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

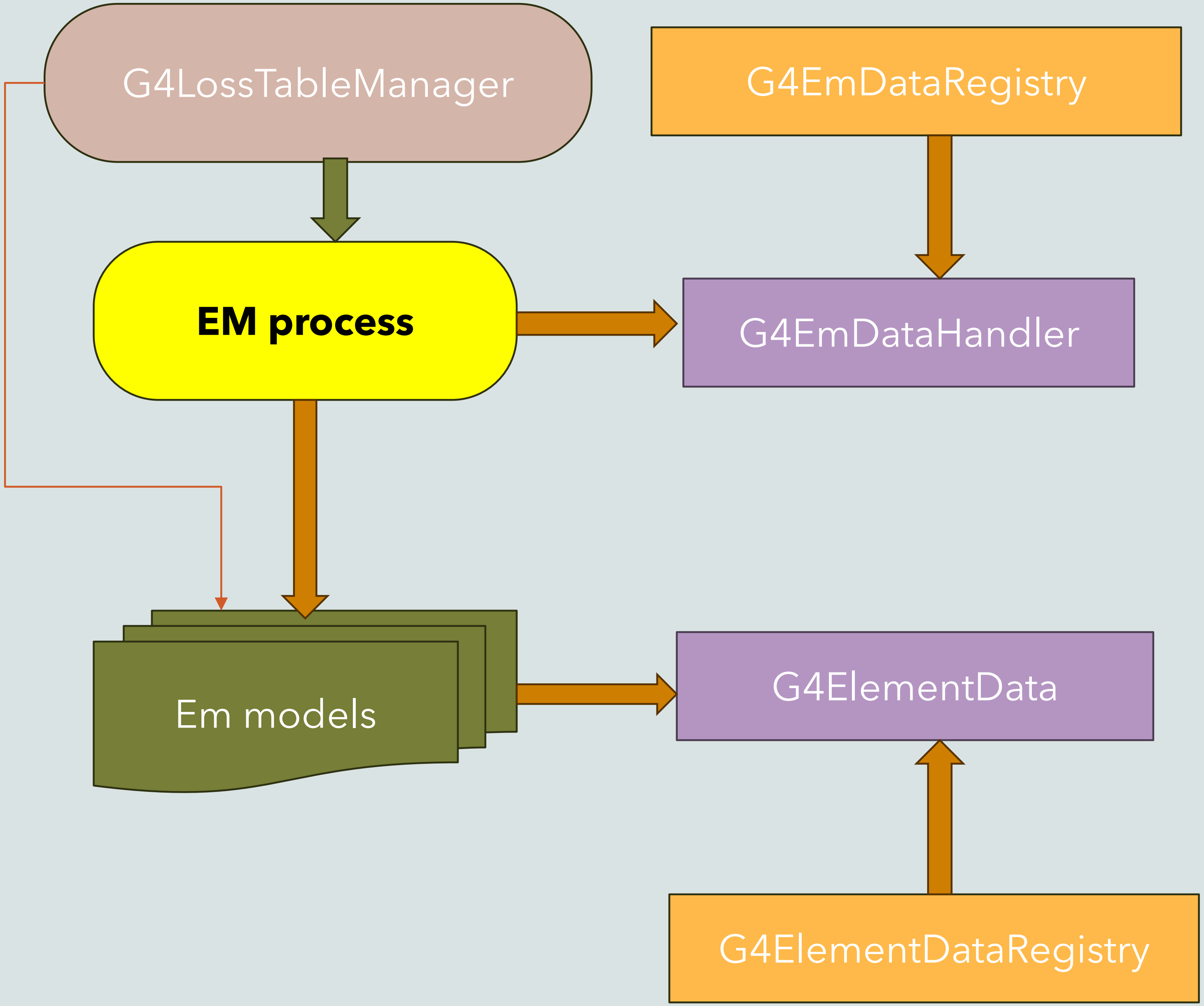
- New dataset G4EMLOW8.6.1
- Initializations of EM tables and data structures are thread safe.
- Full implementation of 3-gamma annihilation and positronium production and decay
- Full implementation of X-Ray scattering and examples
- Alternative EM processes for exotic particles
- Extension of models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

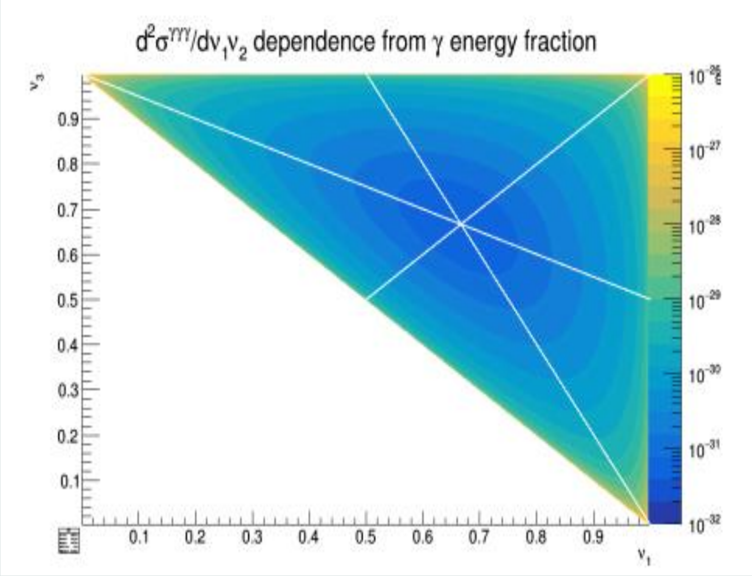
EM data handling for 11.3

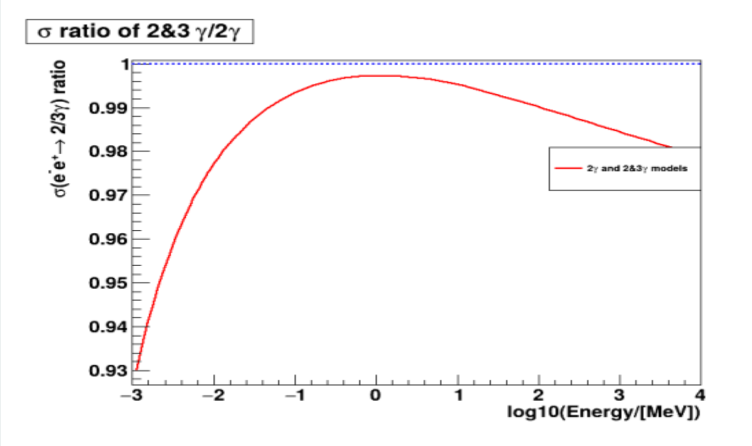
- **Existing G4ElmentDataRegistry**
  - *Keep G4ElementData for EM models*
- **G4LossTableManager define master thread in constructor**
  - *It may be the first working thread*
- **New class G4EmDataRegistry**
  - *singleton to keep shared data from EM processes*
    - Physics tables
    - EM cross section 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





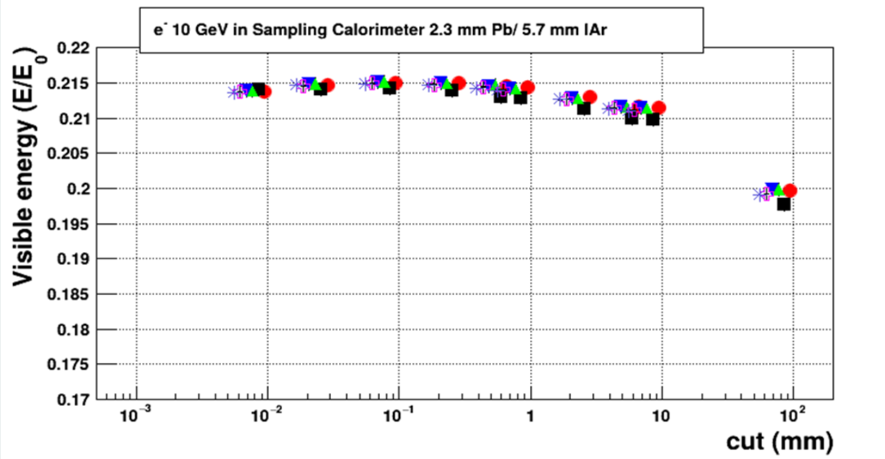
Positron annihilation at rest

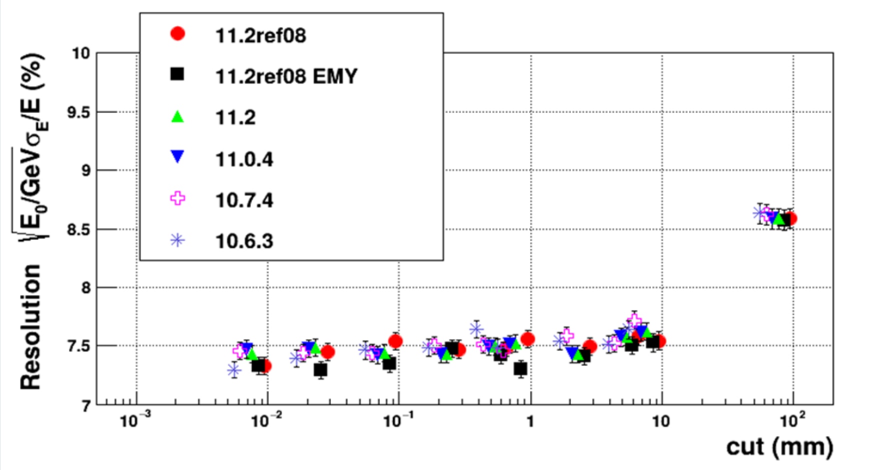
- Creation of positronium at rest concerns mainly medical applications
- A choice of model for sampling of final state is provided via enumerator
  - *G4PositronAtRestModelType*
    - fSimplePositronium
    - fAllisonPositronium
    - fOrePowel
    - fOrePowelPolar
- Selection of positronium model
  - */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*

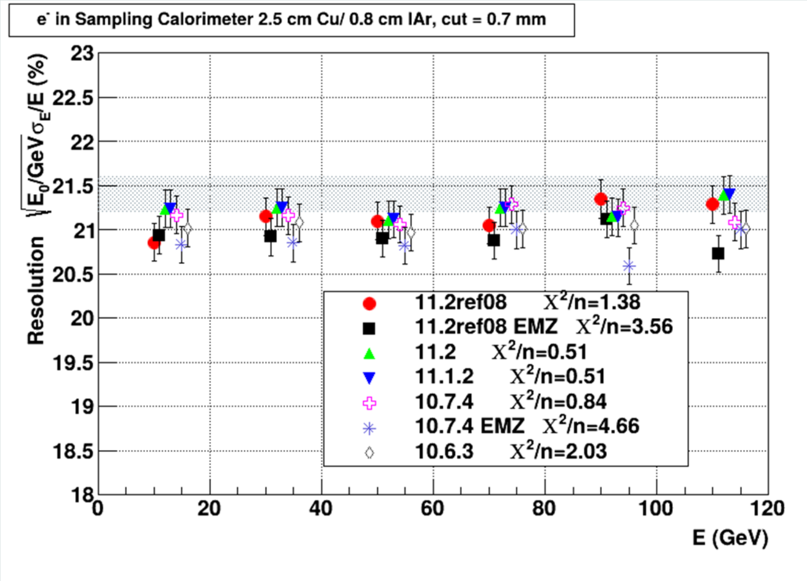
Other new developments

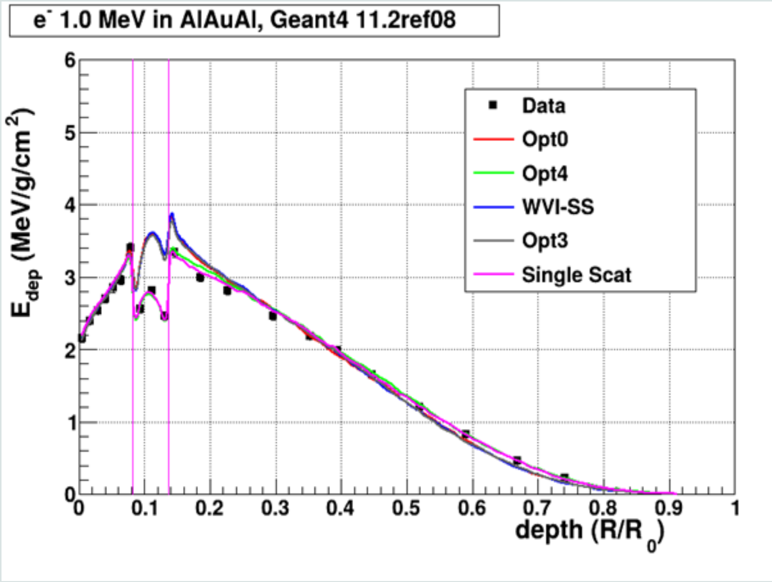
- EPICS2017 data
  - *Since 11.2 these data for Livermore gamma models*
  - *Livermore photo-electric model and Rayleigh scattering models are the default in EM Opt0 physics*
  - *EPICS2017 cross section for gamma conversion is included into Bethe-Heitler model as an option*
    - This model now is not 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*

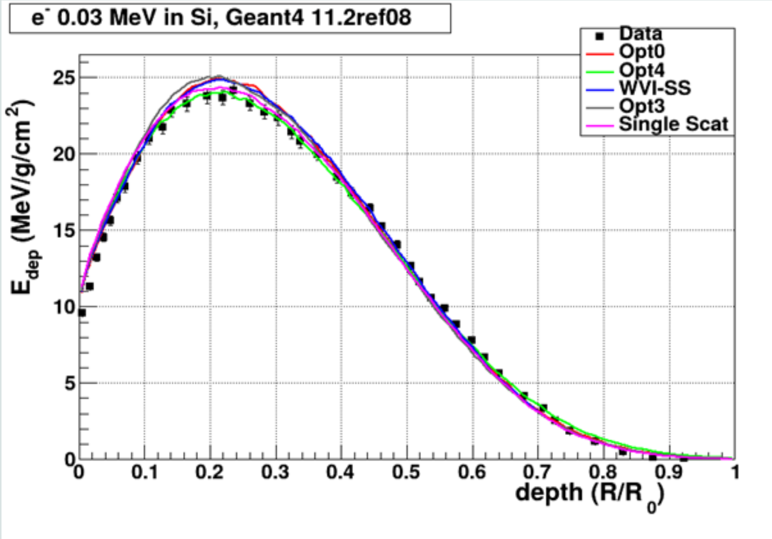
Recent validation results











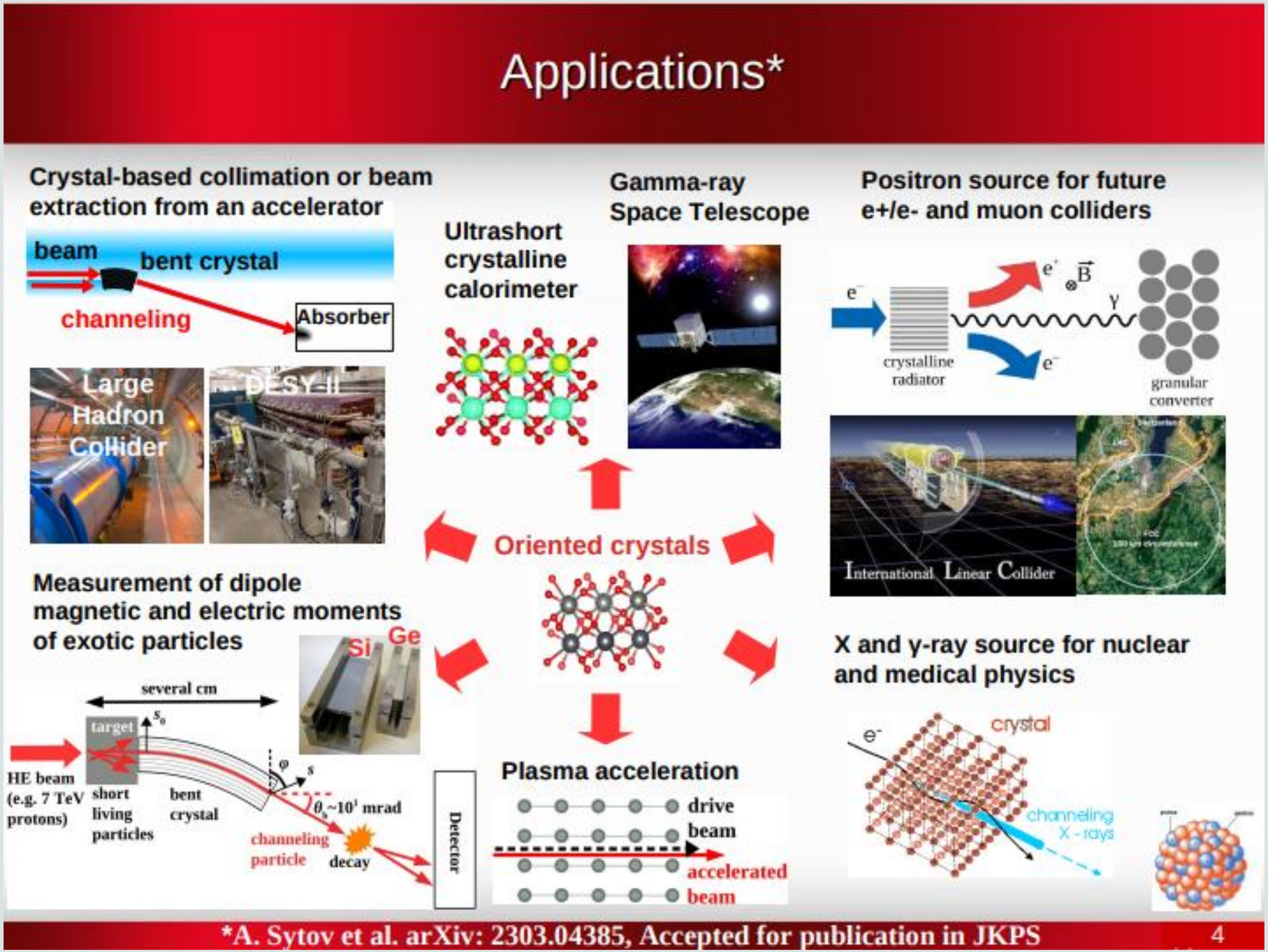
- **There is stability in general for EM calorimetry response simulation from 10.6 to 11.3**
- The only known unstable EM physics is EMY, which was fixed in 11.2.2

Istituto Nazionale di Fisica Nucleare

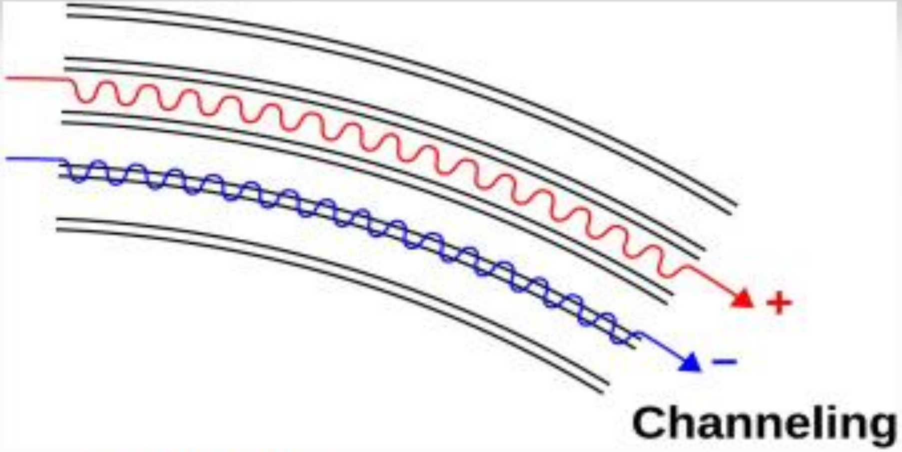
European Commission

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
beam
bent crystal
channeling
Absorber
Large Hadron Collider
DESY-II
Ultrashort crystalline calorimeter
Gamma-ray Space Telescope
Positron source for future e+/e- and muon colliders
crystalline radiator
granular converter
International Linear Collider
Oriented crystals
Measurement of dipole magnetic and electric moments of exotic particles
Si
Ge
several cm
target
HE beam (e.g. 7 TeV protons)
short living particles
bent crystal
channeling particle
decay
Detector
Plasma acceleration
drive beam
accelerated beam
X and γ-ray source for nuclear and medical physics
crystal
channeling X - rays
*A. Sytov et al. arXiv: 2303.04385, Accepted for publication in JKPS
4

Channeling



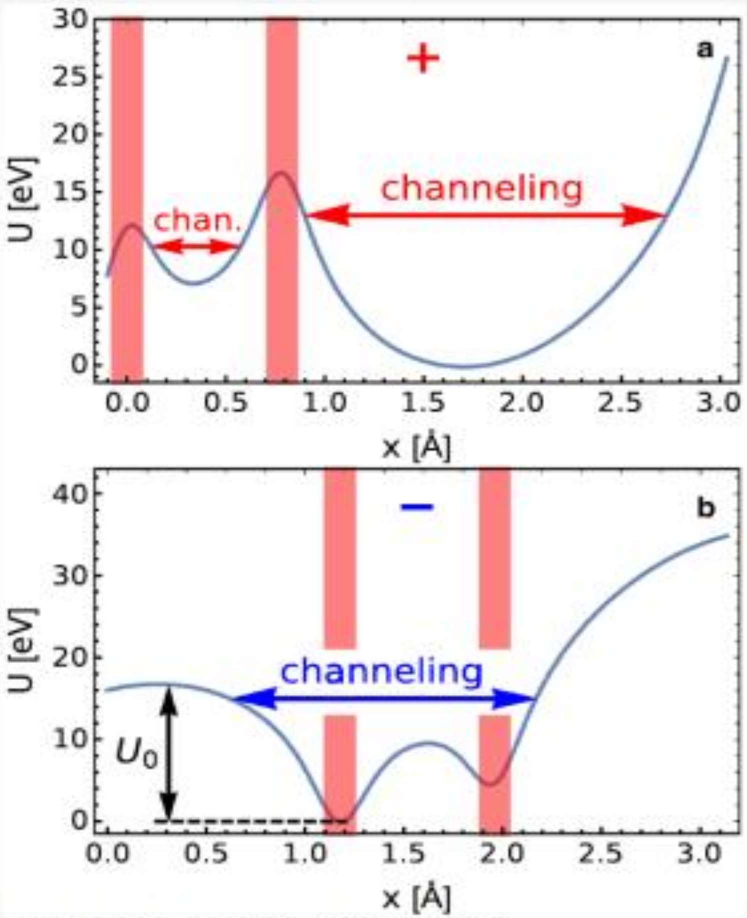
Channeling*:

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

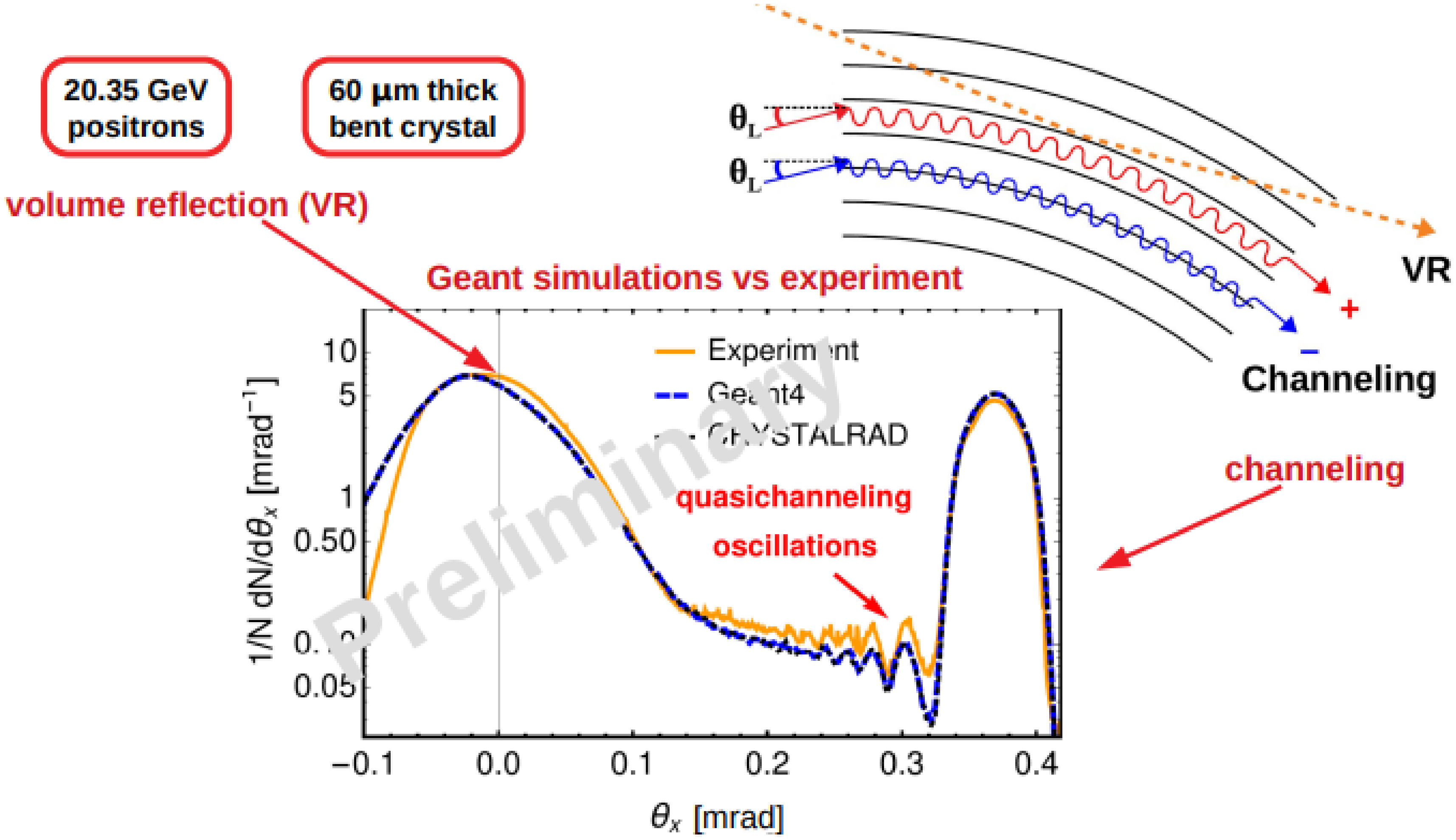


*J. Lindhard, Kgl. Dan. Vid. Selsk. Mat.-Fys. Medd. 34 No 4, 2821–2836 (1965)
E.N. Tsyganov, Fermilab TM-682 (1976)
**A. Sytov et al., Eur. Phys. J. C (2022) 82:197

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

20.35 GeV positrons

60 µm thick bent crystal



To be submitted for publication soon

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

Recent developments in Geant4-DNA

Hoang Tran

Sébastien Incerti

and collaborators

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

Osaka U. 2024

Geant4-DNA in 2024: overview

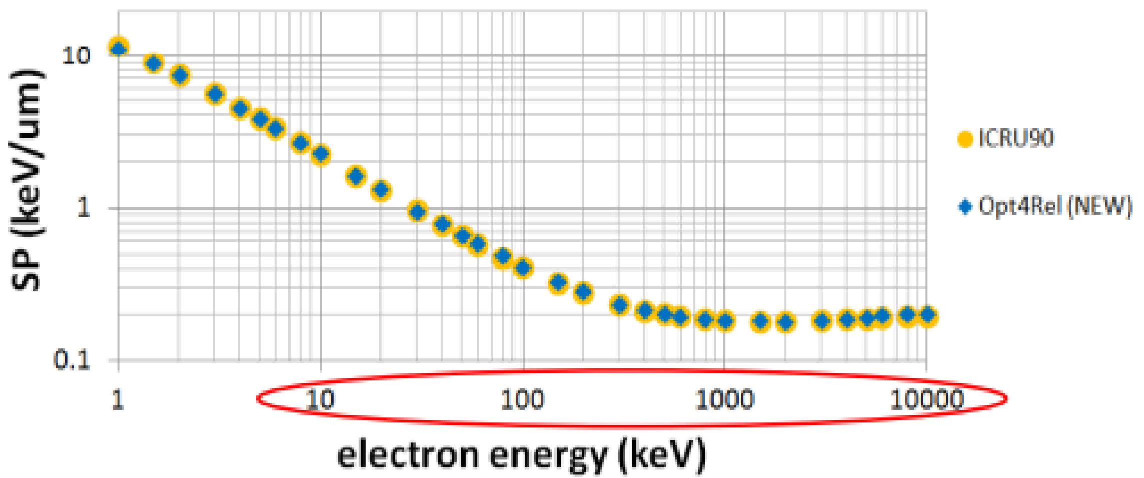
- **Physics (« very low energy » EM Physics)**
  - Update of electron inelastic models for liquid water up to 10 MeV (« dna_option4 » - up to 10 keV) by I. Kyriakou et al. (Ioannina U. team) – paper ready for submission
  - New electron discrete cross section models for O2, N2, CO2 : electronic excitation, 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

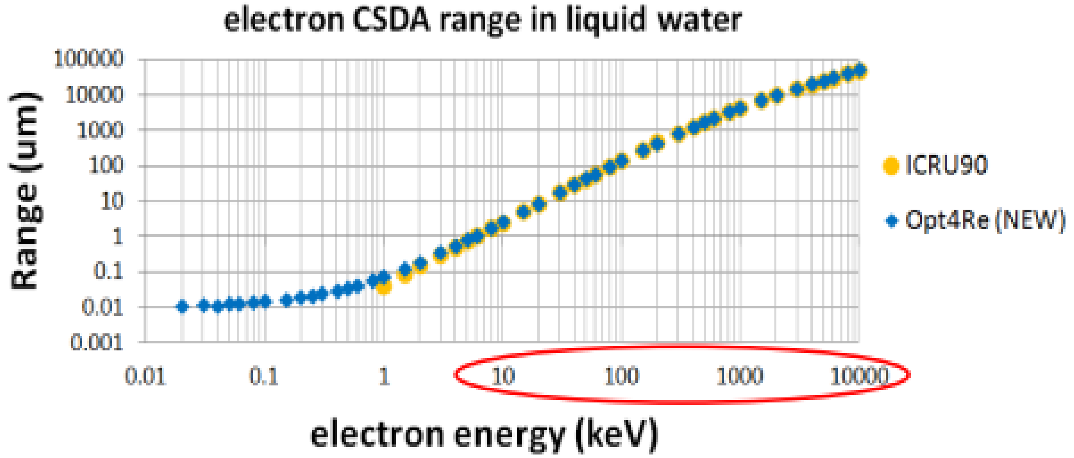
- **Other news**
  - In 2024, reactivated international tutorials « post-COVID » : CNAO, Osaka U., Accra, Bucharest
  - Collaboration Meeting in Osaka U. (thanks again Dousatsu & Takashi !)

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

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



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



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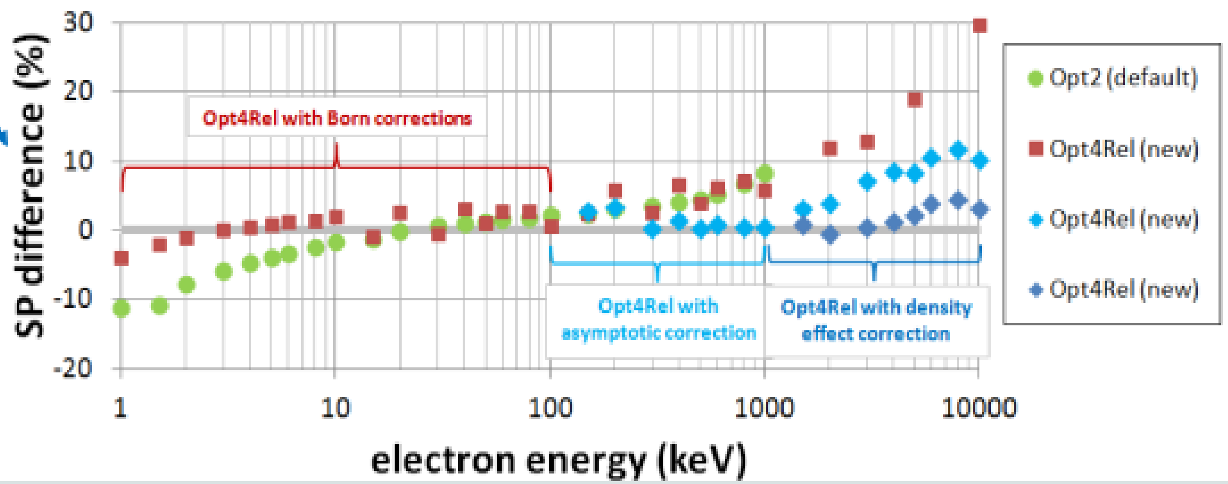


corrections are applied/not applied only within the energy range in which they have an effect larger/smaller than 1% to the electronic stopping power

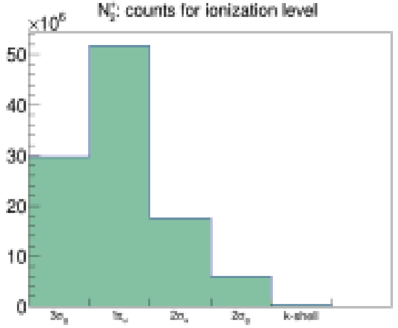
Courtesy of Franceca Nicolati, Carlo Mancini et al. (Roma U.)

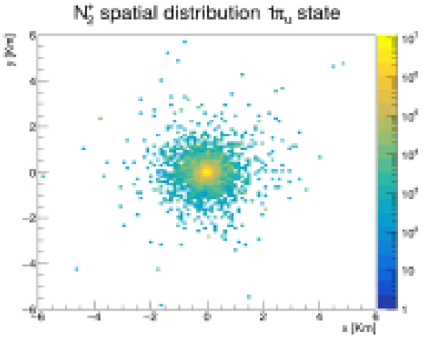
Physics: Geant4-DNA for atmospheric simulations

- 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)

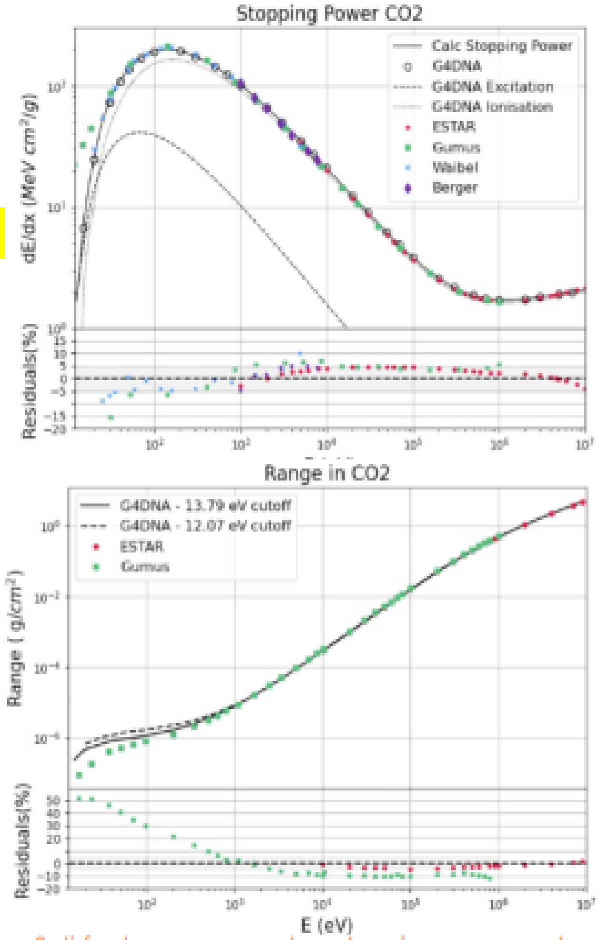
See talk of Francesca Nicolanti, Wed. 16:54

- 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)





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



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

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)

Courtesy of Jose Ramos-Mendez and J. Naoki D-Kondo (UCSF)

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

- Context of **BNCT therapy**: $^{10}B(n,\alpha)^{7}Li$
  - 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 factors[1]
  - **Charge exchange** was obtained using the Classical Trajectory Monte Carlo Method (CTMC) [2]

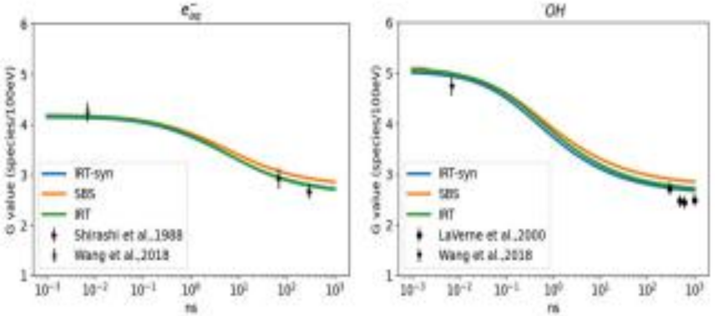
Cross-Section	Based on	Energy Ranges	Applicable to
Ionization	G4DNARuddIonizationExtended	700 eV – 7 GeV	Li^{3+}, Li^{2+}, Li^{1+}, Li^{0}
Excitation	G4DNAMillerGreenExcitationModel	70 eV – 3.5 MeV	Li^{3+}, Li^{2+}, Li^{1+}, Li^{0}
	G4DNABornExcitationModel	3.5 MeV – 700 MeV	Li^{3+}, Li^{2+}, Li^{1+},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

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

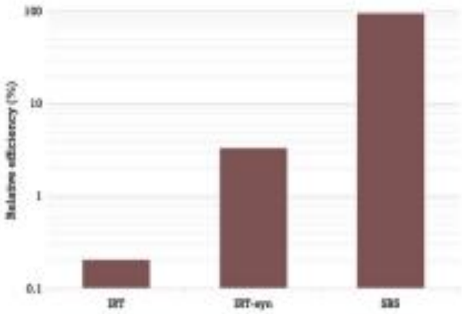
[2] Olson, R. E., & Salop, A. (1977). Charge-transfer and impact-ionization cross sections for fully and partially stripped positive ions colliding with atomic hydrogen. *Physical Review A*, *16*(2), 531–541, https://doi.org/10.1103/PhysRevA.16.531

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 $^{\bullet}OH$ 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

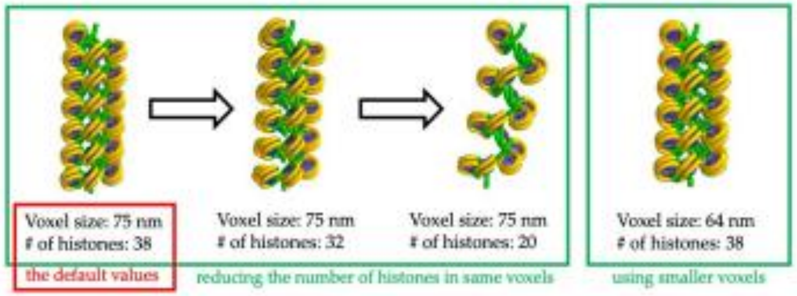
Hoang Ngoc Tran[1] | Jay Archer[2] | Gérard Baldacchino[3,4] | Jeremy M. C. Brown[5] | Flore Chappuis[6] | Giuseppe Antonio Pablo Cirrone[7,8] | Laurent Desorgher[6] | Naoki Dominguez[9] | Serena Fattori[7] | Susanna Guatelli[2] | Vladimir Ivantchenko[10] | José-Ramos Méndez[9] | Petteri Nieminen[11] | Yann Perrot[12] | Dousatsu Sakata[2,13,14] | Giovanni Santin[11] | Wook-Geun Shin[15] | Carmen Villagrasa[12] | Sara Zein[1] | Sebastien Incerti[1]

Abstract

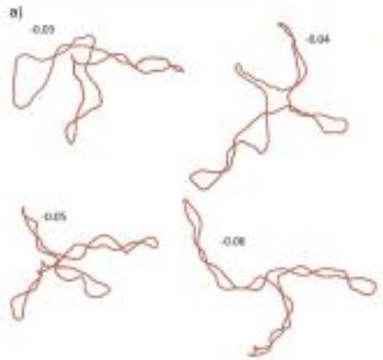
A chemistry module has been implemented in Geant4-DNA since Geant4 version 10.1 to simulate the radiolysis of water after irradiation. It has been used in a number of applications, including the calculation of G-values and early DNA damage, allowing the comparison with experimental data. Since the first 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.

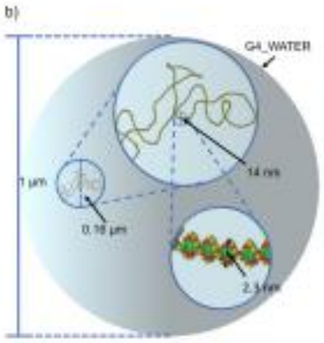
KEYWORDS
Geant4-DNA, radiation chemistry, water radiolysis

Geometries: library



Plasmids

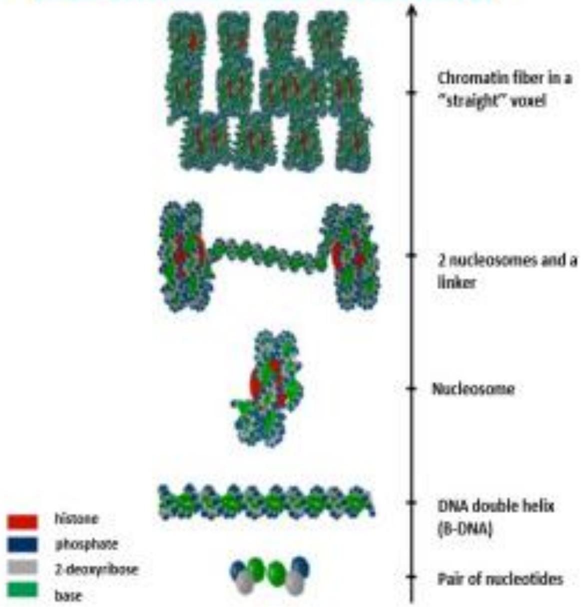


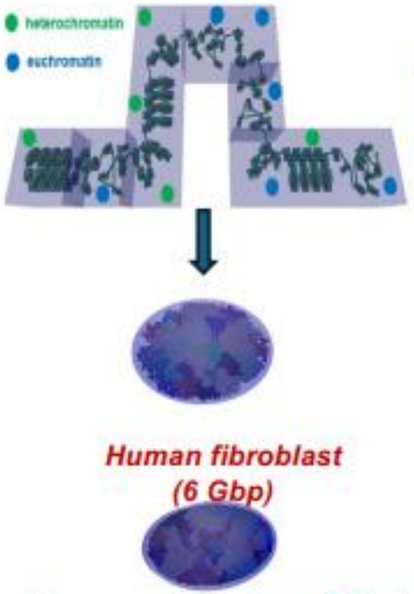


E. coli bacterium

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

Voxels of chromatin



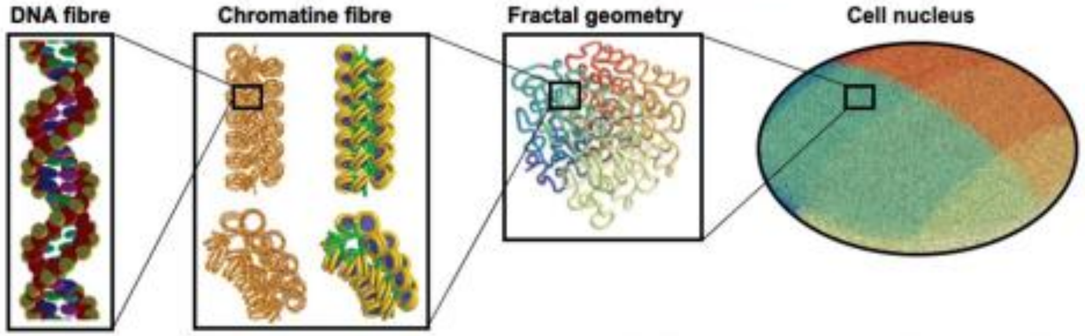


Human fibroblast (6 Gbp)

Human endothelium (6 Gbp)

See talk of Konstantinos Chatzipapas @ TF

Cell nuclei

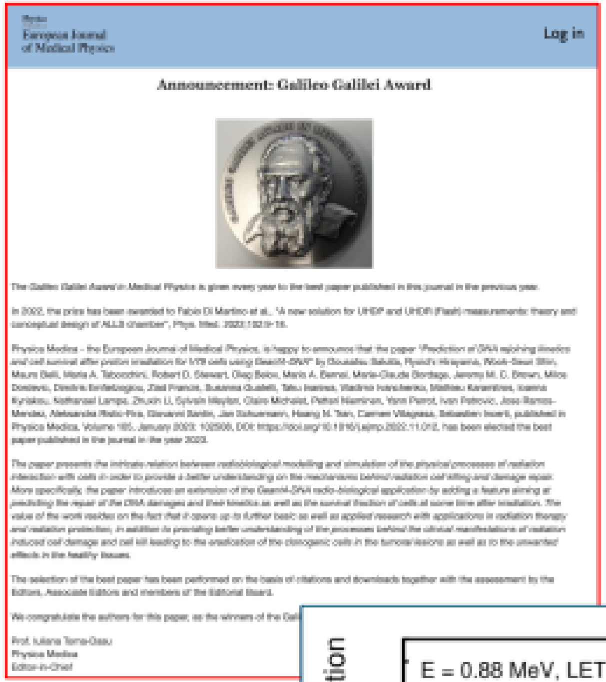


Simulation chain: the « moleculardna » ext. example

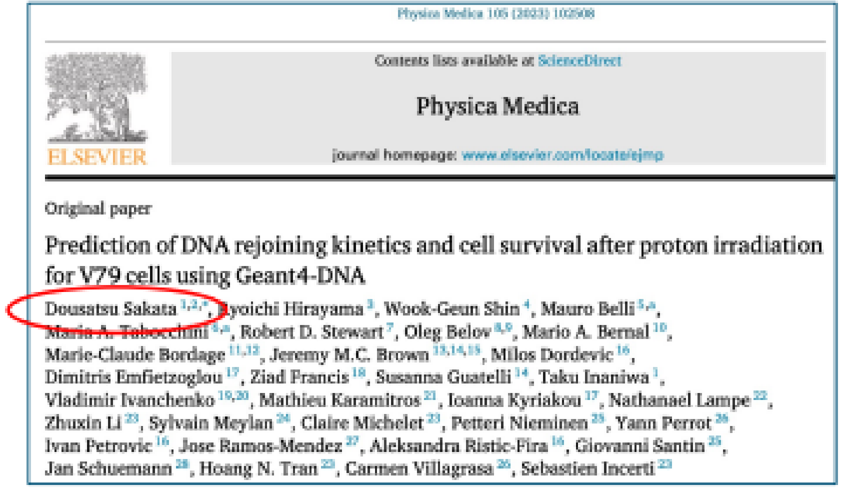
http://moleculardna.org

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

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



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


Physica Medica 105 (2023) 102508

Contents lists available at ScienceDirect

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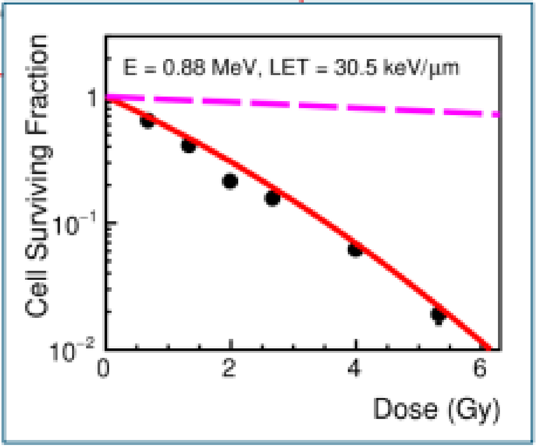
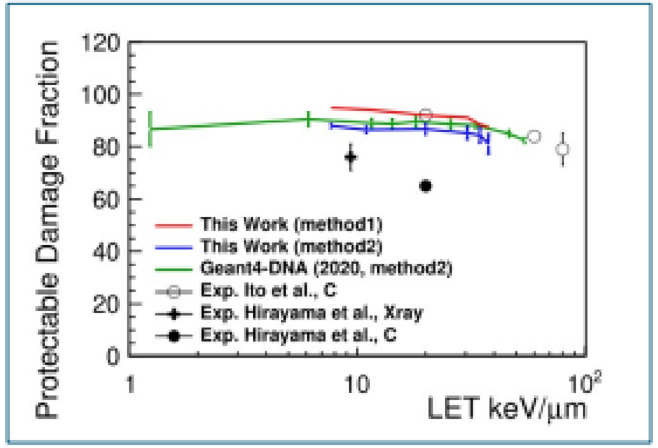
journal homepage: www.elsevier.com/locate/ejmp

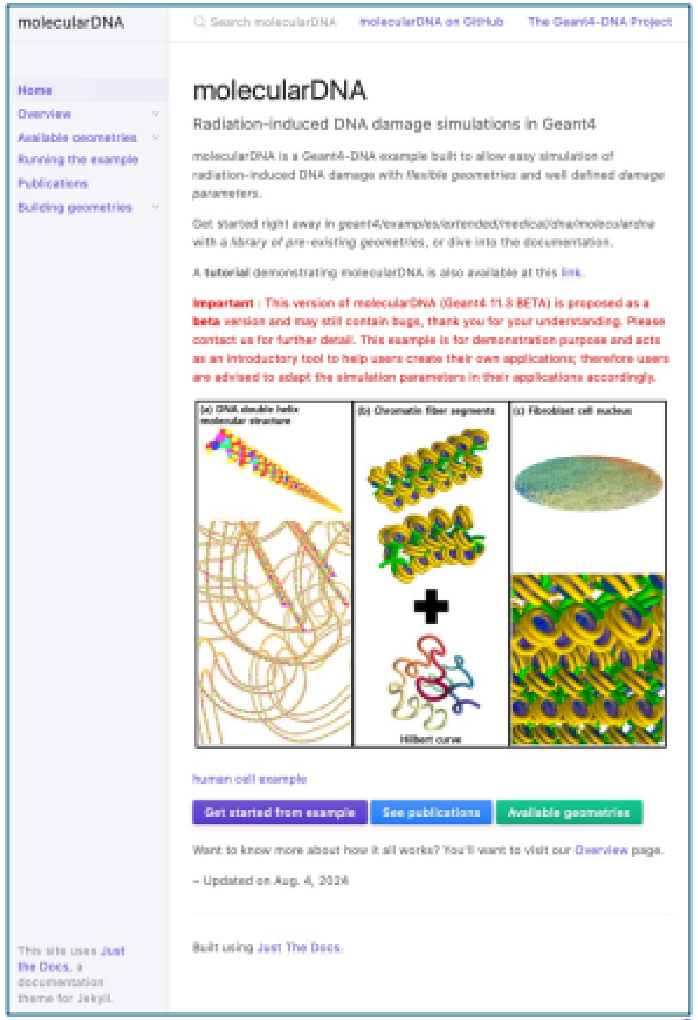
Original paper

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

Dousatsu Sakata, Ryoichi 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 Santin, Jan Schuemann, Hoang N. Tran, Carmen Villagrasa, Sebastien Incerti







Thank you