Simulation of Multiple Coulomb scattering in GEANT4
Single Coulomb scattering

Single Coulomb deflection of a charged particle by a fixed nuclear target.

The cross section is given by the Rutherford formula

$$\frac{d\sigma}{d\Omega} = \frac{r_e^2 Z_p^2 Z^2}{4} \left( \frac{mc}{\beta p} \right) \frac{1}{\sin^4 \theta/2}$$
Multiple Coulomb scattering

Charged particles traversing a finite thickness of matter suffer repeated elastic Coulomb scattering. The cumulative effect of these small angle scatterings is a net deflection from the original particle direction.

If the number of individual collisions is large enough (> 20) the multiple Coulomb scattering angular distribution is gaussian at small angles and like Rutherford scattering at large angles. The Molière theory reproduces rather well this distribution. [Mol48, Bethe53]
Gaussian approximation

The central part of the spatial angular distribution is approximately

\[ P(\theta) \, d\Omega = \frac{1}{2\pi\theta_0^2} \exp \left[ -\frac{\theta^2}{2\theta_0^2} \right] \, d\Omega \]

with

\[ \theta_0 = \frac{13.6 \text{ MeV}}{\beta pc} \, z \, \sqrt{\frac{l}{X_0}} \left[ 1 + 0.038 \ln \left( \frac{l}{X_0} \right) \right] \]

where \( l/X_0 \) is the thickness of the medium measured in radiation lengths \( X_0 \) ([Highland75]).
This formula of $\theta_0$ is from a fit to Molière distribution. It is accurate to $\leq 10\%$ for $10^{-3} < l/X_0 < 10^2$ 

note: the appearance of $X_0$ in the formula is only for convenience.

Others formulas for $\theta_0$ have been developed, starting from the Molière theory. [Lynch91]

**related quantities**

- lateral displacement $r(l)$
- true (or corrected) path length $t(l)$
- projected angular deflection $\theta_{proj}(l)$

they are correlated random variables, for instance needed in Monte Carlo simulation.
Neither the Moliere theory nor the Gaussian approach of MSC give information about the spatial displacement of the particle, they give the scattering angle distribution only. To get a more complete information it is better to start with theory of Lewis which based on the transport equation of charged particles ([Lewis50, Kawrakow98]).
The MSC model used in GEANT4 uses the Lewis theory to simulate the transport of charged particles. In this approach model functions are used to sample the spatial and angle distributions after a step, the theory gives constraints for these model functions (the model functions should give the same moments of the distributions then the theory). The details of the MSC model can be found in the GEANT4 Physics Reference Manual ([PRM]).
Transport of charged particles

A charged particle starts from a given point (origin of the reference frame), moving in a given direction (dir. of the z-axis).

Let $p(r, d, t)$ denote the probability density of finding the particle at the point $r = (x, y, z)$ moving in the direction of the unit vector $d$ after having travelled a path length $t$.

The transport is governed by the transport equation:

$$\frac{\partial p(r, d, t)}{\partial t} + d \cdot \nabla p(r, d, t) = n_{at} \int \left[ p(r, d', t) - p(r, d, t) \right] \frac{d\sigma(\chi)}{d\Omega} d\Omega$$

which can be solved exactly for special cases only.

But this equation can be used to derive different moments of $p$. 
The practical solutions of the particle transport can be classified:

- **detailed (microscopic) simulation**: exact, but time consuming if the energy is not small. Used only for low energy particles.

- **condensed simulation**: simulates the global effects of the collisions during a macroscopic step, but uses approximations.
  EGS, GEANT3 - both use Moliere theory -, GEANT4

- **mixed algorithms**: "hard collisions" are simulated one by one + global effects of the "soft collisions".
  PENELLOPE [Fer93].
MSC model in Geant4, notations

- **true path length or 't' path length** is the total length travelled by the particle. All the physical processes restrict this 't' step.

- **geometrical or 'l' path length** is the straight distance between the starting and endpoint of the step, if there is no magnetic field. The geometry gives a constraint for this 'l' step.

- **path length correction** (transformation) : $t \iff l$
  
  $t \implies l : F(l, t, \lambda)$
  
  $l \implies t : G(t, l, \lambda)$

- **scattering angle distribution**: $f(cos\theta, t, \lambda)$

- **lateral displacement**: $R(t, \lambda)$.
Physics input of the model

first transport mean free path:

\[
\frac{1}{\lambda} = 2\pi n_{at} \int_{-1}^{1} (1 - \cos \chi) \frac{d\sigma(\chi)}{d\Omega} d(\cos \chi)
\]  

(2)

where \(d\sigma(\chi)/d\Omega\) is the differential cross section of the scattering, \(n_{at}\) is the nb of atoms per volume.

i-th transport mean free path is defined similarly with the substitution: \((1 - \cos \chi) \Rightarrow (1 - P_i(cos \chi))\), (i-th Legendre polynomial).

Instead of using the cross section directly the model uses \(\lambda\) and \(\lambda_2\) to calculate the different (spatial and angle) distributions.

Basic assumption of the model: the scattering/transport depend on the physics through a dependence on the \(t/\lambda\) and \(t/\lambda_2\) variables.
Steps of MSC algorithm (are essentially the same for many condensed simulations):

1. selection of step length $\leftrightarrow$ physics processes + geometry 
   (MSC performs the $t \leftrightarrow l$ transformations only)
2. transport to the initial direction: (not MSC business)
3. sample scattering angle $\theta$
4. compute lateral displacement, relocate particle
**STEP 1**

1. take the smallest step length coming from the step
   limitations given by the physics processes (all but MSC)
   \[ t = \min(t_{\text{proc1}}, t_{\text{proc2}}, \ldots, t_{\text{proc}n}) \]

2. do the \( t \to l \) transformation \( F(l, t, \lambda) \mapsto l_{\text{phys}} \)
   done by \texttt{AlongStepGetPhysicalInteractionLength()} of MSC

3. ask step limit \( l_{\text{geom}} \) from geometry

4. take the final (geom.) step size as \( l_{\text{step}} = \min(l_{\text{phys}}, l_{\text{geom}}) \)

5. compute the corresponding true step length
   \[ G(t, l_{\text{step}}, \lambda) \mapsto t_{\text{step}} \]
   done by \texttt{AlongStepDoIt()} of MSC
**Model function** $F(l, t, \lambda)$

Distribution with the theoretical mean values.

\[
F(l, t, \lambda) = \begin{cases} 
(k + 1)/t \ (l/l_0)^k & \text{for } l < l_0 \\
n(k + 1)/t \ [(t - l)/(t - l_0)]^k & \text{for } l \geq l_0 
\end{cases}
\] (3)

where

\[ l_0 = \langle l \rangle + d \ (t - \langle l \rangle) \] (4)

where $\langle l \rangle$ is the mean value of $l$, $d$ is a constant model parameter.

The value of the exponent $k$ is computed from the requirement that $F(l, t, \lambda)$ should give the theoretical mean value for $l$

\[ k = \frac{2 \ < l > - t}{l_0 - \ < l >} \] (5)
The geometrical path length $\Rightarrow$ true path length transformation is performed using the mean values

$$
t = \langle t \rangle = -\lambda \log \left( 1 - \frac{l}{\lambda} \right)
$$

This transformation should be done at volume boundaries only when the final step length comes from the geometry. In all the other cases MSC can take the original value of the true path length!
STEP 3, performed by PostStepDoIt() of MSC

Sample $\theta$ from the model distribution $f(x, t, \lambda) \; (x = \cos \theta)$.

$$f(x, t) = q \{ p f_1(x, t, \lambda) + (1-p) f_2(x, t, \lambda) \} + (1-q) f_3(x, t, \lambda)$$

(7)

$p, q \in [0, 1]$

$f_i(x, t, \lambda)$ are relatively simple functions of $x$ and the variable $\tau = t/\lambda$.

($f_1 \approx$ Gaussian for small angle, $f_2$ has a Rutherford-like tail, $f_3 = \text{const}$).
STEP 4, performed by PostStepDoIt() of MSC compute the mean lateral displacement according to the theoretical formula and change the position of the particle correspondingly.

note: this step is executed only if the particle is ‘far’ from the boundary of the volume.

MSC is a ContinuousDiscreteProcess, until now we have seen AlongStepGetPhysicalInteractionLength() AlongStepDoIt() PostStepDoIt().

What is the task for PostStepGetPhysicalInteractionLength()?

It sets only a ForceFlag in order to ensure that PostStepDoIt() is called at every step.
Simulation results $\Leftrightarrow$ data, the ultimate test of the reliability of MC simulations

- scattering angle distributions
- energy deposit distribution in detectors
- transmission of charged particles ($c_{tr}$, $\theta$ and $T_{tr}$ distr.)
- backscattering of charged particles ($c_{b}$, $\theta$ and $T_{b}$ distr.)
- .....

Geant4 Tutorial - CERN, 13.11.02
L. Urbán (KFKI, Budapest)
Angle distributions, Geant4 $\leftrightarrow$ data

Angular distribution of 15.7 MeV e- after Au foils

- data (18.66 mg/cm²)
- G4 (18.66 mg/cm²)
- data (37.28 mg/cm²)
- G4 (37.28 mg/cm²)
Angular distribution of 15.7 MeV e- after Au foils

- **data (18.66 mg/cm²)**
- **G4 (18.66 mg/cm²)**
- **data (37.28 mg/cm²)**
- **G4 (37.28 mg/cm²)**

**Graph Title:** Angular distribution of 15.7 MeV e- after Au foils

**Axes:**
- **x-axis:** angle (deg)
- **y-axis:** 10⁻¹ to 10⁻⁷

**Legend:**
- Blue circles: data (18.66 mg/cm²)
- Blue line: G4 (18.66 mg/cm²)
- Black circles: data (37.28 mg/cm²)
- Black line: G4 (37.28 mg/cm²)
Angular distribution of 6.56 MeV p after 0.0926 mm Si

- **data**
- **G4**

*(energy loss 1.14 MeV)*
Simulation of Multiple Coulomb scattering in GEANT4

Scattering of 158.6 MeV p in 0.0290 g/cm² Pb

- GEANT4
- Gaussian with measured theta0
- Gaussian with Highland theta0
  mean energy loss 78 keV

angle (deg)
Simulation of Multiple Coulomb scattering in GEANT4

as the previous plot, but GEANT4 $\iff$ GEANT3

Scattering of 158.6 MeV p in 0.0290 g/cm² Pb

angle (deg)
as the previous plot, but GEANT4 $\iff$ GEANT3 with tails.
Simulation of Multiple Coulomb scattering in GEANT4

Scattering of 158.6 MeV p in 20.196 g/cm2 Pb

- GEANT4
- Gaussian with measured theta0
- Highland with T=127.4 MeV

mean energy loss 62.3 MeV
as the previous plot, but GEANT4 $\leftrightarrow$ GEANT3

Scattering of 158.6 MeV p in 20.196 g/cm$^2$ Pb

- GEANT4 Eloss=62.3 MeV
- GEANT3 Eloss=62.4 MeV
Simulation of Multiple Coulomb scattering in GEANT4

Scattering of 241 MeV/c pi+ in 2.16 g/cm² C

- GEANT4
- Gaussian with measured theta₀
  mean energy loss 4.35 MeV
Simulation of Multiple Coulomb scattering in GEANT4

Scattering of 330 MeV/c pi+ in 0.948 g/cm² Pb

- GEANT4
- Gaussian with measured theta0
  mean energy loss 1.06 MeV

projected angle (rad)
Energy deposit distribution in Si detector

Energy deposit of 980 keV e- in 0.3 mm Si

without MSC GEANT4 = GEANT3 → difference comes from the different MSC simulation!
Depth-dose distribution

Energy deposit of 0.5 MeV e- in Al as a function of depth

(error on data ≈ 5 – 10%).
Transmission of e- through layers

Transmission coeff. of 1 MeV e- (Al)

- data
- GEANT4 fr=0.01
- GEANT4 fr=1
- GEANT3

Transmission coeff. (1 keV cut)
Energy spectra of transmitted electrons, G4+data

Energy spectrum of transmitted e\(^{-}\) (Al, T=1 MeV), G4 + data

cut=0.006 mm, fr=0.01

- Red line: 0.32 g/cm\(^2\)
- Black line: 0.22 g/cm\(^2\)
- Blue line: 0.10 g/cm\(^2\)
Energy spectra of transmitted electrons, G3+data

Energy spectrum of transmitted e- (Al, T=1 MeV), G3 + data

- Red line: 0.32 g/cm²
- Black line: 0.22 g/cm²
- Blue line: 0.10 g/cm²

MeV

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1

- 0.10 g/cm²
- 0.22 g/cm²
- 0.32 g/cm²
Backscattering is a difficult problem for condensed simulations. One step to the good direction in the GEANT4 MSC algorithm: limit the step in MSC when entering a volume. Algorithm: 

\[ t_{lim} = f_r \times \max(\lambda, range) \]

where \( f_r \in [0, 1] \). If \( f_r = 1 \) there is no step restriction.

This is NOT the user limit, the step is limited only after entering a volume and the step limit energy and particle dependent!

(Limiting the step length at boundaries is not enough, to get good backscattering we need good angle distribution as well!)
Backscattering of $e^{-} \quad \text{G4+data+G3}$

backscattering coeff. of 60 keV $e^{-}$ for diff. materials

- data
- GEANT4 $fr=0.01$
- GEANT4 $fr=1.$
- GEANT3

$cut = 1 \text{ keV}$

atomic number ($Z$)

GEANT4 Tutorial - CERN, 13.11.02
L. Urbán (KFKI, Budapest)
Backscattering of e- \( \text{G4+data+G3} \)

**Backscattering coeff. of e- (Au, energy dependence)**

(1 keV cut)

![Graph showing backscattering coefficient as a function of energy for electrons in gold. The graph compares data with GEANT4 and GEANT3 simulations.](image-url)
Simulation of Multiple Coulomb scattering in GEANT4

Backscattering of e- G4+data+G3

backscattering coeff. of 40 keV e- (Au)

- data
- GEANT4 fr=0.01
- GEANT4 fr=1
- GEANT3

angle of incidence (deg)
Backscattering of e+ G4+data+G3

backscattering coeff. of 35 keV e+ (Au)

% 100
90
80
70
60
50
40
30
20
10
0

0 10 20 30 40 50 60 70 80 90
angle of incidence(deg)

data
GEANT4 fr=0.01
GEANT3
Simulation of Multiple Coulomb scattering in GEANT4

Backscattering of $e^-$ G4 simulation $\approx$ exp.data not shown here

Energy and angle distribution of backscattered electrons (T0=1 MeV)

![Graph showing energy and angle distribution for different elements (Al, Fe, Sn, Au) with MeV on the y-axis and degrees on the x-axis.](image-url)
Backscattering of e- G4+data

Backscattering coeff. of 40 keV e- (Au)

- data
- GEANT4 fr=0.001
- GEANT4 fr=0.01
- GEANT4 fr=0.1
- GEANT4 fr=1

angle of incidence (deg)

%
Simulation of Multiple Coulomb scattering in GEANT4

Backscattering of e- G3+data

backscattering coeff. of 40 keV e- (Au)

- data
- GEANT3 no stepmax
- GEANT3 stepmax=0.1 range
- GEANT3 stepmax=0.01 range
- GEANT3 stepmax=0.001 range

angle of incidence(deg)

0 10 20 30 40 50 60 70 80 90

0 10 20 30 40 50 50 70 80 90

%
References


[Highland75] V.I.Highland, NIM 129, 497 (1975)


[PRM] GEANT4 Physics Reference Manual,  