

Summary of Parallel session 4A

New EM models and tools

Chairs: V. Ivantchenko and S. Guatelli

< Wed 25/09 >

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09:00

New Geant4-DNA physics models for electrons in DNA-related material (remote)

Marie-Claude Bordage 

F113, Jefferson Lab

09:00 - 09:15


New Geant4-DNA physics models for electrons in gold (remote)

Ioanna Kyriakou 

F113, Jefferson Lab

09:15 - 09:30

Status of MPEXS-DNA

Shogo Okada 

F113, Jefferson Lab

09:30 - 09:45

Geant4-DNA for other solid state materials


Susanna Guatelli 

F113, Jefferson Lab

09:45 - 10:00

10:00


Directional brem splitting

Daren Sawkey 

F113, Jefferson Lab

10:00 - 10:15

X-ray fluorescence with ANSTO libraries

Susanna Guatelli 

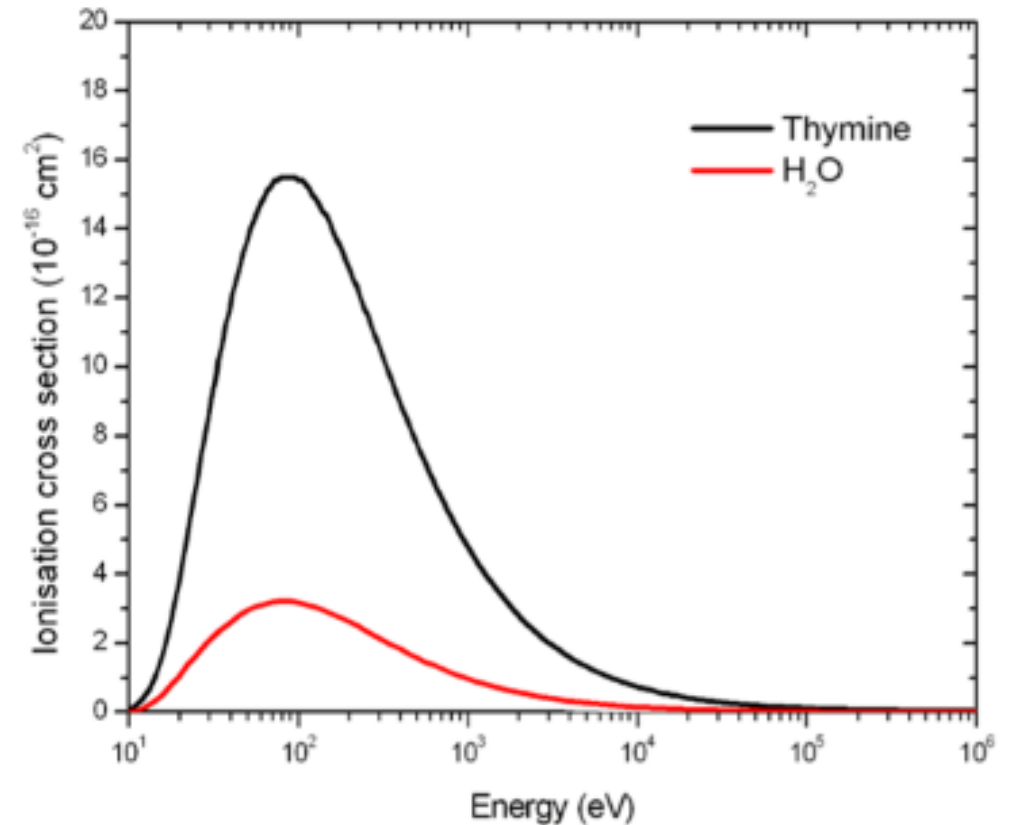
F113, Jefferson Lab

10:15 - 10:30

Recent developments of Geant4-DNA CPA100

- By M.-C. Bordage and S. Incerti
- CPA100 physics models for electrons in **liquid water** already integrated in Geant4 (Geant4-DNA option 6 physics list)
- Currently extension of the Geant4-DNA CPA100-based models to **DNA bases**

Electron ionisation total cross section

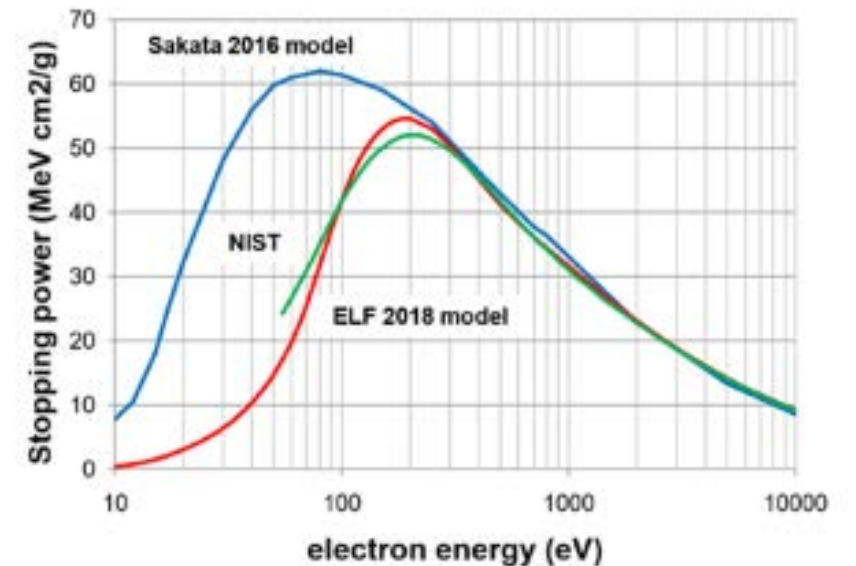
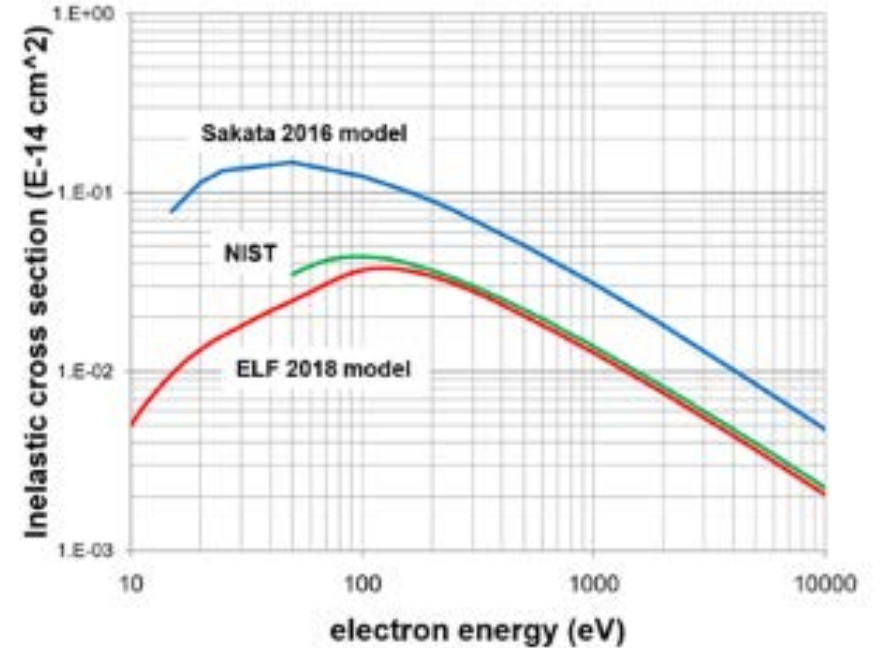


Geant4-DNA extensions to gold

- I. Kyriakou, D. Emfietzoglou, D. Sakata, S. Incerti, S. Guatelli
- Models based on the ELF (energy-loss-function) approach

GNP2016 vs. GNP2018 models

Process	2016 models	2018 models
Elastic	ELSEPA	ELSEPA
Ionization	Rel. Binary Encounter Bethe Vriens	Dielectric
Excitation	Exp.+Dirac B-Spline R Matrix	Dielectric
Plasmon	Quinn	Dielectric
Bremsstrahlung	Seltzer & Berger	Seltzer & Berger

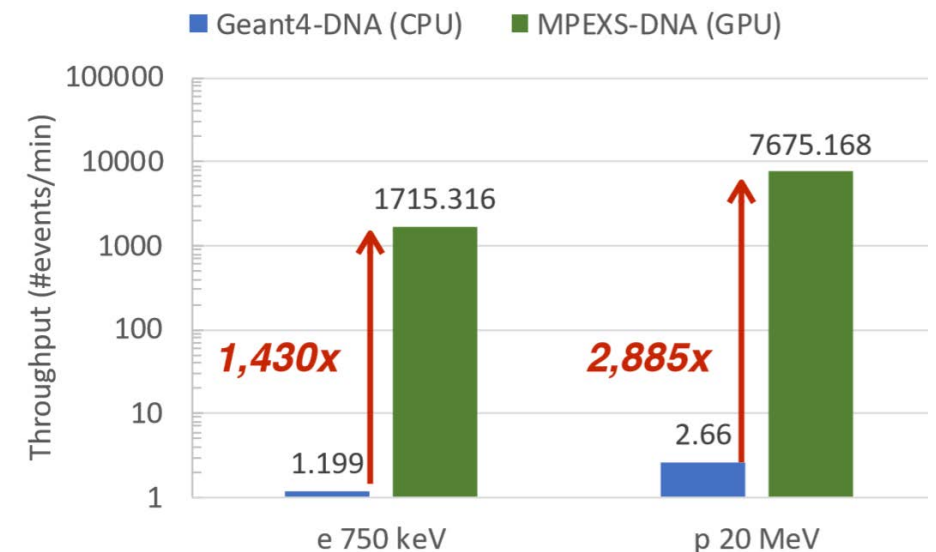
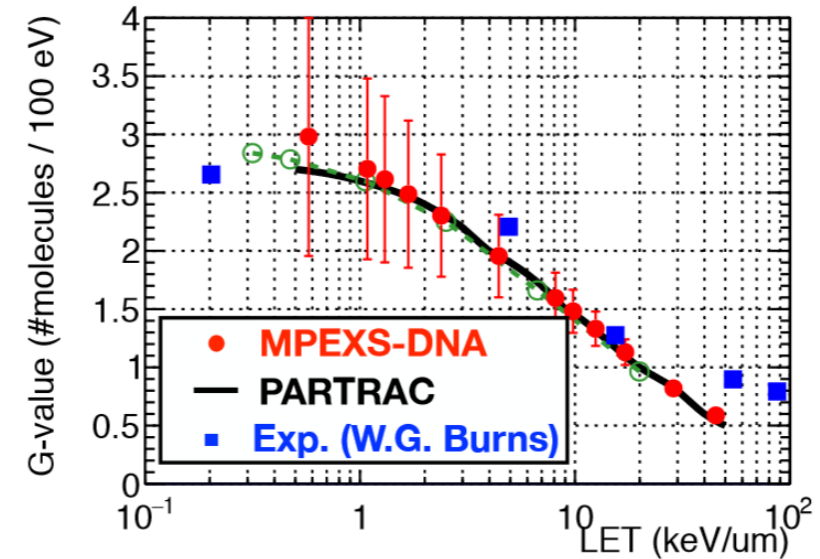


Status of MPEXS-DNA

Reference publication: DOI: 10.1002/mp.13370

- S. Okada, K. Murakami, S. Incerti, K. Amako, T. Sasaki
- MPEXS-DNA: A nanodosimetry simulator running on GPU
 - Most of the physics lists for Geant4-DNA are covered, all Geant4-DNA physico-chemical and chemical processes are implemented
- Current activities:
 - Implementation of an alternative model for Chemistry Stage in Geant4-DNA and MPEXS-DNA
 - Based on I. Plante, DOI: 10.1007/s00411-011-0367-8
 - Quantitative Estimation of DNA Damage Using Clustering Model in Geant4-DNA and MPEXS-DNA

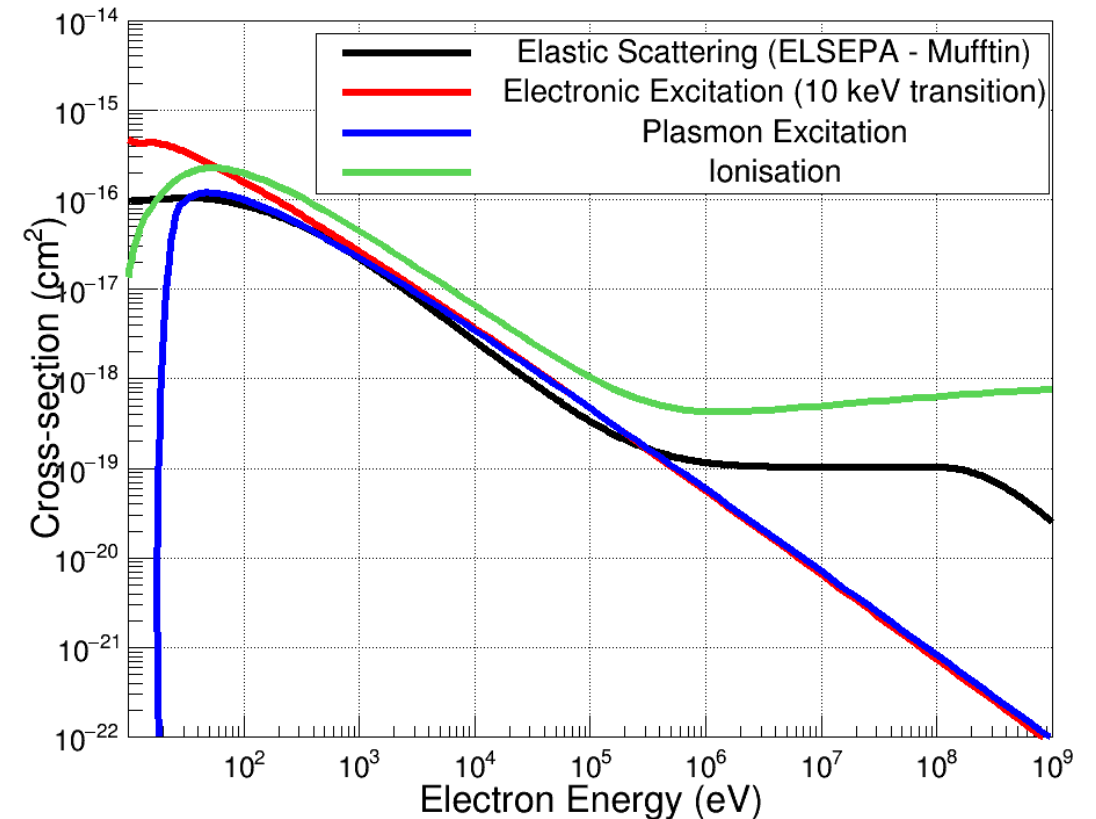
B: LET dependency of G-value for $\cdot\text{OH}$ radicals at 1 μs after proton irradiation



- GPU: NVIDIA, TITAN V
- CPU: Intel, Xeon E5-2643 v2, 3.5 GHz

Geant4-DNA for other solid state materials: graphite

- D. Bolst, D. Sakata, C. Fontes, I. Kyriakou, D. Emfietzoglou, S. Incerti, S. Guatelli
- Elastic scattering: ELSEPA
- Plasmon excitation: Cross section from atomic state using Quinn model
- Ionisation: Relativistic Binary Encounter Bethe Vriens
- Electronic excitation: ACE
- Under development



Same approach of Sakata et al, Journal of Applied Physics, 120 (24), art. no. 244901, 2016

Directional bremsstrahlung splitting in Geant4

- D. Sawkey

- Method:

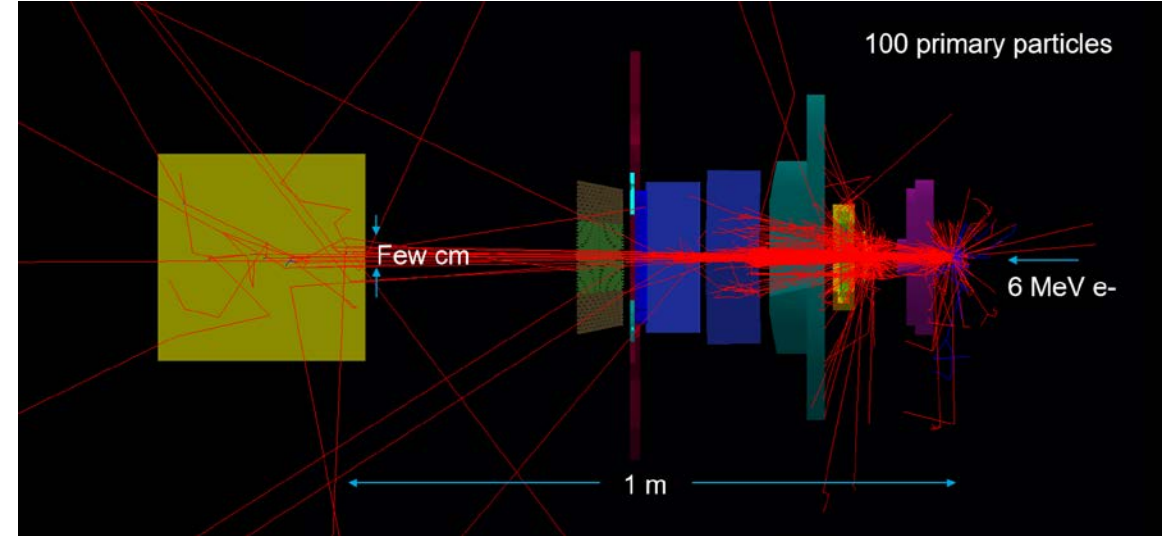
For all interactions producing gammas:

- Split N times (new weight $1/N$)
- Is the gamma going towards target volume?
 - If yes, keep
 - If no, play Russian Roulette (survival probability $1/N$, weight 1)
- All gamma reaching the target volume have weight $1/N$

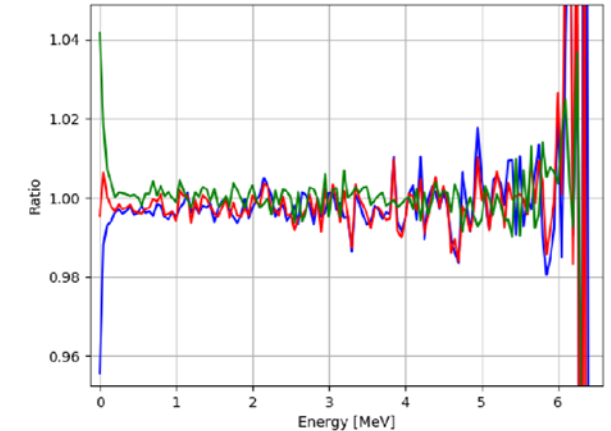
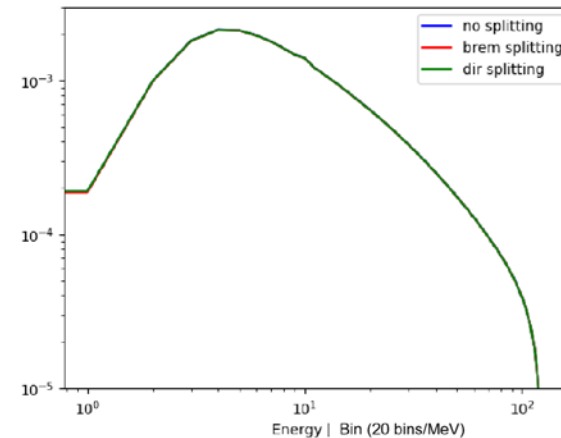
- Work in progress

- Proposal

- Currently store –list of secondaries (`std::vector<G4DynamicParticle*>`)
- Parallel list of weights `std::vector<G4double>`
- Find a more efficient to store the weight . Maybe within `G4DynamicParticle` or `G4Track`???

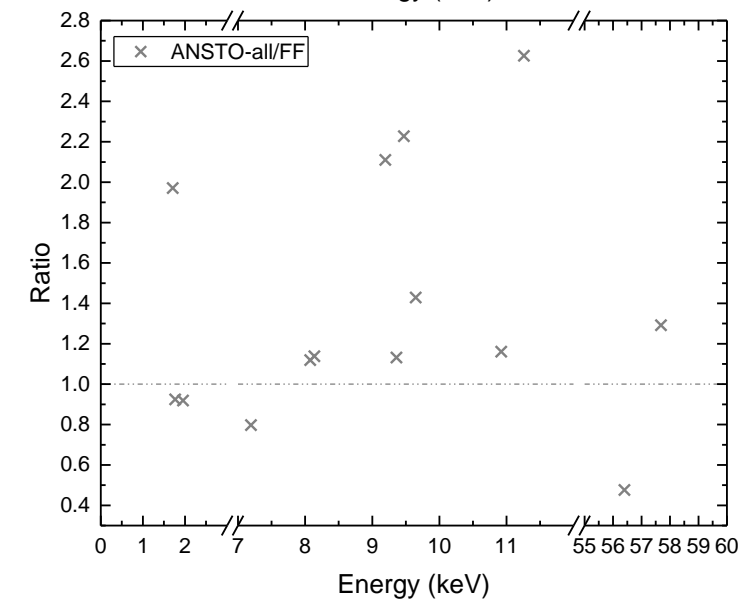
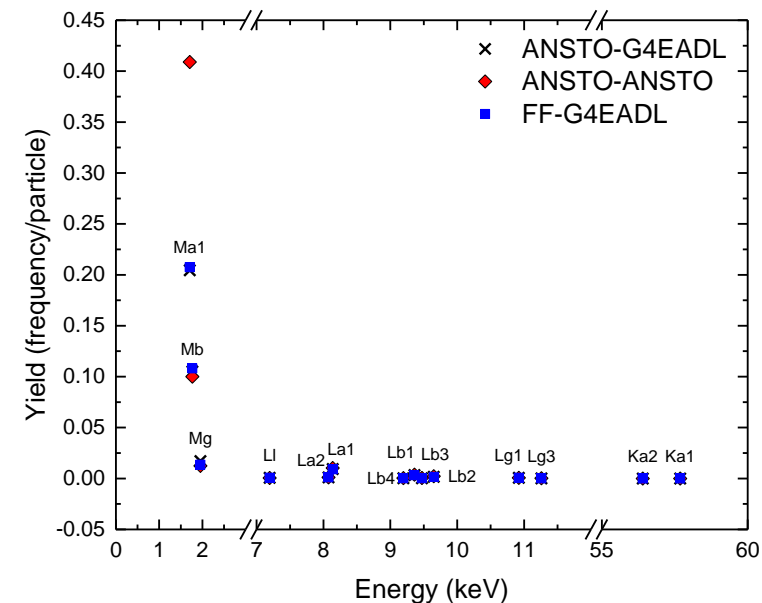


Spectrum at patient plane



X-ray fluorescence with ANSTO libraries

- S. Bakr, J. Archer, A. Rosenfeld, D.D. Cohen, R. Siegele, S. Incerti, V. Ivanchenko, A. Mantero, S. Guatelli
- ionisation cross-sections:
 - Based on Form Factor (Taborda K, L, M 2011-2013)
 - ANSTO PIXE cross section (next public release)
- Transition probabilities:
 - EADL
 - ANSTO-fluo
 - D. D. Cohen, J. Crawford, and R. Siegele, "K, L, and M shell datasets for PIXE spectrum fitting and analysis," Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms, vol. 363, pp. 7–18, 2015.
 - Data library of ANSTO with the same format of EADL (G4EMLOW7.7/fluo)
 - The same binding energies of EADL are adopted
 - The radiative transition probabilities reported in the EADL were calculated according to Hartree Slater (HS) methods, however [Cohen et al 2015] recommends the Hartree-Fock approach for M shell



ANSTO-ANSTO: ANSTO cross section with ANSTO transition probabilities

FF-G4EADL: Form Factor cross sections with EADL (Geant4)

ANSTO-G4EADL: ANSTO cross sections with EADL