

SUMMARY OF EM PARALLEL SESSION

L. Pandola

INFN – Laboratori Nazionali del Sud
on behalf of the EM working group

EM parallel sessions, Sep 17th

- **Two blocks**, to make an easier life across time zones!

09:00	Reconfiguration of G4LowEPPysics for low energy polarised X-/gamma ray transport applications	Jeremy Brown	09:00 - 09:20
	Updates on PIXE	Samer Bakr	09:20 - 09:40
	Geant4 implementation of interference effects in X-ray coherent scattering	Gianfranco Paterno	09:40 - 10:00
10:00	Geant4-DNA datasets for ionization and excitation of liquid water by protons above 100 MeV A. Damián Domínguez Muñoz		
	Discussion about model catalogue	Vladimir Ivantchenko	10:20 - 10:50
16:00	Implementation of the EPICS2017 database for photons in Geant4	Li Zhuxin	16:00 - 16:20
	Geant4 simulation of X-ray transition radiation at small angles	Vladimir Grichine	16:20 - 16:40
	GEANT4 MicroElec module 2021 update	Christophe Inguibert et al.	16:40 - 17:00
17:00	Implementing new physics models for electrons in DNA nucleobases	Sara Zein	17:00 - 17:15
	Mesoscopic model of Water Radiolysis in Geant4-DNA	Ngochoang Tran	17:15 - 17:35

Geant4-DNA

Discussion

Geant4-DNA

Geant4-DNA

DEVELOPMENTS IN EM (STD AND LOWEN)

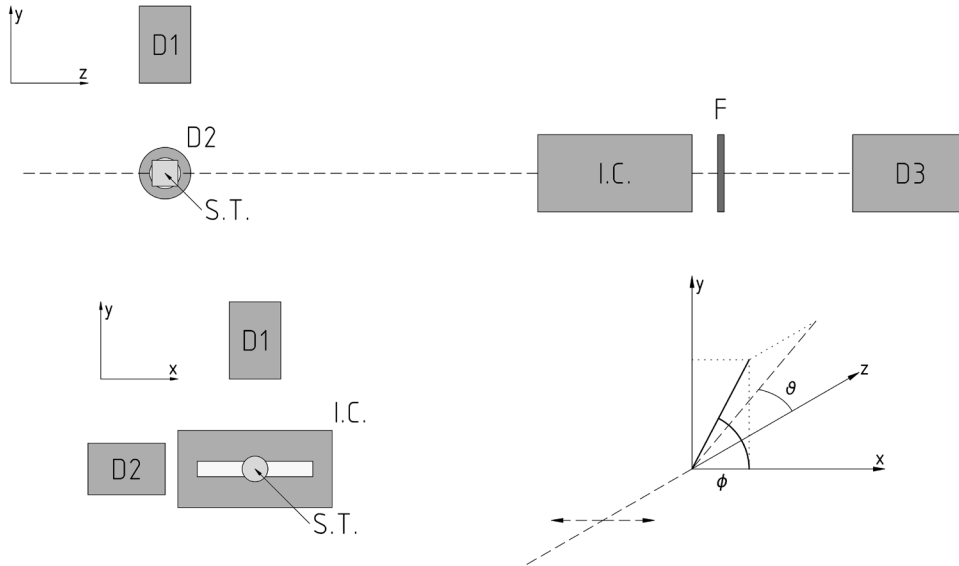
Optimized version of **G4LowEPPhysics** with polarization

Contribution by J. Brown

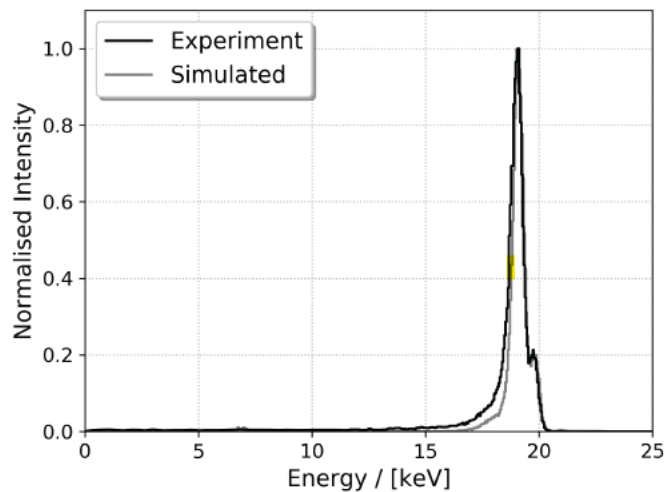
- Specialized version of the **G4LowEPPhysics** for applications with **polarized photons**
 - Electrons and positrons use **opt4**
- Tailored for **astronomy, laser sources, synchrotron**
 - **Polarized gammas, below 10 MeV**
- **Validation** against **experimental data** (SPring-8)
 - Incident x-ray energy 20 and 40 keV on different targets
 - Differences of the order of Geant4 gamma cross sections
 - **Paper on NIM B 502 (2021)**
- **Goal: release in 11.0**
 - Future iteration: enable polarization via **G4EmParameter**

Contribution by J. Brown

Validation

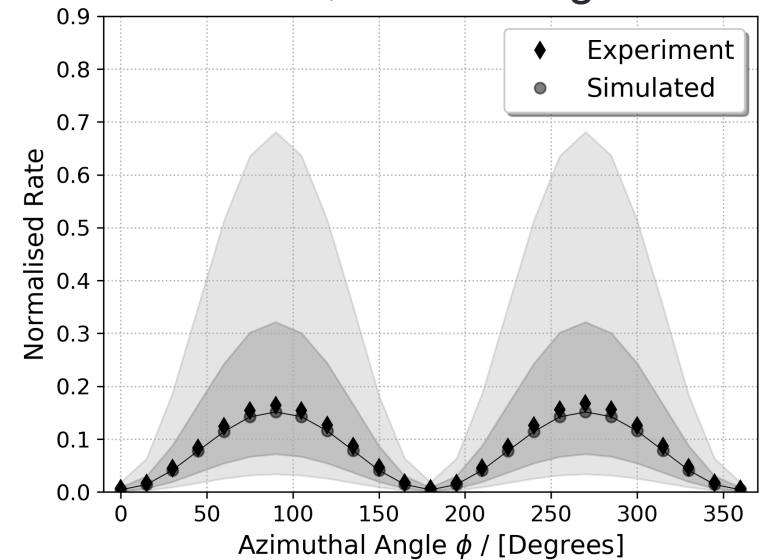


20 keV,
7 mm target

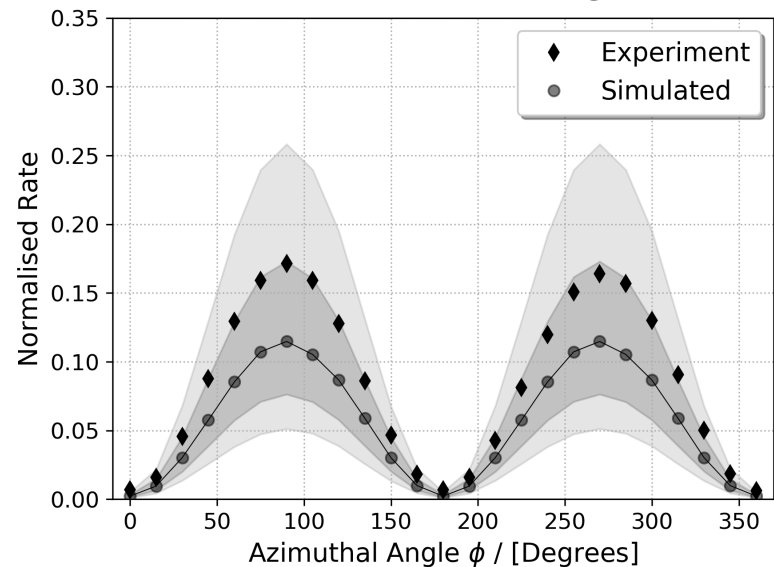


$\phi = 90^\circ$

20 keV, 10 mm target



40 keV, 10 mm target



Updates on PIXE: G4-ANSTO

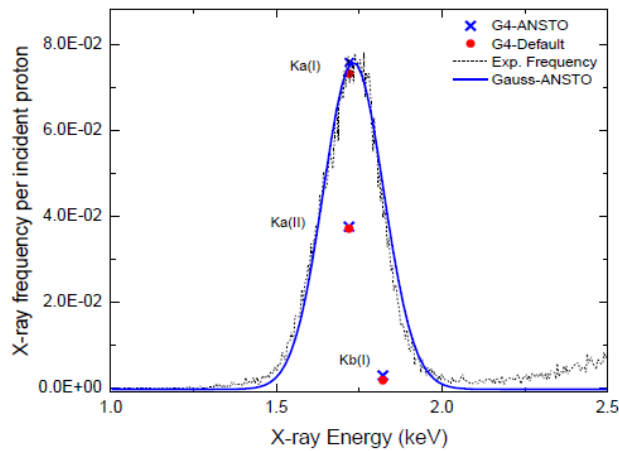
Contribution by S. Bakr

- Describes:
 - **PIXE for alpha and proton ionization** (cross sections available up to **5 MeV**)
 - **Fluorescence yields** (K, L and M shells)
 - Developed and validated by the Australian **ANSTO**
- *Alternative* to the models existing in Geant4
- Validation with **protons** (2 and 3 MeV) and **alphas** (10 MeV) on several **25μm thick targets** (Si, Ti, ...)
 - **TestEm5**
 - Good agreement against data and against G4 default
 - Relaxation using the EADL libraries (default) or the custom ANSTO-HP
 - ANSTO slightly **higher fluorescence yield**
- **Getting ready for 11.0**
 - **New data folder** in **G4LEDATA** and new set of classes in lowenergy, describing the form factors (L, K, M).
 - Extra in **G4LEDATA** → **210MB+24MB**, check if optimizing/compressing
- Paper accepted Sept 13th

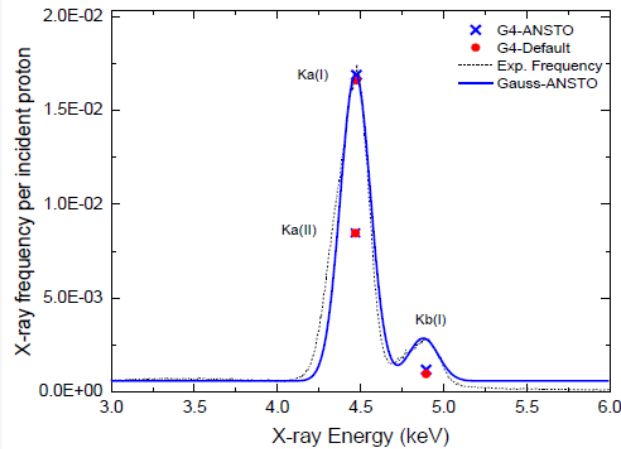
G4-ANSTO

Contribution by S. Bakr

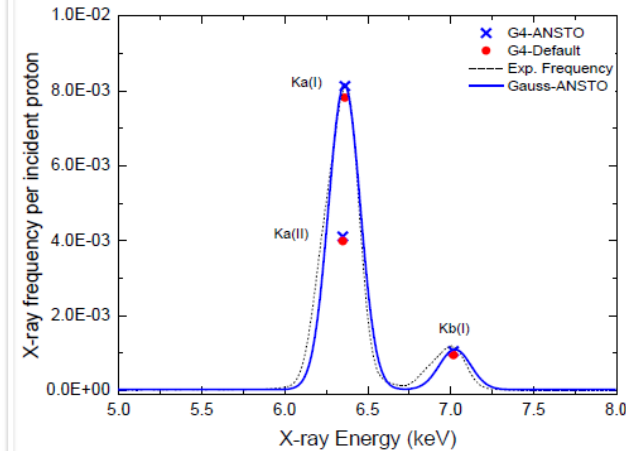
2 MeV proton Si-K, Z=14



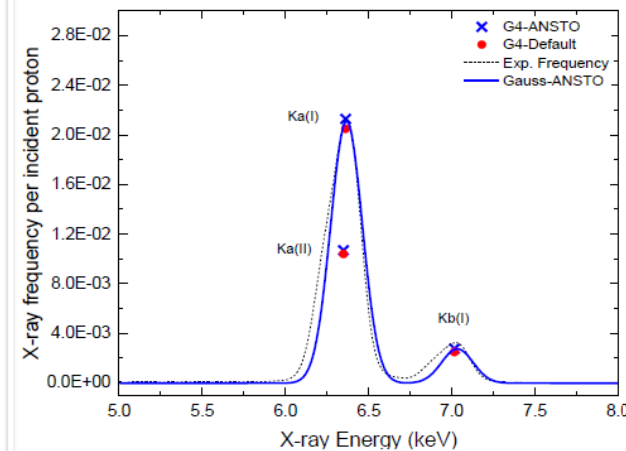
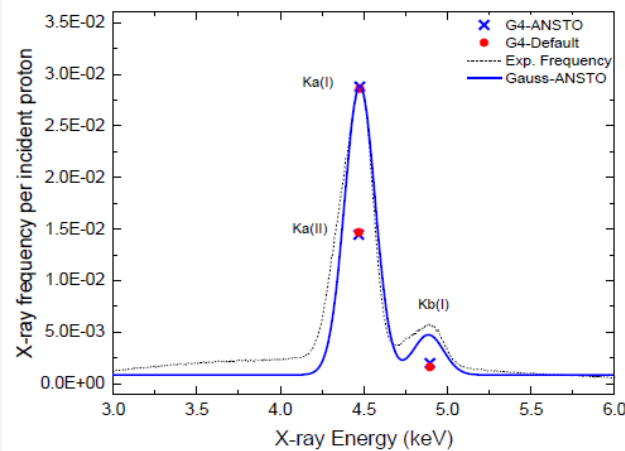
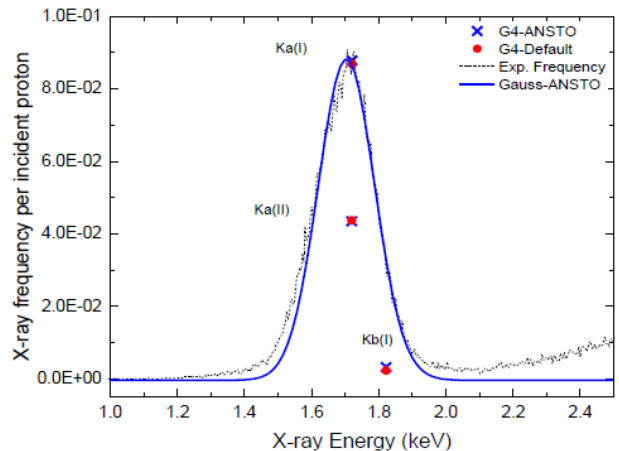
Ti-K, Z=22



Fe-K, Z=26



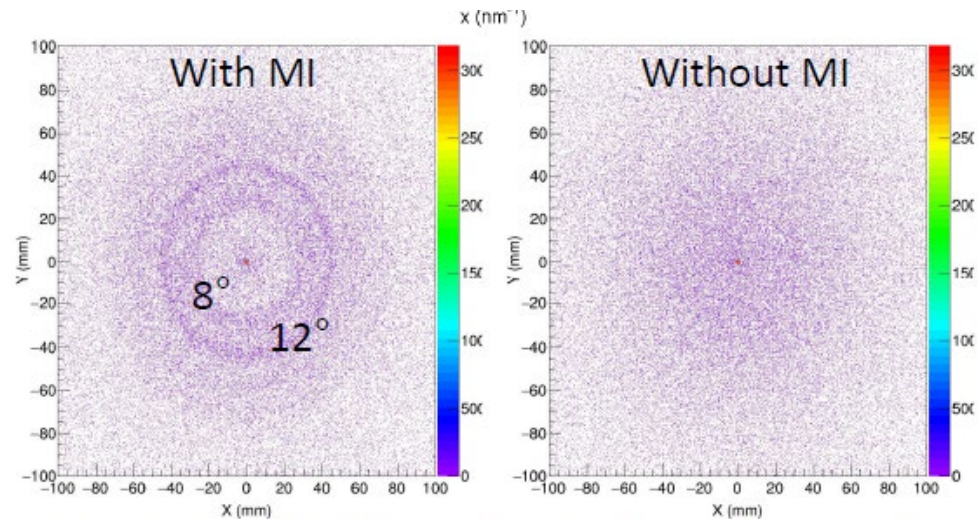
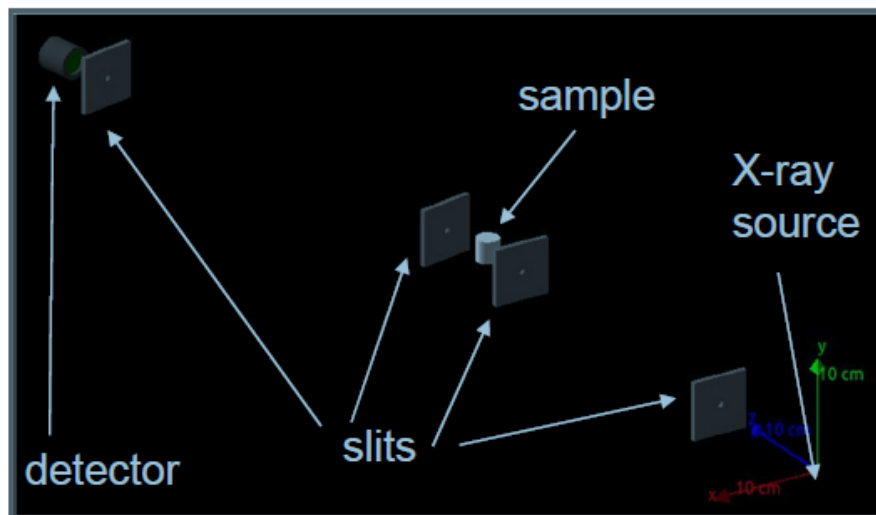
3 MeV proton



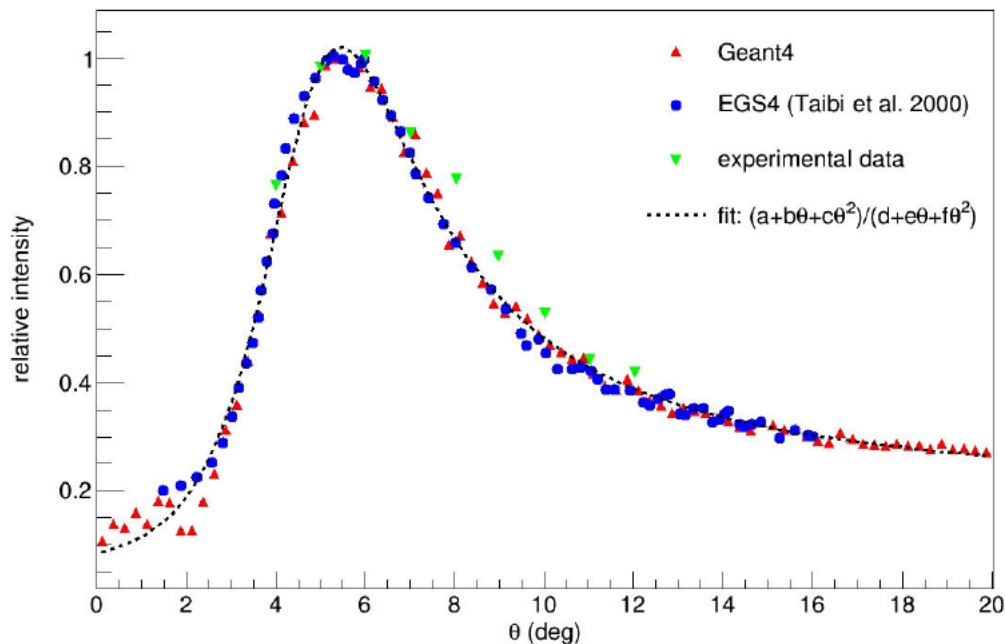
Geant4 implementation of interference effects in X-ray coherent scattering

Contribution by G. Paternò

- Implement **interference effects** in x-ray **coherent scattering**
 - Standard approach disregards possible interference effects
 - Important in **molecules** (especially of biological interest) and at **low-angles**, where coherent scattering dominates over Compton scattering
- **Modified** version of the **Penelope Rayleigh** model
 - **Form factors** can be provided as **external files**; a database of about 40 material of medical interest included in **G4LEDATA**
 - Approach of building any tissue as the **combination of four basic ingredients** (fat, water, collagen, hydroxyapatite)
- Validation against **data** and **past simulations** (EGS4)
- **Released in Geant4 10.7**
 - Functionalities shown in a **dedicated extended example** (**saxs**)
 - **Documentation** available



Scattering of a 20 keV photon beam in a **human breast** sample



Contribution by G. Paternò

Scattering of polychromatic x-rays (60 kVp and filtration of 0.5 mm Cu) from a 5 mm-thick carcinoma sample (data from Evans et al, 1991)

G. Paternò et al. Physica Medica 51 (2018) 64 -70

Implementation of the EPICS2017 database for photons in Geant4

Contribution by Zhuxin Li

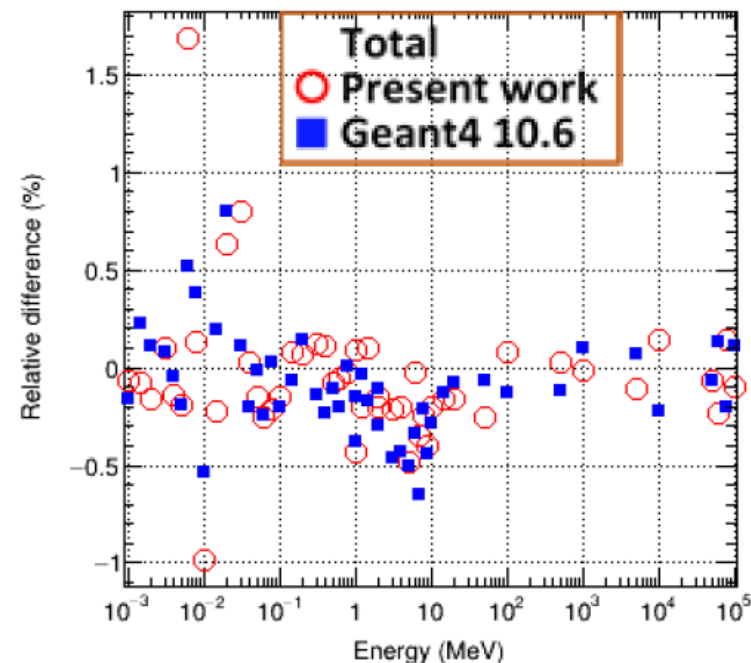
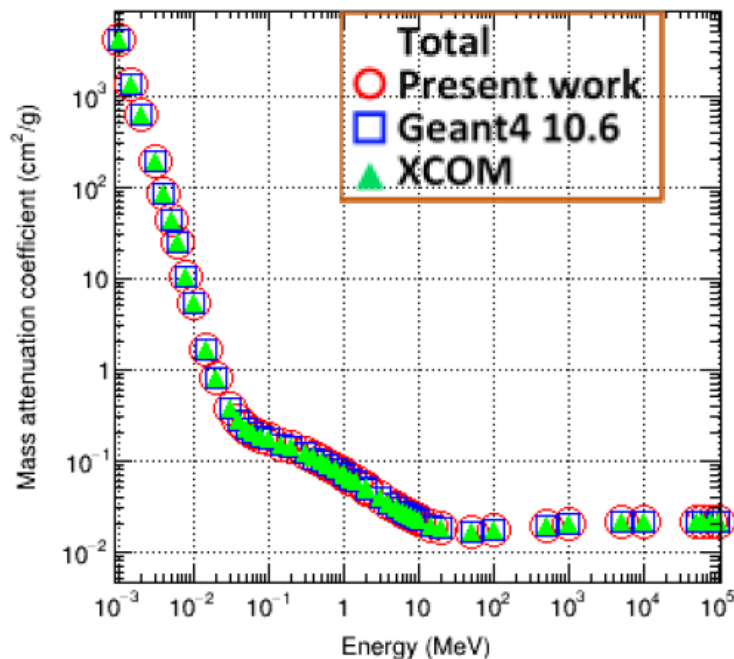
- Migration of the **cross section database** used by the Livermore gamma-ray models from **EPDL97** to **EPICS2017**
 - EPICS2017 has **more data points**, which makes the linear interpolation easier and more robust
 - Significantly **more precise** than before! (esp. low-p Compton)
- For Livermore Compton and Rayleigh models, **scattering functions/form factors** are also updated
 - Difference **up to 10%** with respect to the old version
- Comparative studies using **NIST-XCOM database** (mass attenuation coefficients)
- **Getting ready for 11.0** (GammaConversion already in **10.7**)
 - **Extra data** added in **G4LEDATA**
 - (Check if there is any *unused data* that can be removed)

Benchmarking – EPICS2017

Contribution by Zhuxin Li

Comparative study: mass attenuation coefficient

- ❑ Example: material = water, for total (all processes)
- ❑ A good agreement with XCOM data was observed



Geant4 simulation of X-ray transition radiation at small angles

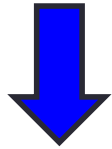
Contribution by V. Grichine

- X-ray **transition radiation** at small angles ($< 1\text{mrad}$)
- Simulation **fails to reproduce** experimental data available from **ATLAS Test Beam**
 - Electrons 20 GeV, regular radiator 30 50- μm -thick mylar foils separated by 2.96 mm air gaps
 - In particular, **peaks at low-angles** are not properly reproduced
- Problem not due to the model itself but to the **limited precision** of the **numerical integration**
 - Simulation reproduces the data if **a finer binning** is used
 - Developed a method/strategy **to adapt the binning dynamically** in order to obtain a good precision
 - Benchmark using **TestEm10**
- **Ready for 11.0**
- **XRT model** will be included in **G4EmExtra** constructor

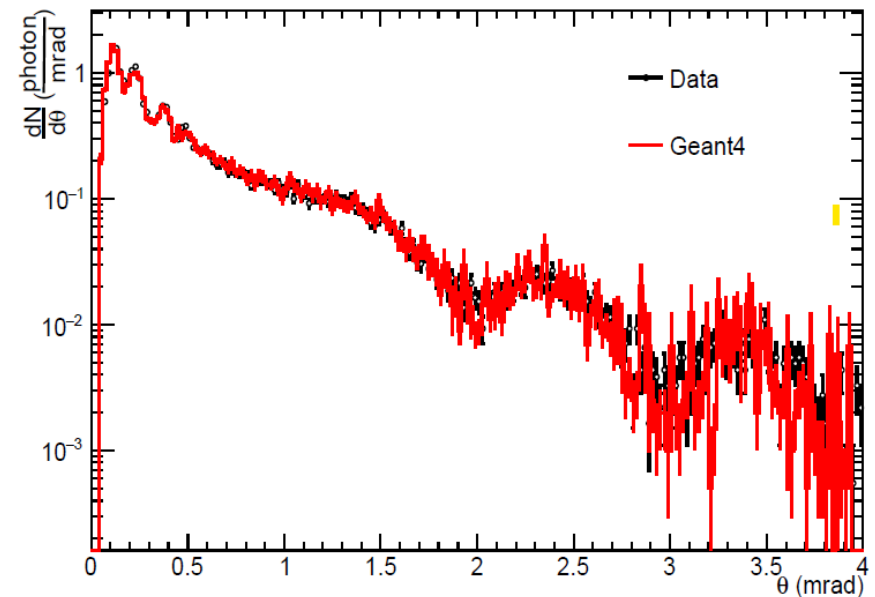
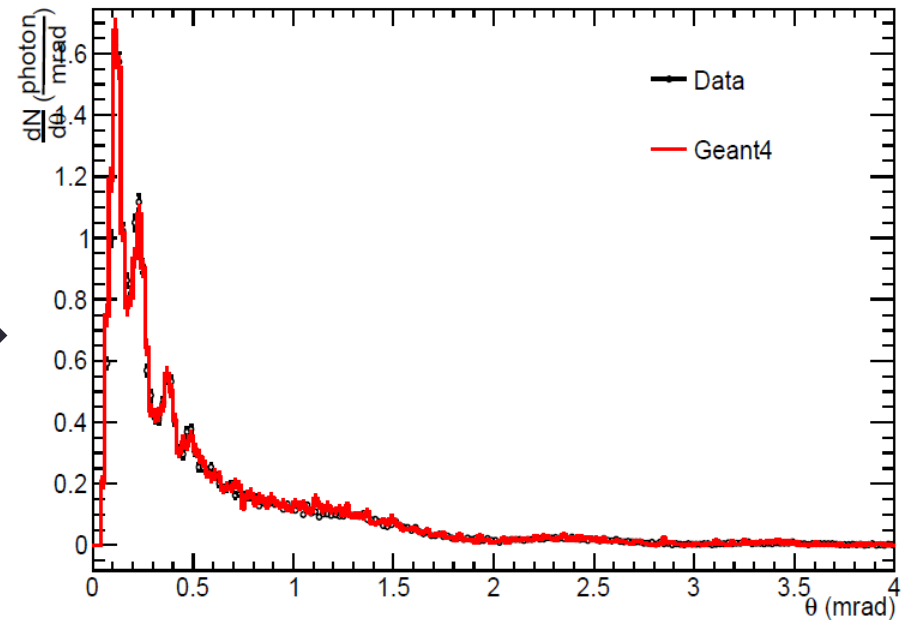
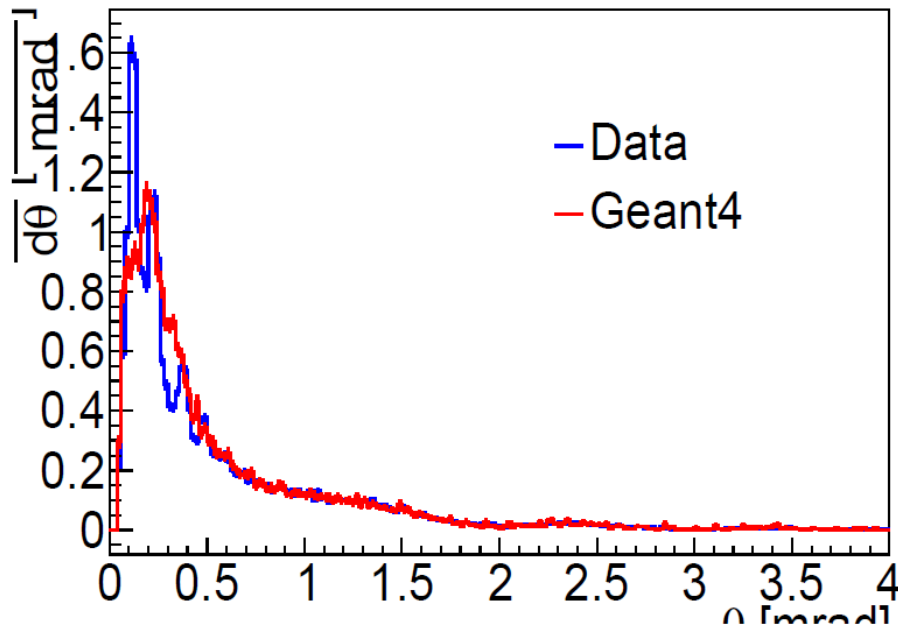
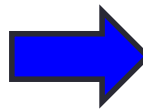
Before and after...

Contribution by V. Grichine

Before



After



GEANT4 MicroElec module 2021 update

Contribution by C. Inguibert & Q.Gibaru

- Update of **MicroElec models** (ONERA group)
 - **Cross section** on dielectric function formalism (down to **few eV e⁻** and **100 eV protons**)
 - Model extended to **16 materials** (11 already in the 11.0.beta, 5 more to come)
 - Elastic e⁻e⁻ database for 92 elements, large gaps (insulators)
- Six **validation papers**, data vs. MicroElec → **good agreement**
- A few **bugs** have been **identified**, most fixed
- **Work-in-progress for 11.0**: bug fixes, reduction of memory footprint, other improvements
- New developments (*post 11.0*):
 - 5 more materials + new examples
 - Transport of **electrons in dielectric materials**

MicroElec - Validation

Both Secondary Electron Emission Yield And Backscattering Emission Yield are Faithfully Reproduced

This work have been published in 6 papers

"Monte-Carlo simulation and analytical expressions for the extrapolated range and transmission rate of low energy electrons [10 eV - 10 keV] in 11 monoatomic materials" Q. Gibaru, C. Inguibert, M. Belhaj, M. Raine, D. Lambert
Applied Surface Science 2021

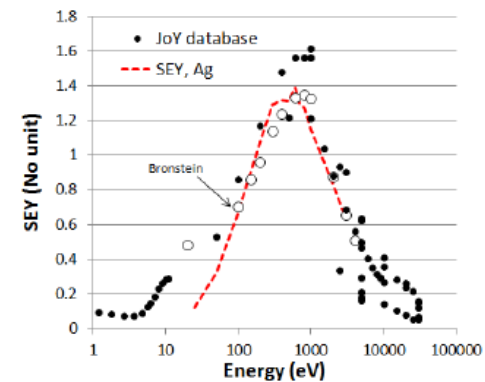
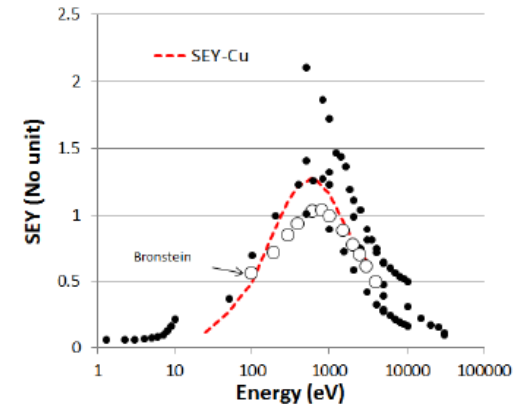
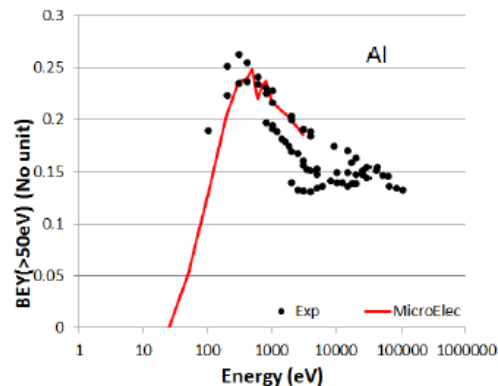
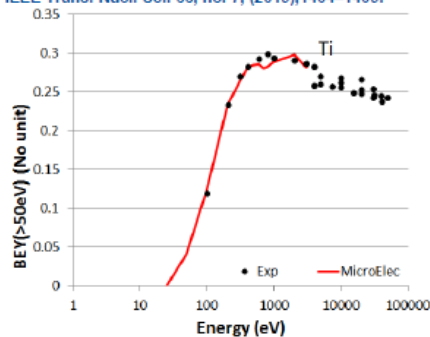
"Role of Electron-induced Coulomb Interactions to the Total SEU Rate during Earth and JUICE Missions" P. Caron, C. Inguibert, L. Artola, N. Baloon, R. Ecoffet
IEEE Trans. Nucl. Sci. 68, no. 8, (2021), 1607–1612.

"Geant4 physics processes for microdosimetry and secondary electron emission simulation: Extension of MicroElec to very low energies and 11 materials (C, Al, Si, Ti, Ni, Cu, Ge, Ag, W, Kapton and SiO₂)"
Q. Gibaru, C. Inguibert, M. Belhaj, J. Puech, M. Raine Nucl. Instr. And Methods 487, (2021), 66-77.

Surface ionizing dose for space application estimated with low energy spectra going down to some hundreds of eV"
C. Inguibert, P. Caron, Q. Gibaru, A. Sicard, N. Baloon, R. Ecoffet IEEE Trans. Nucl. Sci. 68, no. 8, (2021), 1754–1763.

"New SEU modeling method for calibrating target system to multiple radiation particles" P. Caron, C. Inguibert, L. Artola, F. Bezerra, R. Ecoffet
IEEE Trans. Nucl. Sci. 67, no. 1, (2020) 1558–1578.

"Physical Mechanisms of Proton-Induced Single-Event Upset in Integrated Memory Devices" P. Caron ; C. Inguibert ; L. Artola ; R. Ecoffet ; F. Bezerra
IEEE Trans. Nucl. Sci. 66, no. 7, (2019), 1404–1409.



DEVELOPMENTS IN EM (GEANT4-DNA)

Geant4-DNA datasets for ionization and excitation of liquid water by p above 100 MeV

Contribution by D. Dominguez

- Goal: extension of **G4DNAExcitation** and **G4DNAIonisation** for protons to energies **above 100 MeV**
 - Models currently **limited to 100 MeV**
 - Interest in clinical beams **up to 250 MeV**
- **New models** and **data** to cover the region **100-300 MeV**
 - **New cross section dataset** (excitation and ionization) **calculated** from theory (integration of double-differential shell cross sections) and **implemented**
- **Validation**
 - experimental **water vapour** data (< 10 MeV)
 - **stopping power** data (ICRU) and **range** (*no data* at high energy)
- **Getting ready for 11.0** (code & data)
 - Future developments: alphas and hydrogen

Models: development & validation

Contribution by D. Dominguez

DDCS

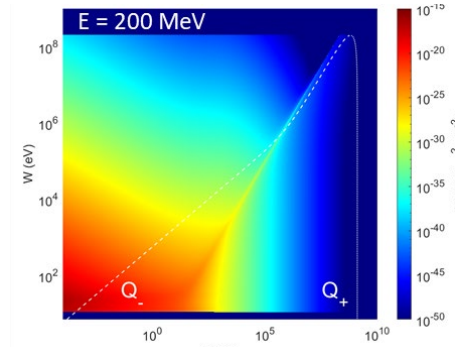
Doubly differential cross section

$$\frac{d^2\sigma}{dWdQ} = \frac{2\pi Z_P^2 e^4}{m_e c^2 \beta^2} \left\{ \frac{2m_e c^2}{WQ(Q + 2m_e c^2)} + \frac{2m_e c^2}{[Q(Q + 2m_e c^2) - W^2]^2} \left[\beta^2 - \frac{W^2}{Q(Q + 2m_e c^2)} \right] \right\} \frac{df(Q, W)}{dW}$$

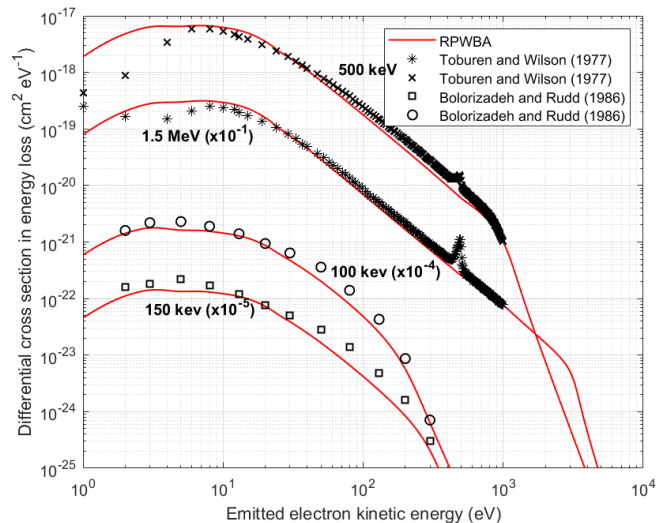
Generalized oscillator strength (GOS)

Response of the material

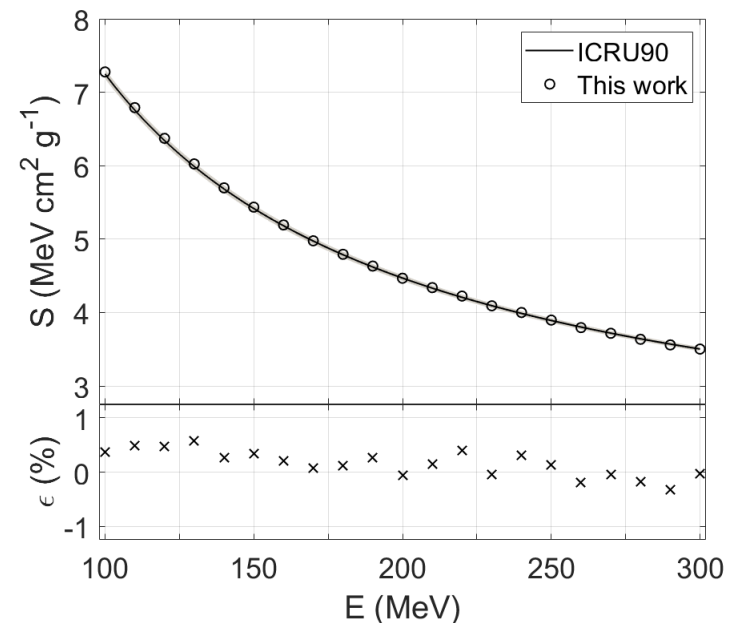
$$\frac{df(Q, W)}{dW}$$



Ionization differential cross section in emitted electron energy



spower example



Implementing new physics models for electrons in DNA nucleobases

Contribution by S. Zein

- Goal: Extend **EmDNA_option6** with **electron interactions** in **water** and **DNA** materials
 - follow approach of **CPA100** code
 - elastic scattering, excitation, ionization (**11 eV - 1 MeV**)
- Testing with examples **spower**, **range** and **mfp** (stopping power, range, inelastic mean free path) and **data** compared **against literature**
- Getting ready for the **June 2022 release**
 - (If tests and validation are completed)

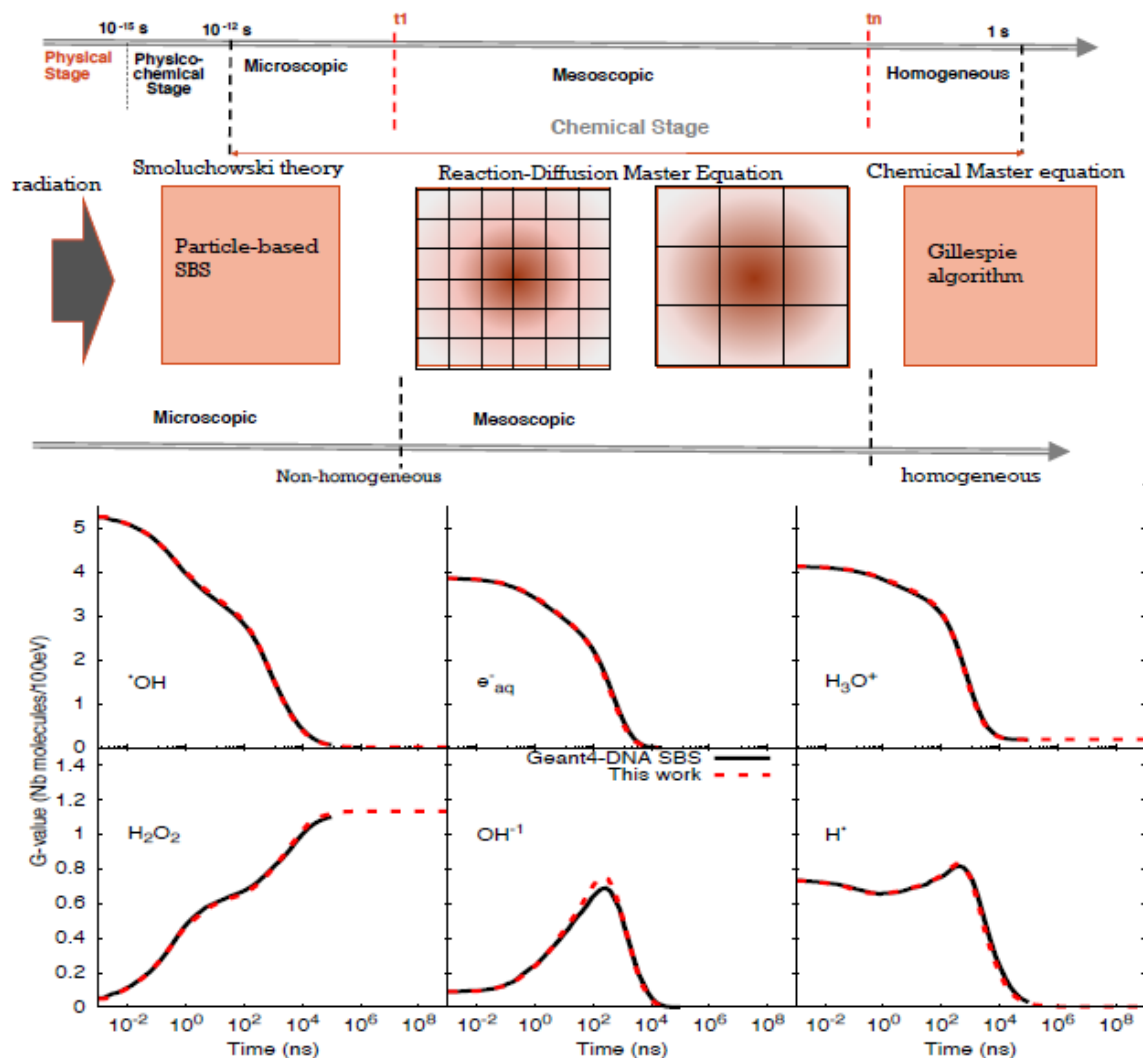
Mesososcopic model of Water Radiolysis in Geant4-DNA

Contribution by N. H. Tran

- **DNA-chemical stage** (important for a number of recent applications, e.g. flash radiotherapy)
 - Need to account for **secondary interactions** over a long time (**1 μ s**)
- Geant4-DNA: Step by Step (SBS) and Independent Reaction Time (IRT) methods \rightarrow *CPU-intensive*
- Test and validate a **Compartment-Based-Model (CBM)**
 - Uses Reaction-Diffusion Master Equation and is **much faster** (factor of 10-1000)
 - Need the **combination of the SBS model** with the **compartment-based model**, and to adapt the size of the **voxel size**
- Stepping algorithm updated
- **Work in progress** to release a **prototype in 11.0**

Validation and benchmarking

Tran et al., Int. J. Mol. Sci. 2021, 22



Contribution by
N. H. Tran