Mihaly Novak, CERN
Vladimir Ivanchenko, CERN
Michel Maire, IN2P3
Sebastien Incerti, IN2P3

on behalf of the Geant4 electromagnetic working group

ELECTROMAGNETIC PHYSICS - 1

3 - 7 September, 2018

Statndard cathegory
Content

- Electromagnetic (EM) physics overview
  - Introduction
  - Structure of Geant4 EM sub-packages
  - Processes and models

- How to invoke EM physics in Geant4?
  - EM Physics lists
  - How to extract physics?

- Few words on some selected standard models
  - Ionisation
  - Multiple scattering

- Where to find help?
Geant4 EM Packages

- **Standard**
  - $\gamma$, $e\pm$ up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV

- **Muons**
  - up to 1 PeV
  - energy loss propagator

- **X-rays**
  - Cherenkov, Scintillation, Synchrotron, etc.

- **High-energy**
  - processes at high energy ($E>10\text{GeV}$)
  - physics for exotic particles

- **Polarisation**
  - simulation of polarized beams

- **Optical**
  - optical photon interactions

- **Low-energy**
  - Livermore library $\gamma$, $e^-$ from 10 eV up to 1 GeV
  - Livermore library based polarized processes
  - PENELLOPE code rewrite, $\gamma$, $e^-$, $e^+$ from 100 eV up to 1 GeV (2008 version)
  - hadrons and ions up to 1 GeV
  - atomic de-excitation (fluorescence + Auger)

- **Geant4-DNA**
  - microdosimetry models for radiobiology (Geant4-DNA project) from 0.025 eV to 10 MeV

- **Adjoint**
  - Reverse Monte Carlo simulation from the volume of interest back to source of radiation

- **Utils**
  - general EM interfaces
Gamma and Electron Transport

- **Photon processes**
  - $\gamma$ conversion into $e^+e^-$ pair
  - Compton scattering
  - Photoelectric effect
  - Rayleigh scattering
  - Gamma-nuclear interaction in hadronic sub-package

- **Electron and positron processes**
  - Ionisation
  - Coulomb scattering
  - Bremsstrahlung
  - Positron annihilation
  - Production of $e^+e^-$ pairs
  - Nuclear interaction in hadronic sub-package

- Suitable for HEP & many other Geant4 applications with electron and gamma beams

Geant4 EM Physics-1, Lund University, Lund, Sweden, 3 - 7 September, 2018
Software Design of EM Physics

- Uniform coherent approach for all EM packages – low energy and high energy models may work together

- A physical interaction or process is described by a process class
  - For example: G4ComptonScattering
    - Assigned to Geant4 particle types in Physics List
  - Three EM base processes:
    - G4VEmProcess
    - G4VEnergyLossProcess
    - G4VMultipleScattering

- A physical process can be simulated according to several models, each model being described by a model class
  - Naming scheme: « G4ModelNameProcessNameModel »
    - For example: G4LivermoreComptonModel or G4PolarizedComptonModel
  - Models can be assigned to certain energy ranges and G4Regions
  - Inherit from G4VEmModel base class

- Model classes provide the computation of
  - Cross section and stopping power
  - Sample selection of atom in compound
  - Final state (kinematics, production of secondaries...)
How to Invoke EM Physics in Geant4?
A Physics list is one of the mandatory user classes. It’s the general interface between the physics, the user needs and the Geant4 kernel.

List of particles: for which EM physics processes are defined:
- $\gamma$, $e^\pm$, $\mu^\pm$, $\pi^\pm$, $K^\pm$, $p$, $\Sigma^\pm$, $\Xi^-$, $\Omega^-$, anti($\Sigma^\pm$, $\Xi^-$, $\Omega^-$)
- $\tau^\pm$, $B^\pm$, $D^\pm$, $D_s^\pm$, $\Lambda_c^+$, $\Sigma_c^+$, $\Sigma_c^{++}$, $\Xi_c^+$, anti($\Lambda_c^+$, $\Sigma_c^+$, $\Sigma_c^{++}$, $\Xi_c^+$)
- $d$, $t$, He3, He4, GenericIon, anti($d$, $t$, He3, He4)

The G4ProcessManager of each particle maintains a list of processes.

Geant4 provides several configurations of EM physics lists called constructors (G4VPhysicsConstructor) in the physics_lists library of Geant4.

These constructors can be included into a modular Physics list in a user application (G4VModularPhysicsList).
- Urban multiple scattering for $e^-/e^+$ below 100 MeV only
  - WentzelVI + Single scattering above (mixed simulation model)
- WentzelVI + single scattering for muons and hadrons
- Urban multiple scattering model for ions

<table>
<thead>
<tr>
<th>Constructor</th>
<th>Components</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>G4EmStandardPhysics</td>
<td>Default (QGSP_BERT, FTFP_BERT...)</td>
<td>ATLAS, and other HEP productions, other applications</td>
</tr>
<tr>
<td>G4EmStandardPhysics_option1</td>
<td>Fast due to simple step limitation, cuts used by photon processes (FTFP_BERT_EMV)</td>
<td>Similar to one used by CMS, good for crystals, not good for sampling calorimeters</td>
</tr>
<tr>
<td>G4EmStandardPhysics_option2</td>
<td>Experimental: updated photon models and bremsstrahlung on top of Opt1</td>
<td>Similar to one used by LHCb</td>
</tr>
</tbody>
</table>
**Combined EM Physics List Constructors**

- **Focus on accuracy instead of maximum simulation speed**
- **Ion stopping model based on the ICRU'73 data**
  - Step limitation for multiple scattering using `UseDistanceToBoundary` option
- **Strong step limitation by the ionisation process defined per particle type**
- **Recommended for hadron/ion therapy, space applications**

<table>
<thead>
<tr>
<th>Constructor</th>
<th>Components</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>G4EmStandardPhysics_option3</td>
<td>Urban MSC model for all particles</td>
<td>Proton/ion therapy</td>
</tr>
<tr>
<td>G4EmStandardPhysics_option4</td>
<td>Most accurate combination of models per particle type, energy range (GS-MSC, Mott correction, error-free stepping)</td>
<td>Goal to have the most accurate EM physics</td>
</tr>
<tr>
<td>G4EmLivermorePhysics</td>
<td>Livermore models for γ, e⁻ below 1 GeV, Standard models above 1 GeV</td>
<td>Livermore low-energy electron and gamma transport</td>
</tr>
<tr>
<td>G4EmPenelopePhysics</td>
<td>Penelope models for γ, e± below 1 GeV, Standard models above 1 GeV</td>
<td>Penelope low-energy e± and gamma transport</td>
</tr>
</tbody>
</table>
## Experimental EM Physics List Constructors to be used only for Validation

<table>
<thead>
<tr>
<th>Constructor</th>
<th>Components</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>G4EmStandardPhysicsGS</td>
<td>Goudsmit-Saunderson multiple scattering model for e+ - below 100 MeV</td>
<td>May be considered as an alternative to standard Opt0</td>
</tr>
<tr>
<td>G4EmStandardPhysicsWVI</td>
<td>WVI + SS combination</td>
<td>Is good for high energy interactions</td>
</tr>
<tr>
<td>G4EmStandardPhysicsSS</td>
<td>Single elastic scattering for all particles</td>
<td>Mainly for validation and verification</td>
</tr>
<tr>
<td>G4EmLowEPPhysics</td>
<td>Monarsh University Compton scattering model, WVI-LE model, potentially GS model</td>
<td>Used new low-energy models</td>
</tr>
<tr>
<td>G4EmLivermorePolarized</td>
<td>Polarized gamma models</td>
<td>An extension of Livermore physics</td>
</tr>
</tbody>
</table>
Specialised Models per G4Region: Example of Geant4-DNA Physics

- Standard EM physics constructor as a base
- **G4EmConfigurator** is used to add Geant4-DNA models
  - Geant4-DNA models are enabled only in the small **G4Region** for energy below 10 MeV
  - Allowing CPU performance optimization
- From Geant4 10.2 new UI commands are provided allowing such configuration of top of any EM constructor described above
Atomic de-excitation effects

- Atomic de-excitation initiated by other EM processes
  - Examples: photo-electric effect, ionisation by e- and ions (eg. PIXE)
  - Leave the atom in an excited state

- EADL (Evaluated Atomic Data Library) contain transition probabilities
  - Radiative: fluorescence
  - Non-radiative:
    - Auger e-: initial and final vacancies in different sub-shells
    - Coster-Kronig e-: identical sub-shells

- Atomic de-excitation simulation is compatible with both Standard & Low Energy EM categories
  - Are enabled via UI commands

- See more in the talk on Low Energy EM physics
User Interfaces and Helper Classes

- Geant4 UI commands to define cuts and other EM parameters
- G4EmCalculator
  - easy access to cross sections and stopping powers (TestEm0)
- G4EmParameters
  - C++ interface to EM options alternative to UI commands
- G4EmSaturation
  - Birks effect (recombination effects)
- G4ElectronIonPair
  - sampling of ionisation clusters in gaseous or silicon detectors
- G4EmConfigurator
  - add models per energy range and geometry region
How to **extract Physics**?

- Possible to retrieve Physics quantities using a **G4EmCalculator** object
- Physics List should be **initialized**
- Example for retrieving the total cross section of a process with name `procName`, for particle and material `matName`

```cpp
#include "G4EmCalculator.hh"
...
G4EmCalculator emCalculator;

G4Material* material =
    G4NistManager::Instance()->FindOrBuildMaterial(matName);
G4double density = material->GetDensity();
G4double massSigma = emCalculator.ComputeCrossSectionPerVolume
    (energy, particle, procName, material)/density;
G4cout << G4BestUnit(massSigma, "Surface/Mass") << G4endl;
```

- A good example: `$G4INSTALL/examples/extended/electromagnetic/TestEm0`
  Look in particular at the **RunAction.cc** class
Comment on Physics Lists

- Physics List may be prepared by any user from scratch
  - At early Geant4 stages this was the recommendation but not now !!!
- Why Geant4 is trying to provide many alternative variants of EM physics constructors?
  - Geant4 physics constructors are validated technically and physically by the Geant4 collaboration for each reference Geant4 version
  - Different user groups and Geant4 developers may communicate their results obtained in the same conditions
Ionisation and multiple scattering are main components of the condense history approach of Monte Carlo simulation.
Hadron and ion ionisation

- Bethe-Bloch formula with corrections used for $E > 2$ MeV

$$\frac{dE}{dx} = 4\pi N e_0 r^2 \frac{z^2}{\beta^2} \left( \ln \frac{2m_e c^2 \beta^2 \gamma^2}{l} - \frac{\beta^2}{2} \left( 1 - \frac{T_c}{T_{\text{max}}} \right) C \right) + \frac{G - \delta - F}{2} + zL_1 + z^2L_2$$

- C – shell correction
- G – Mott correction
- $\delta$ – density correction
- F – finite size correction
- $L_1$ – Barkas correction
- $L_2$ – Bloch correction
- Nuclear stopping
- Ion effective charge

- Bragg peak parameterizations for $E < 2$ MeV
  - ICRU’49 and NIST databases
Simulation of a Step of a Charged Particle

- Values of mean dE/dx, range and cross section of δ-electron production are pre-computed at the initialisation stage of Geant4 and are stored in G4PhysicsTables.

- At run time for each simulation step a spline interpolation is used for interpolation of a table to get mean energy loss.

- At each step a sampling of energy loss fluctuation is performed.
  - The interface to a fluctuation model G4VEmFluctuationModel.

- The cross sections of δ-electron production and bremsstrahlung are used to sample production above the threshold $T_{\text{cut}}$ at PostStep.

- If PIXE de-excitation is active then fluorescence and Auger electron production is sampled AlongStep.

- More on the stepping and the influence of EM processes later !!!
Geant4 Models of Energy Loss Fluctuations

- **Urban model** based on a simple model of particle-atom interaction
  - Current default
  - Atoms are assumed to have only two energy levels $E_1$ and $E_2$
  - Particle-atom interaction can be
    - an excitation of the atom with energy loss $E = E_1 - E_2$
    - an ionization with energy loss distribution $g(E) \sim 1/E^2$

- **PAI model** uses photo absorption cross section data
  - At each step internally all energy transfers below production threshold are sampled to get total energy deposition at a step
    - production of secondary $e^-$ or $\gamma$ only above the threshold
  - Slow model, should be applied for sensitive region of detector only
    - Silicon or gaseous detectors
Step limitation by ionisation process

- To guarantee precision of computation, step size should be limited
- Step limit $S$ is defined by stepping function
  - It takes into account the particle range $R$ and two parameters, $k$ (dRoverRange) and $\rho$ (finalRange)
  - Can be defined via c++ interface or UI command
    - /process/eLoss/StepFunction 0.1 50 um
  - Default values 0.2 and 1 mm
- More on this and its role in stepping later !!!

$$S/R = k + \rho/R \cdot (1-k) \cdot (2-\rho/R)$$
Multiple Scattering (MSC)

- The algorithm performs simulation of many elastic scatterings at a step of a particle
  - The physics processes and the geometry select the step length; MSC performs the \( t \leftrightarrow z \) transformation only
  - Sampling of scattering angle \((\theta, \Phi)\)
  - Computing of displacement and relocation of particle PostStep
- To provide accurate simulation on geometry interface between different materials MSC step limitation is applied
  - Simple
  - UseSafety
  - UseSafetyPlus
  - UseDistanceToBoundary
- Other step limit parameters:
  - RangeFactor – is the most important
  - Geometry factor
  - Skin
- More on this and its role in stepping later !!!
### MSC and Single Scattering Models

<table>
<thead>
<tr>
<th>Model</th>
<th>Particle type</th>
<th>Energy limit</th>
<th>Specifics and applicability</th>
</tr>
</thead>
<tbody>
<tr>
<td>Urban (L. Urban 2006)</td>
<td>Any</td>
<td>-</td>
<td>Default model for electrons and positrons below 100 MeV, (Lewis 1950) approach, tuned to data, used for LHC production.</td>
</tr>
<tr>
<td>Screened Nuclear Recoil (Mendenhall and Weller 2005) TestEm5</td>
<td>p, ions</td>
<td>&lt; 100 MeV/A</td>
<td>Theory based process, providing simulation of nuclear recoil for sampling of radiation damage, focused on precise simulation of effects for space applications</td>
</tr>
<tr>
<td>Goudsmit-Saunderson (M. Novak, latest version 10.4)</td>
<td>e⁺, e⁻</td>
<td>-</td>
<td>Theory based angular distributions (Goudsmit and Saunderson 1950). Mott correction and several stepping option including error-free (Kawrakov et al. 1998), precise electron transport</td>
</tr>
<tr>
<td>Coulomb scattering (2008)</td>
<td>Any</td>
<td>-</td>
<td>Theory based (Wentzel 1927) single scattering model, uses nuclear form-factors (Butkevich et al. 2002), focused on muons and hadrons</td>
</tr>
<tr>
<td>WentzelVI (2009)</td>
<td>Any</td>
<td>-</td>
<td>MSC for small angles, Coulomb Scattering (Wentzel 1927) for large angles, focused on simulation for muons and hadrons; low-energy model is applicable for low-energy e-</td>
</tr>
<tr>
<td>LowEnergyWentzelVI (2014)</td>
<td>Any</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>Electron Coulomb scattering (2012)</td>
<td>e⁺, e⁻</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

**Combined multiple and single scattering model:** G4WentzelVIModel + G4eCoulombScatteringModel

Applied for high energy e⁺⁻, muons, hadrons

Geant4 EM Physics-1, Lund University, Lund, Sweden, 3 - 7 September, 2018
WHERE to Find Help?
List of Main Geant4 Documents and Tools

- **See documentation at:** [https://geant4.web.cern.ch/support](https://geant4.web.cern.ch/support)
  
  a. Introduction to Geant4
  b. Installation Guide
  c. Application Developers
  d. Toolkit Developers Guide
  e. Physics Reference Manual
  f. Physics List Guide
Suggestions

- The list of available **EM processes and models** is maintained by the EM working groups, see more in the EM **web pages**
  - [https://geant4.web.cern.ch/collaboration/working_groups/electromagnetic](https://geant4.web.cern.ch/collaboration/working_groups/electromagnetic)

- Geant4 **extended and advanced examples** show how to use EM processes and models
  - Located in `$G4INSTALL/examples`

- Visit the Geant4 **HyperNews forum**, section “electromagnetic processes” for discussion

- Use Geant4 **bug report system** for problems

- **Your feedback** is always welcome
A web-based verification tool has been developed for easy comparison of EM physics results obtained with different Geant4 version, and with measurements obtained with measurements.

https://geant4-tools.web.cern.ch/geant4-tools/emtesting/
To learn more
$G4INSTALL/examples/extended/electromagnetic

Check basic quantities

Total cross sections, mean free paths ...
Stopping power, particle range ...
Final state: energy spectra, angular distributions
Energy loss fluctuations

TestEm0, Em13, Em14
Em0, Em1, Em5, Em11, Em12
Em14
Em18

Multiple Coulomb scattering

as an isolated mechanism
as a result of particle transport

Em15
Em5

More global verifications

Single layer: transmission, absorption, reflexion, atomic deexcitation, msc
Bragg curve, tallies
Depth dose distribution
Shower shapes, Moliere radius
Sampling calorimeters, energy flow
Crystal calorimeters

Em5
Em7
Em11, Em12
Em2
Em3
Em9

Other specialized programs

High energy muon physics
Other rare, high energy processes
Synchrotron radiation
Transition radiation
Photo-absorption-ionization model

Em17
Em6
Em16
Em8
Em10

Refer to section on extended examples in App. User Guide.
Thank you for your attention!