On the recent DPWA-DCS based Geant4 model for Coulomb scattering

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Outline

Contents

Motivation:

- very accurate *Differential Cross Section* (DCS) for Coulomb scattering of e^-/e^+ on *free atoms* can be computed by using *Dirac Partial Wave Analysis* (DPWA) (using the proper scattering potential; see next slides)
- while these DCS could provide the basis for the most accurate, general (i.e. for all material as long as using the simply additivity rule on the *free atom* DCSs is appropriate) description of the elastic scattering down to very low energies (see later)
- there was no model in `Geant4` (before version `10.7`) making use of these accurate DCSs or could provide similar accuracy (in general)
- I always wanted to implement such a model in `Geant4` to provide a baseline for other e^-/e^+ Coulomb scattering models with more limited precisions (e.g. those based on an exponentially screened Coulomb potential and applying the first Born approximation)

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Relativistic, screened-Rutherford DCS (DCS_{SRF}): (`Geant4` SS; the base GS-MSC)

- scattering of **spinless** e^-/e^+ on **exponentially screened**, **point like Coulomb potential**
- solution of the **relativistic Schrödinger equation** (Klein-Gordon equation) for **spinless** e^-/e^+ under the **first Born approximation**
- simple **analytical DCS** with a single (screening)parameter, efficient angular deflection generation
- limited accuracy

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Mott DCS (DCS_{Mott}):

- scattering of e^-/e^+ on **unscreened**, **point like Coulomb potential**, accounting **spin effects**
- solution of the **Dirac equation** with a point like (unscreened) scattering potential: relativistic Dirac-Coulomb Partial Wave Analysis
- numerical solution i.e. **numerical DCS**
- relatively **accurate** (still point like nucleus) **at higher scattering angles** (that corresponds to close interactions) where the screening is less important
- **less accurate at lower scattering angles** (that corresponds to far interactions) where screening of the potential of the nucleus by the atomic electrons becomes very important

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Combination of these ($DCS_{Mott/RF\times SRF}$): (Mott correction to `Geant4` SS and GS-MSC)

- assume factorisation of the different effects and form the *Mott* to *Rutherford* ratio (both scattering on pure i.e. not screened point potential) and correct the screened Rutherford DCS with this: **includes both spin-relativistic(Mott) and screening(exponential) effects in an approximate way**
- while gives better results compared to any of the above (i.e. better than DCS_{Mott} or DCS_{RF} or DCS_{SRF}), it is still not accurate
- **inaccurate at low scattering angles** where screening by the atomic electrons is important: more accurate than exponential screening is needed
- **inaccurate at lower energies** where the different effects cannot be factorised (especially for higher Z atoms)
- better but still limited accuracy

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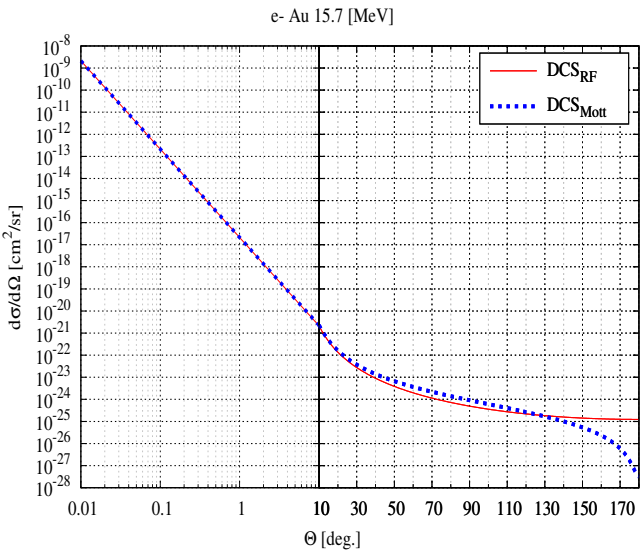

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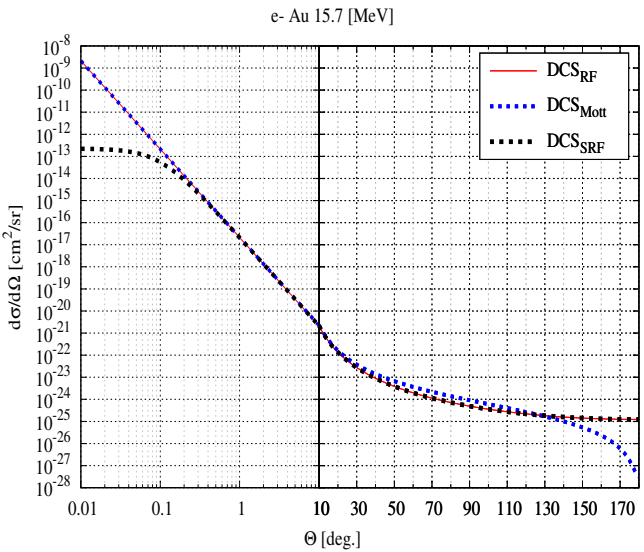

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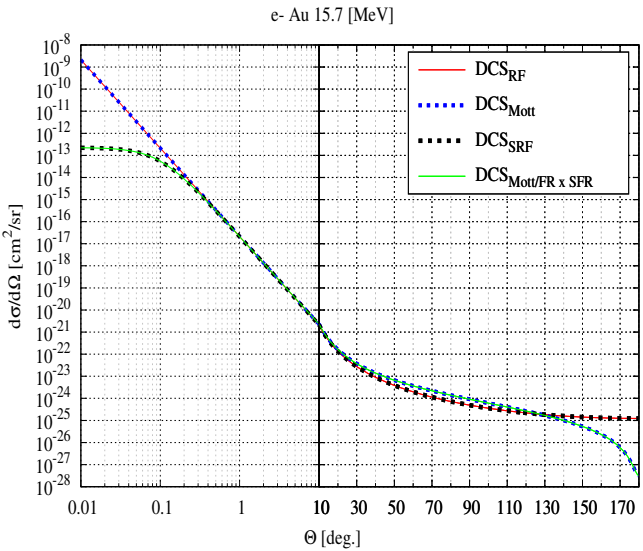

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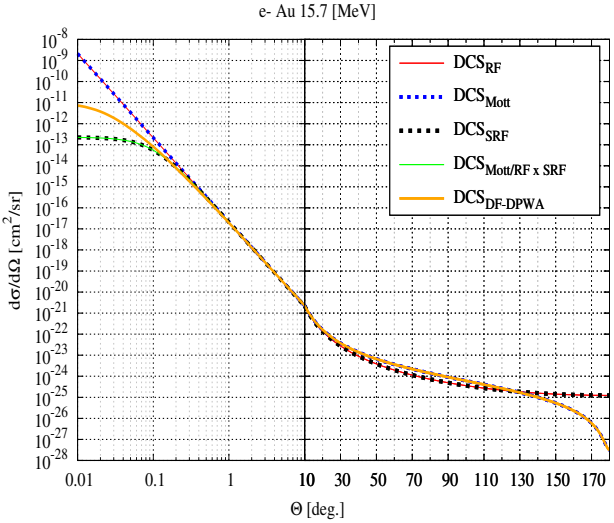

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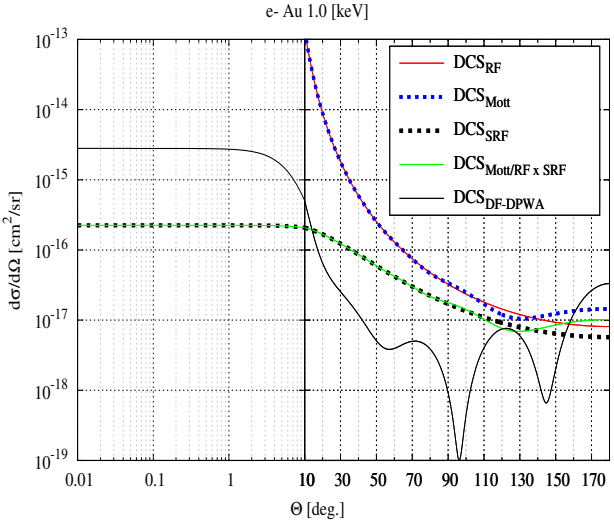

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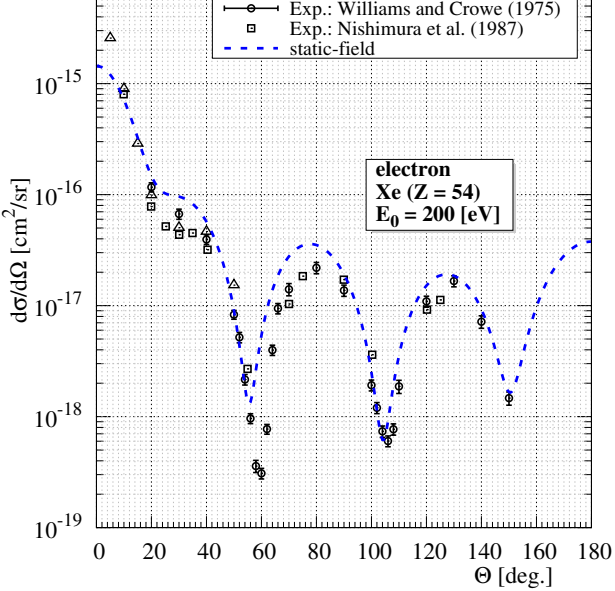

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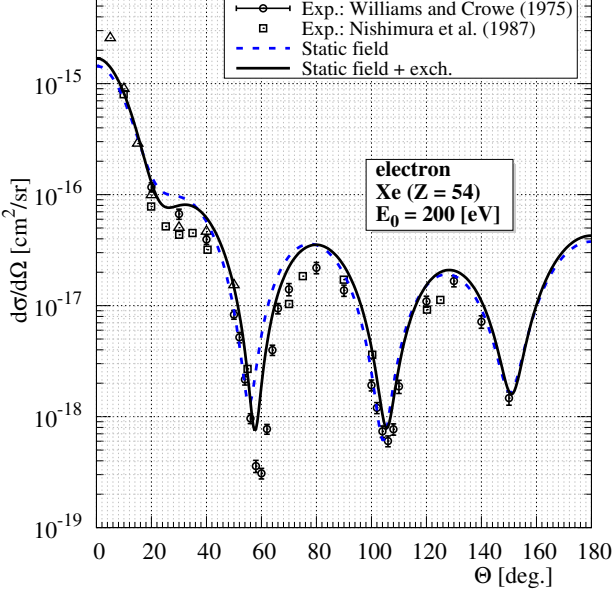

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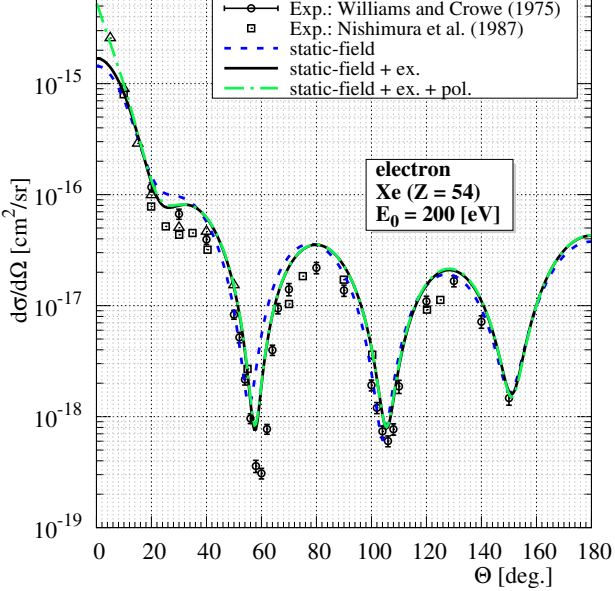

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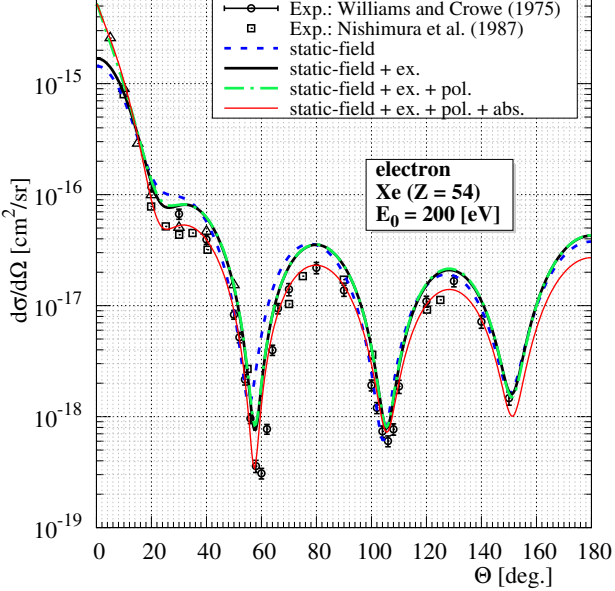

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  - **absorption**: inelastic interaction decreasing the flux of projectiles (not included!)
- **polarisation** and **absorption** *depend on aggregation* effects $\Leftrightarrow$ free atom and additivity rule !
- moreover **absorption** is an inelastic channel so it should not be included in an elastic model (while needs to be accounted when angular distributions are compared to experiments as above)
- one should consider **static-field + exchange correction** with a limit of $\sim$ [keV] for accuracy !!!

Contents

The following settings were used:

- scattering on the ***static-field*** of the nucleus **screened** by the atomic electrons
- by using **Fermi charge distribution** of the nucleus (i.e. instead of a point charge: finite nuclear with a charge distribution) and **electron densities** from the **Dirac-Fock** model of the atom
- ***exchange*** (only for e^- of course), ***correlation-polarization*** (for $E_0 < 10$ [keV]) were applied on the top of the above ***static-field*** approximation
- DCS were computed for **electrons** and **positrons** scattering on ***free atoms*** (described by the above scattering potential) with atomic numbers of $\mathbf{Z = 1\text{-}103}$ and **primary kinetic energies of** $\mathbf{E_0} \in [\mathbf{10eV}, \mathbf{100MeV}]$

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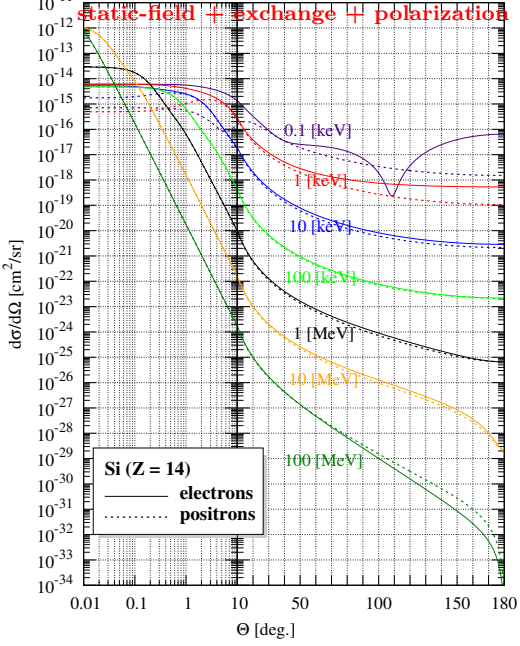
Note:

- ***absorption correction*** **was not included** in the computation since it's an inelastic channel
- scattering on **free atoms** were considered: **general model** i.e. DCS for any materials through the additivity rule
- as a consequence, the **accuracy** of these DCS **might be limited when aggregation effects become important** ($E_0 <\sim [keV]$) i.e. the free atom scattering potential becomes less valid due to the effects of the environment
- also note, that the low energy corrections (e.g. polarisation) are also strongly affected by aggregation effects
- nevertheless, the kinetic energy range was extended down to 10 [eV] (only for for completeness)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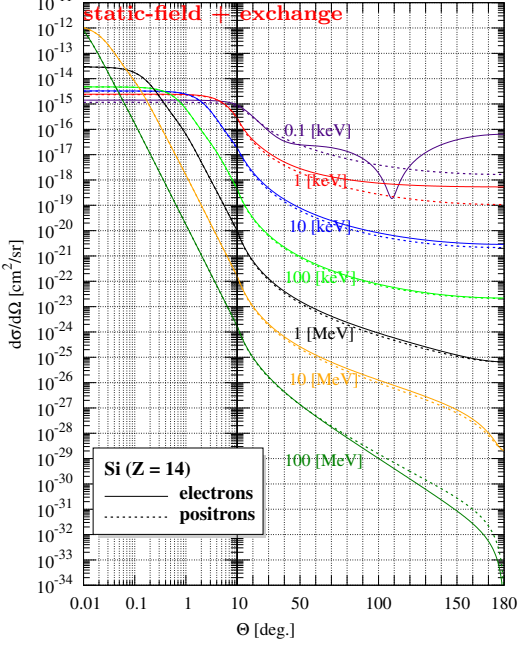
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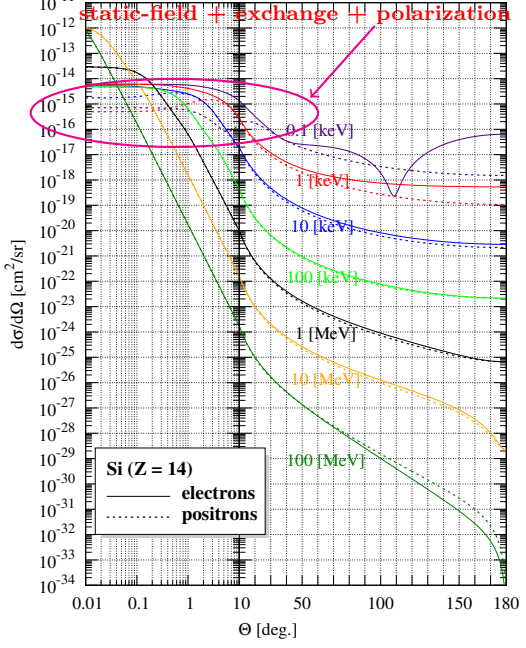
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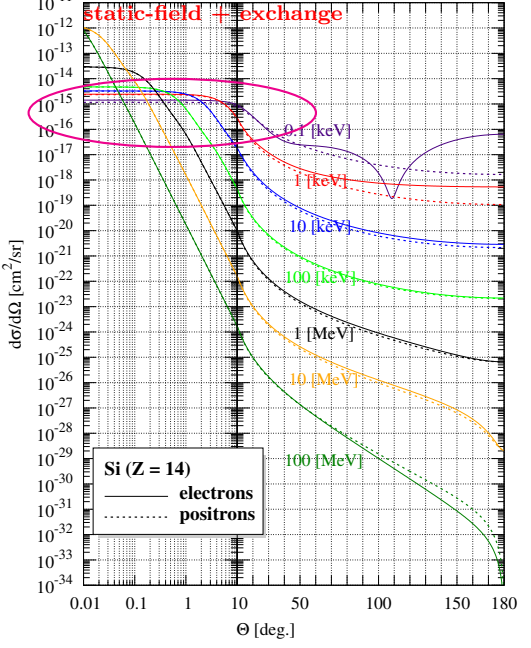
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The G4eDPWAElasticDCS class:

- new class that's responsible for ***handling*** the new numerical DPWA DCS data:
  - **loads** all **DCS data** for a given Z (for the given particle ($e^-/e+$) for all kinetic energies)
  - **computes** (by numerical integral) and **provides** interfaces to obtain **elastic**, **first-** and **second-transport cross sections** for a given **target atom** and **projectile kinetic energy**
  - **provides** interfaces to obtain **samples** (of the cosine) of **polar angle of deflection** in Coulomb scattering **according to the underlying numerical DCSs** [1]
  - **all these** above functionalities (integrated cross sections and sampling of angular deflections) are **also available for restricted polar angle interval** i.e. *for mixed simulation*
    - **mixed simulation** of Coulomb scattering: angular *deflections below* a given *threshold* of scattering *angle* is described by *multiple scattering* (simple *small angle approximation* works fine) while *large angular deflections modelled individually* (analogous to the condensed history description of bremsstrahlung and ionisation)
    - this **requires cross sections** and **sampling of angular deflections over a restricted** (i.e. above threshold) interval of angular deflection

[1] sampling tables have been precomputed, and stored with the DCS data, for fast, accurate sampling based on numerical inversion of the CDF combined either with a binary search (at most 7 steps) or with Walker's alias method for immediate determination of the sampling sub-interval depending if monotonicity is required or not (not discussed today but see more at the *Additional materials* section **here**)

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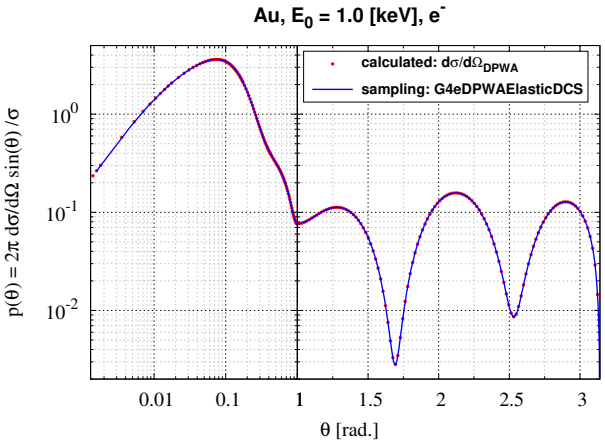

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The G4eDPWACoulombScatteringModel class:

- a model for single Coulomb scattering of e^-/e^+ based on the numerical DPWA DCS data
- makes use of the functionalities provided by the above G4eDPWAElasticDCS class (compact)

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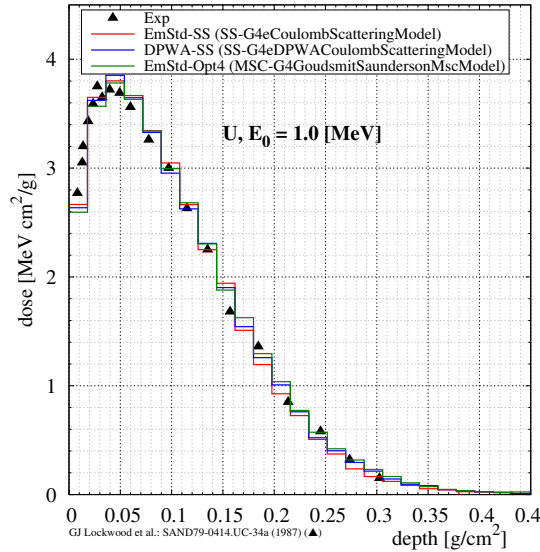
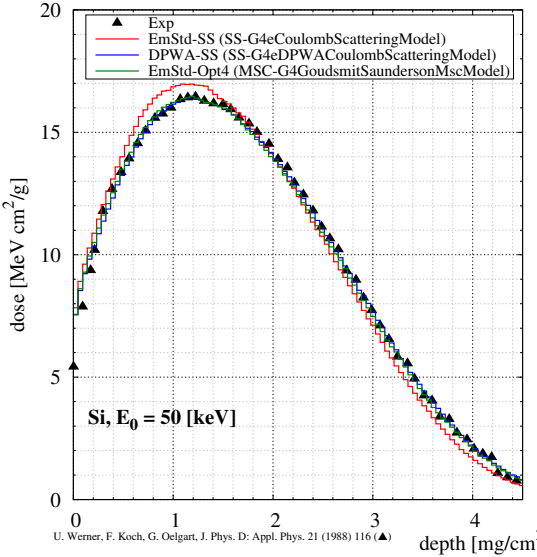
Depth dose profile (EM shower):

- **energy deposit** of $\sim 0.5 - 1$ [MeV] electrons in (semi-infinite) materials such as **U**ranium, **Si**licon or **Be**ryllium **as a function of the depth**


Exp
EmStd-SS (SS-G4eCoulombScatteringModel)
DPWA-SS (SS-G4eDPWACoulombScatteringModel)
EmStd-Opt4 (MSC-G4GoudsmitSaundersonMscModel)
U, E0 = 1.0 [MeV]
dose [MeV cm2/g]
depth [g/cm2]
GJ Lockwood et al.: SAND79-0414.UC-34a (1987) (▲)


Exp
EmStd-SS (SS-G4eCoulombScatteringModel)
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EmStd-Opt4 (MSC-G4GoudsmitSaundersonMscModel)
Si, E0 = 50 [keV]
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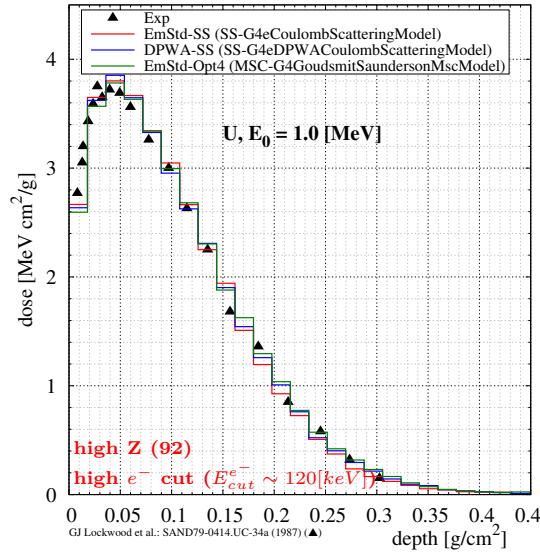
U. Werner, F. Koch, G. Oelgart, J. Phys. D: Appl. Phys. 21 (1988) 116 (▲)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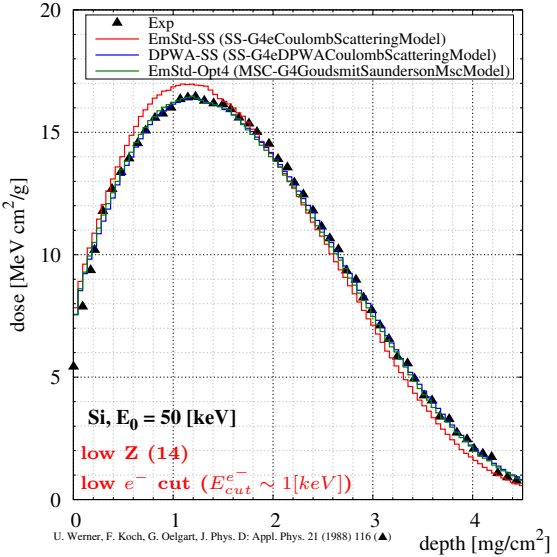
DPWA-SS (SS-G4eDPWACoulombScatteringModel)
EmStd-Opt4 (MSC-G4GoudsmitSaundersonMscModel)
U, E0 = 1.0 [MeV]
high Z (92)
high e− cut (E_cut^e− ∼ 120[keV])
dose [MeV cm2/g]
depth [g/cm2]
GJ Lockwood et al.: SAND79-0414.UC-34a (1987) (▲)


Exp
EmStd-SS (SS-G4eCoulombScatteringModel)
DPWA-SS (SS-G4eDPWACoulombScatteringModel)
EmStd-Opt4 (MSC-G4GoudsmitSaundersonMscModel)
Si, E0 = 50 [keV]
low Z (14)
low e− cut (E_cut^e− ∼ 1[keV])
dose [MeV cm2/g]
depth [mg/cm2]
U. Werner, F. Koch, G. Oelgart, J. Phys. D: Appl. Phys. 21 (1988) 116 (▲)

Depth dose profile (EM shower):

- **energy deposit** of $\sim 0.5 - 1$ [MeV] electrons in (semi-infinite) materials such as **U**ranium, **Si**licon or **Be**ryllium **as a function of the depth**
- production threshold is determined by the thickness of the depth (histogram) slice
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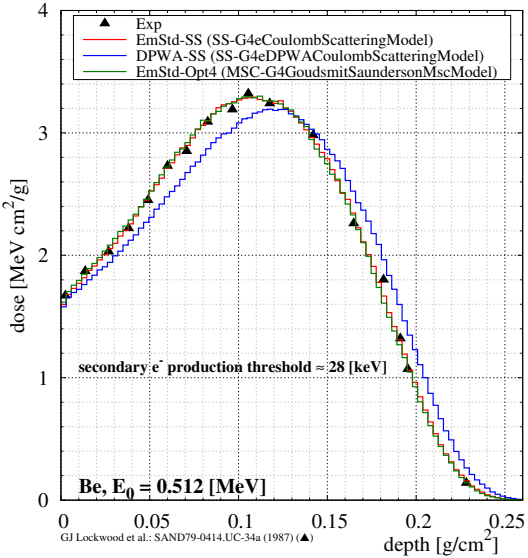

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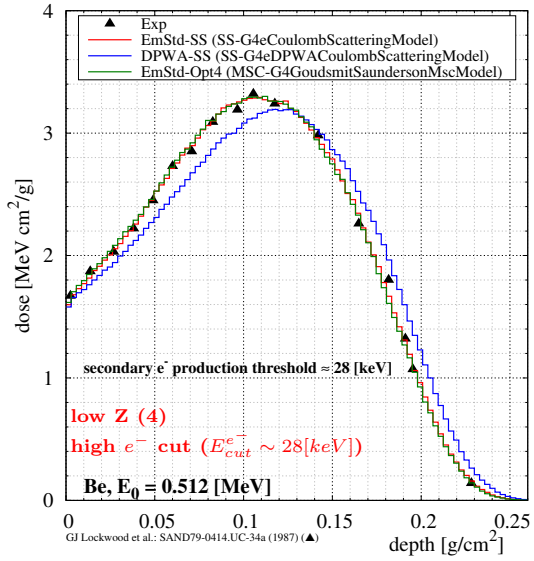
ss of the depth (histogram) slice

l results in case of **U**, the default **S**ingle **S**cattering
h the experimental **Si** data as the others (the new
condary production threshold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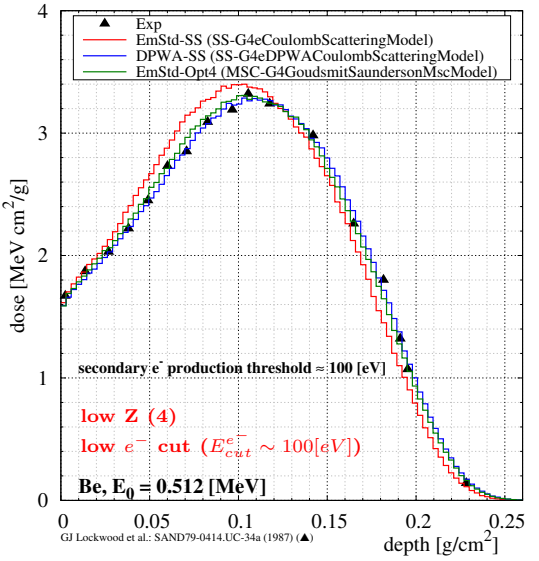
DPWA-SS (SS-G4eDPWACoulombScatteringModel)
EmStd-Opt4 (MSC-G4GoudsmitSaundersonMscModel)
dose [MeV cm^2/g]
depth [g/cm^2]
secondary e$^-$ production threshold ≈ 28 [keV]
low Z (4)
high e^- cut ($E^e_{cut} \sim 28[keV]$)
Be, E$_0$ = 0.512 [MeV]
GJ Lockwood et al.: SAND79-0414.UC-34a (1987) (▲)


Exp
EmStd-SS (SS-G4eCoulombScatteringModel)
DPWA-SS (SS-G4eDPWACoulombScatteringModel)
EmStd-Opt4 (MSC-G4GoudsmitSaundersonMscModel)
dose [MeV cm^2/g]
depth [g/cm^2]
secondary e$^-$ production threshold ≈ 100 [eV]
low Z (4)
low e^- cut ($E^e_{cut} \sim 100[eV]$)
Be, E$_0$ = 0.512 [MeV]
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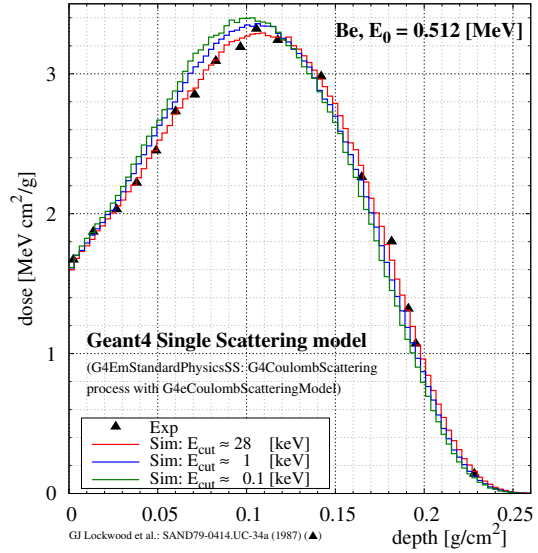
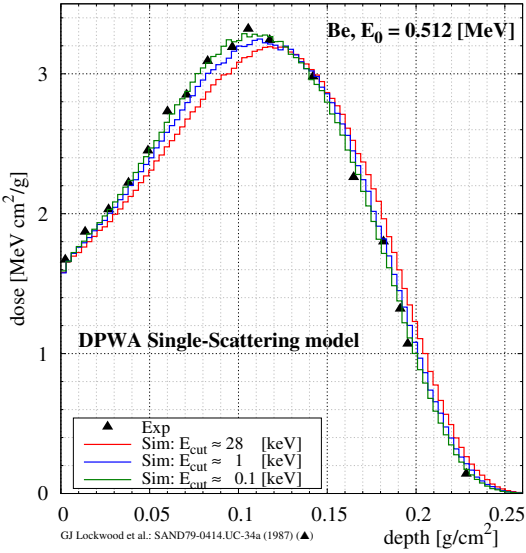

Be, E0 = 0.512 [MeV]
dose [MeV cm2/g]
depth [g/cm2]
Geant4 Single Scattering model
(G4EmStandardPhysicsSS: G4CoulombScattering process with G4eCoulombScatteringModel)
Exp
Sim: Ecut ≈ 28 [keV]
Sim: Ecut ≈ 1 [keV]
Sim: Ecut ≈ 0.1 [keV]
GJ Lockwood et al.: SAND79-0414.UC-34a (1987) (▲)


Be, E0 = 0.512 [MeV]
dose [MeV cm2/g]
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DPWA Single-Scattering model
Exp
Sim: Ecut ≈ 28 [keV]
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Depth dose profile (EM shower):

The problem causing this sensitivity:

- when **condensed history simulation** is used, **sub-threshold ionisations** (and brem. but ionisation is more important now) **are** not **modelled** explicitly but described **as continuous energy losses** along the step (**using** the corresponding restricted stopping power as **a mean energy loss**)
- while the energy loss **fluctuation model accounts the proper distribution of the energy lost in these sub-threshold ionisation** interactions *nothing* takes into account the corresponding angular deflections: **angular deflections in sub-threshold ionisations are not accounted in the simulation**
- while these angular deflections are **negligible in case of higher Z materials** (compared to those related to Coulomb scattering), they become more **important at lower Z cases**
- **this is what we can observe in case of beryllium**: lowering the production threshold, the not accounted deflections, caused by the not modelled sub-threshold ionisation interactions, are less and less so the simulation is getting to be more correct and the result converge to the experimental data

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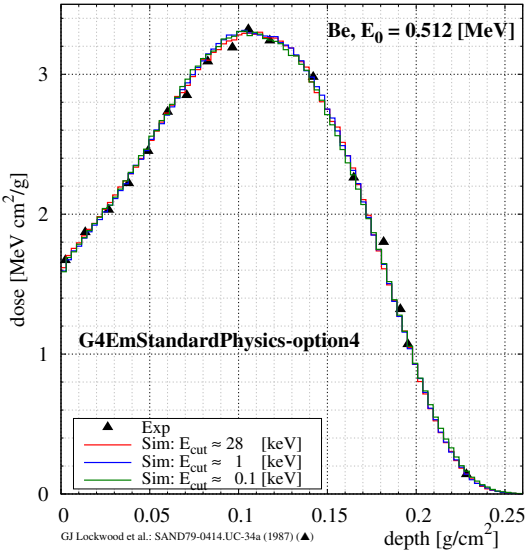
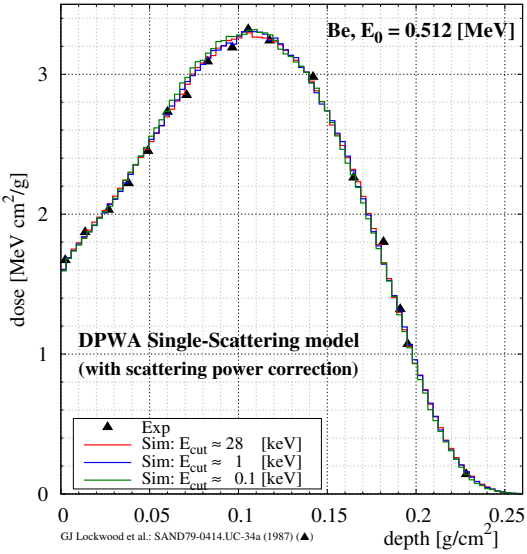

Be, E0 = 0.512 [MeV]
G4EmStandardPhysics-option4
Exp
Sim: Ecut ≈ 28 [keV]
Sim: Ecut ≈ 1 [keV]
Sim: Ecut ≈ 0.1 [keV]
dose [MeV cm2/g]
depth [g/cm2]
GJ Lockwood et al.: SAND79-0414.UC-34a (1987) (▲)


Be, E0 = 0.512 [MeV]
DPWA Single-Scattering model
(with scattering power correction)
Exp
Sim: Ecut ≈ 28 [keV]
Sim: Ecut ≈ 1 [keV]
Sim: Ecut ≈ 0.1 [keV]
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Contents

Summary:

- very accurate *Differential Cross Section* (DCS) for Coulomb scattering of e^-/e^+ on *free atoms* were computed
- the resulted numerical DCS-s are available in `Geant4` since version `10.7` and provide the possibility of developing (single or mixed) simulation models on the most accurate theoretical bases available today
- a single Coulomb scattering model, utilising these DCS data, was developed and available since `Geant4-10.7`
- revealed (again) that need to be careful when combining models, **describing even different interactions**, in our simulation

Questions?