Changes in Geant4 Electromagnetics from Release 4.6.1 to 4.9.1

This document was written by Joseph Perl, who is NOT a member of the Geant4 Electromagnetics Working Group, as an attempt to summarize for his own understanding the changes that have occurred in Geant4 electromagnetics since the publication of the significant paper by E. Poon et. al that used release 4.6.1.

The focus is on changes that would be of relevance to medical physics applications, so:

electron/xray at 5 to 25 MeV

proton/ion at around 160MeV

- Note: may have overlooked some of the changes relevant to proton/ion since the initial focus of this paper was just on electron/xray therapy

imaging (lower energy xrays)

The information contained here was obtained by the close reading of Geant4 Release Notes, the Geant4 Physics Reference Manual, various presentations by the Geant4 EM Group, and from notes found in history files and comments in code.
Vladimir Ivantchenko and Laszlo Urban were kind enough to critique the summary and correct mistakes.

Joseph Perl, February 2008

Summary of Key Changes:

- The original multiple scattering model in Geant4 was based on the Lewis formalism using the main term of the Lewis expansion formula. Results from T. Koi (ILC collaboration) and later from E. Poon et. al. showed that the approach was insufficiently precise. Beginning at Geant4 release 8.0, and tuning in subsequent releases, modifications were made to the model based on ideas from Penelope and EGSnrc including:
  - limit the particle step size near geometry boundaries
  - use correlations between lateral displacement and scattering angle
  - add options to use ‘ plural’ single scattering near boundaries - What is "plural" single scattering?
  - Laszlo's comment:
    - There is no plural single scattering. Near to boundaries plural scattering is used if this option is selected.
    - Steps of this algorithm are as follows:

      sample the number of scatterings n from the step length and the elastic mean free path

      perform the n single scattering and compute the final scattering angle summing up the scatterings.
- SAs an option, single Scattering processes were added which can be used to entirely replace multiple scattering if desired. - Already says "if desired", which is same as what Michel expressed as "As an option"
- Models for energy loss fluctuations were substantially revised.

Detailed Description of Changes:

- Multiple Scattering:
    - Multiple Scattering more significantly limits the step size for the particles. This restriction is undertaken using several criteria, and is applied systematically, in all volumes and materials. In addition a model of the correlation between lateral displacement and final direction has been implemented (see the Physics Reference Manual for further information). As a result, most physical observables become more stable when varying step size limit. (4.8.0) - Aren't we also talking about range cut stability? Not just step size stability?
        - Before release 4.8.0, Multiple Scattering limited the step only after boundary crossings (default value of RangeFactor parameter was 0.2).
        - From release 4.8.0, Multiple Scattering limits the step from the start of the track and after boundary crossings (default value of RangeFactor parameter is 0.02). Results in more steps, so slower, but more stable.
        - From release 4.8.0 to 4.8.1, the additional limitation could be turned off to reproduce pre-4.8.0 behavior by setting the boolean value SetMscStepLimitation to false.
        - From release 4.8.2 onward, this boolean was replaced by an enumerator with the following three step limitation choices:
            Minimal - old algorithm from release 4.7.1 and earlier
                - Associated Enum value is fMinimal

            UseSafety - current default, uses geometrical safety
                - Associated Enum value is fUseSafety

            UseDistanceToBoundary - most advanced, recommended for accuracy in the cases where no magnetic field is set (an important issue since in Geant4, unlike many other Monte Carlo codes, tracking is fully supported within magnetic and electric fields)
                - Associated Enum value is fUseDistanceToBoundary
    - The multiple scattering class for hadrons and ions was separated off from that intended to be used for electrons (4.8.2.). Particles other than e+ and e- are now meant to use G4hMultipleScattering rather than G4MultipleScattering. Difference is that G4hMultipleScattering by default has Minimal step limitation.
    - When step limitation is set to UseDistanceToBoundary, there is an additional option to take smaller steps using Single Scattering near the boundary.
        - This is controlled by the parameter "skin" (4.8.2):
            skin = 0: do not take these additional Single Scattering steps
                - designed for high energy simulations with or without magnetic field

            skin=1: take these additional Single Scattering steps before the boundary at distance d < ~ skin*stepmin where stepmin is the approximate value of the elastic mean free path
                - for precision simulations without magnetic field

(UseDistanceToBoundary doesn't work with field)

skin>1: take these additional Single Scattering steps both before and after the boundary

- same limitations as skin=1, but gives improved results for back scatter

- Default value and logic for setting this default (whether it was set in the physics list versus in the process code) were changed several times between release 4.8.2 and release 4.9.1, but have basically settled down by 4.9.1. Some notes are given here as to how these have changed from release to release, but users of the latest code should basically follow the guidance given in the latter part of this note (where it says to use the predefined EM physics builders).

  In release 4.8.2, skin defaulted to 1 for e+ and e-, 0 for other particles (but was reset to 0 for all particles in many of the predefined physics lists).

  From release 4.8.3, skin defaulted to 0 for all particles
- The EM Coordinators suggest that by release 4.9.1, skin=0 is working well enough that the improvements one would see from skin=1 are visible but not dramatic

  Michel: Do not agree on this statement : true for LHC, certainly not for medical applications.

  Joseph: Please advise what I should write here. I am fine with just removing the above statement, or could have some statement about in which cases skin matters and in which cases not (users would certainly welcome some guidance here)

- Changes to calculations used to translate between true path length and geometrical path length. The purpose is to reduce the step-size dependence of results. (4.6.2)
- Change in the angular distribution for e+/e-: correction to the Highland formula for the width of the central part, changes in the numerical values of some other parameters. (4.6.2, 4.7.0)
- The tail of the angular distribution is now material dependent. (4.8.1)
- The scattering in very thin layers is better than the one in version 8.0 - changed the value of the parameter theta0 (4.8.1)
- The simulation of the back-scattering is improved. (seen by 4.8.1 as combined result of many of the above changes).
- Improved results for large angle scattering; better particle transport near geometry boundaries and less cut dependence for sampling calorimeters. (4.8.2)

- Single Scattering
    - Two processes are now available for users who always want to apply Single Scattering (4.9.1). To use these, replace the multiple scattering processes in the physics lists with one or the other of the following:
        - G4CoulombScattering: for any kind of particle in low-density media
        - G4ScreenNuclearRecoil: alternate process only for protons and ions

- Standard Electromagnetic Processes
    - Energy-loss fluctuations: Reduced area of applicability of the model for simulation of fluctuations at very small steps to provide less step dependent results in solid absorbers. Smoothed out sampling of Gaussian fluctuations, when sigma is much bigger than energy loss. The purpose of both changes is to provide results that are less dependent on step size. For example, for steps down to 0.1 microns (in solid materials) the energy deposition distribution in a thin absorber is not dependent on the step limit. (4.6.2)
    - The model of fluctuations of energy loss was modified again later:
        - G4UniversalFluctuations was improved. Affects all particles except ions (4.9.0)
        - G4IonFluctuations was improved. Affects ions (4.9.1)
    - G4eBremsstrahlungModel: fixed problem of energy loss calculation below 10 MeV. (4.8.1)
    - Sub-Cutoff option added (4.8.1): allows use of smaller cuts in vicinity of a geometrical boundary
    - The EM Coordinators recommend that rather than adjusting step limitation, skin and sub-cutoff values directly, most users should just use one of three predefined EM physics builders (4.9.0)
        - For High Energy Physics:
        -
            emstandard: current best practice for most cases.
                - applies step limitation type UseSafety and skin=0

            emstandard_opt1: faster but less stable against cuts
                - applies step limitation type Minimal

            emstandard_opt2: slowest but most detailed
                - using sub-cutoff options, which enable lower production thresholds for delta-electrons near geometry boundary

            or any ‘standard’ from TestEm series
        -
        - For Medical Physics:

            physics list can be found in
            example/extended/medical/fanoCavity
            Vladimir Objects:
                - "example is dangerous: the example is very specific, physics processes are modified to test this theorem. I would propose to use Physics Lists from other extended examples which are very similar to each other.

    - the selection of option of msc (skin=0, 1...) for medical applications is not obvious. I would not have a strong point that for HEP skin=0, for medical skin>0. The conclusion should be based on numerical results and be quantitative, for example, skin=0 guarantee precision 2%, skin=2 guarantee 1%. For today we not yet ready to clarify these numbers. We need rediscuss that, may be not via e-email but in person.

  Joseph's Comment:

    - The point of this present document is just to summarize changes that have been made that affect medical users. It is not necessary for this document to provide guidance on physics lists. Certainly we need such a document eventually, but I wasn't intending to get into that in this present document. I only included the first comments about recommendations of physics lists because Vladimir made them with such force. Now that I see that they are so controversial, I think we could just leave this out of the present document.

- Low Energy Electromagnetic Processes
    - First iteration towards new models for photoelectric angular distribution: design iteration and re-implementation of non-polarized Sauter-Gavrila distribution (K-shell approximation). (4.6.2)
    - Fixes to tables manipulation, effective charge, graphite problem and Bremsstrahlung low energy edge of the spectrum. (4.7.0)
    - Revision of G4LowEnergyPhotoelectric to allow for new development of precise angular distributions. (4.7.0)