

Numerical DPWA-DCS based Coulomb scattering in Geant4 (Report)

Mihály Novák

7-07-2020

- 1 Motivation
- 2 The Differential Cross Section (DCS)
 - Positioning the theoretical settings
 - The computed DCSs
- 3 Related Geant4 developments
- 4 Some interesting results
- 5 Summary

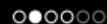
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Motivation:

- 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 is no model in Geant4 that would make 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 base line 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)
- there is a related user requirement assigned to me

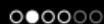
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Relativistic, screened-Rutherford DCS (DCS_{SRF}): (Geant4 SS; the base GS-MS)

- 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}):

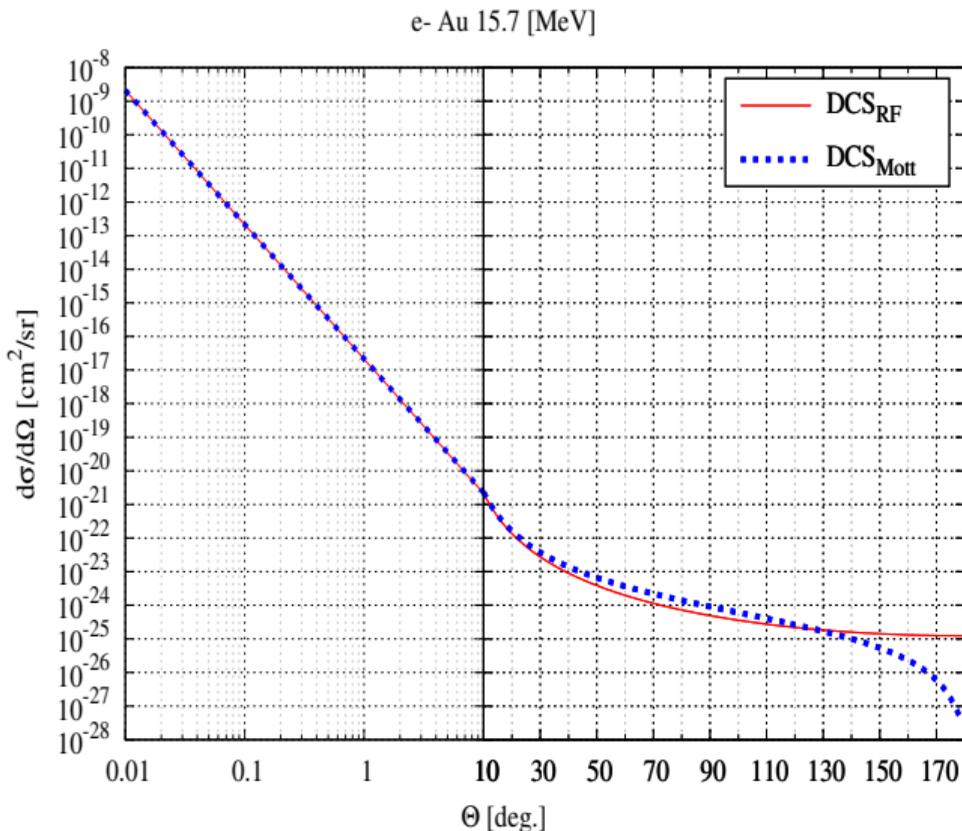
- scattering of e^-/e^+ on **unscreened, point like Coulomb potential**, accounting **spin effects**
- solution of the **Dirac equation** with a point like (unscreened) scattering potential: relativistic Dirac-Coulomb Partial Wave Analysis
- numerical solution i.e. **numerical DCS**
- relatively **accurate** (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

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

- 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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3S-MS-C)

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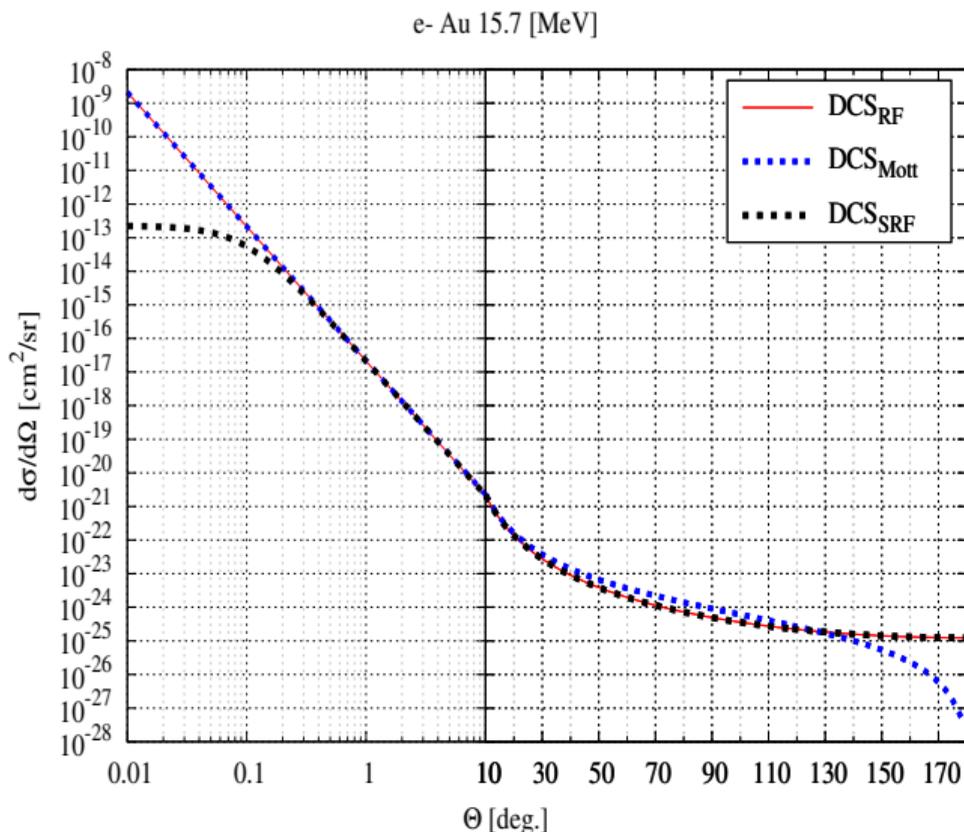
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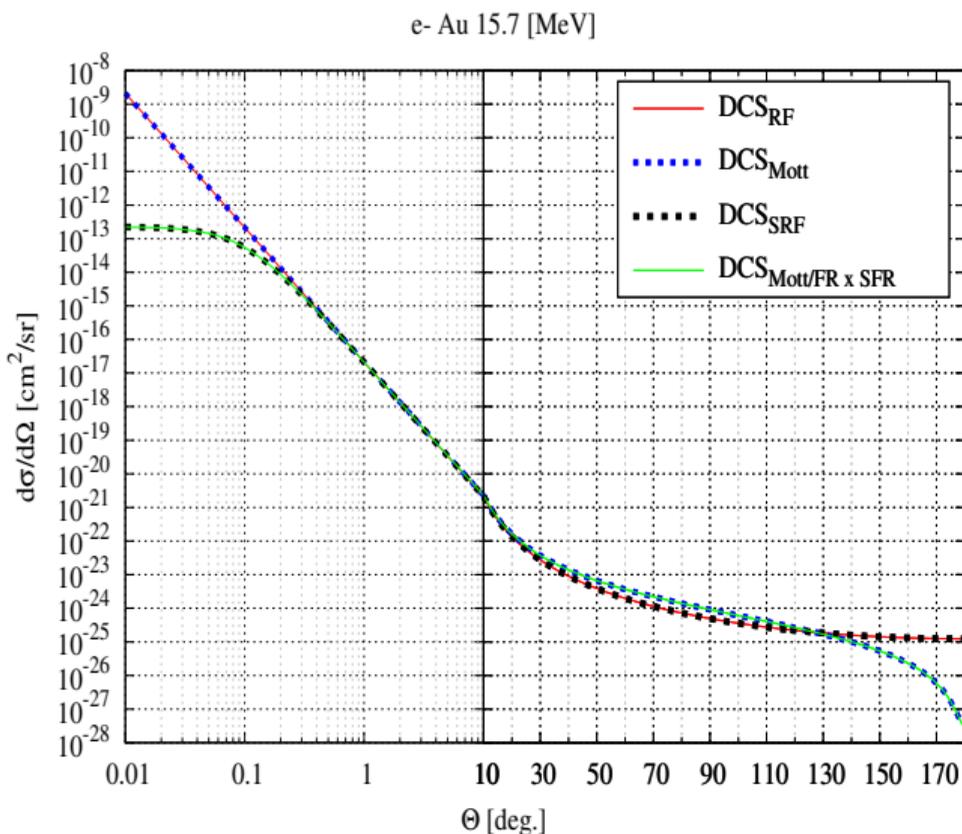
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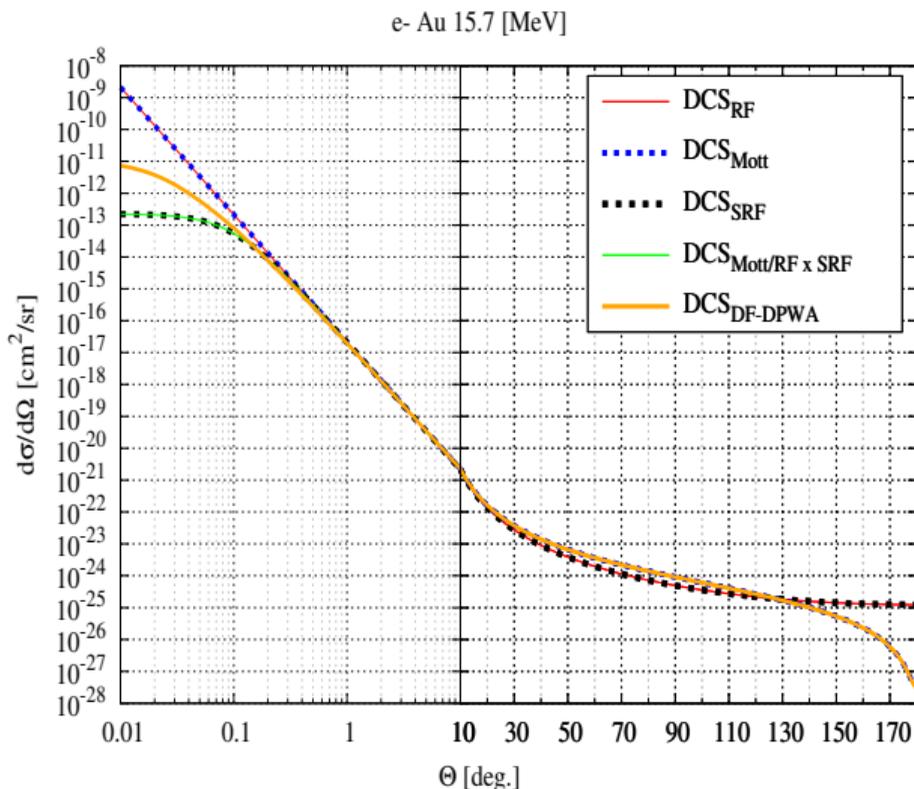
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DF-DPWA-DCS:

- solution of the **Dirac equation**, similarly to the Mott DCS, but instead of scattering on an unscreened, point potential, the (spherically symmetric) potential of the bare nucleus is **screened by using numerical electron densities computed from the Dirac-Fock (DF) model of the atoms**
- this gives the *static-field approximation*: scattering on a **static** (frozen) **field built up by the charge of the nucleus and the atomic electrons**
- screening, actually very **accurate screening** based on the DF electron densities, is included already in the scattering potential (unlike the Mott case) and the scattering equation is solved by using the Dirac Partial Wave Analysis (scattering amplitudes)

DF-DPWA-DCS:

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- screening, actually included already in the scattering equation using the Dirac Pauli-Dirac (DPWA) approximation



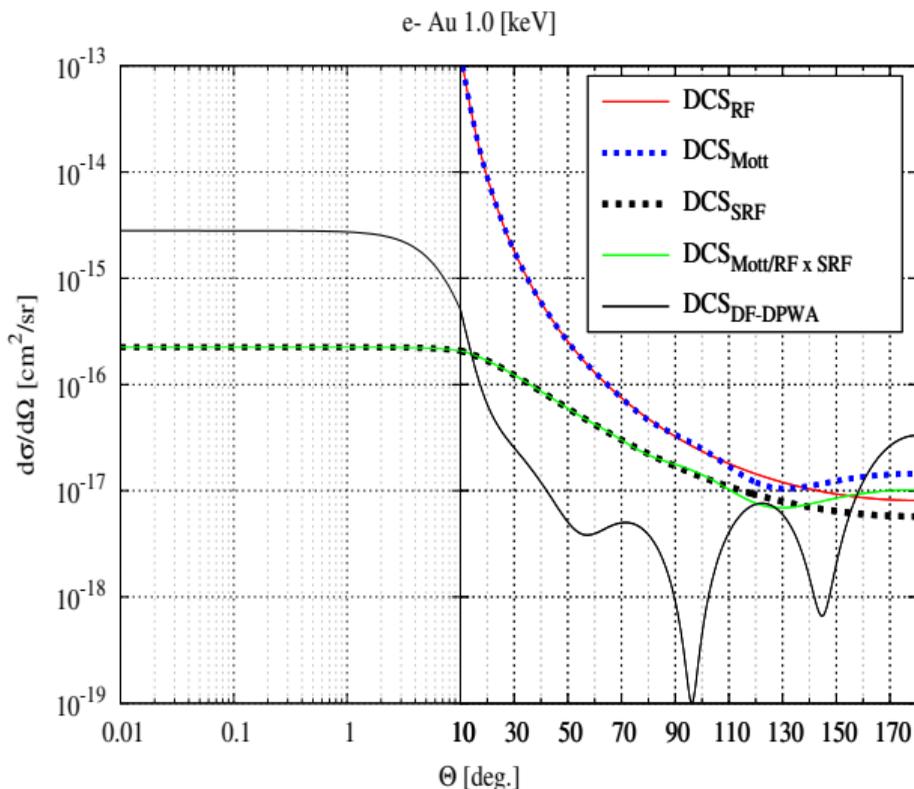
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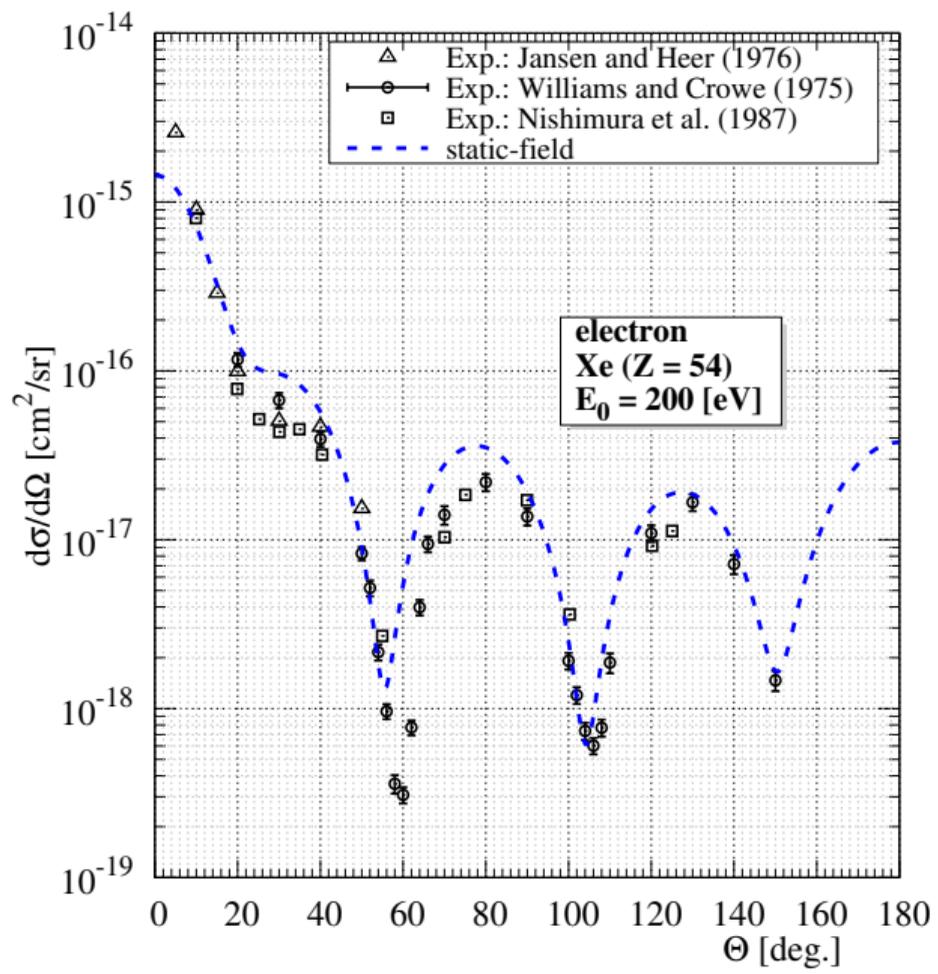
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 - **exchange correction** (e^- , $E < \sim 10[\text{keV}]$): the projectile is not distinguishable from the target electrons
 - **polarisation** (small scattering angles): interaction of the projectile with the dipole induced by itself
 - **absorption**: inelastic interaction decreasing the flux of projectiles (not included!)

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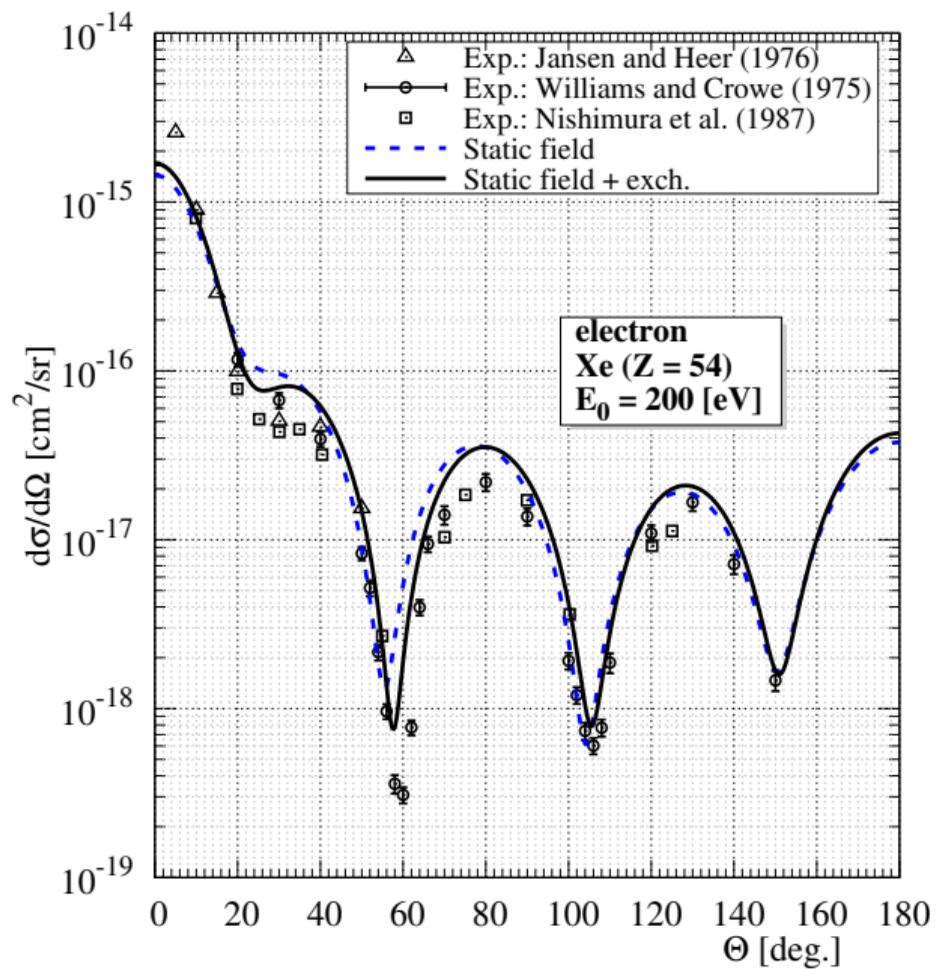
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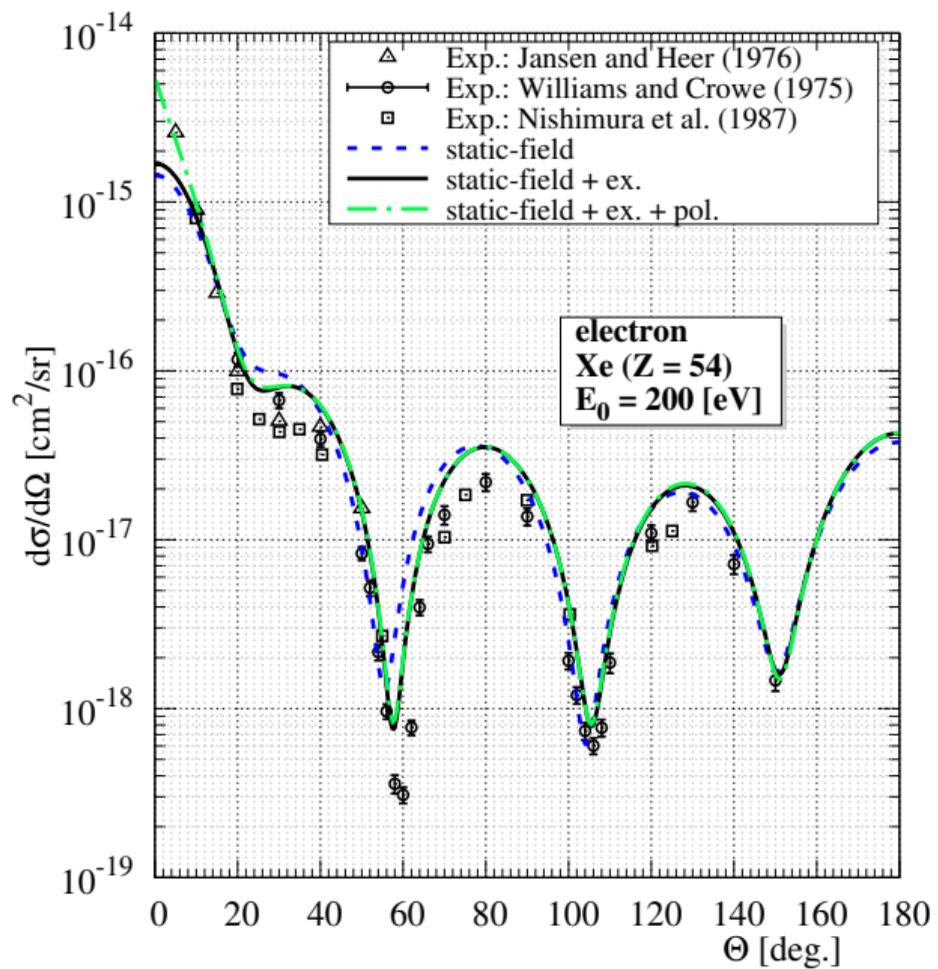
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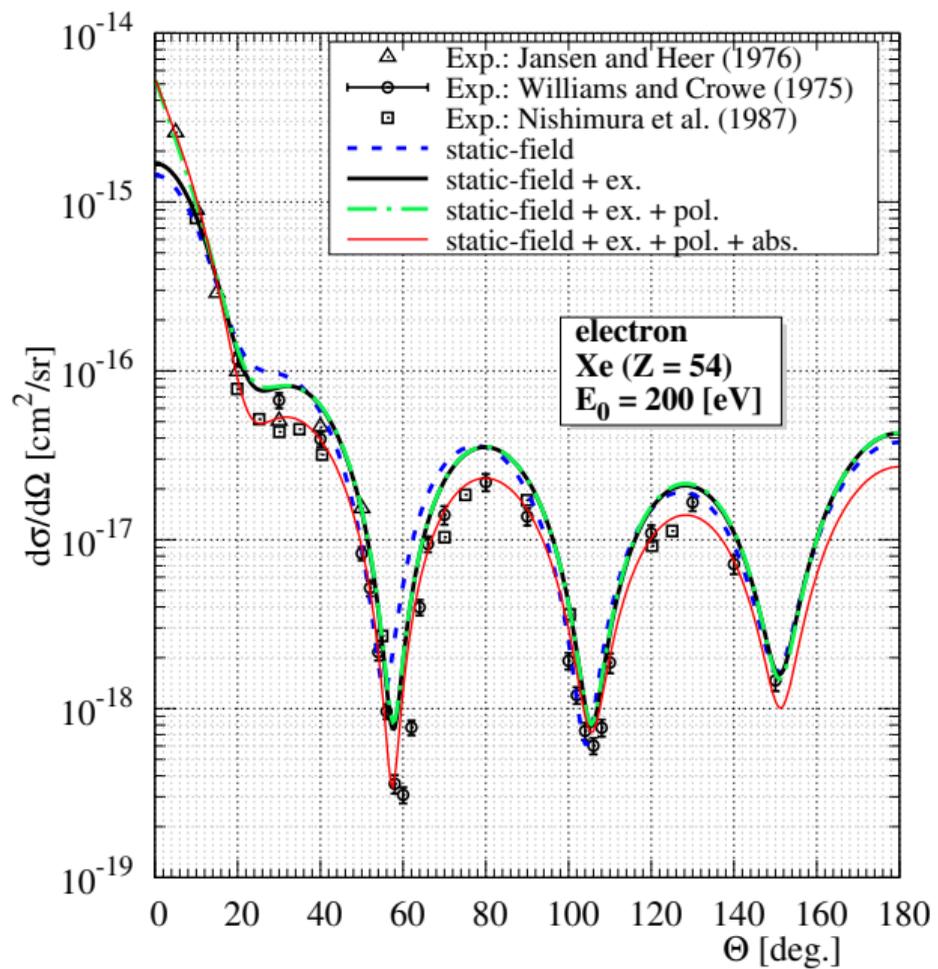
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 - **absorption**: inelastic interaction decreasing the flux of projectiles (not included!)
- **polarisation** and **absorption** *depend on aggregation* effects \Leftrightarrow free atom and additivity rule !
- moreover **absorption** is an inelastic 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 $\sim [\text{keV}]$ for accuracy !!!

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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 **$Z = 1-103$** and **primary kinetic energies of $E_0 \in [10\text{eV}, 100\text{MeV}]$**

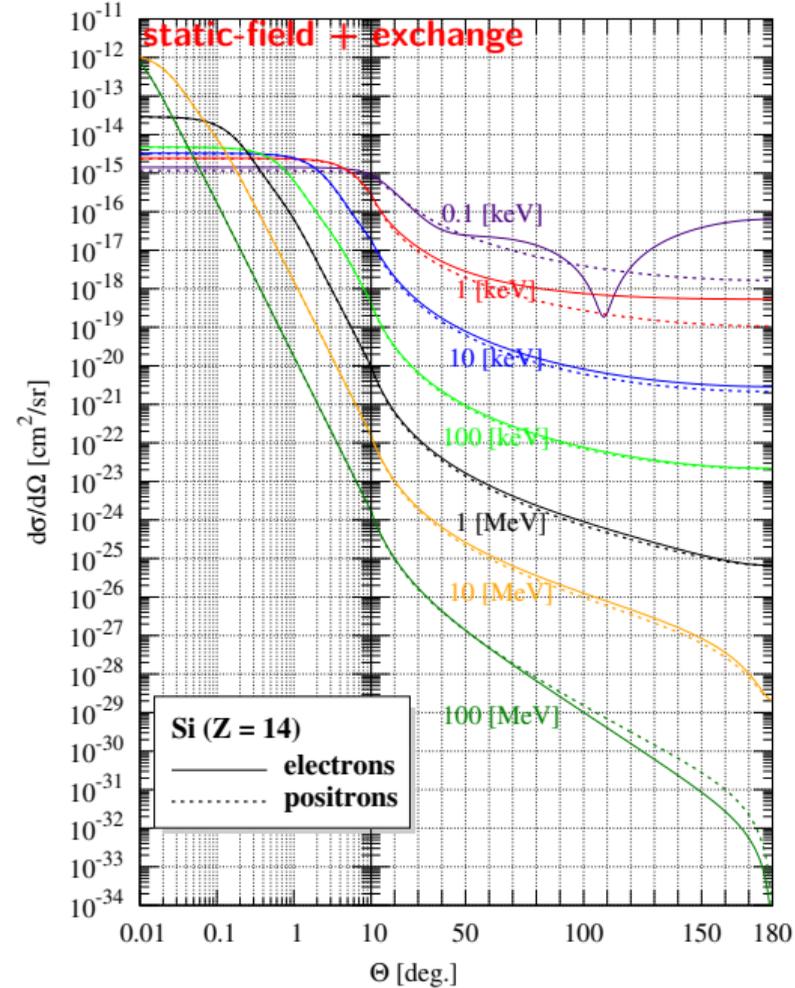
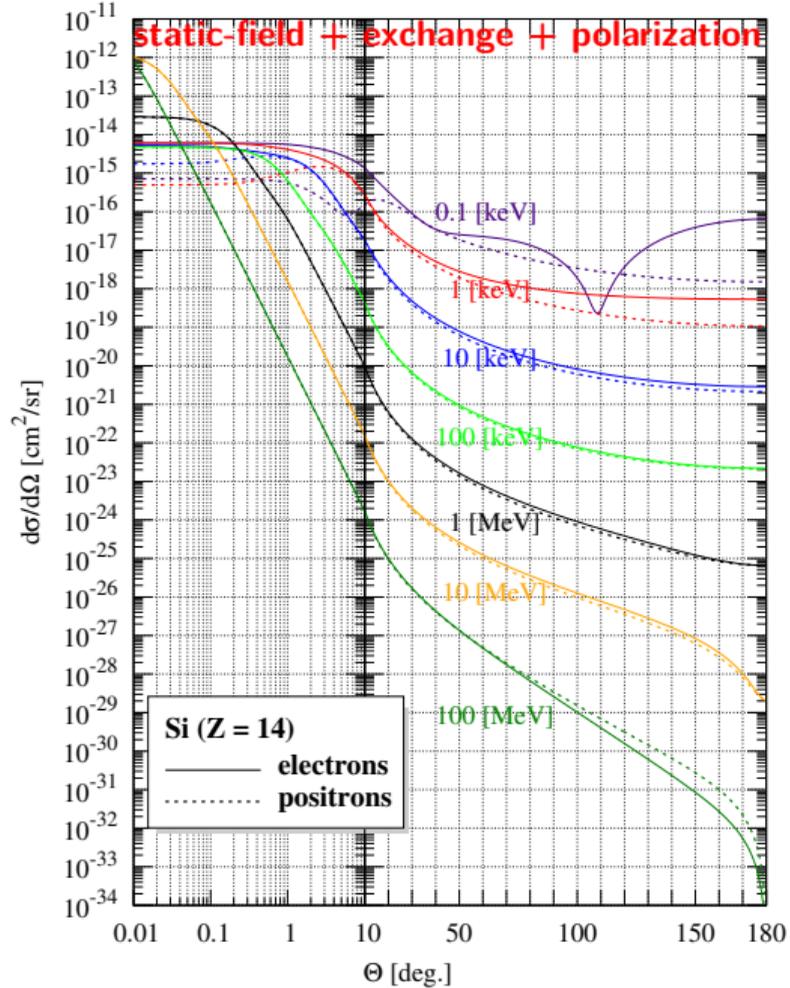


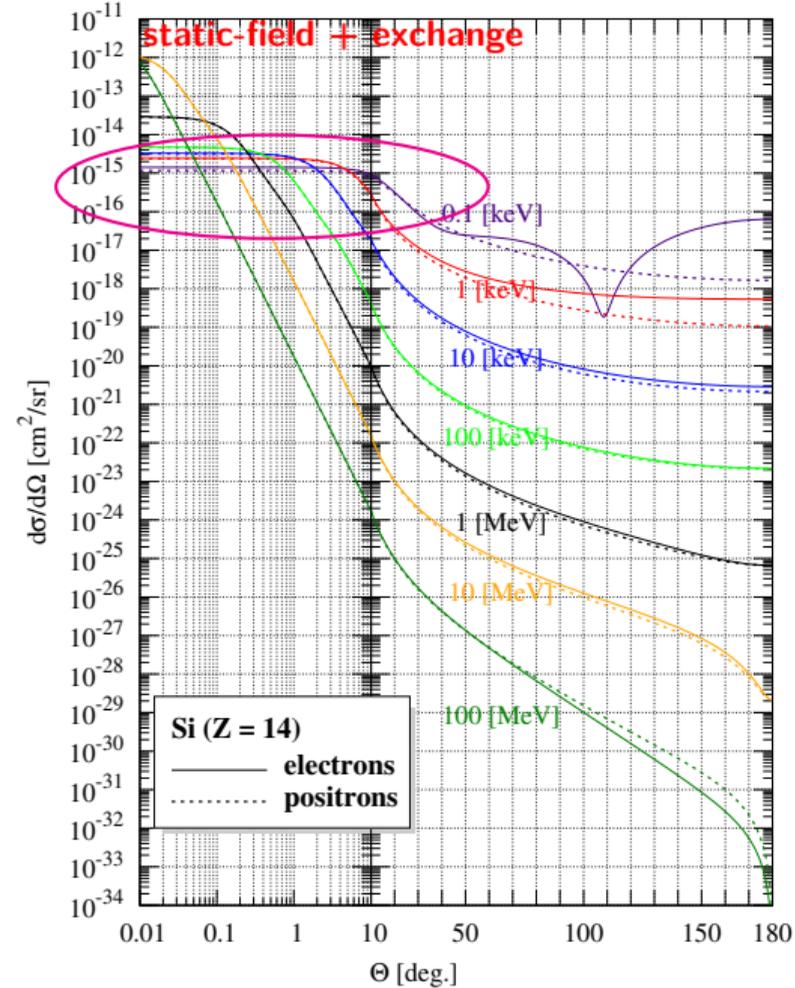
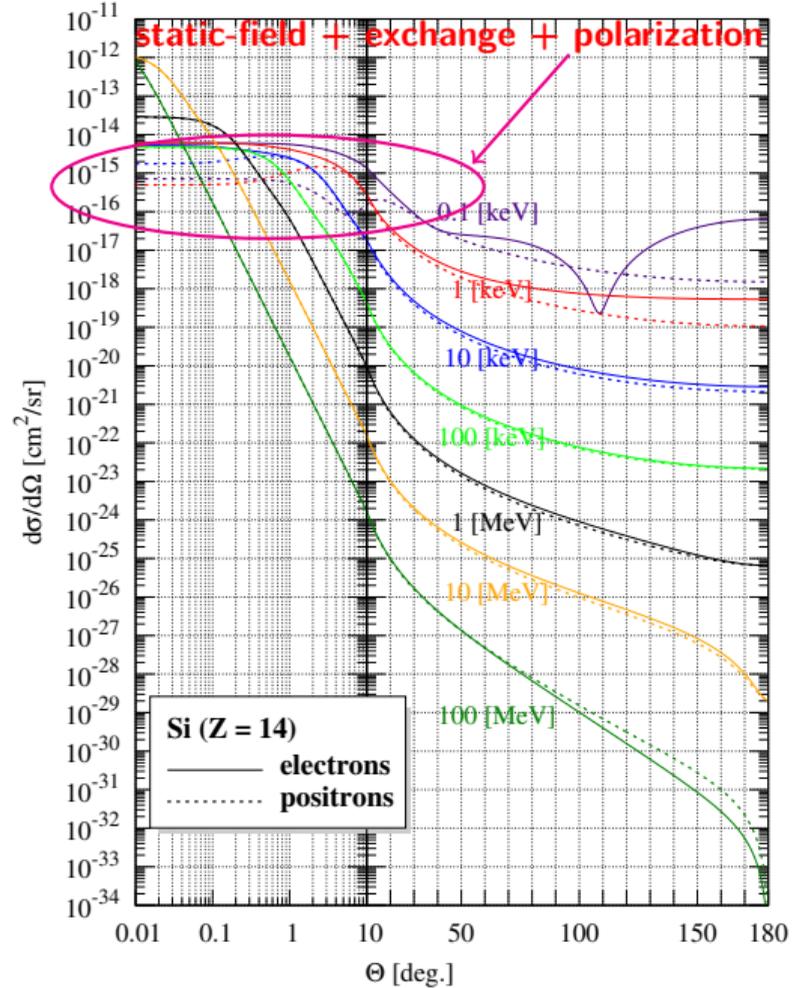
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Note:

- ***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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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
- all the functionalities that developing (either single scattering or mixed) simulation model requires

¹sampling 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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The G4eDPWACoulombScatteringModel class:

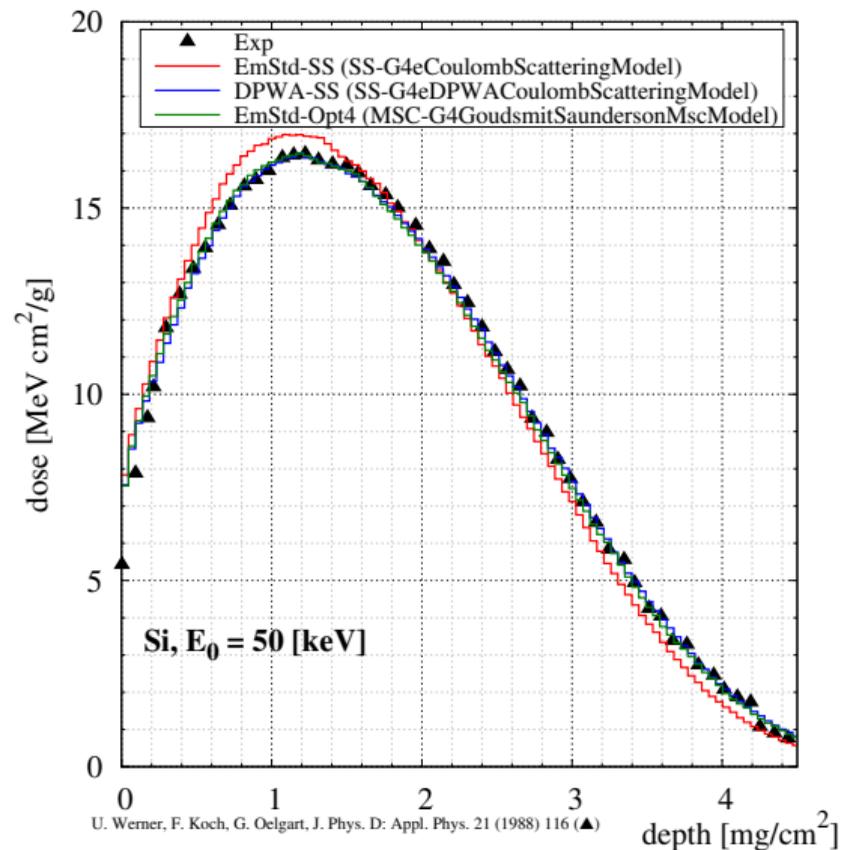
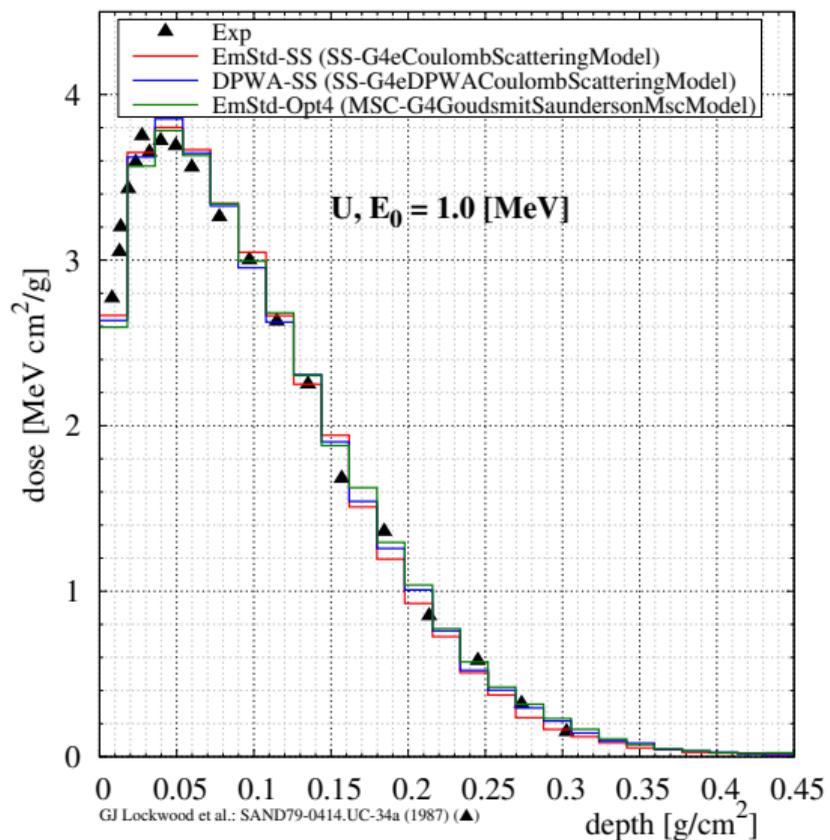
- a model for single Coulomb scattering of e^-/e^+ based on the numerical DPWA DCS data
- makes use of the functionalities provided by the above G4eDPWAElasticDCS class (compact)

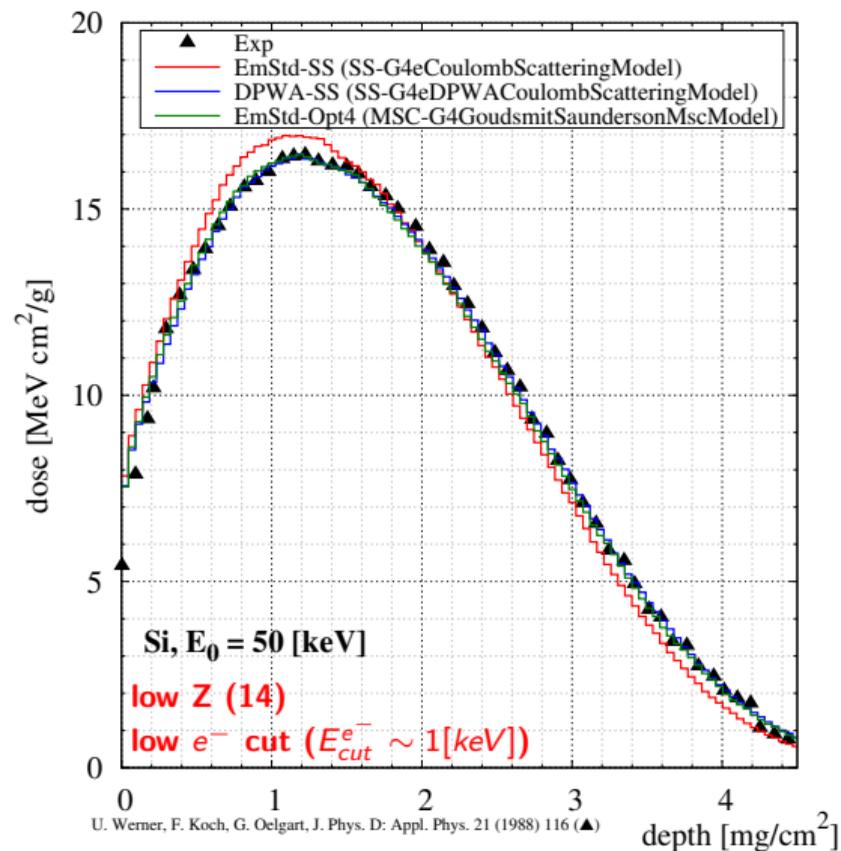
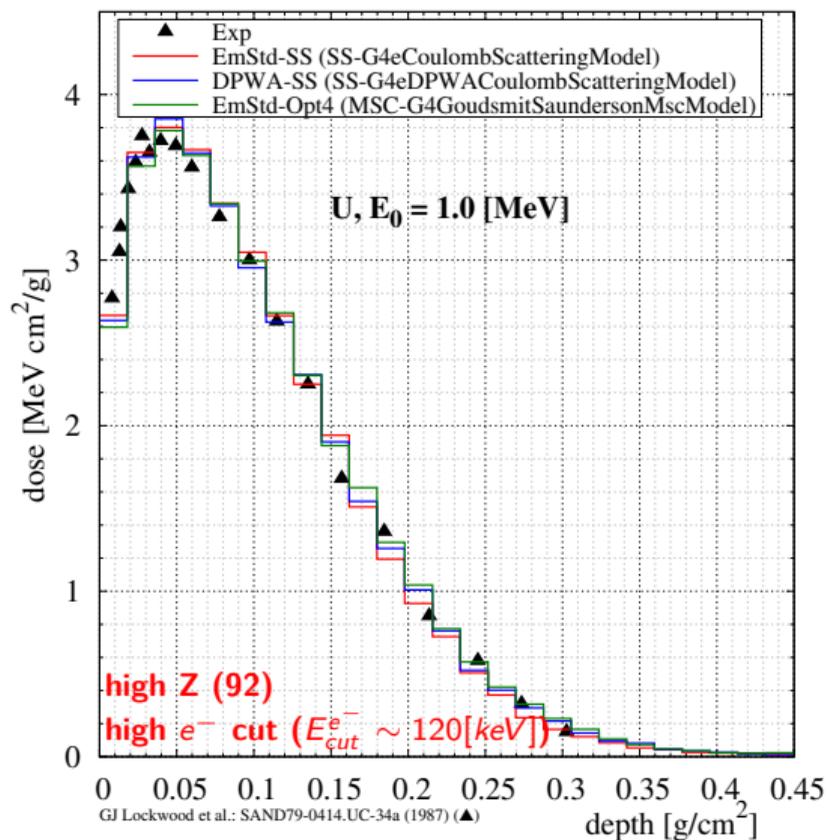
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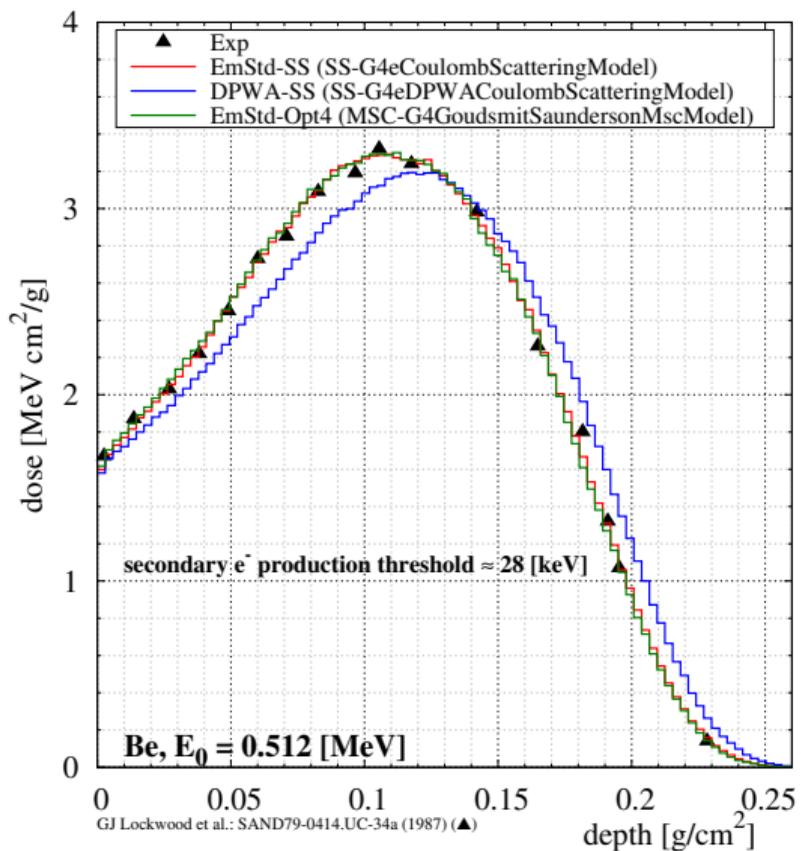
- **energy deposit** of $\sim 0.5 - 1$ [MeV] electrons in (semi-infinite) materials such as **Uranium**, **Silicon** or **Beryllium** as a **function of the depth**





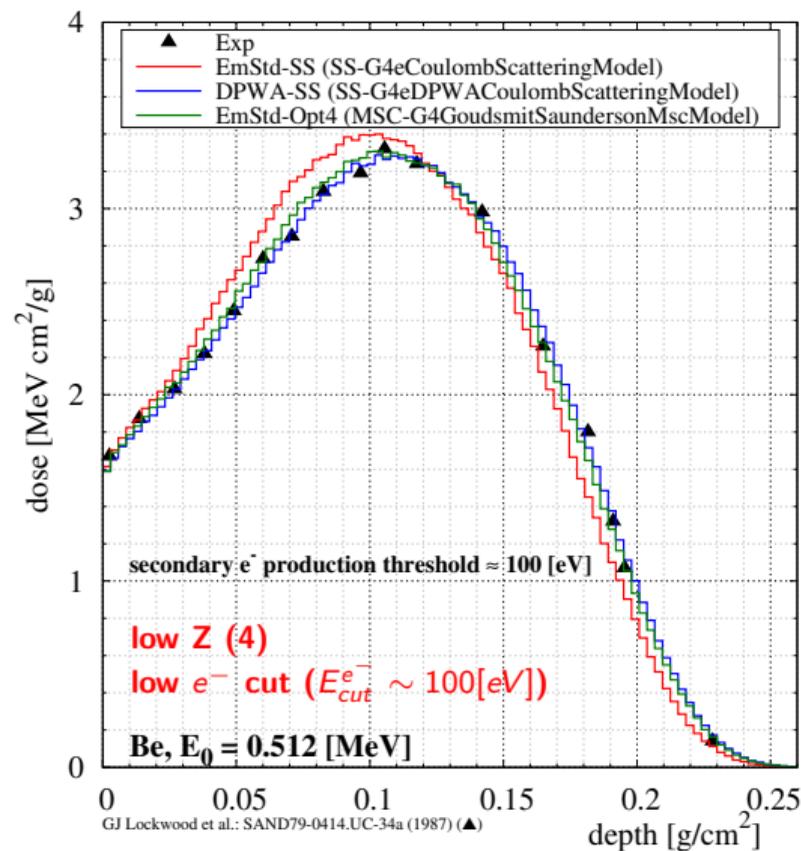
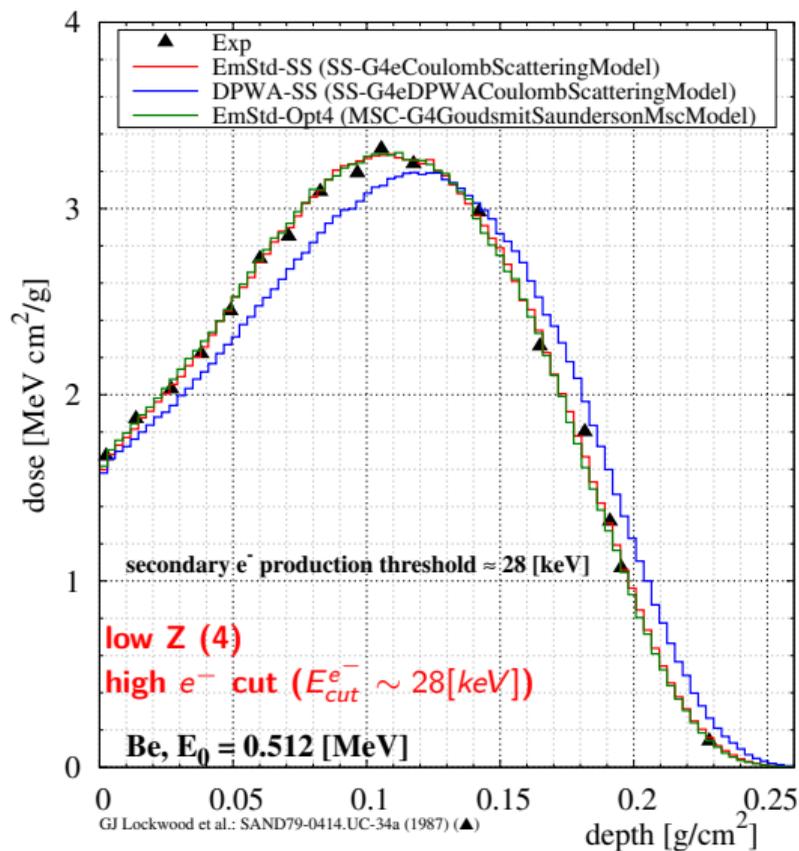
Depth dose profile (EM shower):

- **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
- while all the (investigated) models gives very good results in case of **U**, the default **Single Scattering (SS)** model doesn't provide as good agreement with the experimental **Si** data as the others (the new DPWA-SS and GS-MSD models) in spite of the low secondary production threshold
- this is even stranger in case of **Be**:



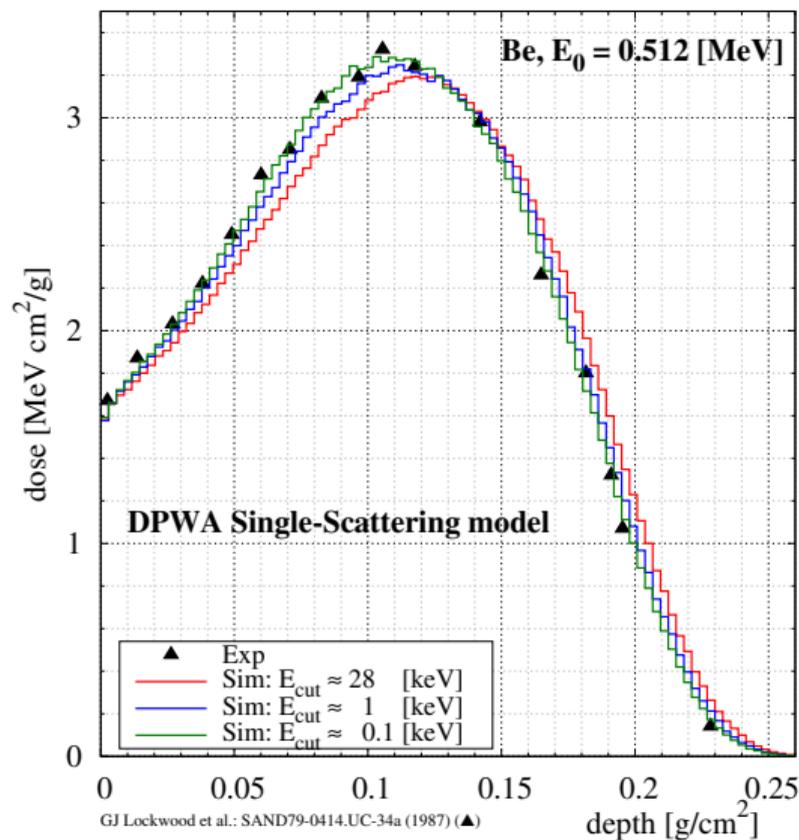
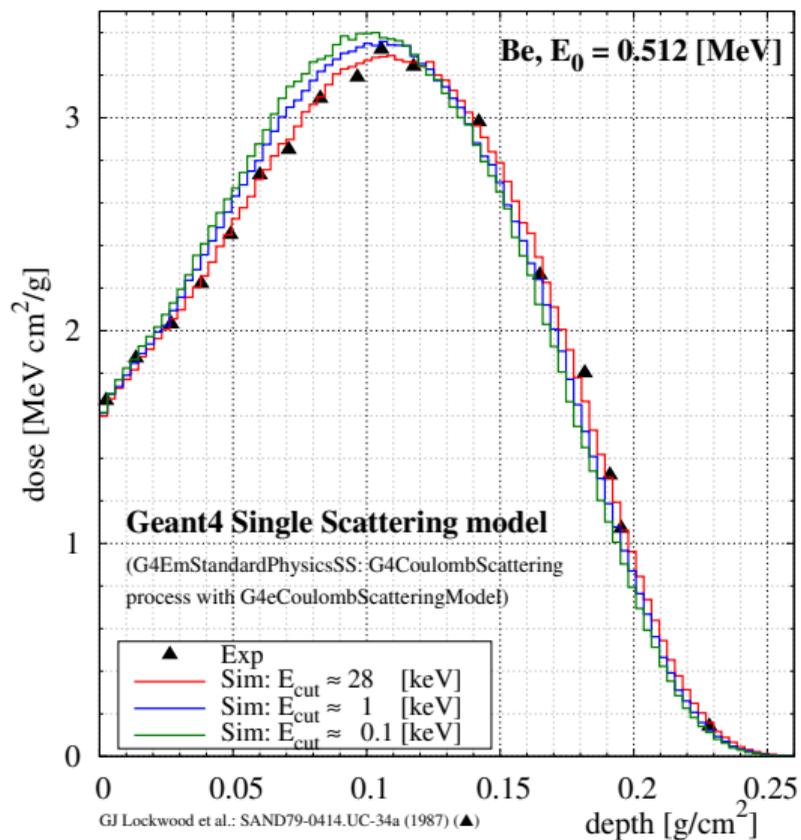
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 - **results** (except GS-MS with its most accurate settings as in Opt4) **sensitive to the production threshold**
 - the new DPWA-SS model **converges to the experiment when lowering the production threshold** (as expected)
 - the SS (the default single scattering model in Geant4) **diverges from the experiment** (incorrect behaviour)

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

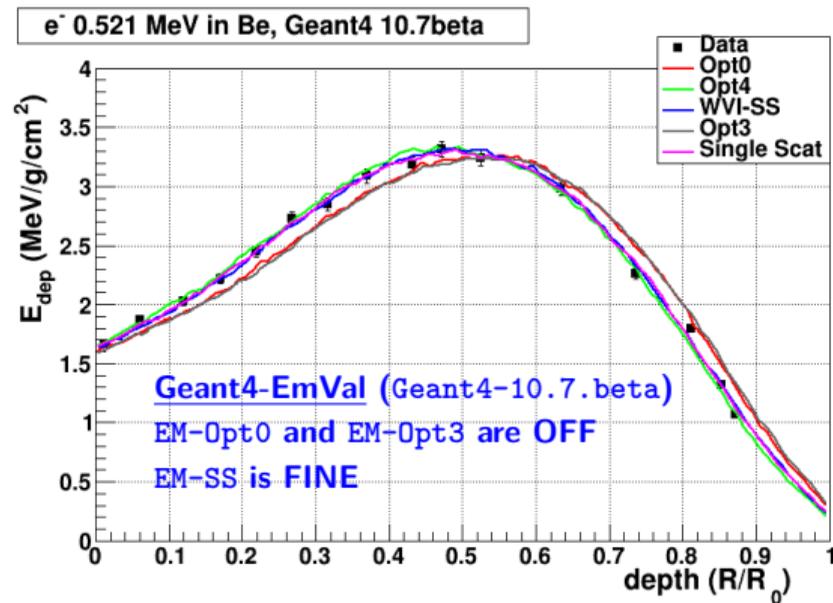
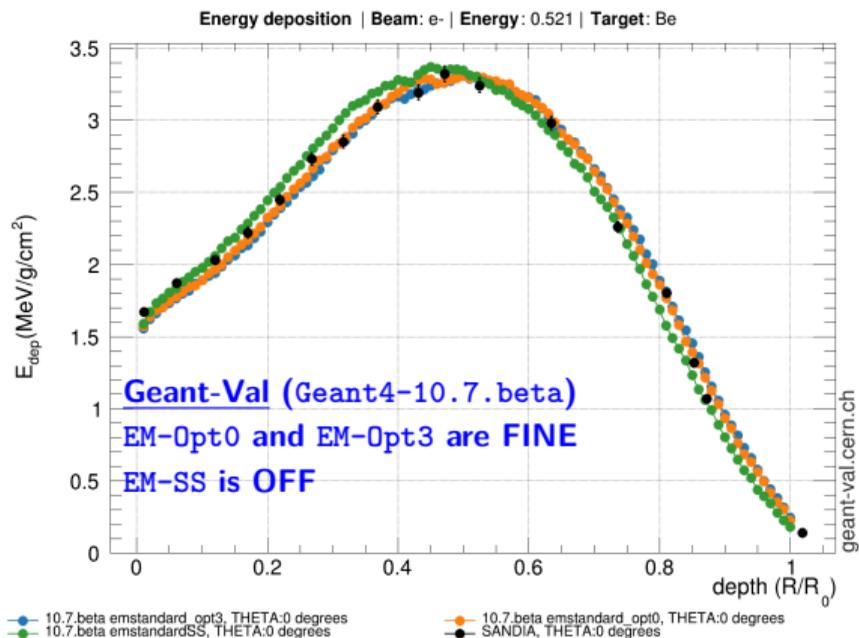
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 - **results** (except GS-MS with its most accurate settings as in `Opt4`) **sensitive to the production threshold**
 - the new DPWA-SS model **converges to the experiment when lowering the production threshold** (as expected)
 - the SS (the default single scattering model in Geant4) **diverges from the experiment** (incorrect behaviour)
 - **angular deflections due to sub-threshold ionisations are not accounted in the simulation**
 - **all physics lists are affected except those using the above GS-MS model** with its most accurate settings: I implemented a **scattering power correction** to account the effects of angular deflections in sub-threshold ionisations (together with the Mott correction)

Depth dose profile (EM shower):



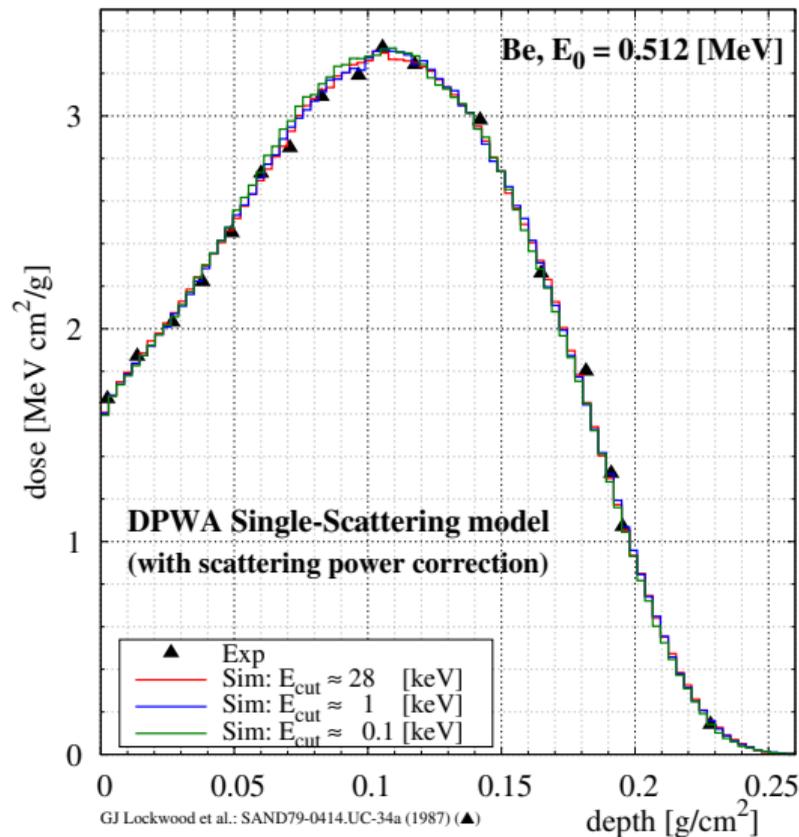
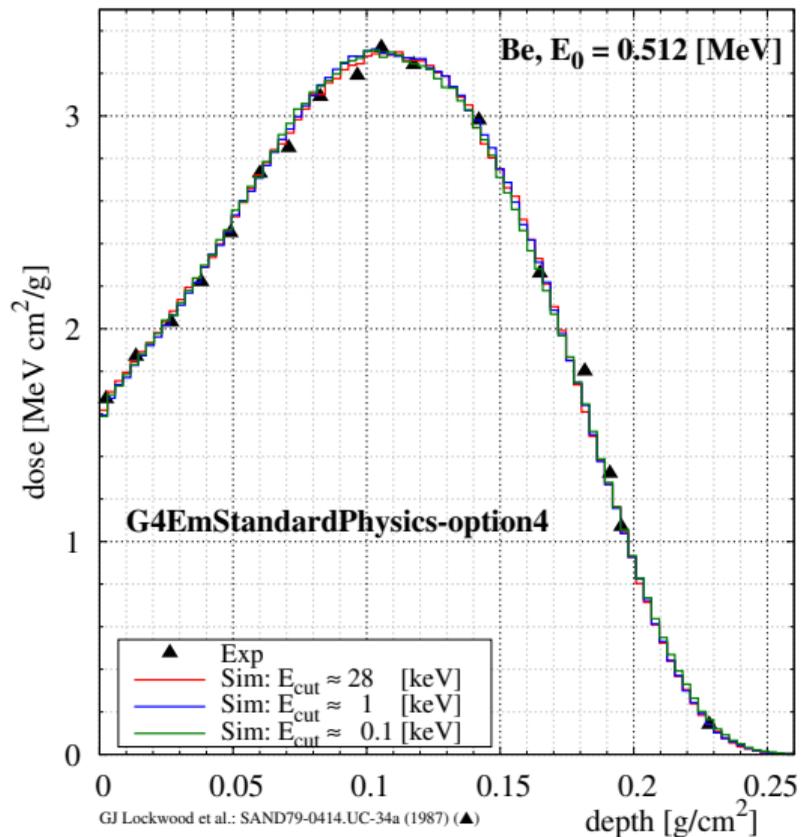
everything is the same but the secondary production threshold → different results/conclusion

Depth dose profile (EM shower):

- **energy deposit** of $\sim 0.5 - 1$ [MeV] electrons in (semi-infinite) materials such as **Uranium**, **Silicon** or **Beryllium as a function of the depth**
- production threshold is determined by the thickness of the depth (histogram) slice
- while all the (investigated) models gives very good results in case of **U**, the default **Single Scattering (SS)** model doesn't provide as good agreement with the experimental **Si** data as the others (the new DPWA-SS and GS-MSc models) in spite of the low secondary production threshold
- this is even stranger in case of **Be**:
 - **results** (except GS-MSc with its most accurate settings as in Opt4) **sensitive to the production threshold**
 - the new DPWA-SS model **converges to the experiment when lowering the production threshold** (as expected)
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 - **the new DPWA-SS model also contains this scattering power correction** (note: should be active only when condensed history simulation is used for ionisation!)



- 1 Motivation
- 2 The Differential Cross Section (DCS)
 - Positioning the theoretical settings
 - The computed DCSs
- 3 Related Geant4 developments
- 4 Some interesting results
- 5 Summary

Summary:

- very accurate Differential Cross Section (DCS) for Coulomb scattering of e^-/e^+ on free atoms have been computed
- the resulted numerical DCS-s are available now in Geant4 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, has been developed and also available now in Geant4
- this development process also revealed some of the weak corners of the current Geant4 EM shower simulation
- further actions might be considered in order to generalise the provided solution to this problems in order to make the shower simulation even more robust