Special EM processes and their role in Geant4-stepping (energy-loss processes and multiple scattering)

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Outline

1. The **G4SteppingManager** and its resposibilities

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3. Pre-step point: step limitation
   - discrete part of the step limit
   - continuous part of the step limitation
   - special continuos processes: transportation, multiple scattering

Outline

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General stepping: `G4SteppingManager`

- A `G4Track` encapsulates both static (`G4ParticleDefinition`) and dynamic properties (energy, momentum, direction,etc.) of a particle
- Geant4 propagates such tracks: one track at a time, step-by-step:
  - from the beginning: first step with a primary or secondary track
  - till the end: particle left the world, particle kinetic energy became zero, dropped below the (user defined) tracking limit or the particle had a destructive interaction (, the user requested to kill the particle)
  - properties of the track (currently under tracking) are updated after each step
  - secondary tracks are pushed into a track stack at each step
- The `G4SteppingManager` is responsible to coordinate one step
  - implements a **general stepping** algorithm: independent from the type of the particle and processes associated to the particle
- We will have a closer look at the step limitation part of this stepping by focusing on charged particles with EM interactions: *Ionization*, *Bremsstrahlung*, *Multiple Scattering* (Why?)

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Ionization and *Bremsstrahlung* are described as *continuous-discrete* interactions:

- secondary electron and gamma production with energy ***below*** the given production energy threshold E^{cut} are **not simulated explicitly**
- instead, these low energy losses described as **continuous** energy losses along the step (i.e. between the pre- and post-step points) based on a mean value
- this mean value is the *restricted stopping power* i.e. mean energy loss in unit step length

$$-\frac{\mathrm{d}E}{\mathrm{d}x}_{\text{rest}}(E;E^{\text{cut}},...) = \int_0^{E^{\text{cut}}} k\frac{\mathrm{d}\sigma}{\mathrm{d}k}(E,..)\mathrm{d}k \tag{1}$$

- secondary electron and gamma production with energy ***above*** the given production energy threshold E^{cut} are **simulated explicitly** as **discrete** interactions
- this discrete interaction probability is determined by the *restricted cross section*

$$\sigma_{\text{rest}}(E;E^{\text{cut}},...) = \int_{E^{\text{cut}}}^{E} \frac{\mathrm{d}\sigma}{\mathrm{d}k}(E,..)\mathrm{d}k \tag{2}$$

that covers interactions only in which the secondary particle will have an energy above the production energy threshold

- the discrete part of the interaction will imply a **discrete step limit** i.e. path length till the next discrete interaction, determined by the **restricted cross section** $\sigma_{\text{rest}}(E; E^{\text{cut}}, ...)$
- the continuous part of the interaction will also imply a **continuous step limit** due to a maximum allowed "**along step energy loss**" value
- due to this "along step energy loss", the particle **kinetic energy** will be **different at the pre- and post-step points**

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First the interactions, that have discrete part, will propose a step length:

- if the target atom density is N and the ***atomic*** interaction ***cross section*** of a process is σ (**assumed to be constant along a step at the moment!**)
- according to the Beer-Lambert law, the p.d.f. of the corresponding ***interaction length*** x (i.e. the probability that the interaction will happen at $x, x+dx$ is $p(x)dx$)

$$p(x) = N\sigma \exp(-xN\sigma) \implies x \in \mathbb{E}\text{xp}(N\sigma) \tag{3}$$

- the mean or expected value of the interaction length x

$$\mathbb{E}(x) = \frac{1}{N\sigma} \equiv \lambda = \frac{1}{\Sigma} \leftarrow x \in \mathbb{E}\text{xp}(N\sigma) \tag{4}$$

  where λ is the ***mean free path*** and $\Sigma = N\sigma = 1/\lambda$ is the ***macroscopic cross section***

- if there are M ***independent interactions*** with the corresponding atomic cross sections $\{\sigma_i\}_{i=1}^M$, mean free paths $\{\lambda_i = 1/N\sigma_i\}_{i=1}^M$, macroscopic cross sections $\{\Sigma_i = N\sigma_i\}_{i=1}^M$ and the M interaction lengths as stochastic variables $\{s_i\}_{i=1}^M$ such that $s_i \in \mathbb{E}\text{xp}(\Sigma_i)$, then the ***shortest interaction length*** i.e. $\eta = \min\{s_1, ..., s_M\}$, $\eta \in \mathbb{E}\text{xp}(\Sigma_t)$, where $\Sigma_t = \sum_{i=1}^M \Sigma_i = \sum_{i=1}^M 1/\lambda_i$ is the ***total macroscopic cross section***

Theorem

If $\{s_1, ..., s_M\}$ *are independent random variables and* $\forall i \in 1, ..., M \;\; s_i \in \mathrm{Exp}(1/\lambda_i)$, *then* $\eta = \min\{s_1, ..., s_M\} \;\in \mathrm{Exp}(\sum_{i=1}^{M} 1/\lambda_i)$

Proof.

By definition, the cumulative distribution function of η as a random variable is equal to the probability that

$$P(\eta < x) = 1 - P(\eta \geq x) = 1 - P(s_1 \geq x, ..., s_N \geq x) = 1 - \prod_{i=1}^{M} P(s_i \geq x)$$
$$= 1 - \prod_{i=1}^{M} (1 - P(s_i < x)) = 1 - \prod_{i=1}^{M} (1 - (1 - \mathrm{e}^{-x/\lambda_i})) = \tag{5}$$
$$1 - \mathrm{e}^{-x\sum_{i=1}^{M} 1/\lambda_i} \implies \eta = \min\{s_1, ..., s_M\} \;\in \mathrm{Exp}(\sum_{i=1}^{M} 1/\lambda_i)$$

□

- usually, the ***total macroscopic cross section*** $\Sigma_t = \sum_{i=1}^{M} \Sigma_i = N \sum_{i=1}^{M} \sigma_i$ is computed and used to sample the path length η to the next discrete interaction point from the exponential distribution, $\eta \in \mathbb{E}\mathrm{xp}(\Sigma_t)$
- then at the post-step point, the type of the discrete interaction is sampled based on the discrete probabilities $p(\mathrm{proc} = i) = \Sigma_i / \Sigma_t$
- in Geant4, ***each discrete process will propose an interaction length*** $s_i \in \mathbb{E}\mathrm{xp}(\Sigma_i \equiv 1/\lambda_i)$ based on their own ***macroscopic cross section*** Σ_i
- then ***the shortest*** $\eta = \min\{s_1, ..., s_M\}$ ***will be selected as discrete step limit***, which is (based on the proof given in the previous slide) equivalent to the previous one
- moreover, with this Geant4 already ***selects the discrete interaction at the pre-step point*** that will(if any[1]) happen at the post-step point i.e. after travelling the path η

[1] there are several cases when the discrete interaction does not happen at all, we will discuss them soon one by one

In case of particles, that have *Ionization* and *Bremsstrahlung*:

- due to the secondary production threshold, the corresponding **restricted macroscopic cross sections** $\Sigma_{\text{rest}}(E; E^{\text{cut}}, \ldots)$ are used to propose the discrete step limit
- due to the continuous part, i.e. the "along step energy losses", the pre-step point E^{pre} and post-step point E^{post} kinetic energies will be different
- the **cross section is not constant along the step**, that must be accounted:
  - a fictive, delta interaction is introduced for each interaction such that, the sum of the real $\Sigma_i^r(E)$ and this delta interaction $\Sigma_i^\delta(E)$ cross section is constant along the step i.e. does not depend on the particle energy

$$\Sigma_i^r(E) + \Sigma_i^\delta(E) = \Sigma_i(\not{E}) \equiv \Sigma_i^{\text{const}} \implies \text{constant along the step} \tag{6}$$

  - and $\Sigma_i^r(E) \leq \Sigma_i^{\text{const}}$ along the step, which implies that $\Sigma_i^{\text{const}} = \max\{\Sigma_i(E)\}$ i.e. maximum along the step
  - this constant macroscopic cross section Σ_i^{const} is used to sample the discrete interaction length(to a real or delta interaction) at the pre-step point
  - at the post-step point, after the along step energy loss is already accounted, the probability that the delta interaction happen is $p(\delta) = 1 - \Sigma_i^r(E^{\text{post}})/\Sigma_i^{\text{const}}$

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So far, the discrete interaction step limits have been considered:

- each discrete process (or discrete part of the process) proposed a step length
- the shortest among these was selected as **the current candidate step length**
- the corresponding process was selected as **the current candidate process**
- **a flag to indicate** that the current candidate step length was proposed by the **discrete part** of the current candidate process
- possible energy loss along the step was considered

At this point, `G4SteppingManager` will ask each continuous part of the processes to propose their own step limits one by one:

- starts with the previous settings regarding the candidate step length, process, and type flag (discrete)
- **each proposed continuous step limit is compared to the current candidate one**
- if the current continuous step limit is shorter than the current candidate, **the candidate step length, process and type flag (continuous)** are updated

continuous part of the step limitation

In case of particles, that have *Ionization* and *Bremsstrahlung* the following continuous step limit function is used:

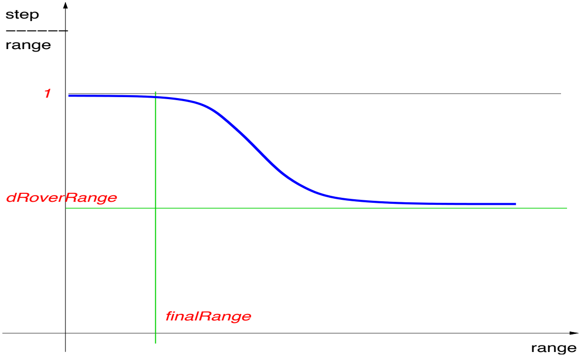
When the particle range $R > \rho_R \equiv finalRange$**:**

$$\Delta S_{lim} = \alpha_R R + \rho_R(1-\alpha_R)\left(2 - \frac{\rho_R}{R}\right)$$

- **default value:** $\rho_R = 1.0[mm]$
- $\alpha_R \equiv dRoverRange$
- **default value:** $\alpha_R = 0.2$
- **at high energies:** $\Delta S_{lim} \approx \alpha_R R$

When the particle range $R < \rho_R$:

- **low energies:** $\Delta S_{lim} = R$



Based on **restricted range**, computed from the **restricted stepping power**!

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special continuos processes: transportation, multiple scattering

So far a candidate physics step length has been selected that is:

- **the current minimum** of the **step length**s, **proposed by all discrete and continuous processes, was selected** as candidate step length
- **it is assumed at this point, that the particle will travel this path length as a straight line along it's original direction**:
  - to the post-step point where the selected discrete interaction takes place ← that discrete interaction proposed the shortest step length
  - to the post-step point where no discrete interaction takes place ← if a continuous interaction proposed the shortest step length

However, there are one or two **special continuous processes left: transportation (always), multiple scattering (possible)**. The end of the step limitation depends:

- if the particle **does not have Coulomb scattering** (**A.**)
- if the particle has **Coulomb scattering** and its **described by** a **single scattering model** i.e. as a **discrete process** (**B.**)
- if the particle has **Coulomb scattering** and its **described by** a **multiple scattering model** i.e. as a **continuous process** (**C.**)

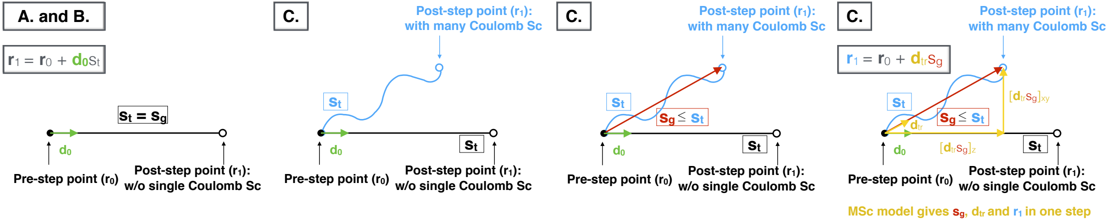
Particles, that do not have Coulomb scattering (**A.**):

- the only remaining (continuous) process is the **transportation** (the last in the list!)
- the above **candidate physical step** length will be **selected** as proposed by the physics since all discrete and all but one (transportation) continuous processes have already proposed their step lengths
- regarding the physics interactions(transportation is still to be called), the particle is supposed to be transported the **selected distance** from the pre-step point **along its original direction**
- **the last continuous process, transportation** will be asked to propose its step limit:
  - if the **particle can be propagated** along its original direction to the selected distance **without hitting volume boundary**, then the **transportation process will accept the proposed step length** (and it will propagate the particle to its proposed post-step point)
  - **otherwise**, the **particle** will be **transported to** the volume **boundary** and the **proposed step length** will be **shortened** by transportation process accordingly

special continuos processes: transportation, multiple scattering

Particles, that have Coulomb scattering and its described by a single scattering model i.e. as a discrete process (**B.**):

- elastic scattering was already accounted in the step limit since it is included in the list of discrete processes
- therefore, everything is the same as in the previous case (**A.**) since the only remaining (continuous) process is the **transportation** (the last in the list!)



Particles, that have Coulomb scattering and its described by a multiple scattering model i.e. as a continuous process (**C.**):

- elastic scattering was removed from the list of discrete interactions $\Longrightarrow$ **elastic scattering is not included in the current step limit** s_t
- therefore, the current candidate step length $\boldsymbol{s_t}$ does not contains the effects of (possible many) elastic scattering
- with elastic scattering, the particle would stop (probably many times) along the currently selected path length $\boldsymbol{s_t}$ and the direction of propagation would change each time
- therefore, the particle would travel the currently selected path length to the next interaction along a curved, zig-zagged trajectory instead of a straight line
- the real post-step point location, the distance (straight line) between the pre- and post step points (**geometrical step length** $\boldsymbol{s_g}$) and final direction of propagation is provided by the Multiple Scattering model

- therefore, before the **transportation (the last), the last but one continuous process, multiple scattering** is asked to provide its step limitation:
  - multiple scattering can further limit the current candidate path length s_t
  - after its own step limitation, multiple scattering will change the current ***true step length*** s_t to the ***geometrical step length*** s_g by computing the corresponding transport distance and ***transport direction*** d_{tr}
- after the **multiple scattering (last but one)**, the **last continuous process, transportation**'s continuous step limitation is invoked, by providing **the transport distance** s_g **instead of the true step length** s_t
- form this point everything is the same as in case of **A.** and **B.**

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- using production cuts is **NOT mandatory** in Genat4: interactions (e.g. *Ionization*) can be described as pure discrete interaction (the appropriate model, process need to be selected)
- using multiple scattering model is **NOT mandatory** neither: single scattering models, processes for elastic scattering are available in Geant4 that will be pure discrete
- using pure discrete processes in the simulation gives exact solution of the transport problem: but **feasible only at low energies!** (below few 100 keV)
- in general, at high energies we need to use condensed history approximation and production cuts to be able to solve the transport problem within acceptable computational time
- these approximations make the transport simulation more complex and naturally introduce some user defined parameters, settings
- understanding more details of these approximations helps the user to provide settings that are the most suitable for their applications
- Geant4 provides several predefined physics lists prepared and maintained by expert physics developers for special application areas

Questions...