

Electromagnetic Physics

http://cern.ch/geant4



Electromagnetic packages in Geant4

- Standard
- Low Energy
- Optical
- Muons
- Different modeling approach
- Specialized according to particle type, energy scope

Electromagnetic physics

- electrons and positrons
- γ, X-ray and optical photons
- muons
- charged hadrons
- ions

High energy extensions

- needed for LHC experiments, cosmic ray experiments...

• Low energy extensions

- fundamental for space and medical applications, dark matter and v experiments, antimatter spectroscopy etc.
- Alternative models for the same process

• Multiple scattering

- energy Bremsstrahlung loss Ionisation
 - Annihilation
 - Photoelectric effect
 - Compton scattering
 - Rayleigh effect
 - g conversion
 - e+e- pair production
 - Synchrotron radiation
 - Transition radiation
 - Cherenkov
 - Refraction
 - Reflection
 - Absorption
 - Scintillation
 - Fluorescence
 - Auger

All obeying to the same abstract Process interface: <u>transparent to tracking</u>



Low Energy Electromagnetic Physics

More information is available from the Geant4 Low Energy Electromagnetic Working Group web site

http://www.ge.infn.it/geant4/lowE/



What is

- A package in the Geant4 electromagnetic package
 - geant4/source/processes/electromagnetic/lowenergy/
- A set of processes extending the coverage of electromagnetic interactions in Geant4 down to "*low*" energy
 - 250 eV (in principle even below this limit)/100 ev for electrons and photons
 - down to the approximately the ionisation potential of the interacting material for hadrons and ions
- A set of processes based on detailed models
 - shell structure of the atom
 - precise angular distributions
- Complementary to the "standard" electromagnetic package

Overview of physics

- Compton scattering
- Rayleigh scattering
- Photoelectric effect
- Pair production
- Bremsstrahlung
- Ionisation
- Polarised Compton
- + atomic relaxation
 - fluorescence
 - Auger effect

following processes leaving a vacancy in an atom

In progress

- More precise angular distributions (Rayleigh, photoelectric, Bremsstrahlung etc.)
- Polarised γ conversion, photoelectric

in two "flavours" of models:

- based on the Livermore Library
- à la Penelope
 - Development plan
 - Driven by user requirements
 - Schedule compatible with available resources

LowE processes based on Livermore Library



Photons and electrons

different approach w.r.t. Geant4 standard e.m. package

- Based on evaluated data libraries from LLNL:
 - EADL (Evaluated Atomic Data Library)
 - EEDL (Evaluated Electrons Data Library)
 - EPDL97 (Evaluated Photons Data Library)

especially formatted for Geant4 distribution (courtesy of D. Cullen, LLNL)

- Validity range: 250 eV 100 GeV
 - The processes can be used down to 100 eV, with degraded accuracy
 - In principle the validity range of the data libraries extends down to $\sim 10 \text{ eV}$
- Elements Z=1 to Z=100
 - Atomic relaxation: Z > 5 (*transition data available in EADL*)

Calculation of cross sections

Interpolation from the data libraries:

$$\log(\sigma(E)) = \frac{\log(\sigma_1)\log(E_2/E) + \log(\sigma_2)\log(E/E_1)}{\log(E_2/E_1)}$$

 E_1 and E_2 are the lower and higher energy for which data (σ_1 and σ_2) are available

Mean free path for a process, at energy E:

$$\lambda = \frac{1}{\sum_{i} \sigma_i(E) \cdot n_i}$$

 n_i = atomic density of the *i*th element contributing to the material composition



Compton scattering

Klein-Nishina
cross section:
$$\frac{d\sigma}{d\Omega} = \frac{1}{4}r_0^2 \frac{hv^2}{hv_0^2} \left[\frac{hv_0}{hv} + \frac{hv}{hv_0} - 2 + 4\cos^2\Theta\right]$$

- Energy distribution of the scattered photon according to the *Klein-Nishina formula*, multiplied by scattering function *F(q)* from EPDL97 data library
- The effect of scattering function becomes significant at <u>low energies</u>
 - suppresses forward scattering
- Angular distribution of the scattered photon and the recoil electron also based on EPDL97

Rayleigh scattering

- Angular distribution: $F(E,q)=[1+\cos^2(q)]\cdot F^2(q)$
 - where F(q) is the energy-dependent form factor obtained from EPDL97
- This process is only available in the *lowenergy* package
 - Not available in the *standard* package

Photoelectric effect

- Cross section
 - Integrated cross section (over the shells) from EPDL + interpolation
 - Shell from which the electron is emitted selected according to the detailed cross sections of the EPDL library
- Final state generation
 - Various angular distribution generators ("naïve", Sauter-Gavrila, Gavrila)
- Deexcitation via the atomic relaxation sub-process
 - Initial vacancy + following chain of vacancies created
- Improved angular distribution in preparation

γ conversion

- The secondary e⁻ and e⁺ energies are sampled using Bethe-Heitler cross sections with Coulomb correction
- e⁻ and e⁺ assumed to have symmetric angular distribution
- Energy and polar angle sampled w.r.t. the incoming photon using Tsai differential cross section
- Azimuthal angle generated isotropically
- Choice of which particle in the pair is e⁻ or e⁺ is made randomly

Photons: mass attenuation coefficient



Comparison against NIST data



$$\chi^2_{\rm N-L}$$
=13.1 – V=20 - p=0.87

20

10

0 07

$$\chi^2_{N-S} = 23.2 - \nu = 15 - p = 0.08$$

LowE accuracy ~ 1%

Photons, evidence of shell effects

photon transmission, Al 1 micrometer



Polarisation

hν

Geant 4







high theta





theory

50

41

Alchen Fals 30 30

.0

Polarisation of a non-polarised photon beam, simulation and theory

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Ratio between intensity with perpendicular and parallel polarisation vector w.r.t. scattering plane, linearly polarised photons

Electron Bremsstrahlung

- Parameterisation of EEDL data
 - 16 parameters for each atom
 - At high energy the parameterisation reproduces the Bethe-Heitler formula
 - Precision is ~ 1.5 %
- Plans
 - Systematic verification over Z and energy



Bremsstrahlung Angular Distributions

Three LowE generators available in GEANT4 6.0 release:

G4ModifiedTsai, G4Generator2BS and G4Generator2BN G4Generator2BN allows a correct treatment at low energies (< 500 keV)



Electron ionisation

- Parameterisation based on 5 parameters for each shell
- Precision of parametrisation is better then 5% for 50 % of shells, less accurate for the remaining shells
- Work in progress to improve the parameterisation and the performance



Electrons: range

Range in various simple and composite materials

Compared to NIST database



G4 Standard

G4 LowE

Electrons - CSDA Range - Aluminium

(Geant4-05-02)



Electrons: dE/dx

Ionisation energy loss in various materials

Compared to Sandia database

More systematic verification planned



Electrons, transmitted

20 keV electrons, 0.32 and 1.04 μm Al



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Energy of the transmitted electron

Geant4 validation vs. NIST database

- All Geant4 physics models of electrons, photons, protons and α compared to NIST database
 - Photoelectric, Compton, Rayleigh, Pair Production cross-sections
 - Photon attenuation coefficients
 - Electron, proton, α stopping power and range
- Quantitative comparison
 - Statistical goodness-of-fit tests
- Other validation projects in progress

NIST Test

- Photon Mass Attenuation Coefficient
- Photon Partial Interaction Coefficient
 - related to the Cross section of a specific photon interaction process
- Electron CSDA range and Stopping Power
- Proton CSDA range and Stopping Power
- α CSDA range and Stopping Power

Elements Be, Al, Si, Fe, Ge, Ag, Cs, Au, Pb, U (span the periodic element table)

Energy range					
photon	1 keV – 100 GeV				
electron	10 keV – 1 GeV				
proton	1 keV – 10 GeV				
α	1 keV – 1 GeV				

Simulation configuration reproducing NIST conditions (ionisation potential, fluctuations, production of secondaries etc.)

Geant 4

Geant4 models: electrons and photons Standard Low Energy EEDL/EPDL Low Energy Penelope

Geant4 models: protons and α Standard Low Energy ICRU49

Low Energy Ziegler 1977 Low Energy Ziegler 1985 Low Energy Ziegler 2000 (Low Energy: free electron gas + parameterisations + Bethe-Bloch)

Dosimetry with Geant4 LowE EM package



Energy deposit in calorimeter

Experimental data

G.J. Lockwood et al.,

"Calorimetric Measurement of Electron Energy Deposition in Extented Media - Theory vs. Experiment", SAND79-0414 UC-34a, 1987.



A. Lechner, M.G. Pia, M. Sudhakar

Geant 4

IEEE NSS 2007 Conf. Rec. - IEEE NPSS Best Student Paper Award

Effect of secondary production threshold

Geant4 Low Energy Electromagnetic

250 eV

EGS

Geant4 Standard Electromagnetic

MCNP

1 keV



Example 5.2. Registration of electromagnetic low energy electron/photon processes.

```
void LowEnPhysicsList::ConstructEM()
theParticleIterator->reset();
while( (*theParticleIterator) () ) {
  G4ParticleDefinition* particle = theParticleIterator->value();
  G4ProcessManager* pmanager = particle->GetProcessManager();
  G4String particleName = particle->GetParticleName();
  if (particleName == "gamma") {
                         = new G4LowEnergyPhotoElectric();
    theLEPhotoElectric
                         = new G4LowEnergyCompton();
    theLECompton
    theLEGammaConversion = new G4LowEnergyGammaConversion();
    theLERayleigh
                        = new G4LowEnergyRayleigh();
    pmanager->AddDiscreteProcess(theLEPhotoElectric);
    pmanager->AddDiscreteProcess(theLECompton);
    pmanager->AddDiscreteProcess(theLERayleigh);
    pmanager->AddDiscreteProcess(theLEGammaConversion);
  3
  else if (particleName == "e-") {
    theLEIonisation = new G4LowEnergyIonisation();
    theLEBremsstrahlung = new G4LowEnergyBremsstrahlung();
    theeminusMultipleScattering = new G4MultipleScattering();
    pmanager->AddProcess(theeminusMultipleScattering,-1,1,1);
    pmanager->AddProcess(theLEIonisation, -1, 2, 2);
    pmanager->AddProcess(theLEBremsstrahlung,-1,-1,3);
```

Processes à la Penelope

- The whole physics content of the Penelope Monte Carlo code has been re-engineered into Geant4 (except for multiple scattering)
 - processes for photons: release 5.2, for electrons: release 6.0
- Physics models by F. Salvat et al.
- Power of the OO technology:
 - extending the software system is easy
 - all processes obey to the same abstract interfaces
 - using new implementations in application code is simple
- Profit of Geant4 advanced geometry modeling, interactive facilities *etc.*
 - same physics as original Penelope

Hadrons and ions

- Variety of models, depending on
 - energy range
 - particle type
 - charge
- Composition of models across the energy range, with different approaches
 - analytical
 - based on data reviews + parameterisations
- Specialised models for fluctuations
- Open to extension and evolution

Hadrons and ions



Interchangeable and transparent access to data sets

Positive charged hadrons

- Bethe-Bloch model of energy loss, E > 2 MeV
- 5 parameterisation models, E < 2 MeV
 - based on Ziegler and ICRU reviews
- 3 models of energy loss fluctuations
- Density correction for high energyShell correction term for intermediate energy



Ziegler and ICRU models

-Chemical effect for compounds

- Nuclear stopping power
- PIXE included





Ziegler and ICRU, Si

-Spin dependent term - Barkas and Bloch terms



Nuclear stopping power



Further activity in progress



Positive charged ions

Scaling: $S_{ion}(T) = Z_{ion}^2 S_p(T_p), T_p = T \frac{m_p}{m_{ion}}$

- $0.01 < \beta < 0.05$ parameterisations, Bragg peak
 - based on Ziegler and ICRU reviews
- $\beta < 0.01$: Free Electron Gas Model

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- Effective charge model
- Nuclear stopping power







Models for antiprotons

- β > 0.5
- $0.01 < \beta < 0.5$
- β < 0.01

Bethe-Bloch formula

Quantum harmonic oscillator model

Free electron gas mode



Options for G4hLowEnergyIonisation

G4hLowEnergyIonisation* hIonisation = new G4hLowEnergyIonisation; hIonisation->Set...();

- •SetHighEnergyForProtonParametrisation(G4double)
- SetLowEnergyForProtonParametrisation(G4double)
- SetHighEnergyForAntiProtonParametrisation(G4double)
- SetLowEnergyForAntiProtonParametrisation(G4double)
- SetElectronicStoppingPowerModel(const G4ParticleDefinition*,const G4String&)
- SetNuclearStoppingPowerModel(const G4String&)
- SetNuclearStoppingOn()
- SetNuclearStoppingOff()
- SetBarkasOn()
- SetBarkasOff()
- SetFluorescence(const G4bool)
- ActivateAugerElectronProduction(G4bool)
- SetCutForSecondaryPhotons(G4double)
- SetCutForSecondaryElectrons(G4double)

Atomic relaxation





Microscopic validation: against reference data

Experimental validation: test beam data, in collaboration with ESA Advanced Concepts & Science Payload Division





Electron emission from Sn - 3 KeV photon Beam



Sn, 3 keV photon beam, electron lines w.r.t. published experimental results

PIXE

- Model based on experimental data
 - Parameterisation of Paul & Sacher data library for ionisation cross sections
 - Uses the EADL-based package of atomic deexcitation for the generation of fluorescence and Auger secondary products
- Current implementation: protons, K-shell



Geant4 parameterisation (solid line)

Experimental data



Further documentation on Geant4 Atomic Relaxation

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

Geant4 Atomic Relaxation

Susanna Guatelli, Alfonso Mantero, Barbara Mascialino, Petteri Nieminen, and Maria Grazia Pia

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IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 3, JUNE 2007

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2007

Validation of Geant4 Atomic Relaxation Against the NIST Physical Reference Data 2007

S. Guatelli, A. Mantero, B. Mascialino, M. G. Pia, and V. Zampichelli

More in preparation (M.G. Pia et al.)





Transition	p-value
KL_2	1
KL_2	1
KM	1
KM_4^2	1
KM_{ϵ}^{\dagger}	1
KN	1
KN_2^2	1
$L_1 M_2$	1
$L_{1}^{1}M_{2}^{2}$	1
L.M.	1
$L_1 M_5^4$	1
$L_1 N_2$	1
$L_1 N_2$	1
L_1N_2	0.997
$L_1 N_2$	1
L ₂ M.	1
$L_2 M_2$	1
$L_2 M_4$	1
L_2N_2 or L_2N_2	1
L_2N_2	1
L ₂ N ₄	1
$L_2 N_4$	1
$L_2 M_1$	1
L_2M_2	1
$L_2 M_2$	1
L	1
L _a M _z	1
L ₂ N ₂ or L ₂ N ₂	1
L _i N ₂	1
L ₂ N ₂	1
\mathbf{L}_{3}	1
<u> </u>	1
	-

Goodness of fit test

Goodness-of-fit test	p-
Anderson-Darling	1 ^{val}
Cramer-von Mises	1 ue
Kolmogorov-Smirnov	1
Kuiper	1
Watson	1

Fluorescence transition probabilities



Experimental reference:

W.T. Elam, B.D. Ravel, J.R. Sieber, *A new atomic database for X-ray spectroscopic calculations,* Radiat. Phys. Chem. 63 (2002) 121–128

Bad but harmless...



25% absolute error \Rightarrow 0.04% error in an experimental use case

Hard to say ...



Controversial experimental data

Hidden for 17 years...



The error is in EADL!

Easy to put a remedy in Geant4 Replace EADL data with Scofield data directly Geant 4 in Geant4 Low Energy data file G4EMLOW

In progress

Extensions down to the eV scale

- In water (for radiobiology studies)
- Other materials (gas, solids)

Difficult domain

- Models must be specialised by material
- Cross sections, final state generation, angular distributions

1st development cycle: Very-low energy extensions

Physics of interactions in water down to the eV scale

Complex domain

- **Physics**: collaboration with theorists
- Technology: innovative design technique introduced in Geant4 (1st time in Monte Carlo)

• Experimental complexity as well

- Scarce experimental data
- Collaboration with experimentalists for model validation
- Geant4 physics validation at low energies is difficult!

S. Chauvie et al., Geant4 physics processes for microdosimetry simulation: design foundation and implementation of the first set of models, IEEE Trans. Nucl. Sci., Vol. 54, no. 6, pp. 2619-2628, Dec. 2007

Geant4-DNA physics processes

Specialised processes for low energy interactions with water

Models in liquid water

- More realistic than water vapour
- Theoretically more challenging
- Hardly any experimental data
- New measurements needed

Status

- 1st β -release Geant 48.12006
- Full release December 2007
- Further extensions in progress

Current focus

– Experimental comparisons

Toolkit: offer a wide choice among available alternative models for each process

Particle	Processes
e⁻	Elastic scattering Excitation Ionisation
р	Charge decrease Excitation Ionisation
Н	Charge increase Ionisation
He++	Charge decrease Excitation Ionisation
He+	Charge decrease Charge increase Excitation Ionisation
He	Charge increase Excitation Ionisation

(Current) Physics Models

	е	р	Н	α He ⁺ He
Elastic	> 7.5 eV Screened Rutherford + empirical <i>Brenner-</i> <i>Zaider</i>			
Excitation	7.5 eV – 10 keV $A_1B_1, B_1A_1,$ Ryd A+B, Ryd C+D, diffuse bands	10 eV – 500 keV Dingfelder 500 keV – 10 MeV Emfietzoglou	100 eV – 10 MeV Dingfelder	Effective charge scaling
Charge Change		100 eV – 10 MeV Dingfelder	100 eV – 10 MeV Dingfelder	from same models as for proton
Ionisation	7 eV – 10 keV <i>Emfietzoglou</i> 1b ₁ , 3a ₁ , 1b ₂ , 2a ₁ + 1a ₁	100 eV – 500 keV <i>Rudd</i> 500 keV – 10 MeV <i>Dingfelder (Born)</i>	100 eV – 10 MeV Dingfelder	Dingfelder

No emotional attachment to any of the models Toolkit: offer a wide choice among many available alternatives

What is behind...

Policy-based class design

- A policy defines a class or class template interface
- Policy host classes are parameterised classes
 - classes that use other classes as a parameter
- Advantage w.r.t. a conventional strategy pattern
 - Policies are not required to inherit from a base class
 - The code is bound at compilation time
 - No need of virtual methods, resulting in faster execution



Weak dependency of the policy and the policy based class on the policy interface

Highly **customizable** design Open to extension

New technique 1st time introduced in Monte Carlo

Geant4-DNA physics process

Handled transparently by Geant4 kernel

G4VProcess (from processes management)

+ AlongStepDolt()

- + AlongStepGetPhysicalInteractionLength()
- + AtRestDolt()
- + AtRestGetPhysicalInteractionLength()

+ PostStepDolt()

- + PostStepGetPhysicalInteractionLength()
- + IsApplicable()



Deprived of any intrinsic physics functionality

Configured by template specialization to acquire physics properties



From cells to plasma...

Proton charge transfer processes for 12 materials

(He, water vapour, N₂, CO, CO₂, hydrocarbons)

Relevant to astrophysics and fusion reactor design



Geant 4

M. Kimura et al., Phys. Rev. A 61, 032708, 2000

How to use policy-based processes

// Definition

typedef G4DNAProcess<G4CrossSectionElasticScreenedRutherford,G4FinalStateElasticScreenedRutherford> ElasticScreenedRutherford; typedef G4DNAProcess<G4CrossSectionElasticScreenedRutherford,G4FinalStateElasticBrennerZaider> ElasticBrennerZaider; typedef G4DNAProcess<G4CrossSectionExcitationEmfietzoglou,G4FinalStateExcitationEmfietzoglou> ExcitationEmfietzoglou; typedef G4DNAProcess<G4CrossSectionExcitationBorn,G4FinalStateExcitationBorn> ExcitationBorn; typedef G4DNAProcess<G4CrossSectionIonisationBorn,G4FinalStateIonisationBorn> IonisationBorn; typedef G4DNAProcess<G4CrossSectionIonisationRudd,G4FinalStateIonisationRudd> IonisationBorn; typedef G4DNAProcess<G4CrossSectionIonisationRudd,G4FinalStateIonisationRudd> IonisationRudd; typedef G4DNAProcess<G4CrossSectionExcitationMillerGreen,G4FinalStateExcitationMillerGreen> ExcitationMillerGreen; typedef G4DNAProcess<G4CrossSectionChargeDecrease,G4FinalStateChargeDecrease> ChargeDecrease; typedef G4DNAProcess<G4CrossSectionChargeIncrease,G4FinalStateChargeIncrease> ChargeIncrease;

// Registration

```
if (particleName == "e-")
```

```
{
```

}

processManager->AddDiscreteProcess(new ExcitationEmfietzoglou); processManager->AddDiscreteProcess(new ElasticScreenedRutherford); processManager->AddDiscreteProcess(new ElasticBrennerZaider); processManager->AddDiscreteProcess(new IonisationBorn);

Physics models and their validation

• S. Chauvie et al.,

Geant4 physics processes for microdosimetry simulation: design foundation and implementation of the first set of models IEEE Trans. Nucl. Sci., vol. 54, no. 6, Dec. 2007

S. Chauvie, P. Nieminen, M. G. Pia
 Geant4 model for the stopping power of low energy negatively charged hadrons
 IEEE Trans. Nucl. Sci., vol. 54, no. 3, pp. 578-584, Jun. 2007

S. Guatelli, A. Mantero, B. Mascialino, P. Nieminen, M. G. Pia
 Geant4 Atomic Relaxation

IEEE Trans. Nucl. Sci., vol. 54, no. 3, pp. 585-593, Jun. 2007

S. Guatelli, A. Mantero, B. Mascialino, P. Nieminen, M. G. Pia, V. Zampichelli
 Validation of Geant4 Atomic Relaxation against the NIST Physical
 Reference Data

IEEE Trans. Nucl. Sci., vol. 54, no. 3, Jun. 2007, pp. 594-603

• K. Amako et al.,

Comparison of Geant4 electromagnetic physics models against the NIST reference data

IEEE Trans. Nucl. Sci., vol. 52, no. 4, pp. 910-918, Aug. 2005

The problem of validation: finding reliable data



Geant 4

To learn more

- Geant4 Physics Reference Manual
- Application Developer Guide
- http://www.ge.infn.it/geant4/lowE



- OO technology provides the mechanism for a rich set of electromagnetic physics models in Geant4
 - further extensions and refinements are possible, without affecting Geant4 kernel or user code
- Two main approaches in Geant4:
 - Standard package
 - Low Energy package

each one offering a variety of models for specialised applications

- Extensive validation activity and results
- More on Physics Reference Manual and web site