach

- “**condensing” several physical interactions** of charged particles into a single virtual step using multiple scattering and energy loss theories.
- Acceleration of the simulation at the cost of accuracy in the modelling of the physical interactions.
- Dosimetry
- **Geant4 EM physics – Geant4 EM Physics Opt 4 recommended for medical physics applications**

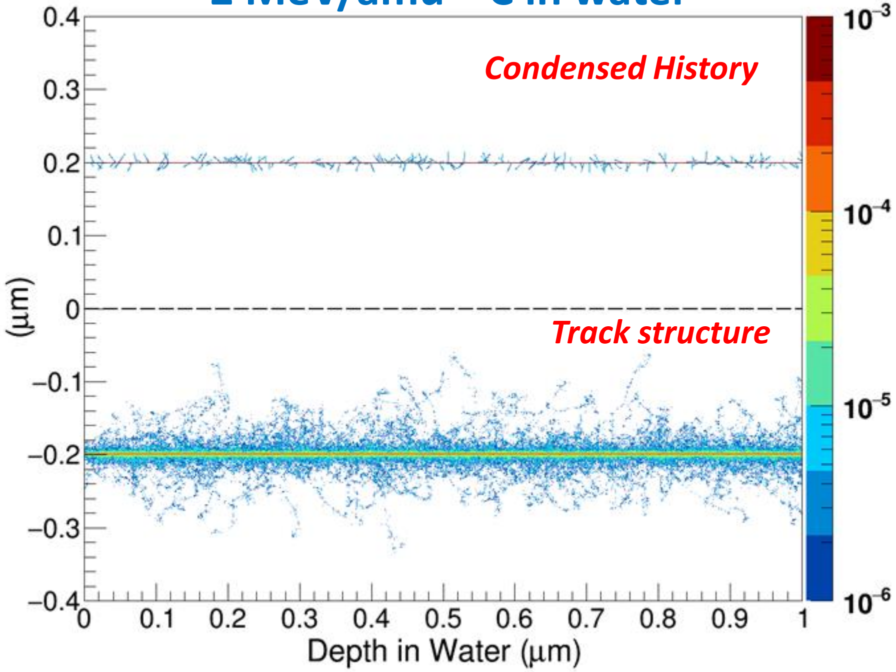
Track structure approach

- All the particle **interactions are modelled one by one**.
- Very detailed description of the track structure but at the cost of being computationally intensive.
- Micro-nanodosimetry
- **Geant4-DNA**



Dosimetry — **Microdosimetry (cellular scale)** — **Nanodosimetry (DNA scale)**

2 MeV/amu ^{12}C in water



Energy deposition in liquid water, in the units of MeV per incident particle, produced by **ten 2 MeV/amu ^{12}C ion tracks**. Figure courtesy of Dr D. Bolst, CMRP, UOW, Australia.

Geant4 EM physics: **Geant4 EM physics list Option 4 (Geant4 11.4)**

Modelling EM interactions of charged particles and photons

- **Rayleigh scattering and photoelectric effect**: Livermore model – EPICS2017 (Electron–Photon Interaction Cross Sections) data libraries (Li, Z, et al. (2022) Physica Medica, 95:94–115).
- **Compton Scattering**:
  - G4LowEPCompton model (to improve low-energy Compton e^- directionality accuracy) for E< 20 MeV (Brown JMC, et al. (2014) "A low energy bound atomic electron Compton scattering model for Geant4" NIM B., 338:77–88.)
  - Klein–Nishina model for E> 20 MeV
- **Gamma conversion**: G4BetheHeitler5DModel (D. Bernard (2013) NIM A. 2013;729:765–780 and 2018; 899:85–93)
- **e- ionisation**: Penelope model for E < 100 keV and Standard Model for E > 100 keV
- **Bremsstrahlung**: Seltzer Berger Model for E < 1 GeV and BremsstrahlungRelModel above
- **Positron interactions** (Standard model)
  - Positronium production (para-/orto-positronium creation) and 3-γ annihilation
- **e^+e^- multiple scattering model**: G4GoudsmitSaundersonMsc Model below 100 MeV and then Wentzel VI model

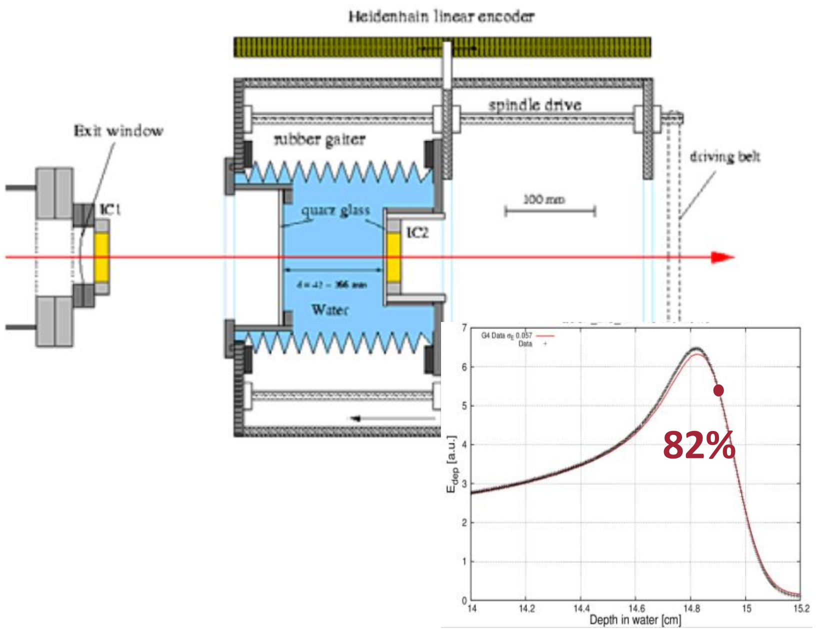
- **Single Coulomb scattering** is invoked for large angle deflections
- **Proton ionisation**: since Geant4 11.1 adoption of ICRU90 data for water, air, graphite. For the other materials, NIST PSTAR data are used if available. If not, ICRU49 is used.
- **Alpha ionisation:** adoption of ICRU90 data. For not available materials, NIST ASTAR.
- **Ionisation model for ions** heavier than Helium: G4LinhardSorensenIonModel , available for the full energy range. It includes includes data from ICRU73, ICRU90 and ICRU49.
  - G4LinhardSorensenIonModel addresses limitations of Bethe–Bloch for heavy ion projectiles in the relativistic regime.
- **Nuclear stopping power** on

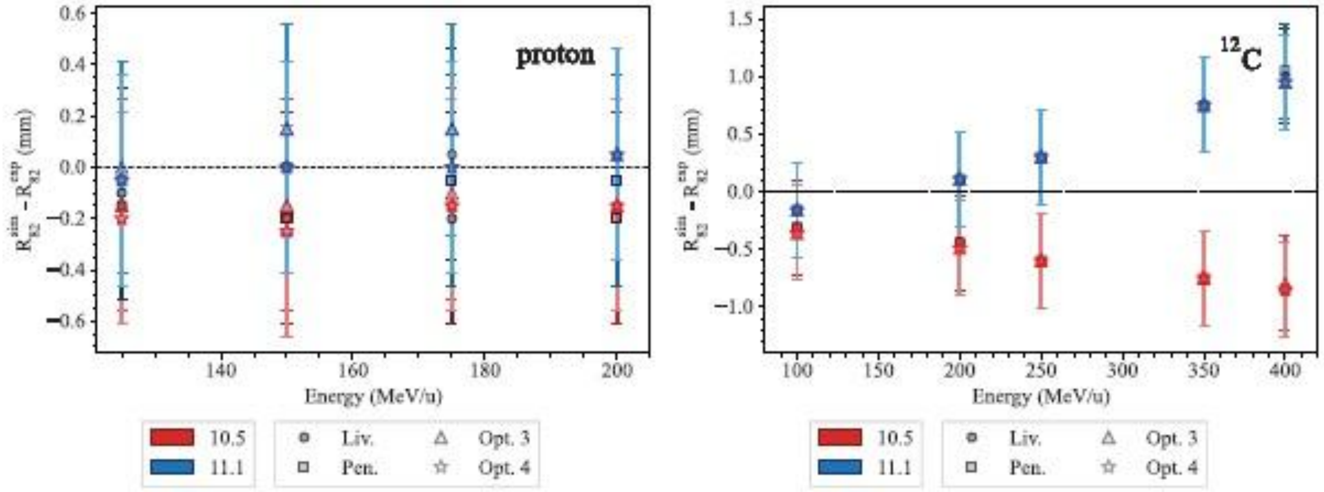
Light IonBragg Curves

By M A Cortés-Giraldo and J. M. Quesada, Sevilla University, Spain

Ref. Data: **D. Schardt et al., GSI Report 2008-1**

QGSP_BIC_HP for hadronic physics, 95% confidence level





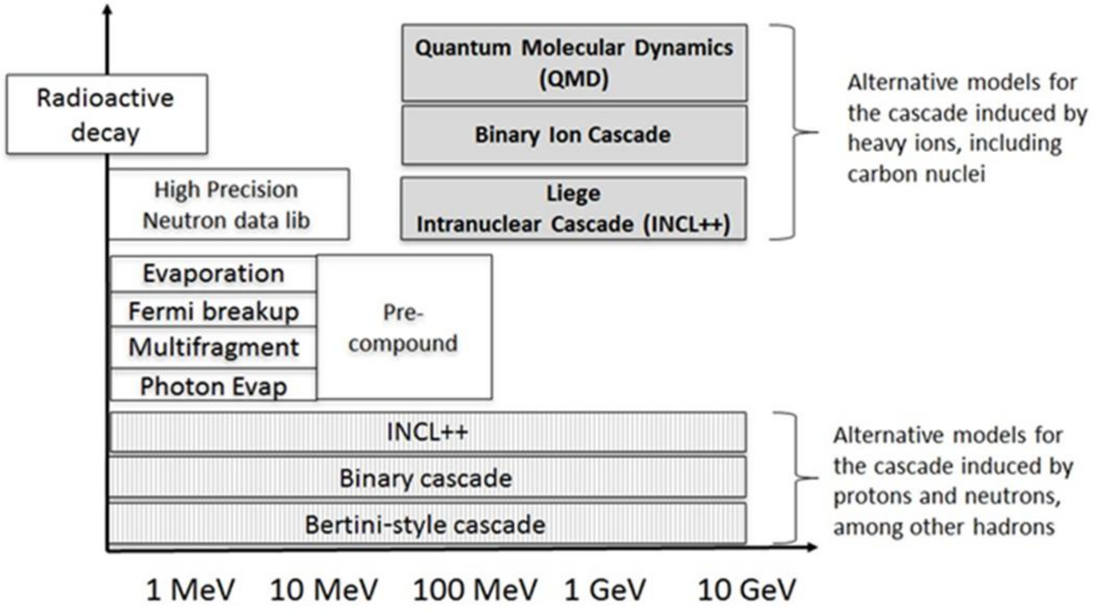
- Initial energy spread adjusted from experimental Bragg curves
- Simplified geometry model for simulation
    - **Depths of 82% distal dose are compared**

- The ^{12}C Bragg Peak position tends to be slightly overestimated In Geant4 11.1, while it was slightly understimated in Geant4 10.5
    - due to the Linhard Sorensen Ion Model, available since Geant4 11.0.
- When compared to Geant4 10.5, Geant4 11.1 produces R_{82} closer to the reference data for 100 and 200 MeV/u ^{12}C ions.
- In the case of 400 MeV/u ^{12}C, the difference of R_{82} is ~ 1 mm with Geant4 11.1 and 0.85 mm with Geant4 10.5.

Geant4 Physics Lists: EM + Hadronic

For proton therapy (recommended):

- QGSP_BIC_HP
  - High Precision data libraries for neutrons with energy < 20 MeV
- QGSP_BIC_AllHP
  - Physics model that uses TALYS-based Evaluated Nuclear Data Library (TENDL). TENDL is based on experimental and calculated results of TALYS nuclear model code to produce a nuclear data library for p, n, ^{2}H, ^{3}H, α and ^{3}He for energies below 200 MeV



For carbon ion therapy:

QGSP_BIC_HP +

- **G4IonBinaryCascade** - LightIonBinaryCascade model (BIC).
- **G4IonQMDPhysics** - Quantum Molecular Dynamics (QMD) model.
- New: G4LiQMDPhysics – Improved QMD model for hadrontherapy
- **G4IonINCLXXPhysics** - Liège Intranuclear-Cascade model (INCL).

Fragmentation models

- BIC: Interaction between a projectile and a single nucleon of the target nucleus interacting in the overlap region as Gaussian wave function
- QMD and LiQMD: All nucleons of the target and projectile, each with their own wave function;
- INCL: Nucleons as a free Fermi gas in a static potential well. Targets and projectiles with $A \leq 18$.

Light Ion Quantum Molecular Dynamics model (LiQMD)

- Improved specifically for hadrontherapy applications
- Y. Sato et al 2022 Phys. Med. Biol. 67, 225001
- Released for the first time in Geant4 11.2
- Available through the *Shielding physics list* with an extra argument: *Shielding(true)*

Physics in Medicine & Biology
IPEM Institute of Physics and Engineering in Medicine

PAPER

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

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Keywords: hadron therapy, fragmentation, quantum molecular dynamics, multi-objective optimization

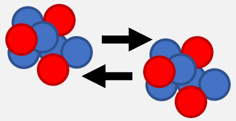
Supplementary material for this article is available online

Update QMD model parameters

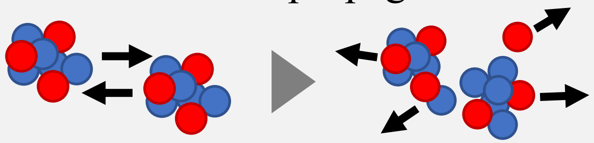
Width of Gaussian wave packet

$$|\phi_i(\boldsymbol{r})|^2 = \frac{1}{(2\pi L)^{3/2}} \exp\left[-\frac{(\boldsymbol{r}-\boldsymbol{r}_i)^2}{2L}\right]$$

Impact parameter



End time of propagation

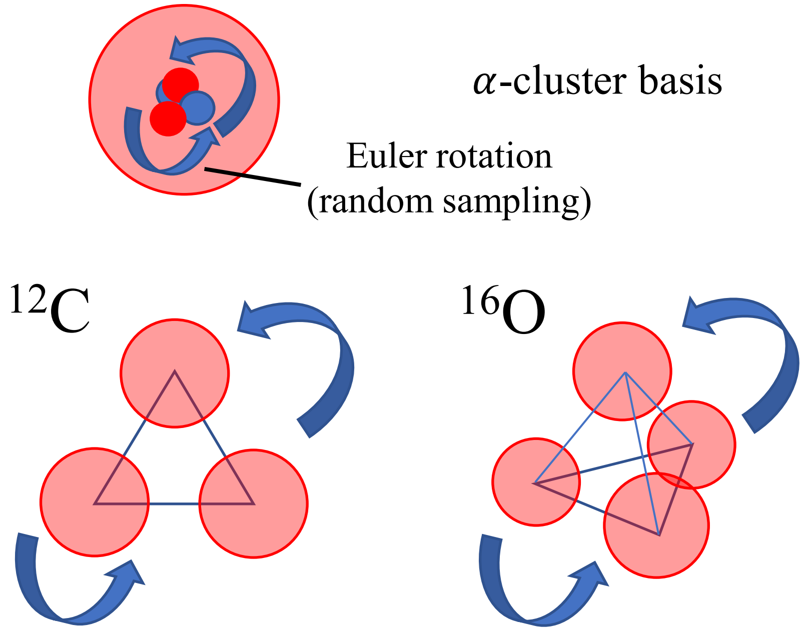


Using a modern Skyrme parameter set

Potential felt by the nucleon:

$$V_i = \frac{A}{2\rho_0}\sum_{j\neq i}\rho_{ij} + \frac{B}{\gamma+1}\frac{1}{\rho_0^\gamma}\left(\sum_{j\neq i}\rho_{ij}\right)^\gamma + \frac{g_0}{2\rho_0}\sum_{j\neq i} f_{sij}\rho_{ij} + \frac{g_\tau}{\rho_0^\eta}\left(\sum_{j\neq i}\rho_{ij}\right)^\eta + \frac{C_s}{2\rho_0}\sum_{j\neq i}\tau_{3,i}\tau_{3,j}\rho_{ij}(1-\kappa_s f_{sij}) + \frac{\alpha\hbar c}{2}\sum_{j\neq i}\frac{1}{|\boldsymbol{R}_i-\boldsymbol{R}_j|}\mathrm{erf}\left(\frac{|\boldsymbol{R}_i-\boldsymbol{R}_j|}{\sqrt{4L}}\right)$$

Ad-hoc incorporation of α-cluster structure



By Yoshi-hide Sato, Akihiro Haga, Tokushima University, Japan, and Collaborators

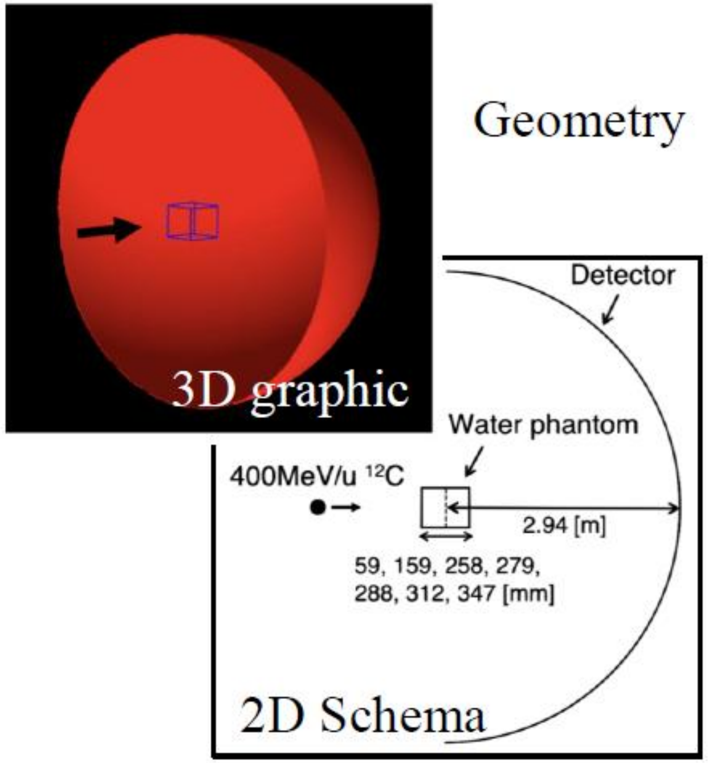
Validation of the LiQMD for C-12 hadrontherapy

By Yoshi-hide Sato, Akihiro Haga, Tokushima University, Japan, and Collaborators

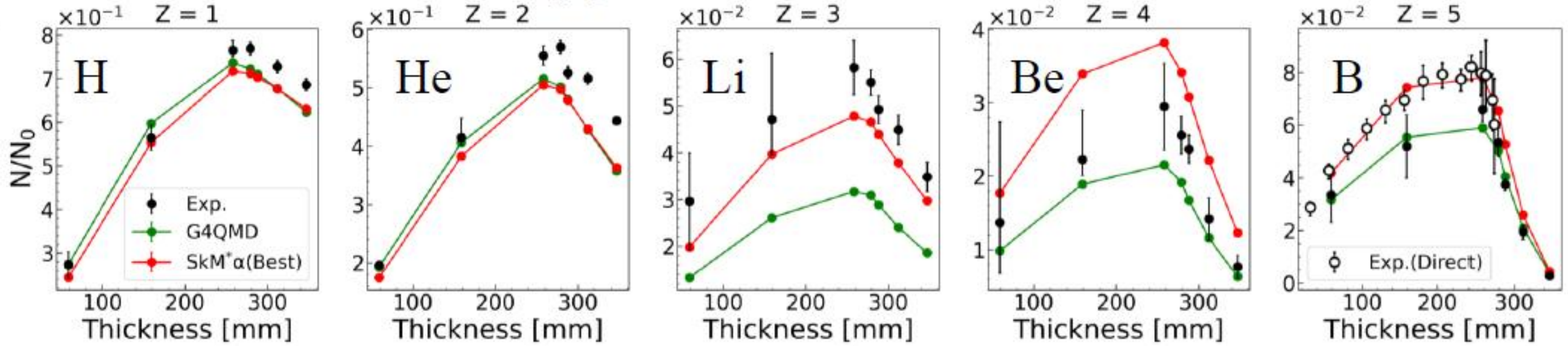
- **Experimental data**
- **QMD (Geant4 v10.7.1)**
- **QMD (Our model)**

Exp data: E. Haettner et al. (2013) PMB, 58 (2013) 8265–8279DOI: 10.1088/0031-9155/58/23/8265

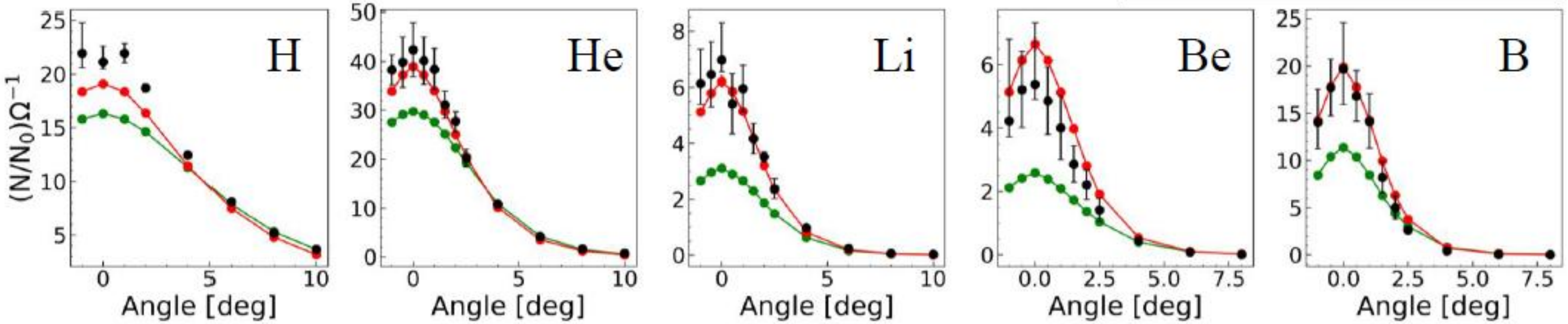
Geometry



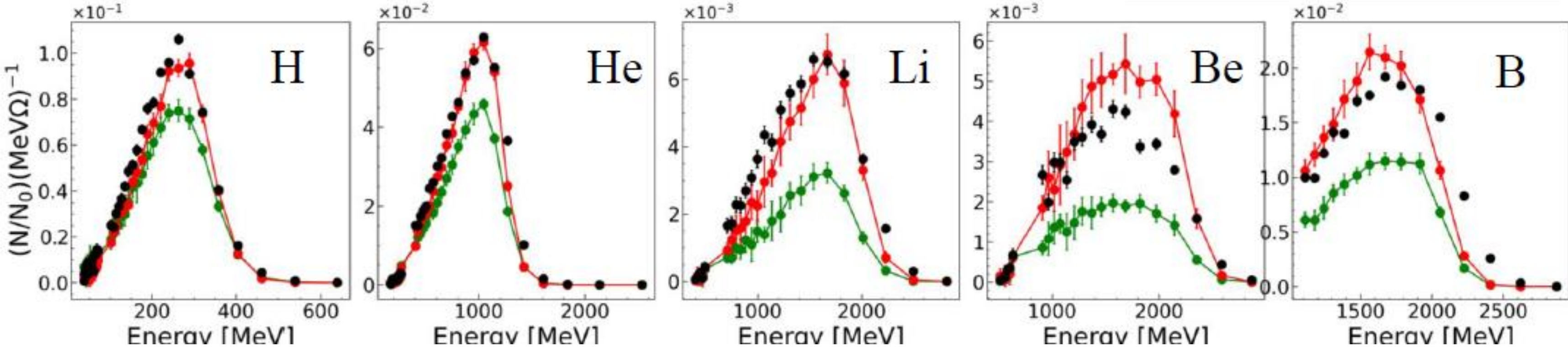
Total fragment yield



Angular distribution



Energy distribution



Validation of LiQMD against exp data

- Validated against exp data for
  - microdosimetry
  - in-vivo PET in ^{12}C therapy (350 MeV/amu ^{12}C ion beam incident on PMMA)
  - Bragg Peak and dose profile, secondary fragments, cross sections of 95 MeV/u ^{12}C ions incident on thin targets (H, C, O, Al, and Ti)
- the **LIQMD model demonstrates better agreement** with experimental measurements for nearly all fragment species compared to the QMD model
- Sato YH, et al. Validation of Light-Ion Quantum Molecular Dynamics (LIQMD) model for hadron therapy. Phys Med. 2024 Dec;128:104850

Validation of LiQMD beyond C-12 therapy

More information can be found at:
Talk by K. Moore "Validation of Geant4 fragmentation models for hadron therapy beyond carbon ion therapy", 2025 Geant4 Collaboration Meeting

- Tested G4 Fragmentation models: BIC, INCL, QMD and LiQMD, Geant 11.3
- By K. Moore, S. Guatelli, D. Bolst (Centre For Medical and Radiation Physics, University of Wollongong) and collaborators

Publication	Beam/s	Beam size	Target	Measurement	Bragg peak (mm)
Matsufuji et al. 2003, PMB	^{12}C - 290 MeV/u ^{20}Ne - 400 MeV/u	100 mm diameter	PMMA	Fragment build up curve	150/150
Haettner et al. 2010, PMB	400 MeV/u	5 mm (FWHM)	Water	Fragment build up curve, Angular and energy distributions	276

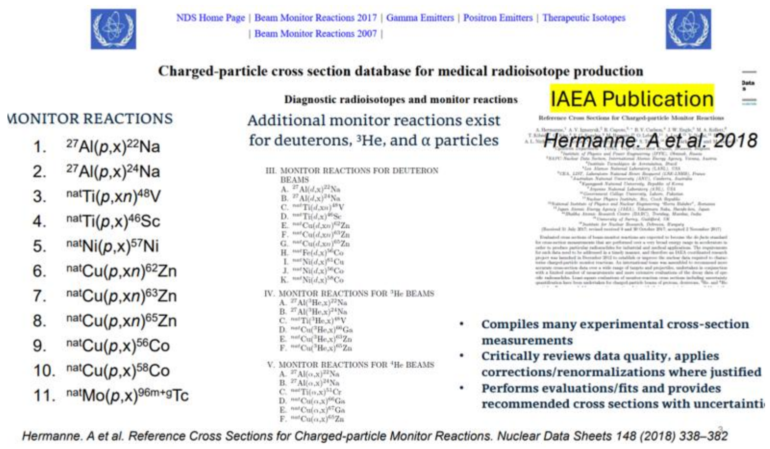
- LiQMD provides the best agreement for 290 MeV/u ^{12}C with a more accurate angular distribution
- It provides the best agreement for most fragments in the case of 400 MeV/u ^{20}Ne
- H and He fragments are of particular interest due to ~10x higher yields and larger ranges and angular spread (healthy tissue)
  - All Geant4 fragmentation models agree within ~20% for H for both C and Ne beams
  - The agreement is within ~60% for He for G4 frag models apart from LiQMD (23 %)

Low Energy (< 20 MeV) Neutrons: Particle HP

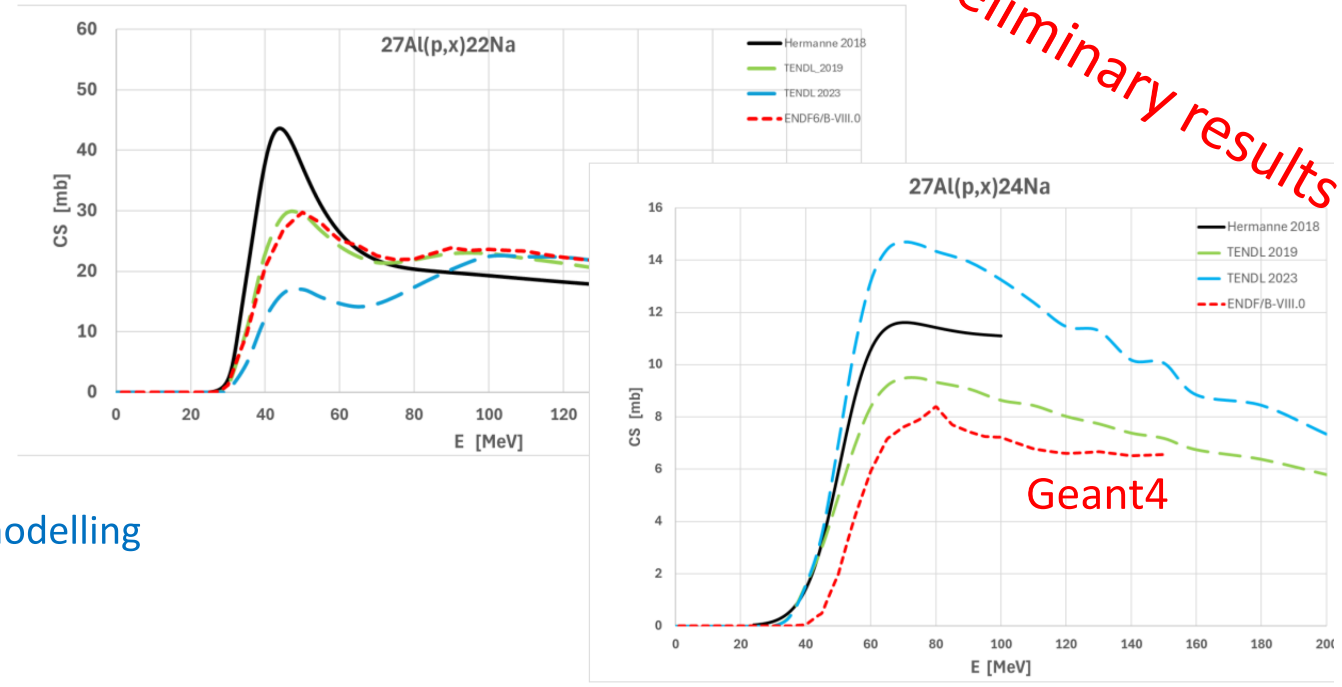
- Major developments of ParticleHP in the past years
  - In G4 11.0 and 11.1, improved treatment of thermal neutrons (< 4 eV):
    - Corrected treatment of the temperature interpolation (G4 11.0) and updated thermal cross-sections in G4NDL-4.7 (G4 11.1)
  - Introduced option in G4 11.2 to model accurately elastic resonant scattering in heavy nuclei
- Technical developments in G4 11.2
    - Introduced for users' convenience _HPT physics lists (i.e. with thermal scattering treatment enabled)

Under development: new monitor-reaction cross sections in Geant4

- IAEA reference database of evaluated monitor-reaction cross sections for protons, deuterons, ^{3}He and α particles (https://www-nds.iaea.org/medical/)
- Geant4 cross-section data are primarily sourced from ENDF/B-VIII.0 and TENDL-2019
- We compare Geant4 data libraries with the IAEA-evaluated dataset (Hermanne et al., 2018) and update them where needed.
- By I. Eliyahu (Soreq NRC), P. Arce (CIEMAT), G. Mentasti (Politecnico Milano) and S. Guatelli (University of Wollongong)



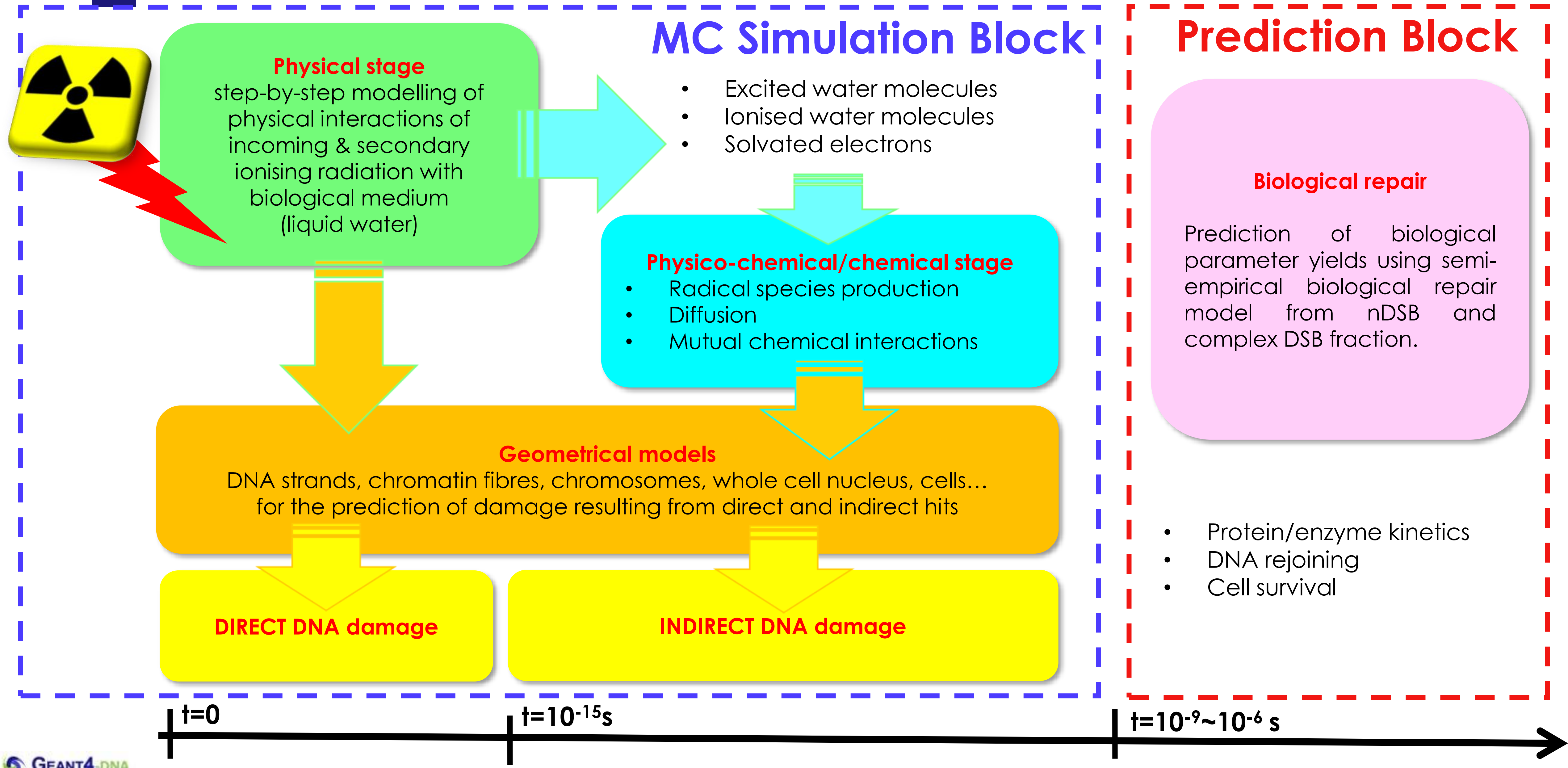
Monitor Reactions for Protons



More information can be found at:

Talk by I. Eliyahu, “Development of IAEA cross sections modelling isotope production”, 2026 Geant4 Collaboration Meeting

The Geant4-DNA approach



Geant4-DNA physics and chemistry

Recommended EM Track Structure physics lists

- **Geant4-DNA processes and models allows the transport in liquid water**
  - Electrons: ionisation, excitation, elastic scattering, vibrational excitation, electron attachment
  - Protons, H (0,+): ionisation, excitation, elastic, charge increase/decrease processes
  - Alpha, He(0,+,2+): ionisation, excitation, elastic, charge increase/decrease
  - Generic ions: ionisation
- **Geant4-DNA Opt2 -** Based on the dielectric theory for e^- ionisation and excitation
- **Geant4-DNA Opt4**
  - Based on the dielectric theory for ionisation and excitation
  - More accurate electron cross sections at lower energies (Kyriakou et al 2016, Journal of Applied Physics, 119(19):194902)
- **Geant4-DNA Opt6**
  - Re-engineering of CPA100 for electrons (Terrissol and Baudre, Radiation Protection Dosimetry, 1990, 31(1-4), 175-177).
  - Binary Encounter model Bethe formalism for ionisation (Kim & Rudd, Physical Review A, 1994, 50(5):3954-67; Bordage et al Physica Medica 2016, 32(12):1833-40).
  - Dielectric theory for electron excitation
  - Same proton, H, He and its charge states, ions physics processes (see Incerti et al, Medical Physics, 2018, 45:e722-e739)

Chemistry component

- **Step-by-Step approach (SBS)** (Karamitros et al, 2011, Prog. in Nucl. Sci. and Tech., 2:503)
  - Transport of chemical species in discrete steps (or time steps Δt) through Brownian motion until a chemical encounter defines a reaction
- **IRT** (Ramos-Méndez et al, 2020, Medical Physics, 47(11):5919-30)
  - Calculation of chemical reaction probability
  - Reaction times can be sampled for every potential pair of reactants.
  - Reactions are then modelled sequentially, starting with those with the shortest reaction time.
  - Products of chemical reactions may undergo further reactions
- **IRT-sync** (Tran et al, 2021, Medical Physics, 48(2):890-901)
  - It uses as the time step the randomly sampled time given by the IRT model until the next expected reaction.
  - After each time step, it is necessary to synchronise the time and position of all diffusing species
  - + access to spatial-temporal information at certain times, for all chemical species, which can then be coupled with information about geometry and boundaries.
- **Mesoscopic (Tran et al. 2021, Int. J. Mol. Sci. 22 (2021) 6023)**
  - **A compartment-based representation that describes the evolution of species through their concentrations in different compartments (voxels).**
  - **Can be used beyond the microsecond and in larger volumes**

Geant4-DNA: recent and next developments

Geant4-DNA Materials: Liquid water, gold, DNA bases (A, T, G, C), sugar, phosphate and precursors of DNA material

- Since Geant4 11:3, generation of multiple-ionised water ions for incident p, α, C
- Since Geant4 11.4, Geant4-DNA physics lists are applicable for all energies and all ions, they combine
  - Geant4 EM Standard physics for all particles for E > 300 MeV/u
  - Geant4 DNA physics for e-, protons, alpha, alpha+, hydrogen, helium, and all ions for E < 300 MeV/u
- **Physics / in progress: extension of energy and material coverage of Geant4-DNA models beyond liquid water:**
  - Electrons in water extended from 10 keV to 10 MeV by I. Kyriakou et al., Appl. Sci. 15 (2025) 1183, to be released
  - Models for electrons in gold by I. Polopetrakis et al., Phys. Med. Biol. 70 (2025) 165019, to be released
  - Models for electrons in N_2, O_2 and CO_2 by F. Nicolanti et al., Phys. Med. 128 (2024) 104838, to be released
  - New discrete e- cross section models for ice water under development by Weizman I.
  - Re-engineering of RITRACKS physics models in Geant4-DNA: J. Archer J et al, 2026, Radiation in Physics and Chemistry, 113461, to be released
- **Chemistry / in progress:** Update of mesoscopic approach development for chemistry / water radiolysis (high dose rates, longer times)
  - On-going (high dose rates, longer times, larger volumes), along with experimental validation
  - Technical feasibility shown here : https://arxiv.org/abs/2409.11993
- **Note : Geant4-MicroElec models**:
  - Adopt the same architecture as Geant4-DNA
  - Mainly for space materials : Be, C, Al, Si, Ti, Fe, Ni, Cu, Ge, Ag, Au, W Kapton, SiO2, Al2O3, TiN, BN.; tested for Silicon

G4-Med tests

By the **Geant4 Medical Simulation Benchmarking Group**
Arce et al (2021), Medical Physics, 48 (1), pp:19-56
Arce et al (2025), Medical Physics, 52 (5), pp:2707-2761

- Geant4-DNA tests
  - Low dose energy electron Dose Point Kernels
  - Microdosimetry
  - Chemistry
- EM physics tests
  - Brachytherapy (Ir-132 and I-125)
  - Electron FLASH radiotherapy
  - MV X-ray radiotherapy test
  - Photon attenuation coeff
  - Electron electronic stopping power
  - Electron backscattering
  - 13 MeV electron forward scattering
  - Bremsstrahlung from thick targets
  - Fano cavity
  - Monoernergetic x-ray internal breast dosimetry

- Hadronic nuclear cross section tests
  - Nucleus-nucleus hadronic inelastic scattering cross sections
  - 62 MeV/u ^{12}C fragmentation
  - Charge-changing cross sections for 300 MeV/u ^{12}C ions
- EM + hadronic physics tests
  - 62 MeV proton beam test (cell survival modelling and averaged LET track)
  - In-vivo PET for carbon ion therapy
  - 67.5 MeV proton Bragg curves in water
  - Light Ion Bragg Peak curves
  - Neutron yield of 113 MeV and 256 MeV protons and 290 MeV/u carbon ions
  - Fragmentation test of a 400 MeV/u ^{12}C ion beam in water

Conclusions

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- Geant4 developments in progress for medical physics community

- Those interested in contributing to the development of Geant4 functionality are encouraged to **contact the Geant4 Collaboration**

- Acknowledgements

I would like to thank **V. Ivantchenko (CERN and Tomsk State U.), S. Incerti and H. Tran (Bordeaux CNRS - IN2P3 & Bordeaux U)** for their contribution to this talk

Thank you!