



What's new in 11.3

Electromagnetic physics part

*V. Ivantchenko, CERN & Tomsk State University**

for the Geant4 EM physics group

12 December 2024



** grant of Government (Agreement No. 075-15-2024-667)*

New features prepared for 11.3

- ❖ New dataset G4EMLOW8.6.1
- ❖ Initializations of EM tables and data structures are thread safe.
- ❖ Full implementation of 3-gamma annihilation and positronium production and decay
- ❖ Full implementation of X-Ray scattering and examples
- ❖ Alternative EM processes for exotic particles
- ❖ Extension of models and examples for channeling
- ❖ New DNA developments

Main infrastructure change in 2024

- ❖ In 2023 we were struggled with the problem of initialization and destroy of shared data in EM models
- ❖ **Lessons learned:**
 - ❖ *static data is a very delicate approach - should not be used if possible*
 - ❖ *Instead of deletion of static data in model or process classes we should use register mechanism allowing to keep shared data until the end of the job*
 - ❖ **The work was started for 11.2 using G4ElementData structure**
 - ❖ Data may be accessed via name
 - ❖ Data will be deleted end of job by the dedicated register classes
 - ❖ If a dataset accessed via the register class, then this dataset should not be static

EM data handling for 11.3

❖ Existing `G4ElementDataRegistry`

❖ Keep `G4ElementData` for EM models

❖ `G4LossTableManager` define master thread in constructor

❖ It may be the first working thread

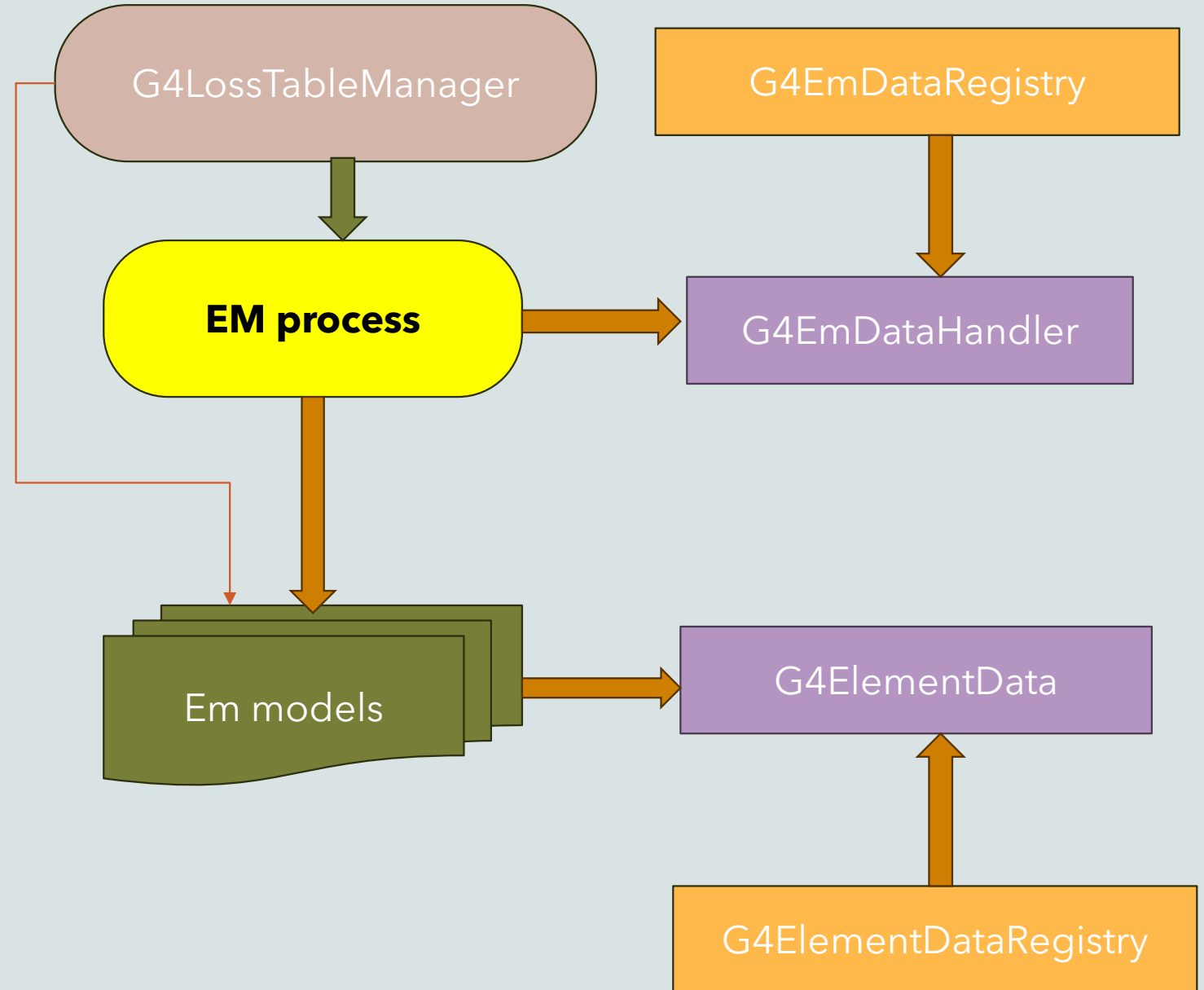
❖ New class `G4EmDataRegistry`

❖ singleton to keep shared data from EM processes

❖ Physics tables

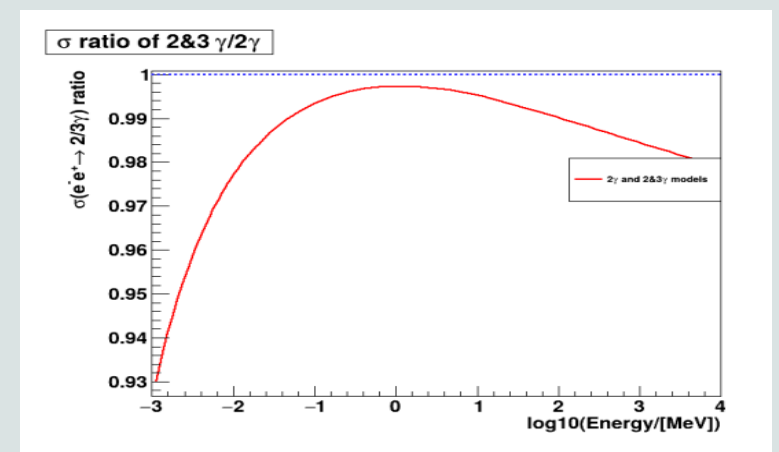
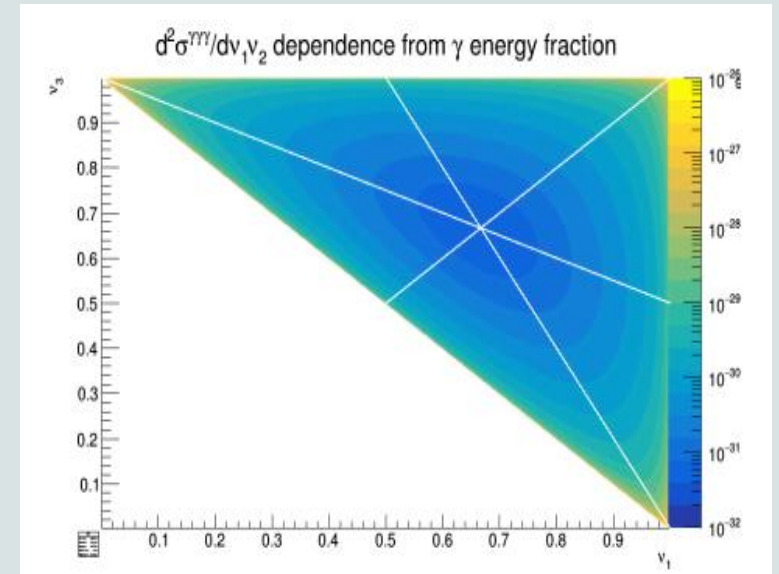
❖ EM cross section shape data

❖ this class is responsible for deletion of `G4EmDataHandlers`



Positron 3- gamma annihilation on fly

- ❖ Pending project for many years
 - ❖ *problems in sampling of final state when a positron become low-energy*
- ❖ Positron 3-gamma annihilation was developed in the framework of CERN summer school projects
- ❖ Design iteration for 11.3 - simulation on fly and at rest are fully independent now
 - ❖ *3-gamma annihilation on fly concerns mainly HEP applications - shower shape may be affected on per mile level*
 - ❖ `/process/em/lowestTripletEnergy 10 MeV`



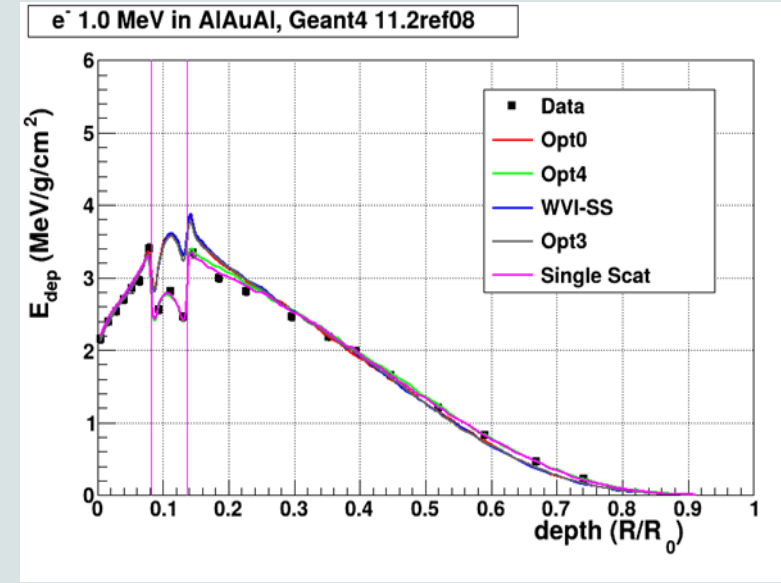
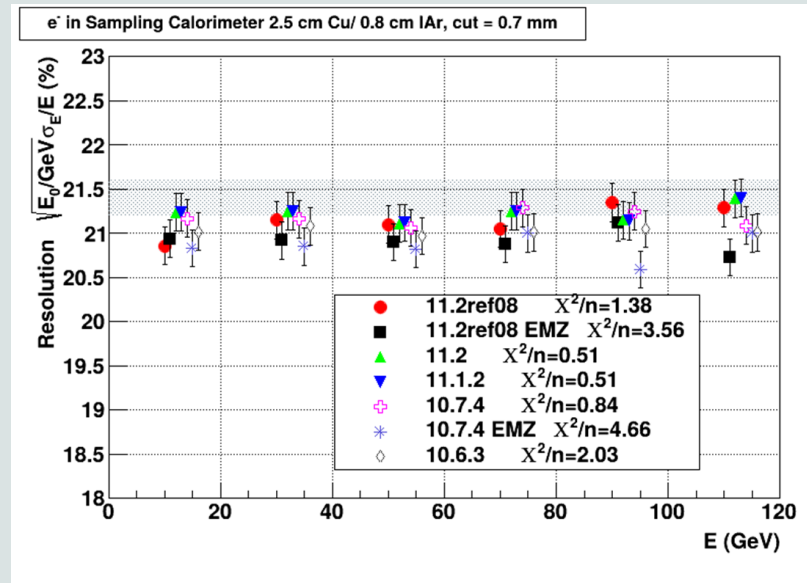
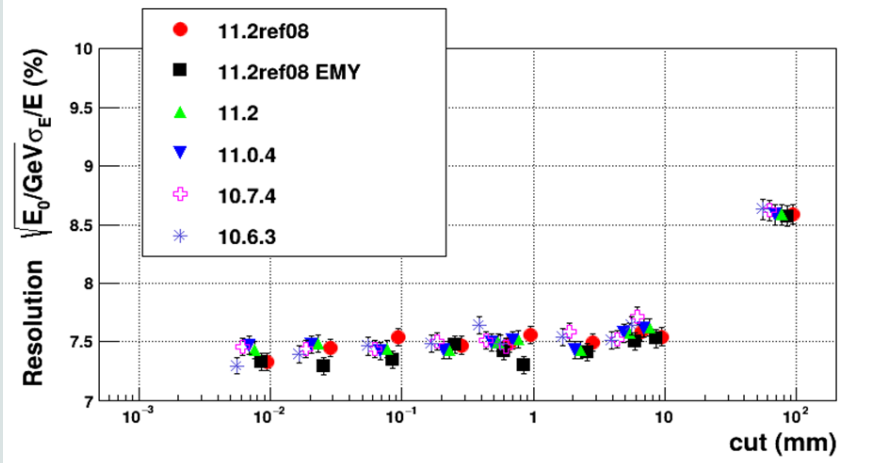
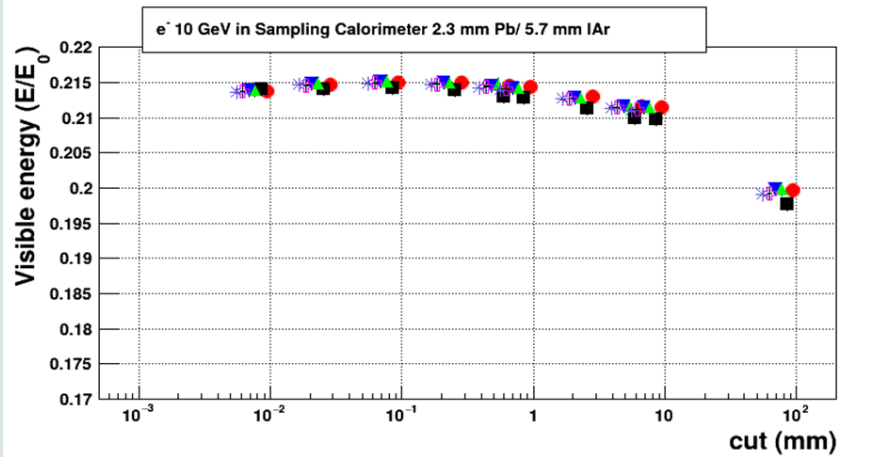
Positron annihilation at rest

- ❖ Creation of positronium at rest concerns mainly medical applications
- ❖ A choice of model for sampling of final state is provided via enumerator
 - ❖ *G4PositronAtRestModelType*
 - ❖ fSimplePositronium
 - ❖ fAllisonPositronium
 - ❖ fOrePowel
 - ❖ fOrePowelPolar
- ❖ Selection of positronium model
 - ❖ */process/em/setPositronAtRestModel Allison* - variant of selection
 - ❖ *Simple* is the current default - annihilation at rest into 2 gamma
 - ❖ *Allison* uses only two gamma Allison model but considers Doppler broadening
 - ❖ *OrePowell* for 2 gamma uses Allison, for 3 gamma - OrePowell model
 - ❖ *Quantum entanglement is applied only on 2 first gamma*
- ❖ Probability of para-/orto-positronium creation and decay defined by G4Material property
 - ❖ */material/g4/ortoPositroniumFraction G4WATER 0.05*

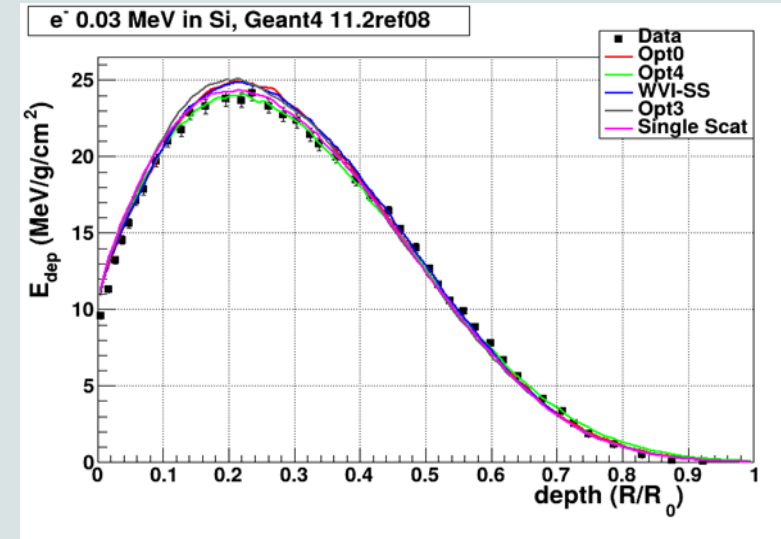
Other new developments

- ❖ EPICS2017 data
 - ❖ Since 11.2 these data for Livermore gamma models
 - ❖ Livermore photo-electric model and Rayleigh scattering models are the default in EM Opt0 physics
 - ❖ EPICS2017 cross section for gamma conversion is included into Bethe-Heitler model as an option
 - ❖ This model now is not used in any physics configurations but only in tests
- ❖ New EM models for exotic particle transport
 - ❖ *G4DynamicParticleIonisation*
 - ❖ *G4DynamicParticleMSC*
 - ❖ *G4DynamicParticleFluctuation*
 - ❖ *G4ParticleDefinition* is not used in these models, only *G4DynamicParticle* data
 - ❖ All computation on fly - no tables stored
 - ❖ *G4ChargedUnknownPhysics* - builder to be added on top of any Physics List

Recent validation results



- ❖ There is stability in general for EM calorimetry response simulation from 10.6 to 11.3
- ❖ The only known unstable EM physics is EMY, which was fixed in 11.2.2





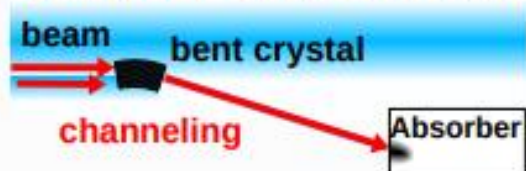
Geant4 ab-initio models on channelling, channelling radiation, and coherent pair production in oriented crystals

A. Sytov et al.



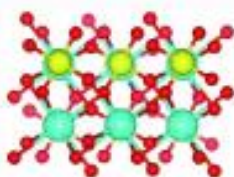
Applications*

Crystal-based collimation or beam extraction from an accelerator

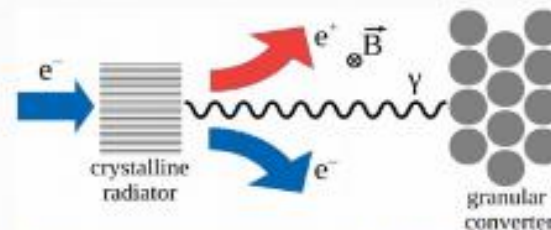


Gamma-ray Space Telescope

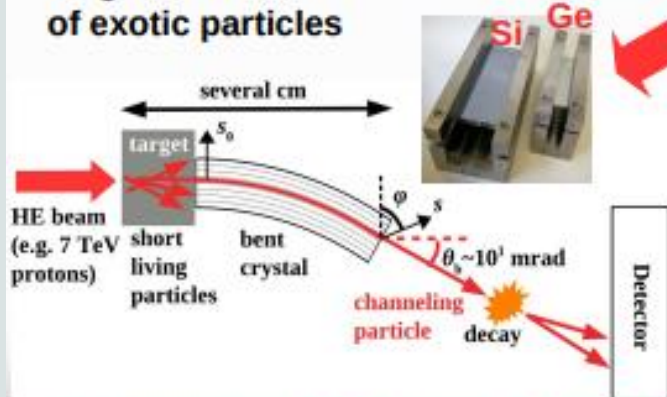
Ultrashort crystalline calorimeter



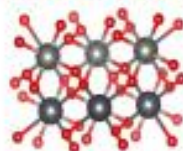
Positron source for future e⁺/e⁻ and muon colliders



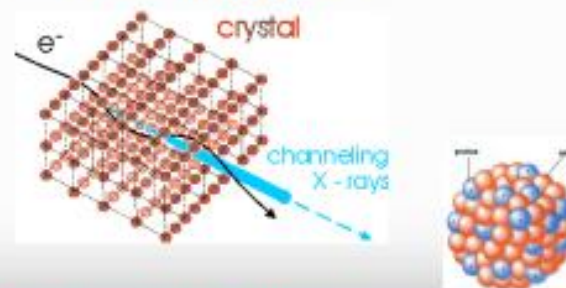
Measurement of dipole magnetic and electric moments of exotic particles



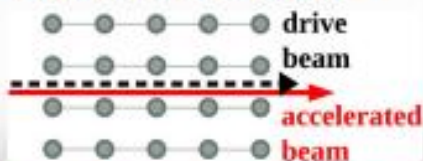
Oriented crystals



X and γ -ray source for nuclear and medical physics

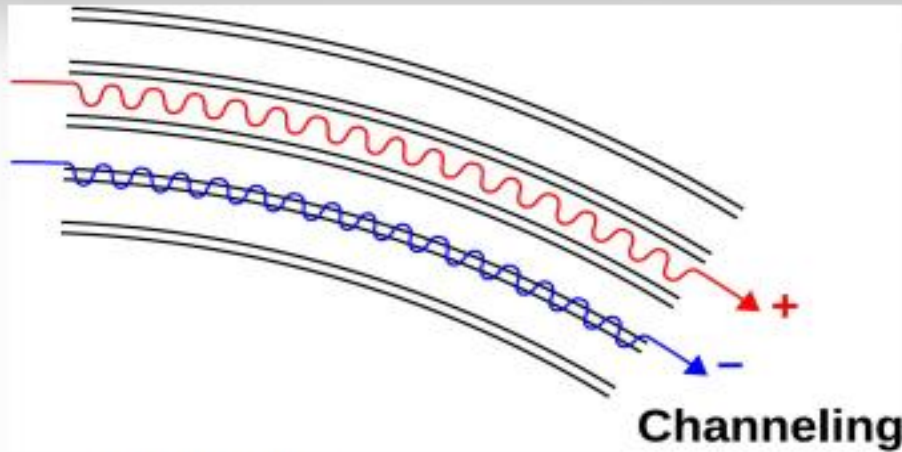


Plasma acceleration



*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS

Channeling



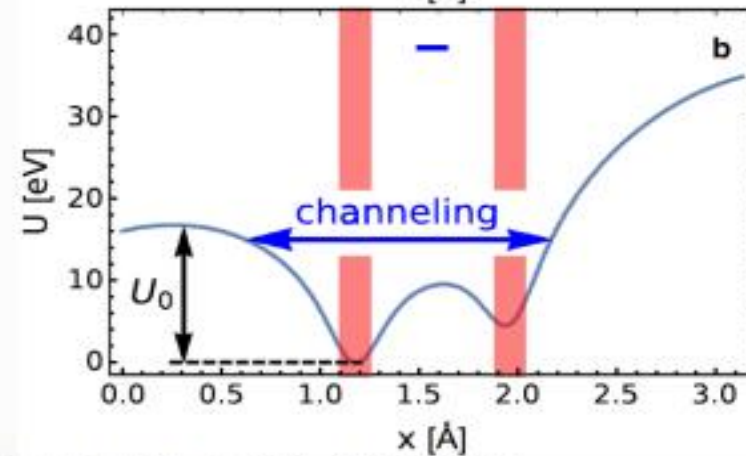
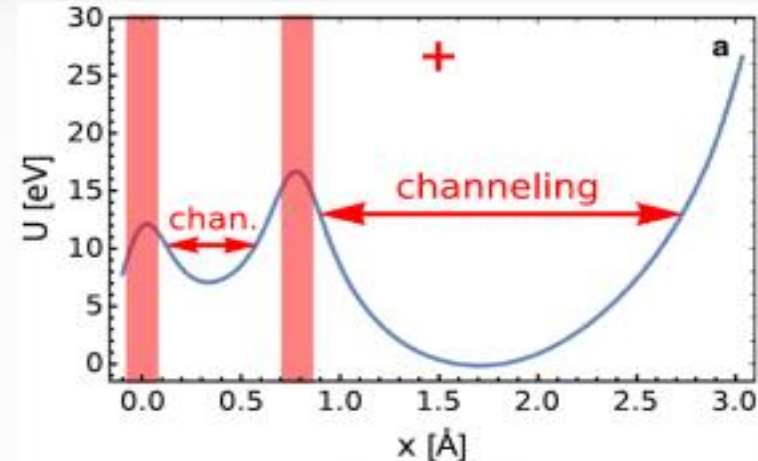
Channeling*:

Charge particle penetration through a monocrystal along its atomic planes/axes

trajectory equation:

$$\frac{d^2x}{dz^2} + \frac{U'_{pl\ x}}{pv} + \frac{1}{R} = 0$$

Interplanar potential



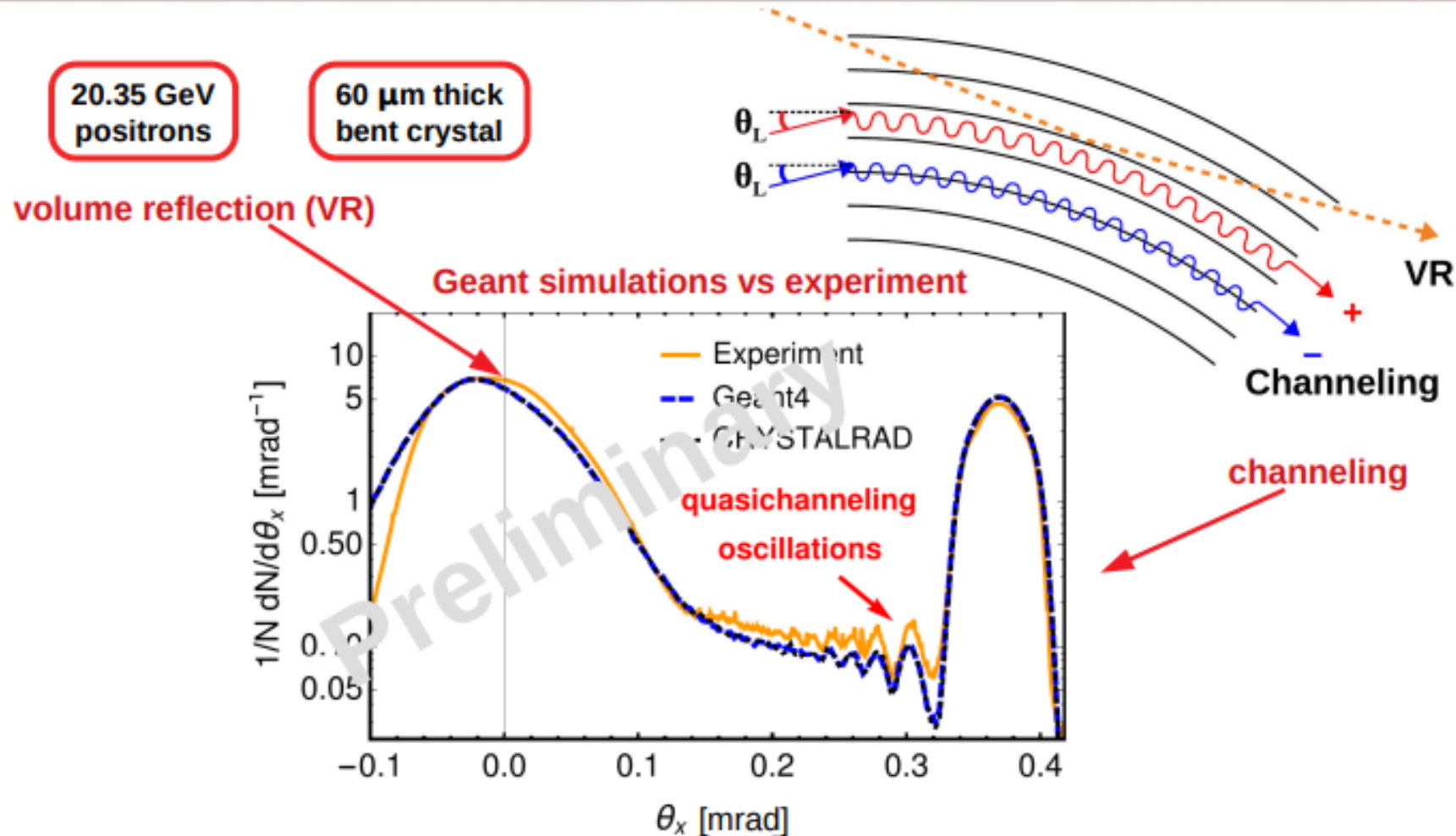
*J. Lindhard, Kgl. Dan. Vid. Selsk. Mat.-Fys. Medd. 34 No 4, 2821–2836 (1965)

E.N. Tsyganov, Fermilab TM-682 (1976)

**A. Sytov et al., Eur. Phys. J. C (2022) 82:197

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More Geant4 channeling model validation: quasichanneling oscillations* at SLAC FACET Facility



To be submitted for publication soon

*T. N. Wistisen, ... and A. Svytoy, Phys. Rev. Lett. 119, 024801 (2017)

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Recent developments in Geant4-DNA

Hoang Tran

Sébastien Inceri

and collaborators

Laboratoire de Physique des deux infinis – Bordeaux
CNRS - IN2P3 & Bordeaux U.
France



Geant4-DNA in 2024: overview



■ Physics (« very low energy » EM Physics)

- Update of **electron inelastic models for liquid water up to 10 MeV** (« dna_option4 » - up to 10 keV) by **I. Kyriakou et al. (Ioannina U. team)** – paper ready for submission
- New **electron discrete cross section models for O₂, N₂, CO₂** : electronic excitation, ionisation, elastic by **F. Nicolanti et al. (Roma U. team)** – recently published and not yet released (<https://doi.org/10.1016/j.ejmp.2023.102661>) - **towards atmospheric physico-chemistry applications**
- New **Lithium discrete cross section models for liquid water** : excitation ionisation, charge gain / loss by **J. Ramos-Mendez et al. (USCF team)** – recently published and not yet released (<https://doi.org/10.1088/1361-6560/ad5f72>) - paves the way to other (selected) ions

■ Chemistry

- Complete **review of Geant4/Geant4-DNA chemistry features (covering the 2012-2024 period)** by **H. Tran et al.** published in Med. Phys. 51 (2024) 5873–5889 (<https://doi.org/10.1002/mp.17256>)
- **Prototype software** for the simulation of **water radiolysis under multi-pulse irradiation** by **A. Le et al.** - <https://arxiv.org/abs/2409.11993>

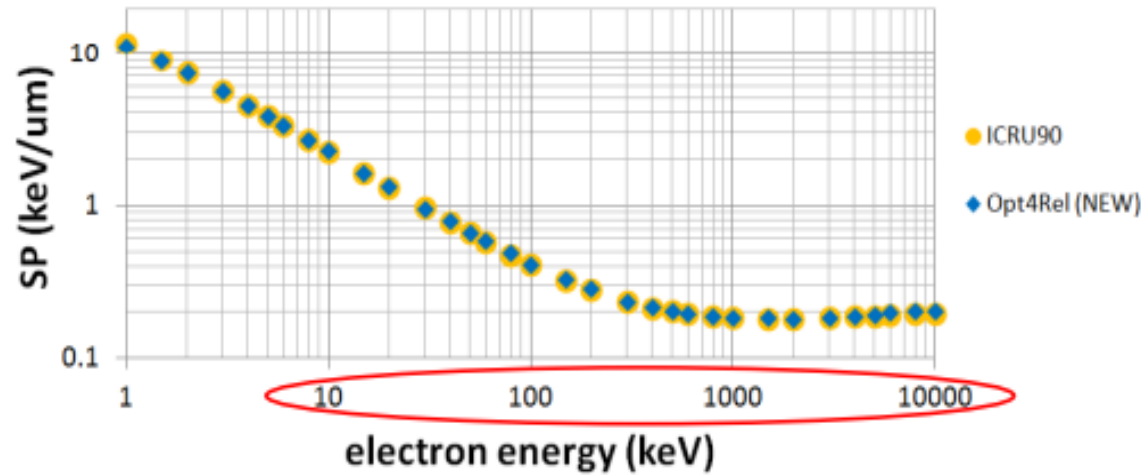
■ Other news

- In 2024, reactivated international **tutorials « post-COVID »** : **CNAO, Osaka U., Accra, Bucharest**
- **Collaboration Meeting** in Osaka U. (thanks again **Dousatsu & Takashi** !)

Physics: updated (discrete) electron physics (« dna_option4 »)

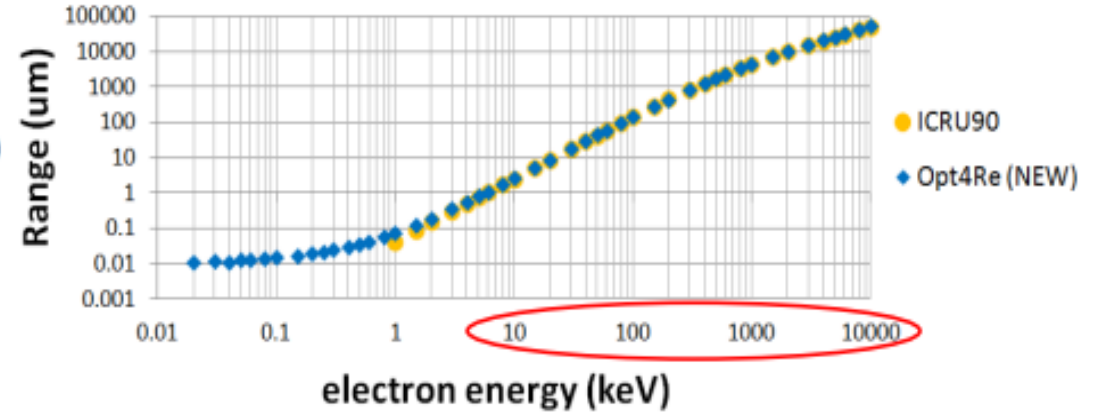
Courtesy of Ioanna Kyriakou et al.
(with ESA / BioRad3 support)

electronic stopping power (SP) of liquid water

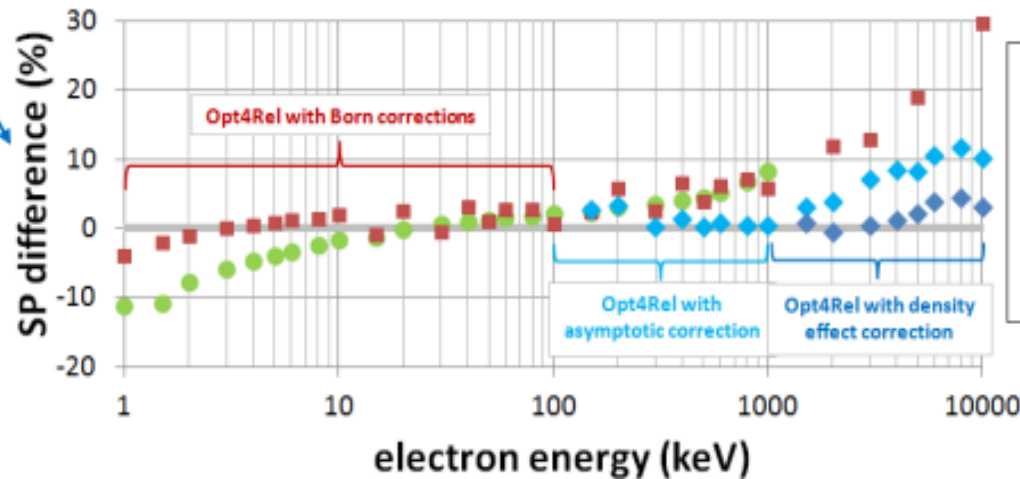


New model (Opt4Rel) within 5% from ICRU up to 10MeV

electron CSDA range in liquid water



New model (Opt4Rel) within 5% from ICRU up to 10MeV



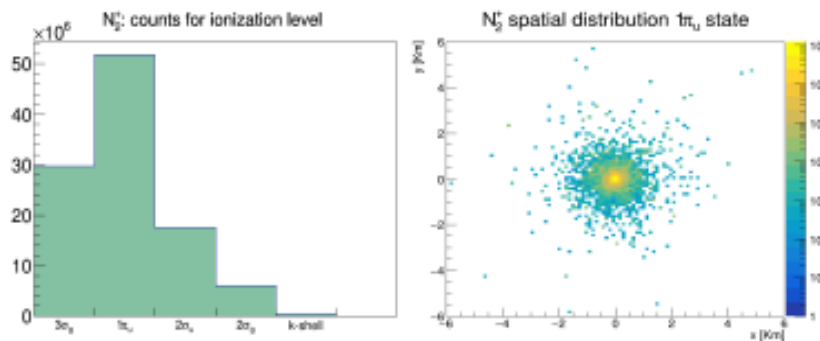
corrections are applied/not applied only within the energy range in which they have an effect larger/smaller than 1% to the electronic stopping power

Physics: Geant4-DNA for atmospheric simulations



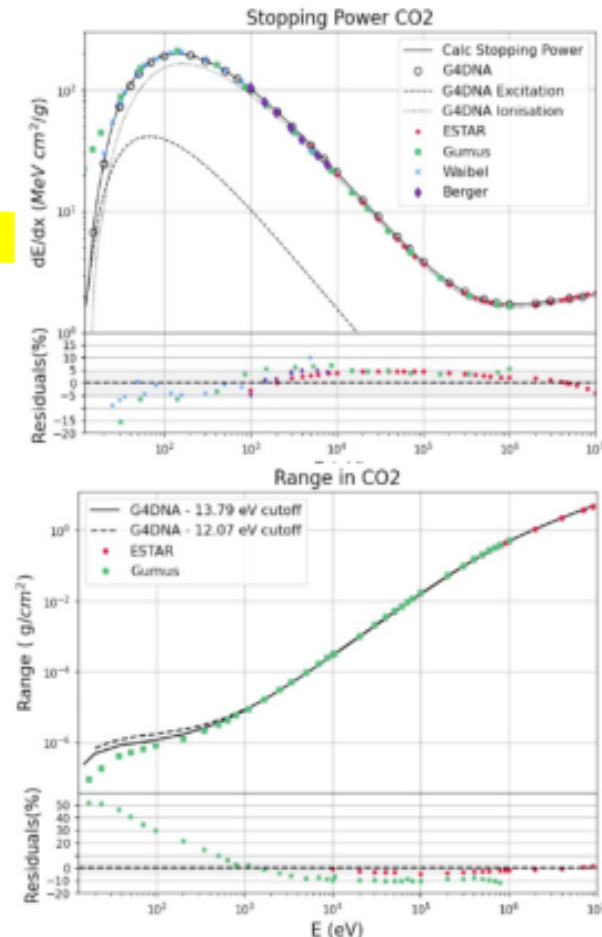
- Cross sections for **electrons impact on N_2 , O_2 , CO_2** molecules have been implemented in Geant4-DNA (energy range: 10 eV – 10 MeV)
- 3 physics model classes:
 - **Elastic** scattering (Independent Atomic Model with Screening Coefficients)
 - **Ionisation** (Relativistic Binary Encounter Bethe Model)
 - **Excitation** (Porter's formula with fitted parameters)
- Ranges and stopping powers verified vs NIST
- A Geant4-DNA simulation in a **thin atmospheric layer** to simulate ionization by secondary cosmic electrons has been written and is ready to run
- **Physico-chemistry dissociation process** has been included through the dissociation branching ratios for N_2 and O_2 (subsequent verification is still needed)

See talk of Francesca Nicolanti, Wed. 16:54



Work in progress:
Extend cross sections to
positrons
(10 eV – 10 MeV)

Model details: F. Nicolanti, et al, Phys Med. 2023 Sep 11;114:102661 [\(link\)](#)
Model implementations: F. Nicolanti, et al, Accepted by Phys Med. (2024)



Satisfactory agreement on stopping power and ranges for incident energies exceeding 200 eV

Physics: lithium Ions Cross-Sections for Geant4-DNA (1)

- Context of **BNCT therapy**: $^{10}\text{B}(n,\alpha)^7\text{Li}$
 - New classes are required in Geant4-DNA for using new XS for **ionization, excitation and charge exchange** processes.
 - New particles are needed for the different states of Li. **A particle template might help** to create these new states.
- Data was obtained for all the charge states of lithium ions
 - **ionization and excitation** were obtained by weighting the Li^{3+} cross-sections by effective charge factors¹
 - **Charge exchange** was obtained using the Classical Trajectory Monte Carlo Method (CTMC)²

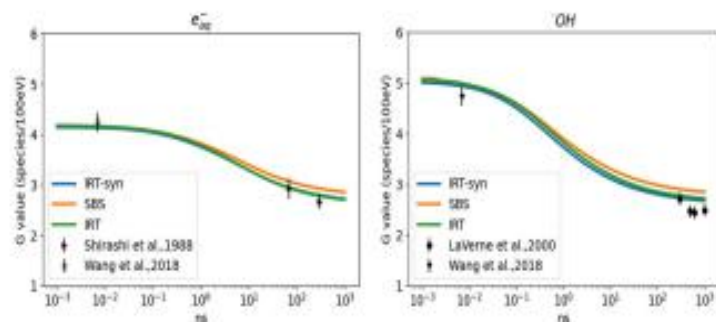
Cross-Section	Based on	Energy Ranges	Applicable to
Ionization	G4DNARuddIonizationExtended	700 eV – 7 GeV	Li^{3+} , Li^{2+} , Li^{1+} , Li^0
Excitation	G4DNAMillerGreenExcitationModel	70 eV – 3.5 MeV	Li^{3+} , Li^{2+} , Li^{1+} , Li^0
	G4DNABornExcitationModel	3.5 MeV – 700 MeV	Li^{3+} , Li^{2+} , Li^{1+} , Li^0
Charge Increase	CTMC	7 keV – 70 MeV	Li^{2+} , Li^{1+} , Li^0
Charge Decrease	CTMC	7 keV – 70 MeV	Li^{3+} , Li^{2+} , Li^{1+}

¹R.H. Garvey, C. H. J. and A. E. S. G. (1975). Independent-particle-model potentials for atoms and ions with $36 < Z \leq 54$ and a modified Thomas-Fermi atomic energy formula*. *Physical Review A*, 12(4), 1144–1152, <https://doi.org/10.1080/00431672.1975.9931783>

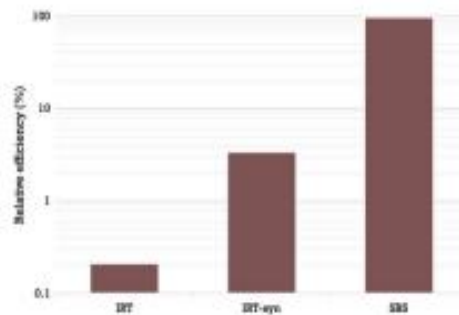
²Olson, R. E., & Salop, A. (1977). Charge-transfer and impact-ionization cross sections for fully and partially stripped positive ions colliding with atomic hydrogen. *Physical Review A*, 16(2), 531–541, <https://doi.org/10.1103/PhysRevA.16.531>

Chemistry: full review (2012-2024)

- Special Report in free access
 - Med. Phys. 51 (2024) 5873–5889
(<https://doi.org/10.1002/mp.17256>)
- Detailed review of
 - 4 alternative approaches
 - **Step-by-step** : tracking but slow
 - **Independent Reaction Time** : fast but no tracking
 - **Independent Reaction Time « synchronized »** : hybrid
 - **Mesoscopic** : beyond the us...
 - **Extended examples** for the simulation of water radiolysis : **chem***, **scavenger**, **UHDR**



G-values of e_{aq}^- and *OH as a function of time for the IRT, IRT-syn, and SBS models, considering 9 chemical reactions for 1 MeV



Relative computation times for IRT, IRT-syn, and SBS.

Received: 19 January 2024 | Revised: 17 May 2024 | Accepted: 25 May 2024
DOI: 10.1002/mp.17256

SPECIAL REPORT

MEDICAL PHYSICS

Review of chemical models and applications in Geant4-DNA: Report from the ESA BioRad III Project

Hoang Ngoc Tran¹ | Jay Archer² | Gérard Baldacchino^{3,4} |
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Laurent Desorgher⁹ | Naoki Dominguez¹⁰ | Serena Fattori¹¹ |
Susanna Guatelli¹² | Vladimir Ivantchenko¹³ | José-Ramos Méndez⁹ |
Petteri Nieminen¹¹ | Yann Perrot¹² | Dousatsu Sakata^{2,13,14} | Giovanni Santin¹¹ |
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R01CA187003, R01CA208419

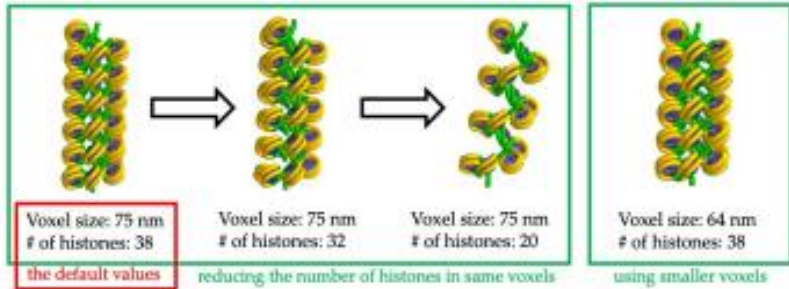
Abstract

A chemistry module has been implemented in Geant4-DNA since Geant4 version 10.1 to simulate the radiolysis of water after irradiation. It has been used in a number of applications, including the calculation of G-values and early DNA damage, allowing the comparison with experimental data. Since the first version, numerous modifications have been made to the module to improve the computational efficiency and extend the simulation to homogeneous kinetics in bulk solution. With these new developments, new applications have been proposed and released as Geant4 examples, showing how to use chemical processes and models. This work reviews the models implemented and application developments for modeling water radiolysis in Geant4-DNA as reported in the ESA BioRad III Project.

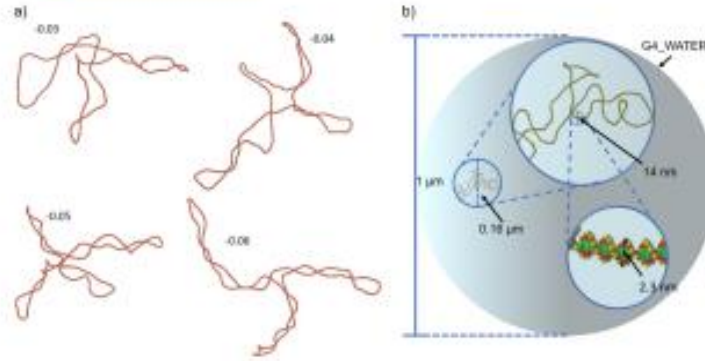
KEYWORDS

Geant4-DNA, radiation chemistry, water radiolysis

Geometries: library



Plasmids

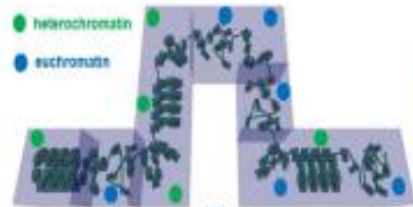
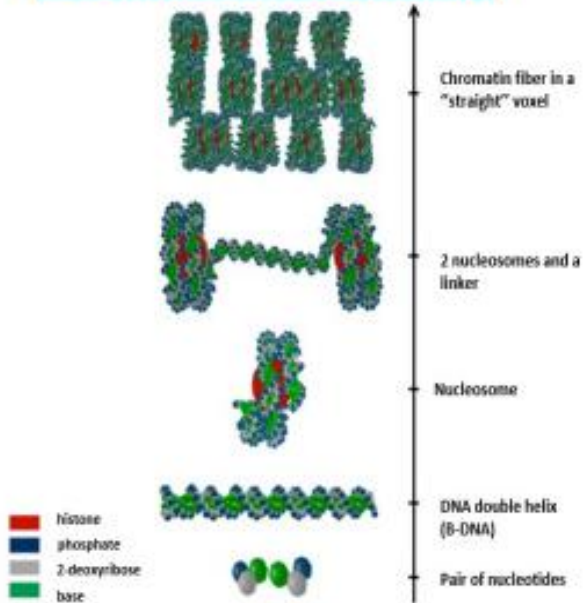


E. coli bacterium



Made available in the "moleculardna" and "dsbandrepair" examples

Voxels of chromatin

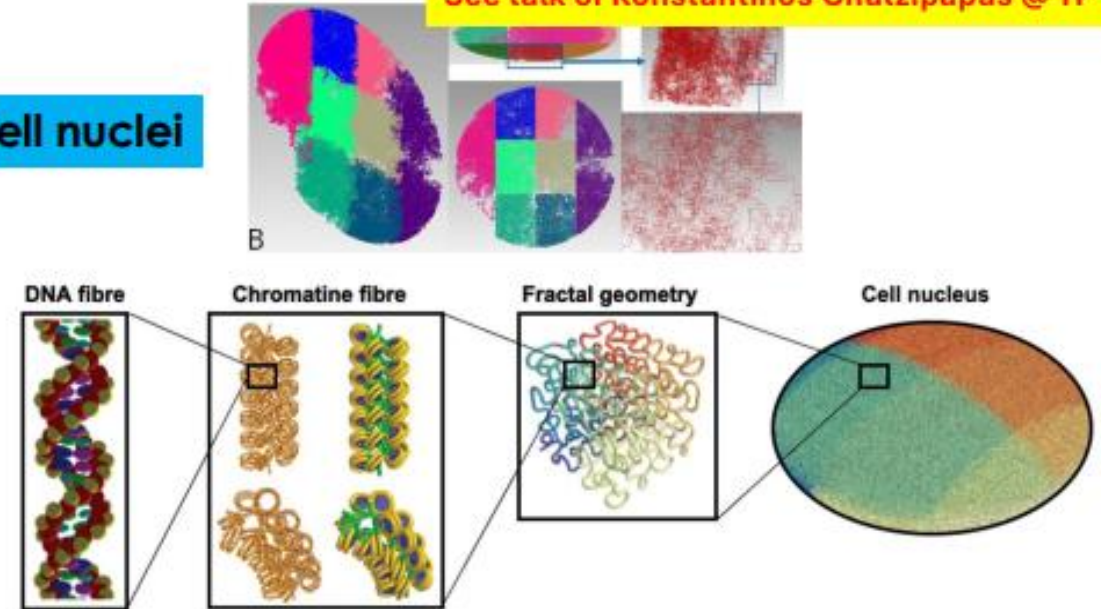


Cell nuclei

Human fibroblast (6 Gbp)

Human endothelium (6 Gbp)

See talk of Konstantinos Chatzipapas @ TF



Simulation chain: the « molecularDNA » ext. example

<http://moleculardna.org>

A Geant4-DNA integral chain (physics, chemistry, geometry, DNA damage, repair & cell survival)

<https://doi.org/10.1016/j.ejmp.2022.11.012>

<https://www.efomp.org/index.php?r=news/view&id=338>

European Journal of Medical Physics

Announcement: Galileo Galilei Award



The Galileo Award in Medical Physics is given every year to the best paper published in this journal in the previous year. In 2022, the prize has been awarded to Fabio Di Martino et al., "A new solution for UHPF and UHDR (Flash) measurements: theory and conceptual design of ALL3 chamber", Phys. Med. 2022; 132:9-18.

Physica Medica – the European Journal of Medical Physics, is happy to announce that the paper "Prediction of DNA rejoining kinetics and cell survival after proton irradiation for V79 cells using Geant4-DNA" by Dousatsu Sakata, Taroichi Hirayama, Wook-Geun Shin, Mauro Belli, Maria A. Tabocchini, Robert D. Stewart, Oleg Belov, Mario A. Bernal, Marie-Claude Bordage, Jeremy M. C. Brown, Milos Dordevic, Dimitris Emfietzoglou, Ziad Francis, Susanna Guatelli, Taku Inaniwa, Vladimir Ivanchenko, Mathieu Karamitros, Ioanna Kyriakou, Nathanael Lampe, Zhuxin Li, Sylvain Meylan, Claire Michelet, Petteri Nieminen, Yann Perrot, Ivan Petrovic, Jose Ramos-Mendez, Aleksandra Ristic-Fira, Giovanni Santini, Jan Schuemann, Hoang N. Tran, Carmen Villagrasa, Sebastien Incerti, published in Physica Medica, Volume 135, January 2022; 102506, DOI: <https://doi.org/10.1016/j.ejmp.2022.11.012>, has been elected the best paper published in the journal in the year 2022.

The paper presents the intimate relation between radiobiological modeling and simulation of the physical processes of radiation interaction with cells in order to provide a better understanding on the mechanisms behind radiation cell killing and damage repair. More specifically, the paper introduces an extension of the Geant4-DNA radio-biological application by adding a feature aiming at simulating the repair of the DNA damages and their kinetics as well as the survival fraction of cells at some time after irradiation. The value of the work reaches on the fact that it opens up to further basic as well as applied research with applications in radiation therapy and radiation protection, in addition to providing better understanding of the processes behind the clinical manifestations of radiation induced cell damage and cell kill leading to the eradication of the clonogenic cells in the tumour lesions as well as to the unwanted effects in the healthy tissues.

The selection of the best paper has been performed on the basis of citations and downloads together with the assessment by the Editors, Associate Editors and members of the Editorial Board.

We congratulate the authors for this paper, as the winners of the Galileo Award.

Prof. Juliana Toma-Ganu
Physica Medica
Editor-in-Chief

Physica Medica 105 (2023) 102508

Contents lists available at ScienceDirect

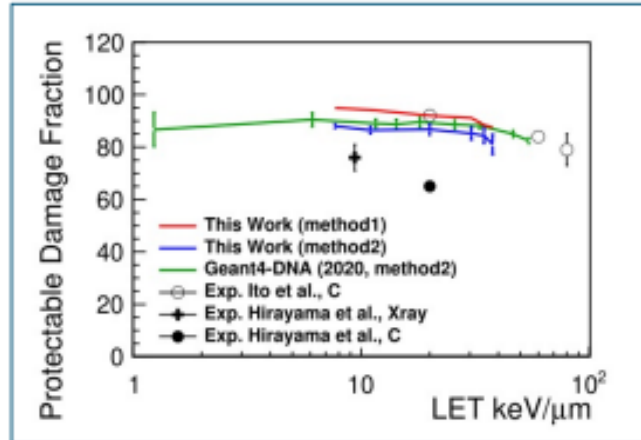
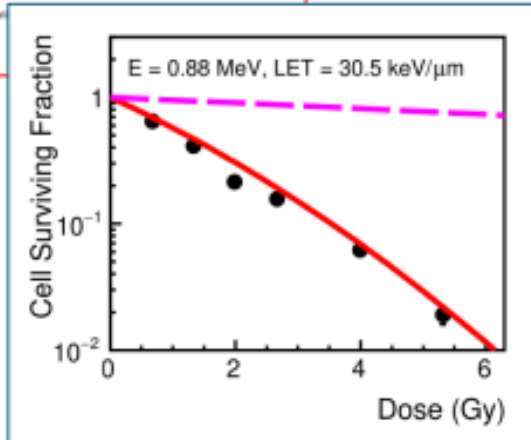
Physica Medica

journal homepage: www.elsevier.com/locate/ejmp

Original paper

Prediction of DNA rejoining kinetics and cell survival after proton irradiation for V79 cells using Geant4-DNA

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molecularDNA

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molecularDNA

Radiation-induced DNA damage simulations in Geant4

molecularDNA is a Geant4-DNA example built to allow easy simulation of radiation-induced DNA damage with flexible geometries and well defined damage parameters.

Get started right away in [geant4examples/extended/medical/dna/moleculardna](#) with a library of pre-existing geometries, or dive into the documentation.

A tutorial demonstrating molecularDNA is also available at this [link](#).

Important : This version of molecularDNA (Geant4 11.3 BETA) is proposed as a beta version and may still contain bugs, thank you for your understanding. Please contact us for further details. This example is for demonstration purpose and acts as an introductory tool to help users create their own applications; therefore users are advised to adapt the simulation parameters in their applications accordingly.

human cell example

Get started from example See publications Available geometries

Want to know more about how it all works? You'll want to visit our Overview page.

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