SUMMARY OF SESSIONS 1A & 2A

L. Pandola
INFN – Laboratori Nazionali del Sud
on behalf of the EM working groups

Session 1A: New EM physics models

- D. Bernard, New 5D gamma conversion model
- A. Alkin, New model of 3-gamma annihilation
- S. Dosatsu, Model for simulation of gold nanoparticles
  - Talking given by I. Kyriakou
- S. Guatelli, New PIXE cross sections and validation of Auger electrons

G4BetheHeitler5DModel: a new 5D gamma conversion model

Slide from D. Bernard

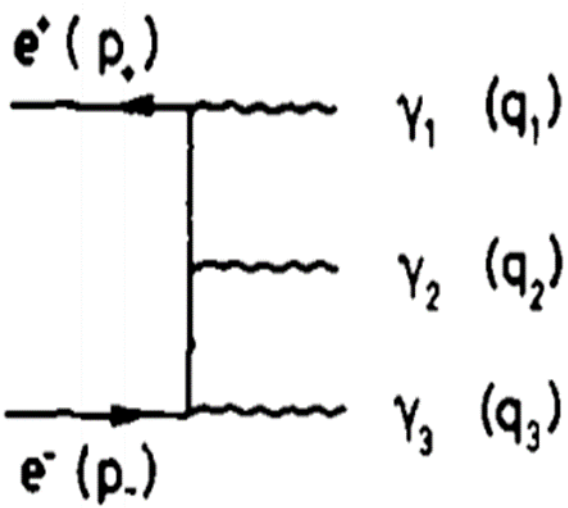
- First physics model that samples the exact (5D) Bethe-Heitler differential cross section
  - Exact target-recoil-momentum distribution
  - Exact (linear) polarisation asymmetry
  - Strict energy-momentum conservation
- G4EmLowEPPhysics (E < 80 GeV)
  - Inherits total cross section from G4BetheHeitlerModel
  - We provide **`SampleSecondaries()`**
- Generator parameters
  - Isolated charged target (no screening) / target in atom (e^- field screening)
  - Polarised (photon polarisation vector zero) or non-polarized (not zero) conversion
  - Pure nuclear / pure triplet / natural (Z / 1) mixture conversion.
- Nucl. Instrum. Meth., A 899 (2018) 85

Geant4 simulation of positron annihilation into 2 and 3 gamma

Slide from A. Alkin

- Andrei Alkin, CERN summer school student, Lomonosov Moscow State University
- Supervisor: V.N. Ivanchenko, Tomsk State University & CERN

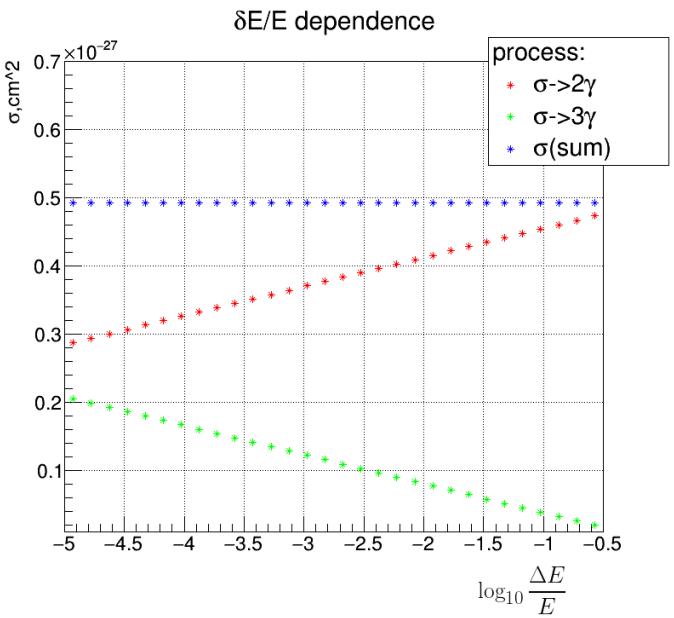
- 3γ-annihilation process at high energy affects high energy shower shape in EM and hadronic calorimeters
- 3γ-annihilation process at rest affects simulation for positron tomography
- This process may provide background for search of light dark matter particles



Current status

Slide from A. Alkin

- The smaller the ΔE-threshold - the greater the proportion of events with 3γ
- Total cross-section remains const



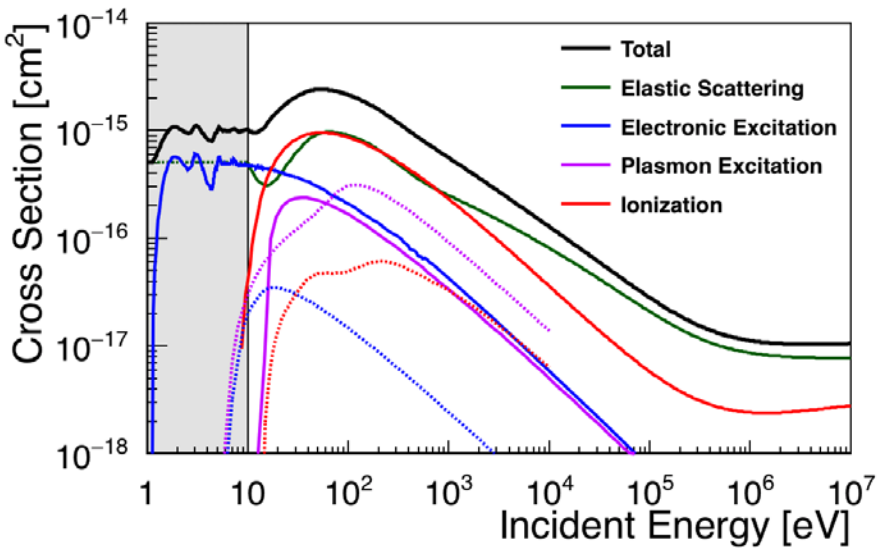
A method of introducing the 3γ-annihilation of electron-positron pair as a next to leading order correction to 2γ-annihilation is proposed.

The 1st version of the model class and unit test to study cross section and final state generation are available.

We plan to deliver new model for Geant4 10.5.

2018 Electron physics models for Gold

Slide from S. Dousatsu



Total cross sections of **Di-Electric**
Theory is shown in **dashed line**.

Physics	Model	
Elastic	PWA (ELSEPA)	10 eV – 1GeV
Ionization	**Di-Electric** Relativistic BEB-V	10 eV – 10 keV 10 keV – 1 GeV
Excitation	**Di-Electric** Exp. +Dirac B-spline RM	10 eV – 10 keV 10 keV – 1 GeV
Plasmon Excitation	**Di-Electric** Quinn	10 eV – 10 keV 10 keV – 1 GeV
Bremsstrahlung	Seltzer and Berger Model	10 eV – 1GeV

Energy Range of the di-electric models
10 eV < E < 10 keV

Summary

Slide from S. Dousatsu

(1) New alternative Geant4-DNA physics models based on Di-Electric theory **have been implemented**.

(2) Electron Physics models for GNP have been improved on **stopping power**.

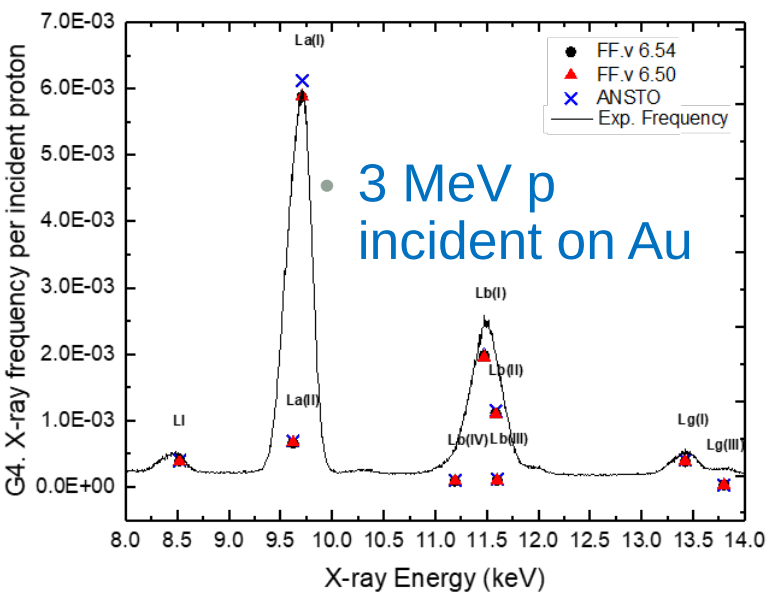
(3) The new DE physics models **demonstrate high dose enhancement** around Au-nanoparticles below 10 um from GNP center.

(4) GS MSC model shows high back-scattering in macroscopic volume, but not in microscopic volume.

PIXE Ionisation Cross Sections

Slide from S. Guatelli

- ANSTO ECPSSR theory
  - Plane wave Born Approx, with corrections for energy loss, Coulomb deflection of the projectile, perturbed stationary states of the target atoms, relativistic nature of the inner electrons
  - Tabulated in Cohen & Harrigan, At. Data Nucl. Data Tables 33 (1985) 255.
  - Agreement with experimental data
    - Few % for K-shell, 5-15% for L-shell, 10-50% for M- shell
- Implemented in Geant4 PIXE module for protons and alpha particles



- 3 MeV p incident on Au

Next step:

- Include ANSTO cross section for carbon ions

  The use of the ANSTO ECPSSR for ions heavier than α particles is more accurate than using $\sigma_{ion}(E)=Q^2\cdot\sigma_p(E\cdot M_p/M_{ion})$
- Validate against experimental measurements at ANSTO

Next stage: Implement recommended approach for X-ray emission

Slide from S. Guatelli

Recommended in Cohen DD, Crawford J, Siegele R. K, L, and M shell datasets for PIXE spectrum fitting and analysis. NIM B. 2015, 363, pp. 7-18.

W_K: Krause(1979), based on experimental measurements

W_L: Campbell (2003) and (2009)

W_M: Dirac Fock theoretical data

K and L shell emission rates: Salem (1974)

M shell emission rate: Dirac Fock theoretical data set. Compilation of Chauhan and Puri – At. Data nucl. Data Tables 94(2008) 38-49

C-K transitions: Chauhan and Puri – At. Data nucl. Data Tables 94(2008) 38-49

$$^{1}\sigma^{X}_{L_p} = \sigma^{I}_{1}\omega_1 \frac{\Gamma_{L_p}}{\Gamma_{L_1}}$$

$$^{2}\sigma^{X}_{L_p} = (\sigma^{I}_{1} f_{12} + \sigma^{I}_{2})\omega_2 \frac{\Gamma_{L_p}}{\Gamma_{L_2}}$$

$$^{3}\sigma^{X}_{L_p} = (\sigma^{I}_{1}(f_{12}f_{23} + f_{13} + f'_{13}) + \sigma^{I}_{2}f_{23} + \sigma^{I}_{3})\omega_3 \frac{\Gamma_{L_p}}{\Gamma_{L_3}}$$

Still to understand which approach to adopt

Validation of Auger e- emission w.r.t. exp. results and theoretical data

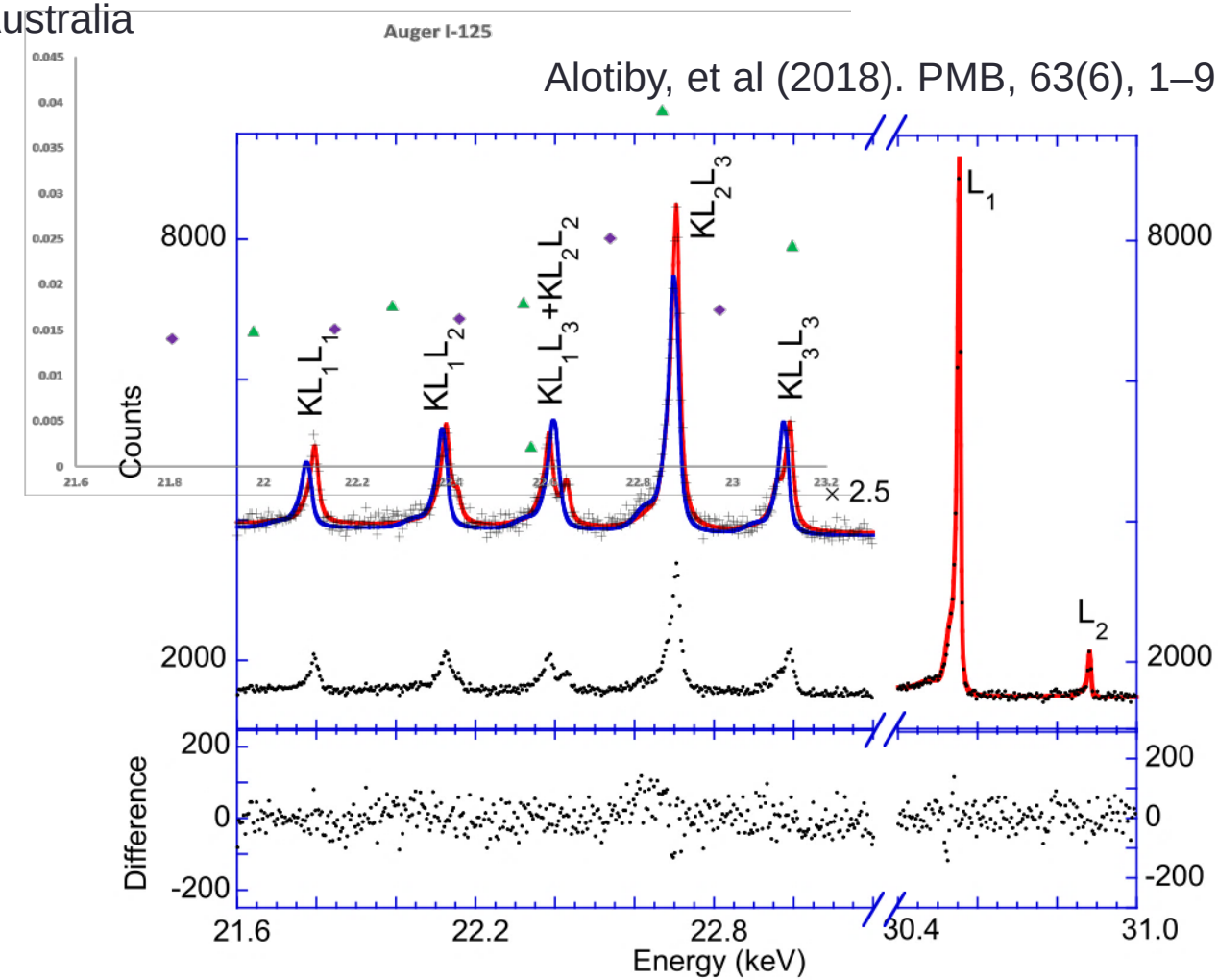
Slide from S. Guatelli

Authors: S. Bakr and S. Guatelli, CMRP, University of Wollongong
T. Kibedi, ANU, Canberra, Australia

Alotiby, et al (2018). PMB, 63(6), 1–9.

~0.15 keV shift observed for EADL/Geant4

Initiated discussion with Vladimir and Marilena



Session 2A: New EM validation results

- I. Kyriakou, Geant4 low-energy models for electron transport in liquid water X
- M. Omer, New low energy elastic model for gammas
- M.C. Bordage, CPA100 models for Geant4-DNA
- S. Guatelli, Validation of the Geant4 EM physics for modelling high energy synchrotron beamlines

Geant4 low-energy models for electron transport in liquid water

Slide from I. Kyriakou

Ioanna Kyriakou, Univ. of Ioannina, Greece and co-workers

- Systematic comparison of the available EM physics models of Geant4 (**Standard Opt4, Livermore, Penelope, Geant4-DNA Opt4**) for the simulation of low-energy electron tracks in liquid water
- Simulations of penetration and dose-point-kernel (DPK) for electrons with initial energy from 100 eV to 10 keV
- Investigation of the effect of tracking (and production) cut and the step-size limit in the condensed-history models

Slide from I. Kyriakou

Summary of main results

- For sub-keV electrons differences between the condensed-history models (Standard Opt4, Livermore, Penelope) and the DNA (Opt4) model are significant (up to ~100% or more); differences become negligible above 5-10 keV
- Livermore has the best agreement with DNA (Opt4) and it is the most stable to step-size variations
- Increasing the tracking (and production) cut from 10 eV to 100 eV for speeding up the simulation can be safely used for electrons above 1 keV
- **Main suggestion**: It is worth using Livermore ionization for electrons below 1 MeV in Standard Opt4 EM physics instead of Penelope.

JAEA Elastic Scattering Model

Slide from M. Omer

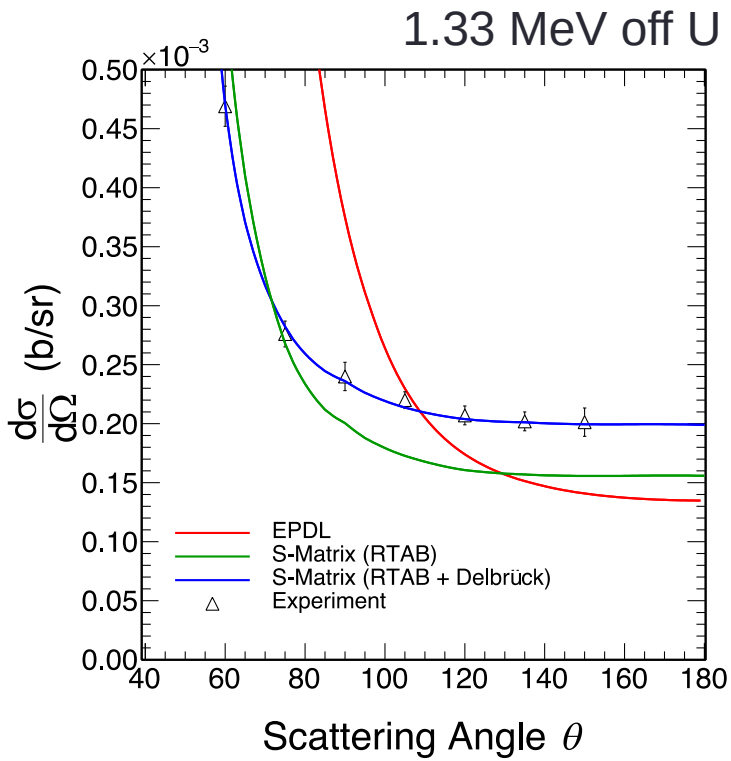
- A new alternative model for G4RayleighScattering improving accuracy of gamma-ray elastic scattering up to 3 MeV.
- Main Improvements:
  - Including the QED nonlinear effect (Delbrück scattering) for the first time.
  - Use the scattering matrix cross section for Rayleigh scattering, much more accurate than the form factor approximation based on evaluated photon data library (EPDL).
  - Handle the interference among all scattering mechanisms.
  - Fix the inconsistency of angular distribution at large scattering angles and high Z elements.
  - Much better agreement with experimental data.

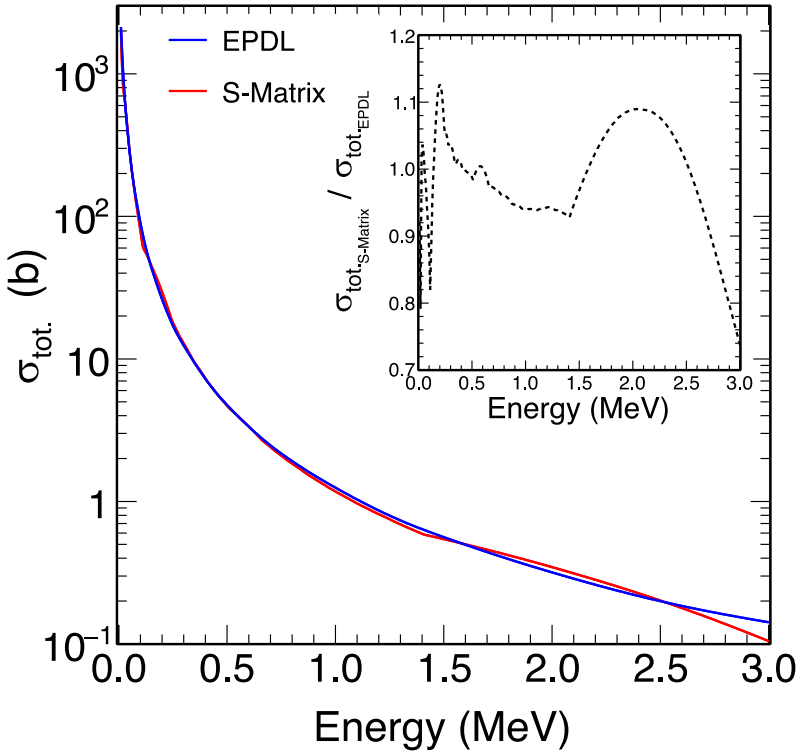
Nucl. Instrum. Meth. B 405 (2017) 43.

JAEA Elastic Scattering Model

Slide from M. Omer

- Rayleigh scattering cannot account for the elastic scattering measured experimentally
- Total cross section is changed by adding Delbrück scattering.
  - The change is up to 20% at 3 MeV.
- Reasonable computational performance with much better accuracy



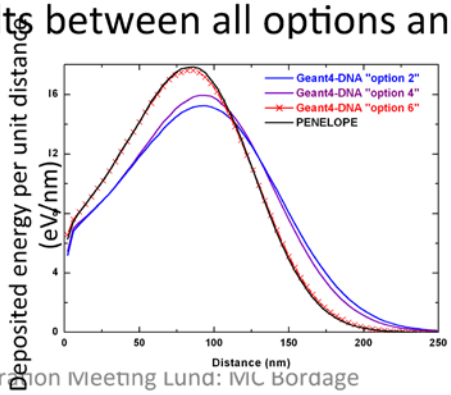


CPA100 models for Geant4-DNA

Slide from M. C. Bordage

- Impact of physics models (option2, option4, option6 (=CPA100 models) in H_2O on the calculations of
  - basic quantities (11 eV – 250 keV)
    - Number of interactions: big differences in the number of excitations
    - ranges: smallest with option6
  - dosimetric quantities (and comparisons with Penelope code in track-structure version).
    - DPK: option6 gives less diffusion
      - Low energy: good agreement between option6 and Penelope
      - High energy: close results between all options and Penelope

2 keV



CPA100 models for Geant4-DNA

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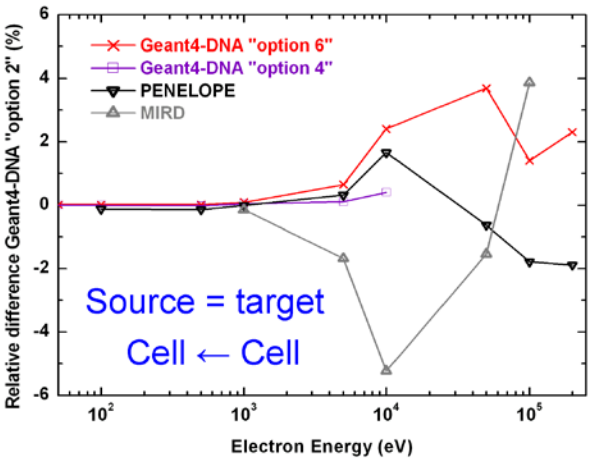
- Impact of physics models (option2, option4, option6 (=CPA100 models) in H_2O on the calculations of

  - dosimetric quantities (and comparisons with Penelope code in track-structure version).

    - S-value (comparison also with MIRD reference data)
      - Monoenergetic electrons
      - Auger emitters

✓ Differences are function, not only of the incident energy but mainly of the configuration source-target.

✓ Important differences are observed with MIRD data.



- Electron interaction physics models in the 4 DNA bases (preliminary results) for elastic scattering and ionization

Validation of the G4 EM physics for modelling high energy synchrotron beamlines

Matthew Cameron, Andrew Dipuglia, Dr. Susanna Guatelli, Dr. Jeremy Davis, Assoc. Prof. Michael Lerch

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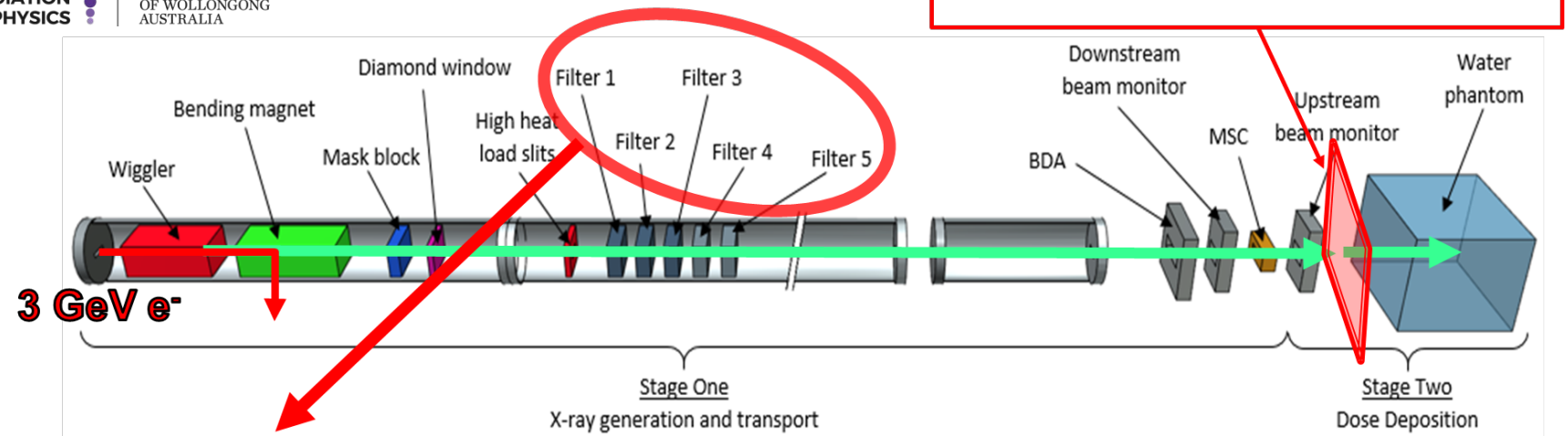
Slide from S. Guatelli

Phase Space Position, Momentum, Polarisation, Energy, Weighting



	High Dose Rate (HDR)	Medium Dose Rate (MDR)	Low Dose Rate (LDR)
Filter 1	C (0.45 mm)		
Filter 2	C (1.49 mm) 45°		
Filter 3	C (10 mm) 45°		
Filter 4	Al (2 mm) 45°	Cu (1 mm) 45°	Al (2 mm) 45°
Filter 5	Cu (1 mm) 45°	Cu (1 mm) 45°	Mo (2 mm) 45°

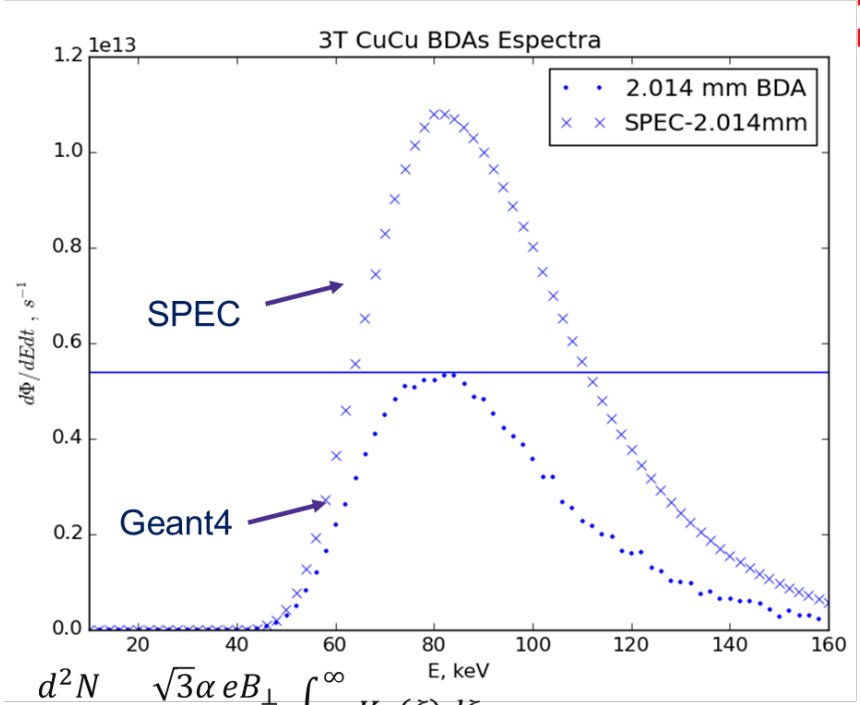
Livermore Polarised Physics, Geant4 9.6.patch4

Absolute comparison

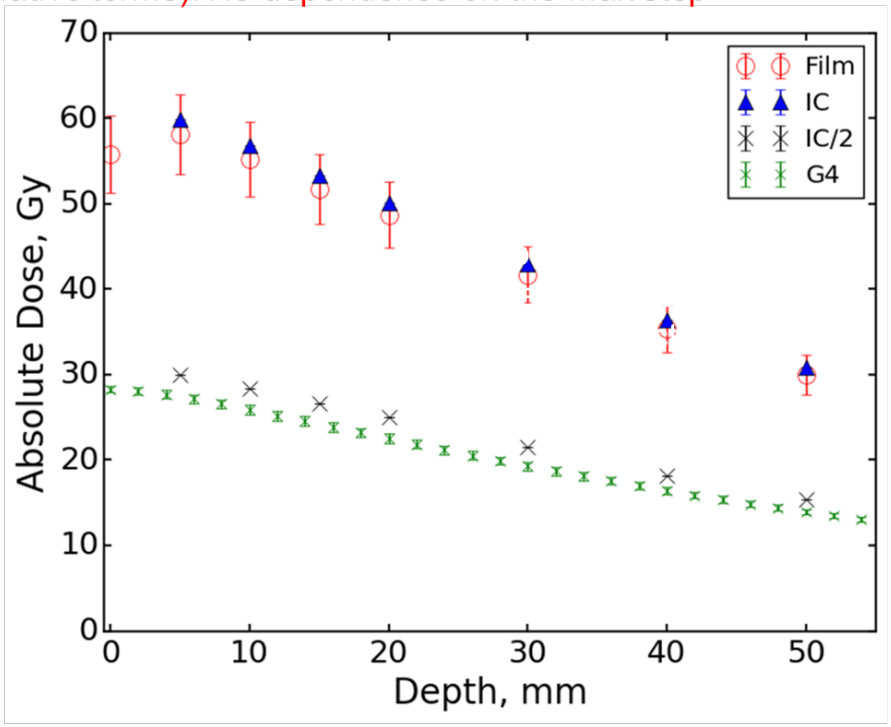
Slide from S. Guatelli

- Geant4.10.2.p02, G4EMLivermorePolarisedPhysics
- Wiggler model: G4SinusoidalMagField in laboratory vacuum

We get a discrepancy of about ~50% when comparing to reference data in absolute terms (good agreement in relative terms). No dependence on the max step



$$\frac{d^2N}{dsdx} = \frac{\sqrt{3}\alpha}{2\pi}\frac{eB_\perp}{mc}\int_x^\infty K_{\frac{5}{3}}(\xi)d\xi$$



Comparison of photon fluence to SPEC, Stevenson et al. 2017 J. Sync. Rad. 24, pp. 110-141.

Comparison to in-house experimental measurements