Some special EM physics topics:

III. On the Multiple Coulomb Scattering

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Geneva (Switzerland), 30 March 2021

- Some special EM physics modelling topic to be discussed:
  - I. using secondary production thresholds (2 weeks ago)
  - II. the corresponding stepping and its parameters (last week)
  - III. multiple Coulomb scattering (today)

- There are some ongoing optimisations in which these might help
- We also have some pending issues (regarding the “cuts”, MSC)
- After some discussions with Marilena, it seemed to be a good idea to start working on these together by arranging these meetings
- These informal discussions might also help to tighten our collaboration

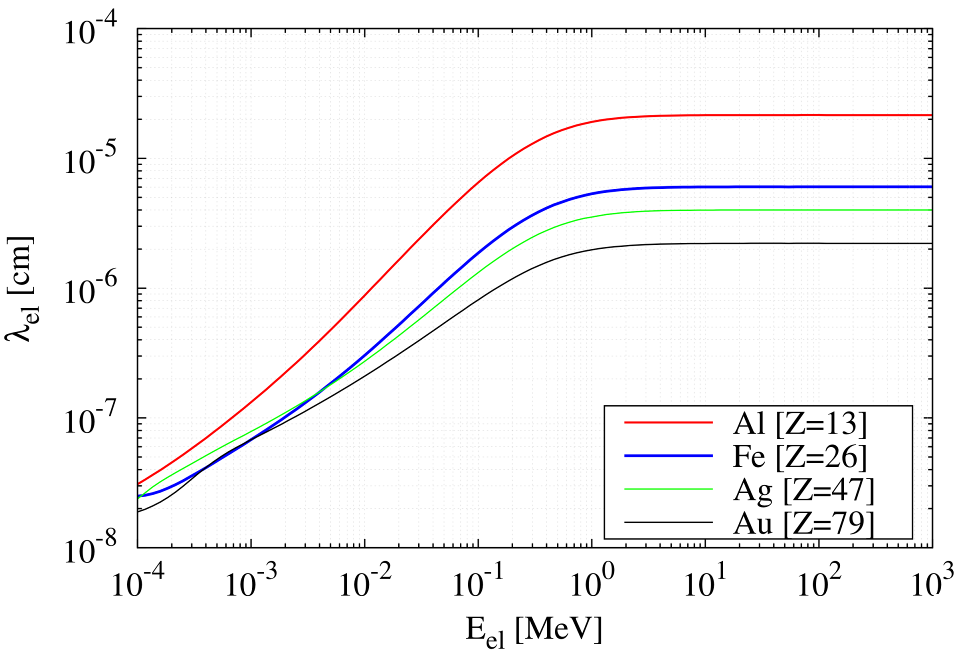
- III. Multiple Coulomb scattering (today)
  - Why do we need to use MCS model?
  - What the MSC model provides?
  - What makes it challenging?
  - Some notes on the `Geant4` MSC models and step limits.
  - Some notes on the `Geant4 EMZ` v.s. `default` EM physics options.

WHY DO WE NEED TO USE MSC MODEL?

Why do we need to use MSC model? 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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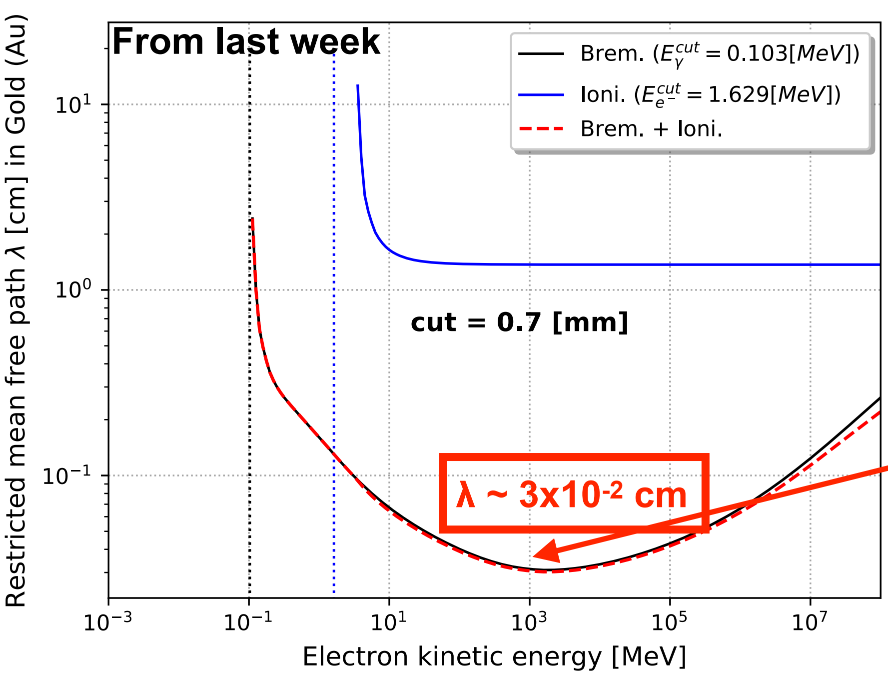
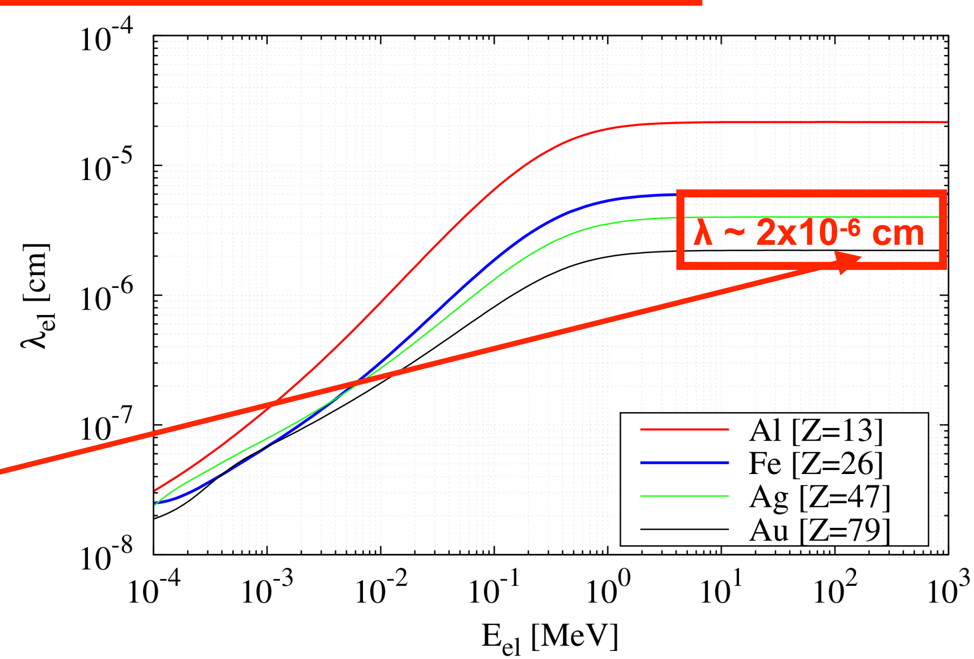
15 000 x more elastic scattering than anything else at 1 [GeV]!





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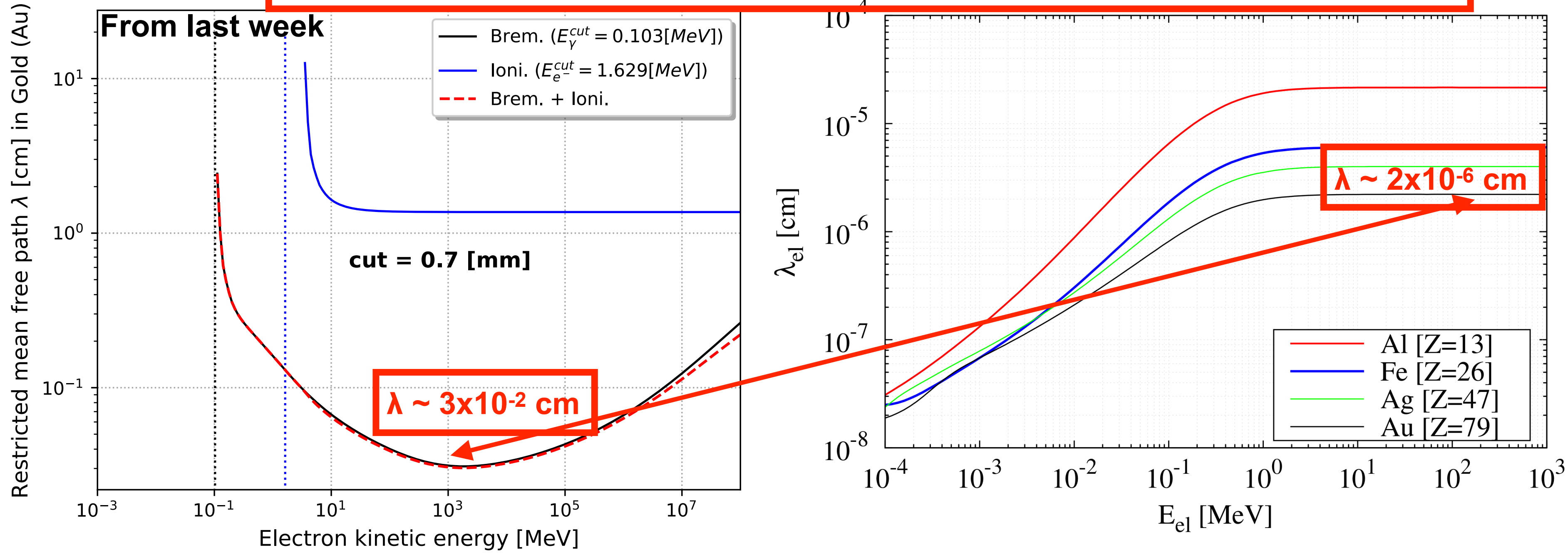

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2. **condensed history simulation**: relies on a **multiple scattering (MSC) model** that accounts the **net effects of many elastic scattering in one step**
   - each particle track is simulated by allowing to make individual **steps** that are **much 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 can be views as **stochastic models** used within the simulation

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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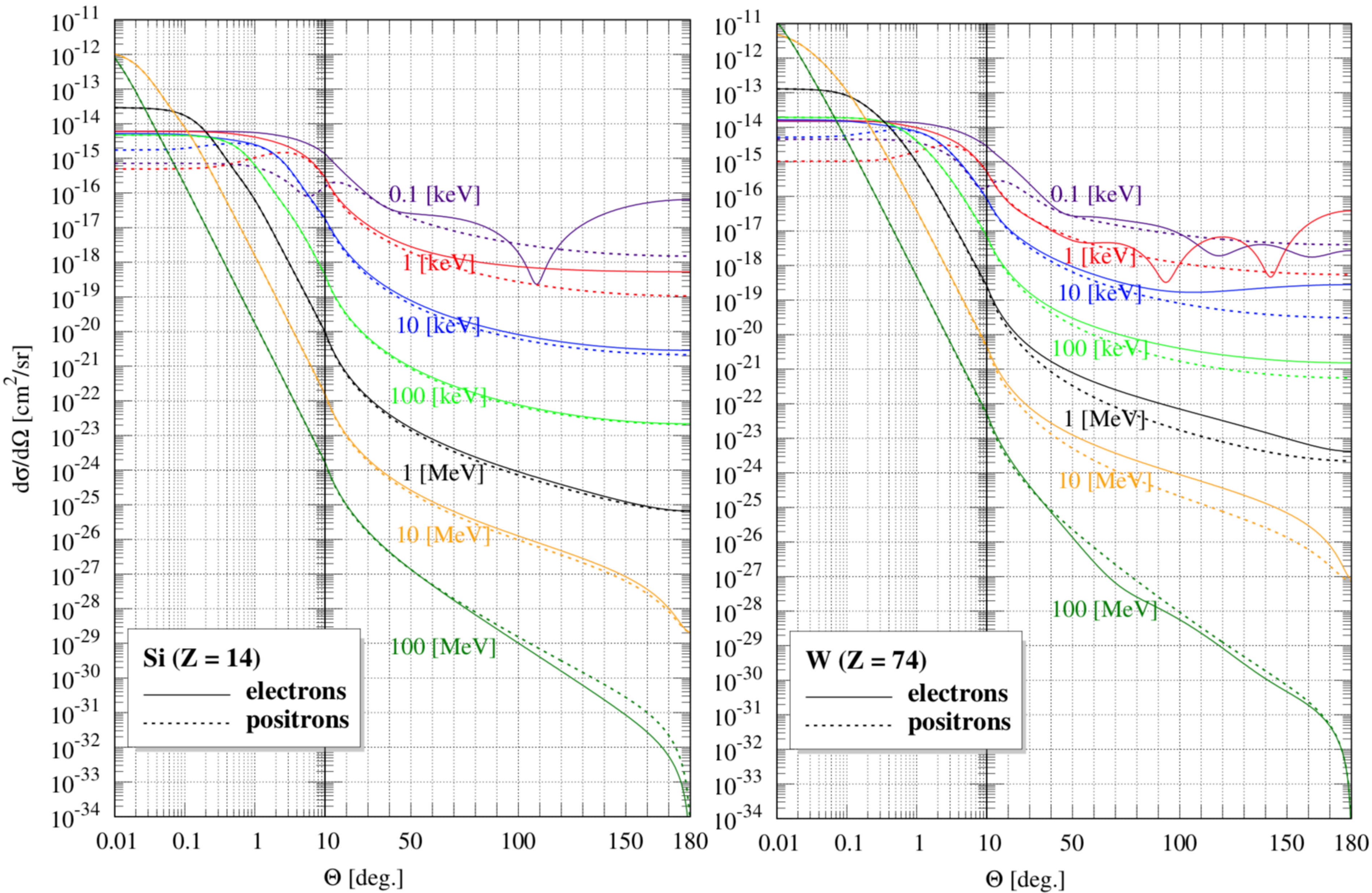

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     - many things become simpler in a *"small angle approximation"*
   - **using** detailed, **event by event simulation to describe *high*(*er*) *angle scattering*** events
   - a similar idea to that used in case of ionisation and bremsstrahlung
   - 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

WHAT THE MSC MODEL PROVIDES

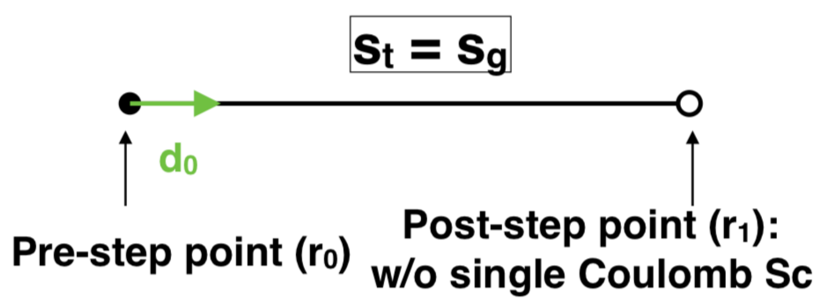
What MSC provides?

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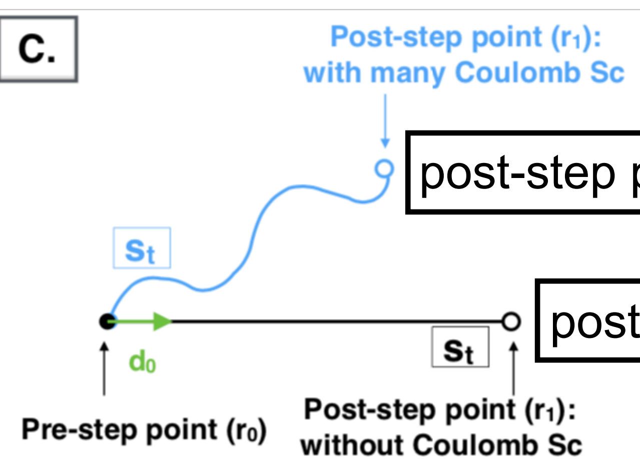
- Particles **with Coulomb** scattering described by **multiple-scattering** model (**C**):

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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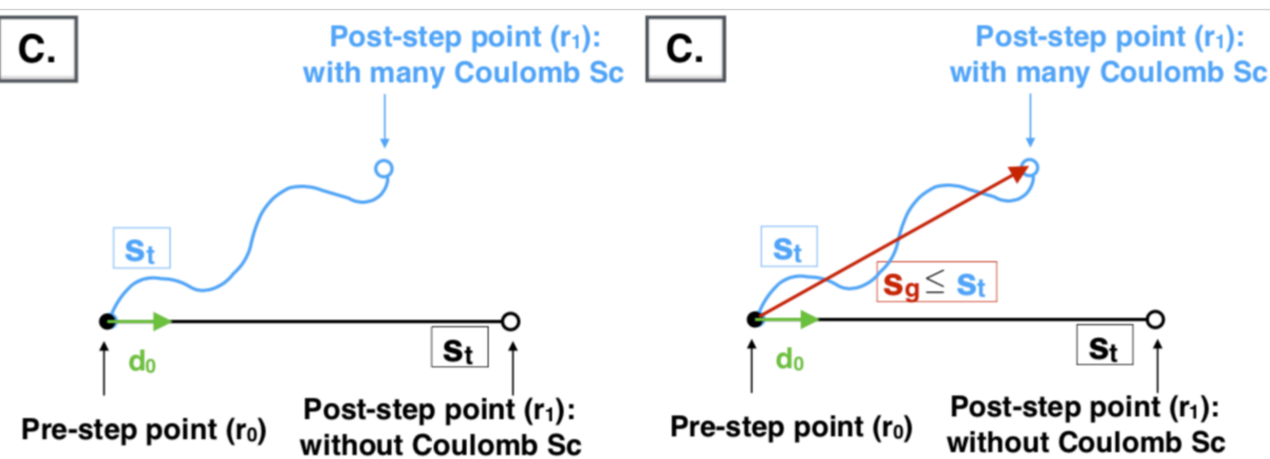

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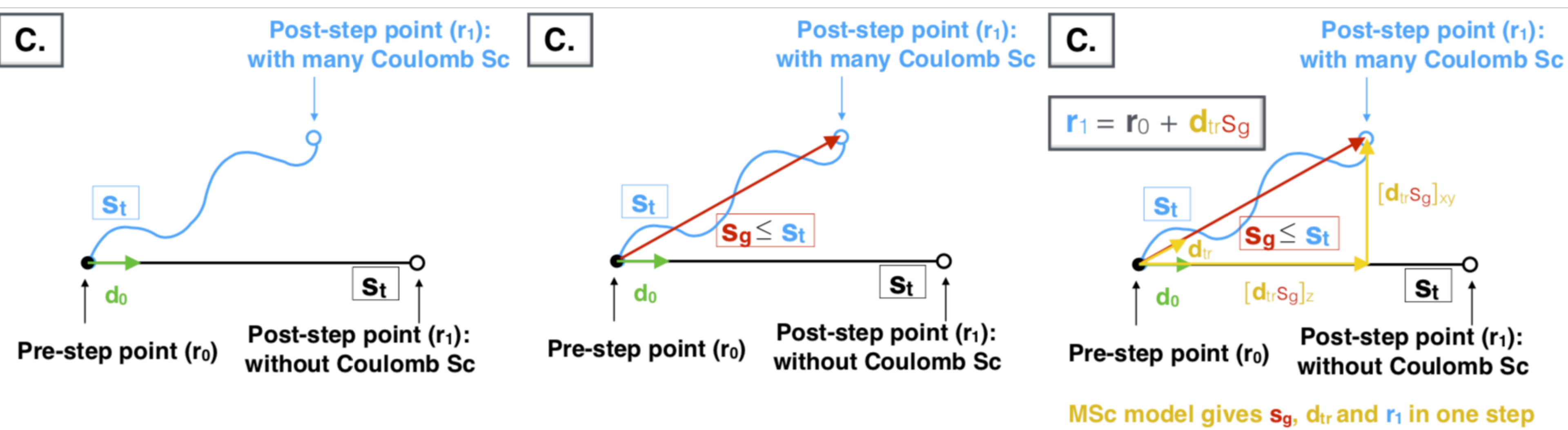

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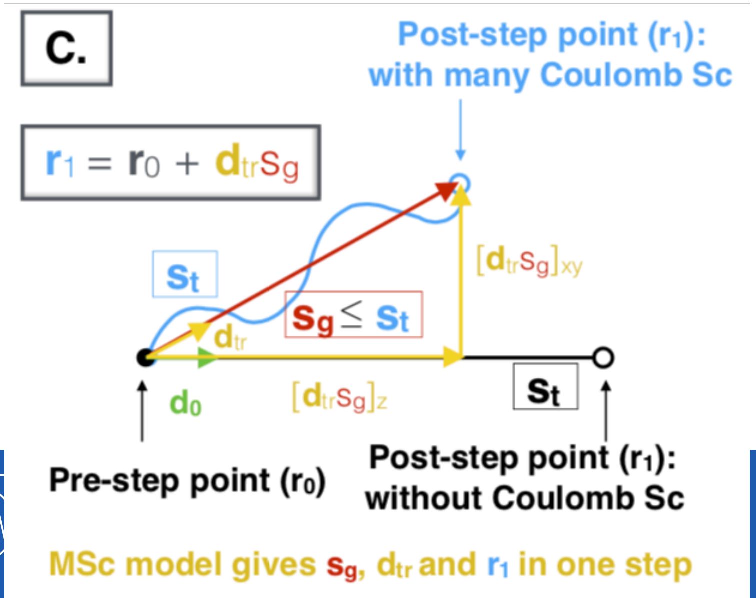
  - MSC provides:
    - ✦ the projection of the transport vector along the original direction ($[d_{tr}s_g]_z$)
    - ✦ the vector of displacement along the perpendicular plane ($[d_{tr}s_g]_{xy}$)
    - ✦ the final direction at the real post-step point (results of many angular deflections)
    - ✦ all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

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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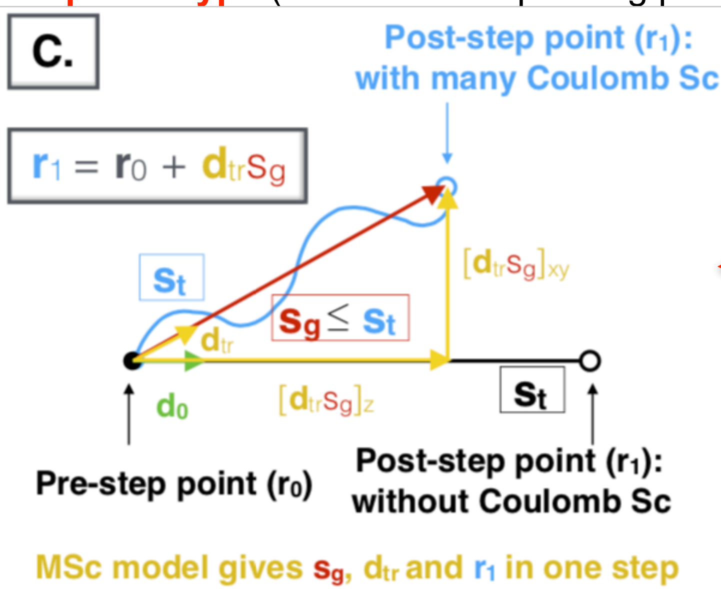
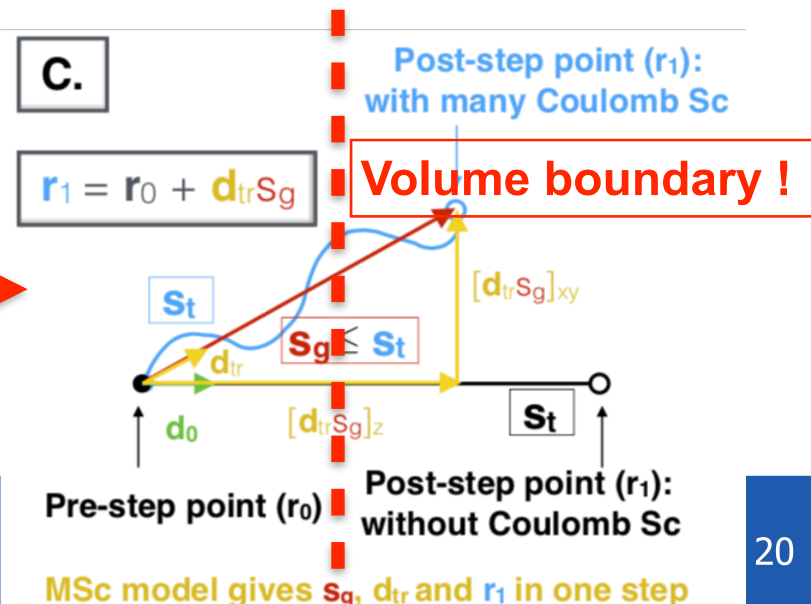
  - however, eventually **the particle might travel a shorter distance** (than $[d_{tr}s_g]_z$) along the original direction **due to hitting a volume boundary**: $s_g' < s_g$ not consistent anymore with s_t :
    - ✦ MSC needs to (re-)**estimate the corresponding true step length s_t'** (inaccuracy)
    - ✦ 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.

SOME NOTES ON THE GEANT4 MSC MODELS AND STEP LIMITS

Some notes on the `Geant4` MSC models and 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**

- 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 step limits

- <u>the default EM physics constructors</u>: 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**

- <u>the **`EMV, EMX`** physics constructors</u>: 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`**)

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