Version 11.2.p01

Electromagnetic Physics I and II

Special topic: Multiple Coulomb scattering (MSC)

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Geant4 Tutorial at Jefferson Lab
27 March 2024

- Electromagnetic (EM) physics overview
  - Introduction, structure of Geant4 EM physics
  - Standard EM physics constructors
- Special EM topics:
  - Secondary production thresholds:
    - in Geant4
    - energy loss fluctuation
    - continuous step limit to to energy loss
    - v.s. tracking cut, `G4UserLimit`, step function
  - EM models per detector region
  - Atomic de-excitation
  - Multiple Coulomb scattering
    - dedicated material

Electromagnetic Physics: special topics

MULTIPLE COULOMB SCATTERING (MSC)

- <u>Multiple Coulomb scattering (MSC)</u>
  - Why should we use MCS models?
  - What the MSC model provides?
  - What makes it challenging?
  - Some notes on the **`Geant4`** MSC models and step limits.
  - Some notes on the **`Geant4 EMZ`** v.s. **`default`** EM physics options.

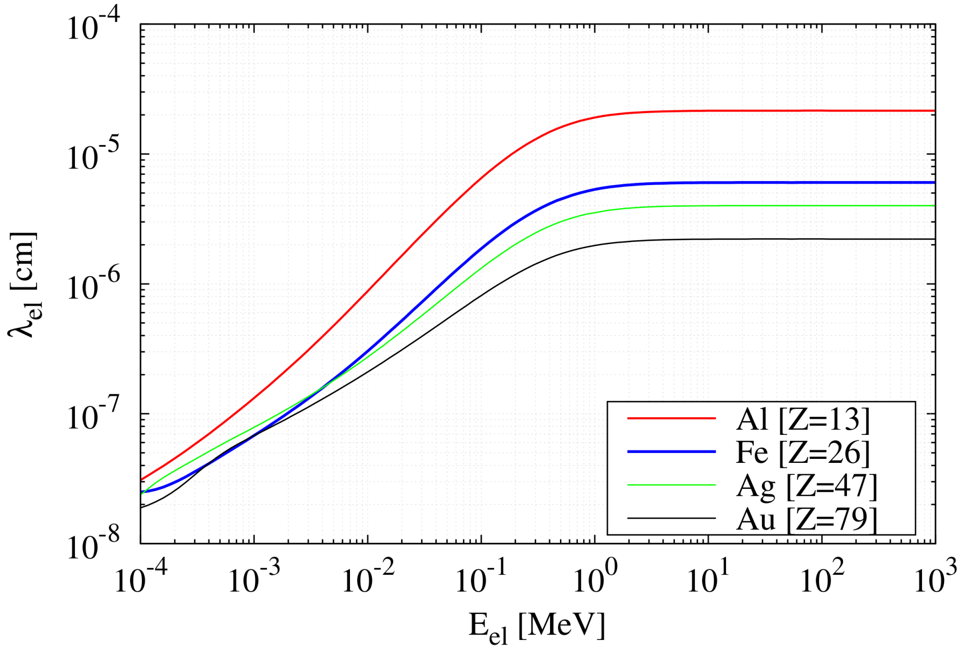
Multiple coulomb scattering (MSC)

WHY SHOULD WE USE MSC MODELS?

Why should we use MSC models? What are the alternatives?

Coulomb scattering: **elastic scattering of charged particles** (e^-/e^+) **on a Coulomb potential** (central field of the nucleus screened by the atomic electrons)

1. detailed simulation: **event-by-event modelling** of elastic scattering is **feasible only if** the mean **number of interactions per track is below few hundred**
   - this limits the applicability of the **detailed simulation** model **only** for e^-/e^+ with relatively **low kinetic energies** (becomes very inefficient otherwise)**:**
     - **E_{kin} < ~100-200 keV**: low mean number of elastic scattering along the path
     - **thin targets:** short path resulting resulting again low mean number of elastic scattering



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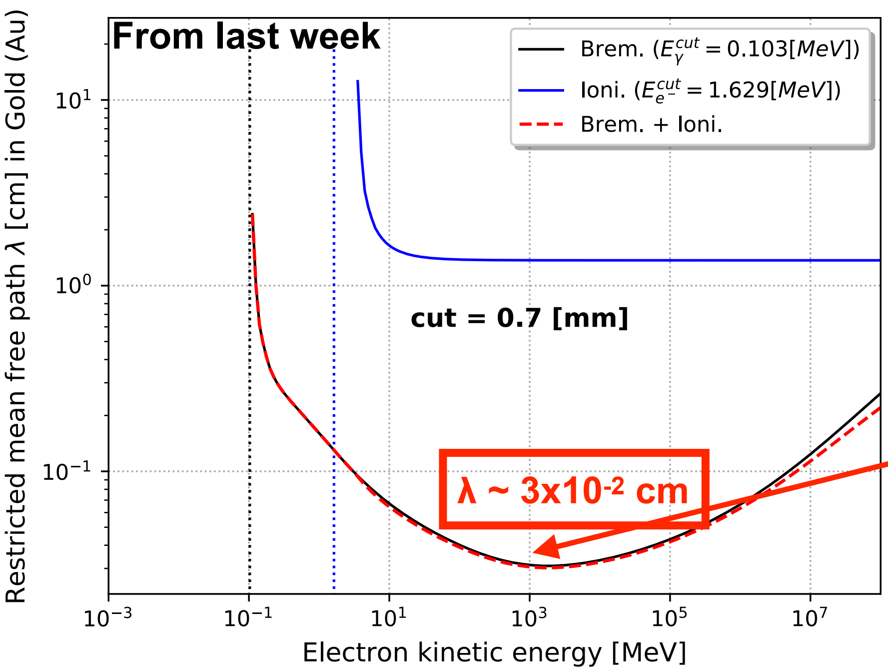
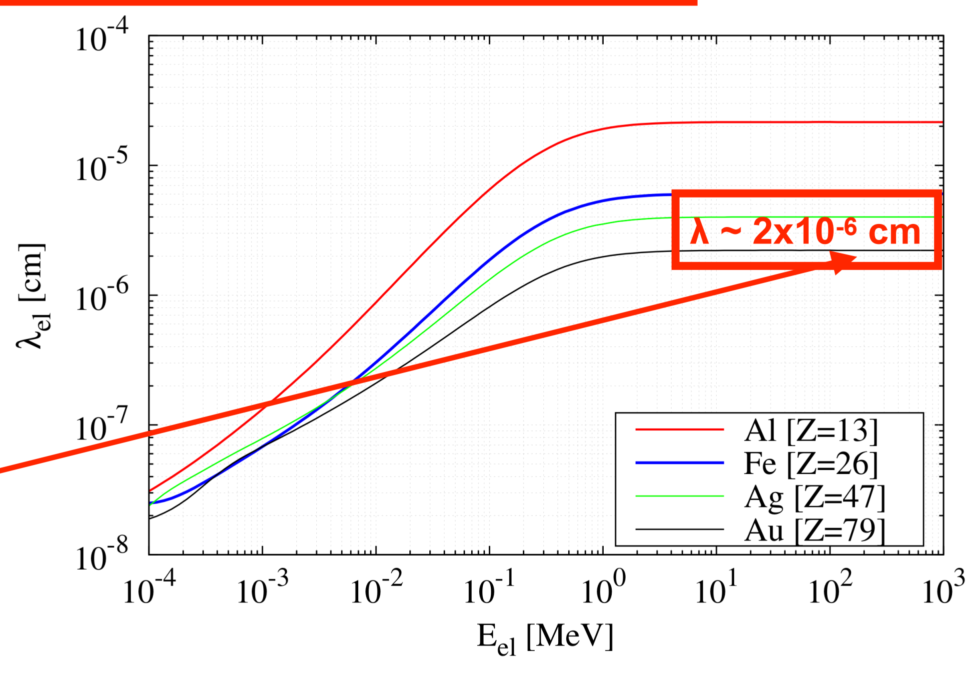
15 000 x more elastic scattering than anything else at 1 [GeV]!





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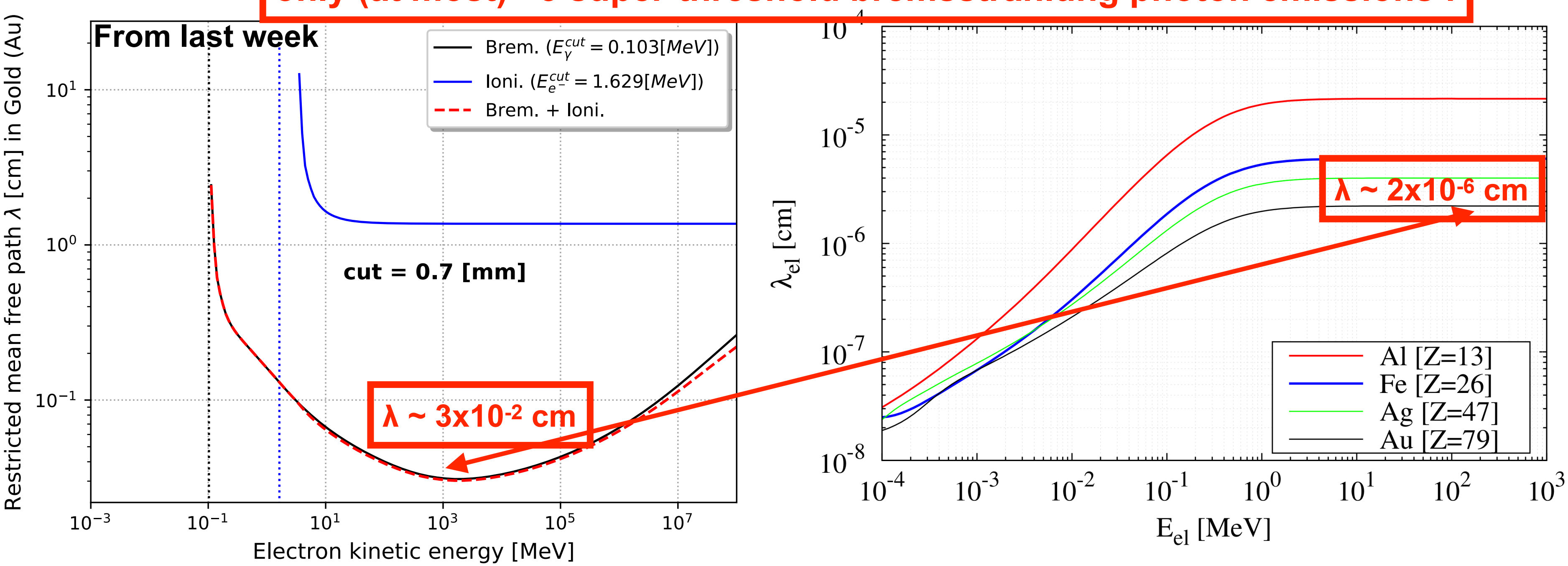
50 000 elastic scattering on 1 [mm] path when E_{kin} > ~1 [MeV] while only (at most) ~3 super-threshold bremsstrahlung photon emissions !



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   50 000 elastic scattering on 1 [mm] path when E_{kin} > ~1 [MeV] while only (at most) ~3 super-threshold bremsstrahlung photon emissions !

2. **condensed history simulation**: relies on a **multiple scattering (MSC) model** that accounts the **net effects of many elastic scattering in one step**
   - each particle track is simulated by allowing to make individual **steps** that are **much larger than the** average **step** length **between** two successive **elastic interactions**
   - the step length is computed *"without considering"* the many elastic events along
   - then the net **effects of these high number of elastic interactions,** such as angular deflection and spacial displacement, are **given by an MSC model at each individual** (condensed history) simulation **step**
   - MSC models are **stochastic models** used within the stochastic simulation itself

3. **mixed simulation**: a **fusion of the two previous** approaches

- **using** special **MSC model** (with a limited scattering angle approximation) **to describe *small angle scatterings*** along a step by exploiting:
    - the DCS for elastic scattering is strongly peaked to the forward directions
    - many things become simpler in a *"small angle approximation"*

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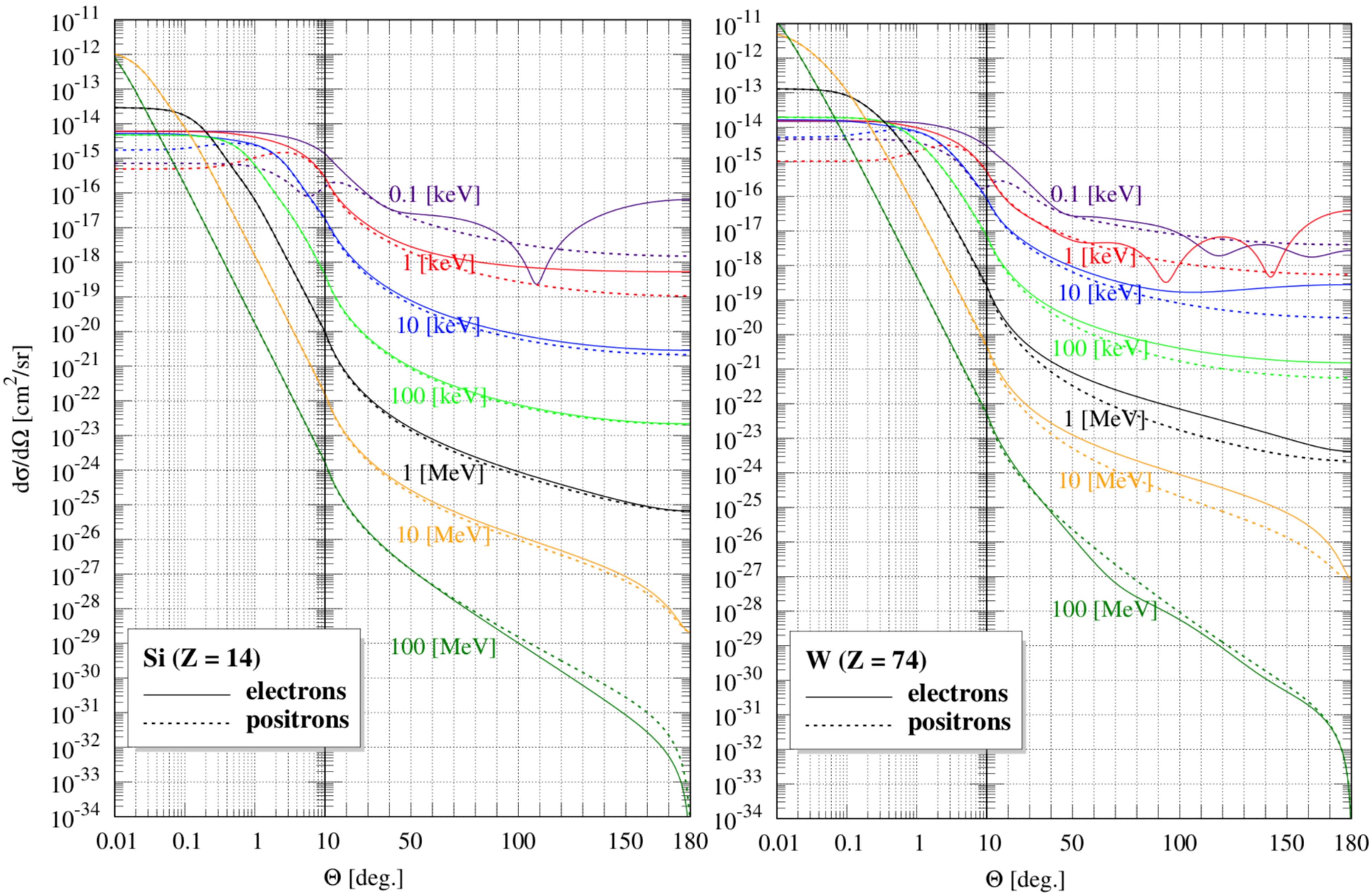

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  - the DCS for elastic scattering is strongly peaked to the forward directions
  - many things become simpler in a *"small angle approximation"*
- **using** detailed, **event by event simulation to describe *high*(*er*) *angle scattering*** events
- a similar idea to that used in case of ionisation and bremsstrahlung
- while a great idea that makes possible accurate simulation, significantly less efficient than using an MSC model: high angle scattering events (i.e. detailed simulation) starts to dominate very quickly with decreasing e^-/e^+ kinetic energies

Multiple coulomb scattering (MSC)

WHAT THE MSC MODEL PROVIDES?

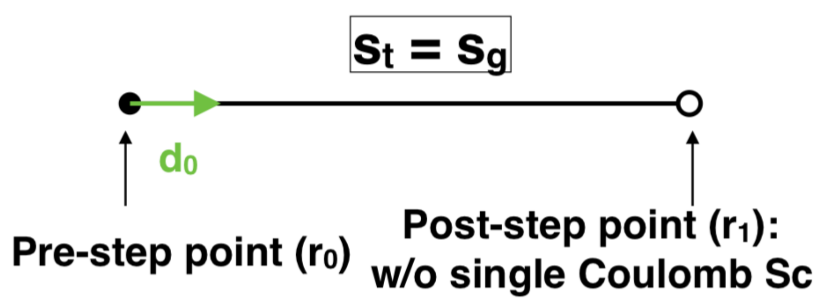
What MSC provides?

<u>A step with a particle</u> <u>(assuming no field):</u> **in an infinite volume** !

- Particles **without Coulomb** scattering process (**A**):
  - moves from the pre- to the post step point **along straight line**
- Particles **with Coulomb** scattering described by **single-scattering** model (**B**):
  - the corresponding cross section participated in the (discrete) step limit
  - moves from the pre- to the post step point **along straight line**
  - where the single Coulomb scattering event might or might not happen (depending if that limited the step or not)

A. and B.

$$\mathbf{r}_1 = \mathbf{r}_0 + \mathbf{d}_0 s_t$$



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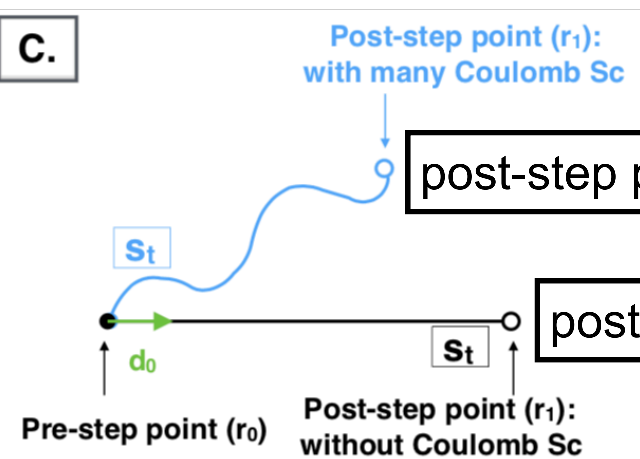
- Particles **with Coulomb** scattering described by **multiple-scattering** model (**C**):

Note: $\mathbf{s_t}$ is the step length determined by all possible physics (e.g. till the next discrete, bremsstrahlung photon emission).



post-step point: **with considering Coulomb sc.**

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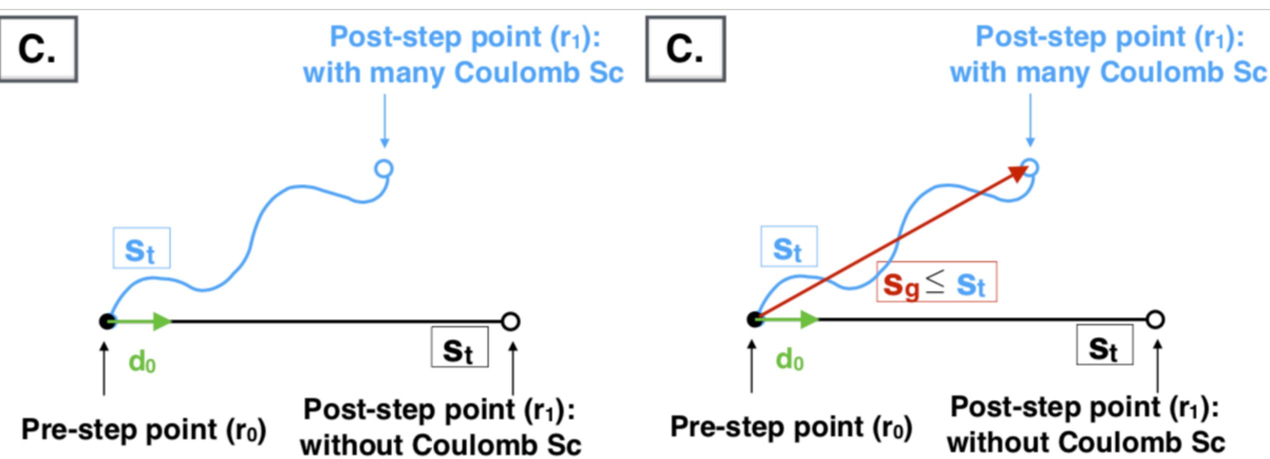

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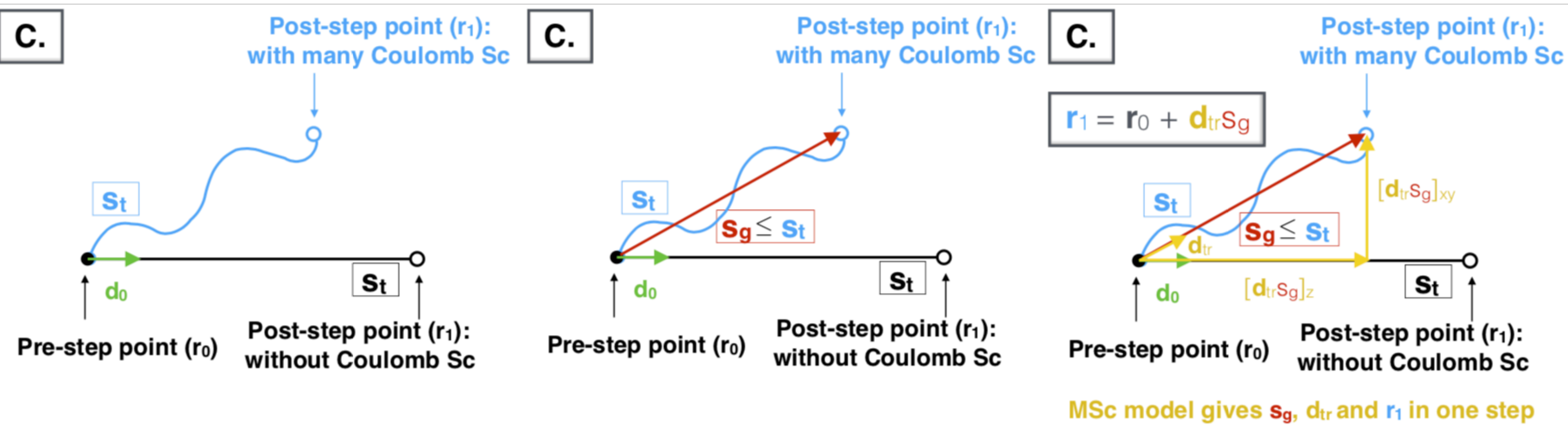

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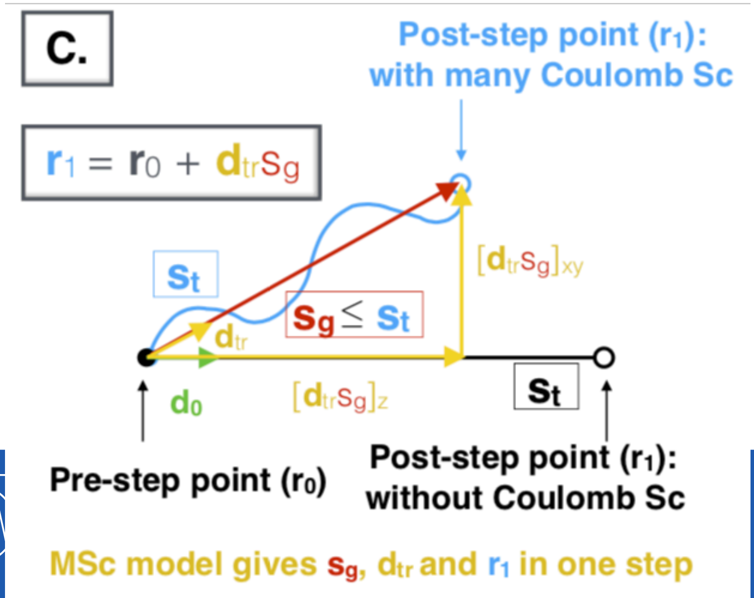
- Particles **with Coulomb** scattering described by **multiple-scattering** model (**C**):
  - MSC provides:
    - ✦ the projection of the transport vector along the original direction ($[d_{tr}s_g]_z$)
    - ✦ the vector of displacement along the perpendicular plane ($[d_{tr}s_g]_{xy}$)
    - ✦ the final direction at the real post-step point (results of many angular deflections)
    - ✦ all these in one step (i.e. without computing the individual interactions)

Multiple coulomb scattering (MSC)

WHAT MAKES IT CHALLENGING?

What makes it challenging?

- **Finite volumes**:
  - **at the pre-step point**, the MSC model needs to compute **everything**, including **the s_g geometrical step length** (transport distance), **based on the s_t true step length:** from s_t to s_g



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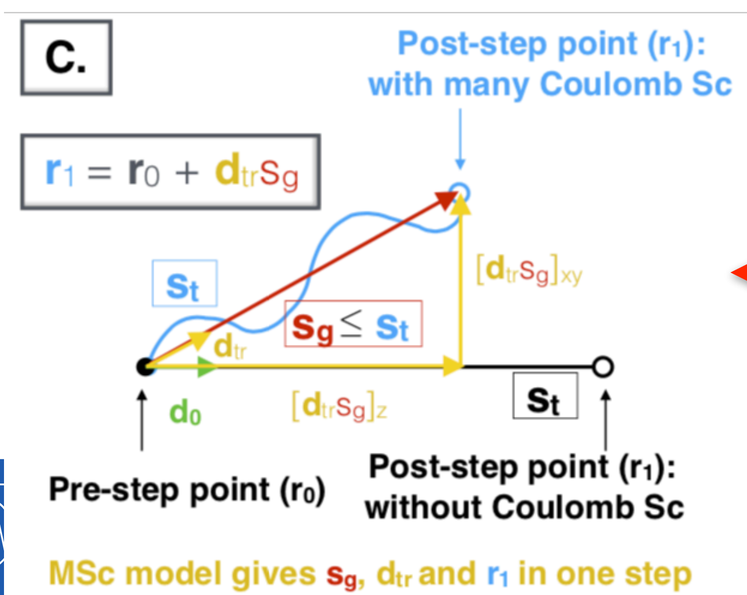
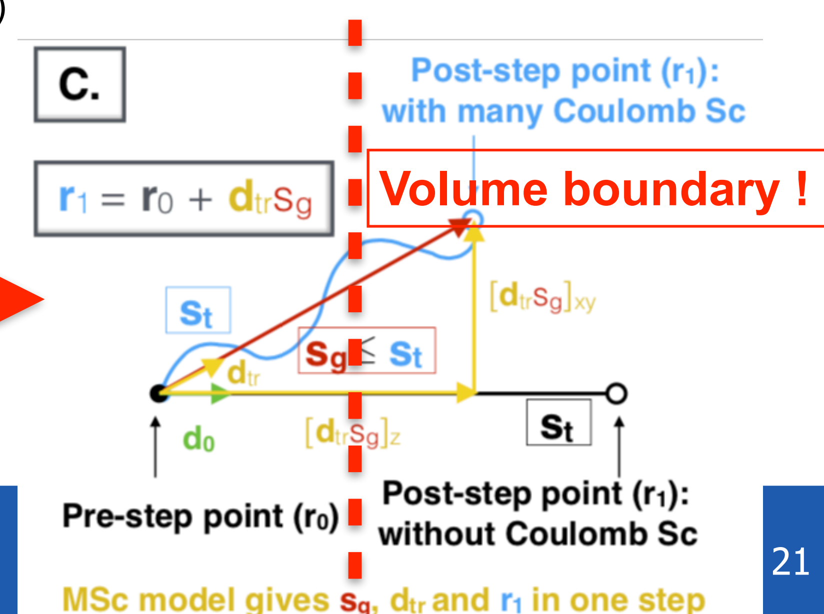
  - however, eventually **the particle might travel a shorter distance** (than $[d_{tr}s_g]_z$) along the original direction **due to hitting a volume boundary**: $s_g' < s_g$ not consistent anymore with s_t :
    - ✦ MSC needs to (re-)**estimate the corresponding true step length s_t'** (inaccuracy)
    - ✦ the **post-step point is on** the volume **boundary**: **no displacement** that results **incorrect final position**
  - each such case is a **clear mistake** in the particle transport: more such mistakes ➡ **less accurate EM shower**
  - **MSC processes** (the models) **impose** an additional **limit on the step** in order to minimise/avoid these mistakes
  - **different** type of **MSC step limits**: tries to relax this step limit (➡ **faster simulation**) ⟺ **maintain accuracy**
    - ✦ **very strong effects** both **to the speed and accuracy of the EM shower simulation**
    - ✦ the main difference, between **the `Geant4` EM physics options** (EMY, EMZ, etc.), **is the MSC model and its step limit type** (and the corresponding parameter values)





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- There are several additional challenges that affects the accuracy, complexity of the MSC model and/or the speed of the simulation:
  - accuracy of the MSC angular distributions and the underlying DCS for elastic scattering
  - accuracy of the displacement algorithm, energy loss correction, etc.
  - stepping must be robust in case of field, large and small volumes, etc.

Multiple coulomb scattering (MSC)

SOME NOTES ON THE GEANT4 MSC MODELS AND THE CORRESPONDING STEP LIMITS

Some notes on the **Geant4** MSC models and the corresponding step limits

- **MSC models**:
  - the two main models for describing e^-/e^+ multiple Coulomb scattering: **G4UrbanMscModel** and **G4GoudsmitSaundersonMscModel**
  - while **G4UrbanMscModel** is an empirical model the **G4GoudsmitSaundersonMscModel** is based on solid theoretical foundations with several higher order corrections providing the most accurate description
  - **G4UrbanMscModel** is the model used in most cases of EM physics constructors (default, EMV, EMX, EMY)
  - **G4GoudsmitSaundersonMscModel** is used in EM physics constructors (EMZ, LIV, PEN, _GS)
  - the MSC stepping algorithm and its parameters are the main differences in these options

- the **EMZ, LIV, PEN** EM physics constructors: **the most accurate EM physics simulation** **(EMZ)**
  - the **G4GoudsmitSaundersonMscModel** is used **with its most accurate settings**
  - the MSC **step limit** is the **UseSafetyPlus** (special version for the GS model):
    - ✦ the MSC step limit is computed based on the safety value
    - ✦ the algorithm switches to single scattering near the volume boundary (**Skin**, measured in elastic MFP units)
    - ✦ makes possible a stepping and **tracking of e^-/e^+ that is free from any errors**
    - ✦ **can be** very **slow** in case of several boundary crossing
  - **UseMottCorrection**: **all** the **higher order corrections** (Mott correction to the angular distributions, scattering power correction, etc.) **are active** (only for the GS MSC model)
  - the corresponding UI commands (the default values in these EM constructors):
    - **/process/msc/StepLimit UseSafetyPlus**
    - **/process/msc/Skin 3**
    - **/process/msc/UseMottCorrection true**

Some notes on the **Geant4** MSC models and the corresponding step limits

- the **EMY** EM physics constructors: **less accurate but a bit faster**
  - the **G4UrbanMscModel** is used **with the UseDistanceToBoundary MSC step limit** type:
    - ✦ the MSC step limit is computed by using the distance to the volume boundary along the current direction
    - ✦ this distance is shortened in order to try to avoid hitting the boundary
    - ✦ the algorithm switches to single scattering near the volume boundary (**Skin**, measured in elastic MFP units)
  - additional step limit components are also used, among which the most important is a kind of heuristic:
    - ✦ the **maximum of a fraction of the initial range (RangeFactor)** of the particle (when entered in the current volume) and **a fraction of the safety** (**SafetyFactor**)
  - the faster than the previous but can lead to errors (especially in case of magnetic field)
  - one can use exactly the same step limit and settings even with the GS MSC model
  - the corresponding UI commands (the default values in this EM constructors):
    - **/process/msc/StepLimit UseDistanceToBoundary**
    - **/process/msc/Skin 1**
    - **/process/msc/RangeFactor 0.04**
    - **/process/msc/SafetyFactor 0.6**

Some notes on the **Geant4** MSC models and the corresponding step limits

- the default EM physics constructors: **less accurate but faster** **(a stronger compromise on accuracy for gaining speed)**
  - the **G4UrbanMscModel** is used **with the UseSafety MSC step limit** type:
    - ✦ there is no single scattering steps near the volume boundary (less accurate boundary crossing)
  - the heuristic is relaxed further (in case of e^-/e^+):
    - ✦ a **function of the fraction of the initial range (RangeFactor)** is used letting the particles to go for a longer step (when it is though to be possible)
  - the **_GS** EM physics constructor provides the same physics setting, including the MSC stepping algorithm and parameters but using the **G4GoudsmitSaundersonMscModel** instead of the **G4UrbanMscModel** model for e^-/e^+
  - the corresponding UI commands (the default values in this EM constructors):
    - **/process/msc/StepLimit UseSafety**
    - **/process/msc/RangeFactor 0.04**
    - **/process/msc/SafetyFactor 0.6**

- the **EMV, EMX** physics constructors: should be used only in case of very large volumes **(a kind of "don't case" setting)**
  - large range factor value (**RangeFactor 0.2**) very relaxed MSC step limit (**Minimal**)
  - on the top of this, displacement is turned OFF in case of **EMX**
  - (while **ApplyCuts** is turned ON in case of **EMV**)

Multiple coulomb scattering (MSC)

SOME NOTES ON THE `GEANT4 EMZ` V.S. `DEFAULT` EM PHYSICS OPTIONS

Some notes on the `Geant4 EMZ` v.s. `default` EM physics options

- as mentioned, main difference between the EM options is the model used for describing the MSC of e^-/e^+, its settings, especially the MSC step limit algorithm
- there are of course additional differences when using moving from the `default` to the direction of `EMZ`: more accurate (more complex) models are used in case of several interactions, different step function parameters in the energy loss related step limit, atomic relaxation is activated, etc.
- when **tuning the EM physics** settings:
  - use `EMZ` to see the most accurate physics simulation results that can be achieved
  - perform the same simulation with the `default` or other relaxed EM physics options to see the gap between the physics accuracy and computing time
  - start to refine the relaxed EM physics constructor settings in order to increase/relax the accuracy and/or the computing time of the simulation

- if you are **happy with the accuracy given by the** `default` **EM settings**, you might **try to relax even further that settings** in order **to gain seed** while the accuracy do not change much:
  - e.g. **increase the MSC range factor** from 0.04 to 0.06 relaxing further the MSC step limits, leading to s**maller number of simulation step** with e^-/e^+ which can **significantly reduce the computing time**
  - keep doing this **as long as** the effects of the corresponding increased rate of MSC related errors (hitting boundary) **do not change much your results**
  - keep in mind that **different EM models can be used in different detector regions**, that provides the possibility for **refining the stepping according to** e.g. **the granularity** of the detector

Some notes on the `Geant4 EMZ` v.s. `default` EM physics options

- if one would like to **decrease the accuracy gap between** the results given by **`EMZ` and the `default` EM physics** constructors **while keeping the computing time under control**:
  - first the origin(s) of the main difference(s) need to be identified
  - keeping in mind, that:
    - ✦ the **main difference** between the EM options **is the MSC model for e-/e+ and its settings**
    - ✦ the `_GS` EM option has the same physics as the `default`, except the MSC model for e-/e+ that is the same as in `EMZ`
    - ✦ but keep in mind, that `_GS` option has **as relaxed MSC stepping algorithm as in the `default`** (actually a bit even more relaxed with a range factor of 0.06 instead of the 0.04)
  - one can easily confirm that the main source of the difference between the results obtain with the `default` and `EMZ` options is indeed the description of the e-/e+ MSC by:
    - ✦ starting from the original `_GS` EM option, **gradually apply more accurate settings** of the underlying **`G4GoudsmitSaundersonMscModel`** in order **to bring closer** and closer to its usage in `EMZ`:
      1. first use the error free stepping: `/process/msc/StepLimit UseSafetyPlus`
      2. if the results are still deviate from that of `EMZ`: `/process/msc/Skin 3`
      3. if the results are still deviate from that of `EMZ`: `/process/msc/UseMottCorrection true`
    - ✦ the above settings brings accuracy of `_GS` EM option from the `default` to that of similar to `EMZ` in most cases !
  - there are different possibilities depending on the results of the above: if those, especially 1. brings the required accuracy:
    - ✦ one might try the `UseDistanceToBoundary` that is a bit relaxed MSC step limit with even decreased values of the `RangeFactor` (< 0.06 - 0.04) and/or higher value of the `Skin` (e.g. 2, 3)
    - ✦ or even the more relaxed `UseSafety` MSC step limit combined with a smaller value of the `RangeFactor` (< 0.06 - 0.04) and/or `SafetyFactor` (< 0.6)

THAT'S IT FOR TODAY