

IEEE Nuclear Science Symposium and Medical Imaging Conference Short Course

Simulation Techniques Using Geant4

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This course exploits training material developed by several Geant4 Collaboration members: thanks to all of them!



Hadronic Physics

Basic concepts of simulation with Geant4 a s a general purpose Monte Carlo toolkit



Hadronic physics challenge

- Even though there is an underlying theory (QCD), applying it is much more difficult than applying QED for simulating EM interactions
- We must deal with at least three energy régimes:
 - Chiral perturbation theory (< 100 MeV)
 - Resonance and cascade region (100 MeV 20 GeV)
 - QCD strings (> 20 GeV)
- Within each regime there are several (sub)-models:
 - Many of these are phenomenological

Geant4 approach to hadronics

- Provide a general model framework that allows implementation of processes and models at many levels
- Separate models and processes in framework:
 - Hadronic models and cross sections implement processes → multiple models for the same process (e.g. in different energy ranges)
- Provide processes containing:
 - Many possible models and cross sections
 - Default cross sections for each model

Models still under development

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Geant4 strategy in hadronics

- Provide several optional models and cross section sets in each energy region
- Let the user decide which physics is best:
 - Complex task handled in physics lists → set of physics models attached to the various particles (in given energy ranges)
- Validate new models against experimental data:
 - Extensive and systematic validation program
- Understand the trade-off between performance, physics and general applicability vs. energy

The Geant4 physics lists

- A key point for the user is to choose the proper physics list for his/her own specific application.
- To start:
 - have a look at the physics lists of the advanced examples released with Geant4
 - use one of the educated guess physics lists provided by Geant4 for different use cases

Information to help users choosing the proper physics list is available

http://geant4.cern.ch/support/proc_mod_catalog/

physics_lists/physicsLists.shtml

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Geant4 process

- A process uses cross sections to decide when and where an interaction will occur:
 - GetPhysicalInteractionLength()
 - Many processes will be in competition (one of them will be chosen)
- A process uses an interaction model to generate the final state:
 - DoIt()
- Three types of process (possibly mixed):
 - AtRest, AlongStep (continuous), PostStep
- Each particle has its own process manager
- Each process has a set of models coordinated with energy range manager

Hadronic process

- At rest
 - Stopped muon, pion, kaon, anti-proton
 - Radioactive decay
 - Particle decay (decay-in-flight is PostStep)
- Elastic
 - Same process to handle all long-lived hadrons (multiple models available)
- Inelastic
 - Different processes for each hadron (possibly with multiple models vs. energy)
 - Photo-nuclear, electro-nuclear, mu-nuclear
- Capture
 - Pion- and kaon- in flight, neutron

Geant 4Fission

Hadronic cross sections



Cross sections

- Default cross section sets are provided for each type of hadronic process:
 - Fission, capture, elastic, inelastic
- Can be overridden or completely replaced
- Different types of cross section sets:
 - Some contain only a few numbers to parameterize cross section
 - Some represent large databases (data driven models)
- Cross section management
 - GetCrossSection() \rightarrow sees last set loaded for energy range

Alternative cross sections

• To be used for specific applications, or for a given particle in a given energy range, for instance:

Low energy neutrons

- elastic, inelastic, fission and capture (< 20 MeV)
- Neutron and proton inelastic cross sections
 - 20 MeV < E < 20 GeV
- Ion-nucleus reaction cross sections (several models)
 - Good for E/A < 1 GeV
- Isotope production data
 - E < 100 MeV
- Photo-nuclear cross sections

Information on the available cross sections http://geant4.cern.ch/support/proc_mod_catalog/cross_sections Geant4 Course - M. G. Pia

Final states of hadronic processes: overview of the available models



Different types of models

- Data driven models
- Parametrisation driven models
- Theory driven models

Information on the available models at:

http://geant4.cern.ch/support/proc_mod_catalog/models

Models in hadronic framework



Data driven models (1/2)

• Characterized by using data directly:

- Cross sections
- Angular distribution
- Multiplicity and final states
- To get interaction length and final state, models just interpolate data read from a database:
 - Usually linear interpolation of cross section, and Legendre polynomials

• Examples:

- Coherent elastic scattering (pp, np, nn)
- Radioactive decay (T1/2 and decay channels)
- Neutrons (E < 20 MeV), for isotopes and/or natural elements

Transport of low-energy neutrons

- The energy coverage of these models is from thermal energies to 20 MeV
- The modeling is based on the data formats of ENDF/B-VI, and all distributions of this standard data format are implemented
- Includes cross sections and final state information for elastic and inelastic scattering, capture, fission and isotope production
- The file system is used in order to allow granular access to, and flexibility in, the use of the cross-sections for different isotopes, and channels
- Code in directory: /source/processes/hadronic/models/neutron_hp Geant4 Course - M. G. Pia

G4NeutronHPInelastic

• Currently supported **final states** are:

- (n,ng) (discrete and continuum), (n,n2p), (n,nd), (n,nt), (n,n3He), (n,na), (n,nd2a), (n,nt2a), (n,n2p), (n,n2a), (n,n3a), (n,2na), (n,2np), (n,2nd), (n,2na), (n,2n2a), (n,nX), (n,3n), (n,3np), (n,3na), (n,4n), (n,p), (n,pd), (n,pa), (n,2p),(n,d),(n,da), (n,d2a), (n,dt), (n,t), (n,t2a), (n,3He), (n,a), (n,2a) and (n,3a)
- Available channels for a target isotope depend on the database files in the inelastic/FS directory
- Secondary distribution probabilities are supported
 - isotropic emission
 - discrete two-body kinematics
 - N-body phase-space distribution
 - continuum energy-angle distributions
 - Legendre polynomials and tabulation distribution
 - Kalbach-Mann systematic $A + a \rightarrow C \rightarrow B + b$, C:compound nucleus

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G4NDL (Geant4 Neutron Data Library)

• The data include both **cross sections** and **final states**

- directory \$G4NEUTRONHPDATA
- The data are based on evaluated data libraries
 - Brond-2.1, CENDL2.2, EFF-3, ENDF/B-VI.0, 1, 4, FENDL/E2.0, JEF2.2, JENDL-FF, JENDL-3.1,2, MENDL-2
- The data format is similar ENDF, however it is not the same
- Additional environment variables to control NeutronHP processes:
 - G4NEUTRONHP_NEGLECT_DOPPLER to neglect Doppler broadening (speeds the simulation up),
 - G4NEUTRONHP_SKIP_MISSING_ISOTOPES to force the exact isotope file (do not use natural composition if the file is not available)

Parametrisation driven models

- Depend on both data and theory:
 - Parameterize cross sections, multiplicities, angular distributions
 - Fit of experimental data with appropriate parameterizations, plus some theory
- Final states determined by theory, sampling:
 - Use conservation laws to get charge, energy, etc.
- Examples:
 - Fission
 - Capture
 - LEP, GEISHA-based HEP models \rightarrow see next slide

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Parametrisation driven models

- Based on GEISHA package of GEANT 3.21
- Two sets of models for inelastic scattering of particles in flight:
 - Low energy models LEP: E < 30 GeV
 - /hadronic/models/low_energy
 - High energy models HEP: 10 GeV < E < 15 TeV
 - /hadronic/models/high_energy
- LEP and HEP can be applied to p, n, p, K, L, S, Ξ, a, t and d
- Original approach to primary interaction, nuclear excitation, intra-nuclear cascade and evaporation is kept

Parametrisation driven models

- After the initial interaction of a hadron with nucleons in the nucleus:
 - highly excited hadrons fragmented into more hadrons
 - residual clusters decayed in nucleons and p's
 - remnant nucleus is de-excited by emission of p, n, d, t and a
- LEP and HEP models are fast in terms of CPU but not very detailed
 - to have a more precise simulation, one should use cascade models
- Fission, capture and coherent elastic scattering are also modeled through parameterised models

Hadron elastic scattering

- Parameterized GHEISHA-style (G4LElastic)
 - classical scattering (not all relativistic)
 - simple parameterization of cross section, angular distribution
 - can be used for all long-lived hadron projectiles, all energies
- Alternative (specialized) models for coherent elastic scattering:
 - G4LEpp for (p,p), (n,n): taken from detailed phase-shift analysis, good up to 1.2 GeV
 - G4LEnp for (n,p): same as above
 - G4HadronElastic for (h,A): nuclear model details included as well as interference effects, good for 1 GeV and above, all long-lived hadrons
 - G4QElastic for (p,A), (n,A): parameterization of experimental data by M. Kossov, part of CHIPS modeling

Theory driven models

- Dominated by theory
 - QCD, strings, chiral perturbation theory
- Data used mainly for normalization and validation
- Final states determined by sampling theoretical distributions
- Combined use defined in PhysicsList:
 - Parton string models at high energies,
 - Intra-nuclear transport models at intermediate energies
 - Statistical break-up models for de-excitation...

Theory driven models

- Parton string
 - Projectiles with E > 5 GeV (up to 100 TeV)
 - de-excitation either by CHIPS or pre-compound models
- Chiral invariant phase space, CHIPS
 - All energies
 - Quark-level event generator for the fragmentation of hadronic systems into hadrons
 - Interactions between hadrons are treated as purely kinematic effects of quark exchange
 - Decay of excited hadronic systems is treated as the fusion of two quark-partons within the system
 - Includes non-relativistic phase space of nucleons to explain evaporation

Nuclear de-excitation and break-up Geant 4 Geant 4 Geant 4

FRITIOF-based models

- Handles the formation of strings in the initial collision of a hadron with a nucleon in the nucleus. String fragmentation into hadrons is handled by the Lund fragmentation model.
- De-excitation of the remnant nucleus is handled either by the CHIPS models or by precompound models (see next slides)
- Handles p, n, pions and kaons
- From 15 GeV to 100 TeV

Area of theory-driven models under active development

Bertini cascade

- Collection of theory driven models with parameterisation features:
 - /hadronic/models/cascade
- Intermediate energies ~1 MeV 10 GeV
- Models included:
 - Bertini intra-nuclear cascade (INC) model with excitons
 - Pre-equilibrium model
 - Nucleus explosion model
 - Fission model
 - Evaporation model
- Slower but more detailed than parameterized models

Bertini cascade

- For A>4 a nucleus model is composed of three concentric spheres
- Impulse distribution in each region follows
 Fermi distribution with zero temperature
- Particle treated: p,n, pions, photon evaporation and nuclear isotope remnats
- Final states, will be included for K⁺, K⁻, K⁰, K⁰-bar, Λ, Σ⁺, Σ⁰, Σ⁻, Ξ⁰ and Ξ⁻



Schematic presentation of the intra-nuclear cascade. A hadron with 400 MeV energy is forming an INC history. Crosses present the Pauli exclusion principle in action.

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Binary cascade

- The nucleus is explicitly modeled in **G4BinaryCascade**
 - Nucleons have momentum and are placed in space
 - Momentum taken into account for scattering
 - Hadron-nucleon collisions including re-scattering
 - Particles follow curved trajectories in nuclear potential
 - At end of cascade, the nucleus and exciton system is passed to preequilibrium model (precompound \rightarrow see next slides)
- Binary cascade model handles incident p, n and π
 - valid for incident p, n from 0 to <10 GeV
 - valid for incident π + π from 0 to 1.3 GeV
- A variant of the model, **G4BinaryLightIonReaction**, is valid for incident light ions

Liège cascade model

• INCL 4.2 cascade model (Liège cascade)

 re-engineered from FORTRAN into C hadronic/models/incl

- Handles primary p, n, p, d, t, 3He and α
- Valid from 200 MeV to 3 GeV and for target nuclei from C to U
- Uses ABLA or HETC models for nuclear evaporation below 200 MeV
 - produce p, n, α and nuclear fragments

Area under active development

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Precompound model

 G4PrecompoundModel is used for nucleon-nucleus interactions at low energy and as nuclear deexcitation model within higher-energy models

- e.g. FRITIOF, parameterized, cascades, parton strings ...

- Valid for p,n up to 170 MeV
- Takes a nucleus from a highly-excited state down to equilibrium energy by emitting p, n, d, t, 3He and a
- Once equilibrium is reached, other models called to take care of nuclear evaporation and break-up
- Alternative to CHIPS-based de-excitation

Evaporation models

- Geant4 provides several different implementations for evaporation models:
 - G4Evaporation (default), HETC evaporation, INUCL evaporation and ABLA
- Models predict the final state as results of an excited nucleus break-up by evaporation
 - takes as input A, Z, 4-momentum, angular-momentum, excitation energy
 - produces p, n, g, d, t and α
 - fission of heavy nuclei with A > 65

Hadronic model inventory

http://geant4.cern.ch/support/proc_mod_catalog/models



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I MeV 10 MeV 100 MeV 1 GeV 10 GeV 100 GeV 1 TeV

Ion inelastic interactions

- Many cross section formulae for N-N collisions are included in Geant4
 - Tripathi, Shen, Kox and Sihver
- These are empirical and parameterized formulae with theoretical insights
- G4GeneralSpaceNNCrossSection was prepared to assist users in selecting the appropriate cross section formula
- Final state according to models: G4BinaryLightlon (variant of Binary cascade), G4WilsonAbrasion or G4EMDissociation

G4WilsonAbrasionModel and G4Wilson AblationModel

- G4WilsonAbrasionModel is a simplified macroscopic model for nuclear-nuclear interactions based largely on geometric arguments
- The speed of the simulation is found to be faster than models such as G4BinaryCascade, but at the cost of accuracy
- A nuclear ablation has been developed to provide a better approximation for the final nuclear fragment from an abrasion interaction → deexcitation of nuclear prefragments

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Radioactive decay

- To simulate the decay of radioactive nuclei
- Empirical and data-driven model
- α , β +, β decay and electron capture are implemented
- Data derived from Evaluated Nuclear Structure Data File (ENSDF)
 - nuclear half-lives, level structure for the parent or daughter nuclide, nuclear decay branching ratios, Q-value of the decay process → directory \$G4RADIOACTIVEDATA
- If the daughter of a nuclear decay is an excited isomer, its prompt nuclear de-excitation is treated using the G4PhotonEvapolation → database of γ lines and nuclear levels in \$G4LEVELGAMMADATA
- Internal conversion is also implemented

Using Geant4 hadronic physics



Physics Lists

- The user **must implement a physics list**:
 - Derive a class from G4VUserPhysicsList
 - Define the particles required \rightarrow ConstructParticle()
 - Register models and cross sections with processes and processes with particles \rightarrow ConstructPhysics()
 - Set secondary production cuts \rightarrow SetCuts()
 - In main(), register your physics list with the Run Manager

• Care is required:

- Multiple models, cross sections allowed per process
- No single model covers all energies, or all particles
- Choice of model is heavily dependent on physics studied

Ready-available PhysicsLists

- It is not easy to figure out what is the appropriate physics list for one's own application
 - usually a problem for newcomers!
- 1. Use the **physics lists** of the advanced examples released with Geant4 (many use-cases covered)
- 2. Ready-to-use hadronic physics lists available for different common use-cases, e.g.:
 - Low and high energy nucleon penetration shielding
 - Medical neutron applications
 - Low background experiments (underground)

Info to help users to choose the proper physics list: http://geant4.cern.ch/support/proc_mod_catalog/

physics_lists/physicsLists.shtml

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Webpage for reference physics lists



Given the toolkit nature of Geant4, a choice of physics processes is available. The choices offer either different detail of physics modeling or different physics modeling descriptions. It is the choice of the user to decide how much detail in the physics modeling is needed, weighing the detail against cpu performance. A user can construct his own physics list, or use one of the physics lists offered below, or modify any of the offered physics lists.

Reference Physics Lists

Please see the <u>detailed description</u> for a full description of all reference physics lists including our current understanding of physics performance. The reference physics lists are part of the Geant4 source code and are distributed as an integral part of Geant4 from the <u>Geant4 download area</u>. Physics lists include those originally named 'educated guess physics lists'. Nearly all these lists are suitable for all primary particles and for a wide range of energies. There are four families of lists:

- · LHEP or parameterised modeling of hadronic interactions.
- · QGS, or lists based on a modeling using Quark Gluon String model for high energy hadronic interactions of protons, neutrons, pions, and Kaons.
- FTF, or lists based on a modeling using the FTF model for high energy hadronic interactions of protons, neutrons, pions, and Kaons; FTF is FRITIOF like string model.
- · several more specialised lists.

All of the lists in the first three families share components to attach certain types of processes to groups of particles. The classes of components are:

- · electromagnetic interactions for all particles and electromagnetic processes for leptons and gammas. Three different settings are offered
 - · the default setting using standard parameters tuned for best physics performance
 - using parameters optimised for better CPU performance at the cost slightly less precise physics. This is identified in physics lists by the extension _EMV.
 - · a set of experimental parameters, used by physics lists with the extension _EMX
- Inelastic interactions for hadrons
- Elastic scattering of hadrons off nuclei
- · Capture at rest for negative charged hadrons and muons
- · Decay of unstable particles in flight and at rest
- specialised treatment of low energy neutrons (< 20MeV)

Physics Lists in Geant4 examples

Other Physics Lists

Code Example

```
G4ParticleDefinition* proton=
                                               retrieve the
G4Proton::ProtonDefinition();
                                             process manager
G4ProcessManager* protonProcessManager =
                                                for proton
proton->GetProcessManager();
```

// Elastic scattering create the **process G4HadronElasticProcess*** protonElasticProcess = for elastic new G4HadronElasticProcess(); scattering

```
G4LElastic* protonElasticModel =
                                      LE parametrized model for
new G4LElastic();
```

```
protonElasticProcess->
RegisterMe(protonElasticModel);
```

```
elastic scattering
```

```
register the model to
     the process
```

```
protonProcessManager->
```

```
AddDiscreteProcess (protonElasticProcess);
```

attach the process to proton

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Code example

// Inelastic scattering creates the **G4ProtonInelasticProcess*** protonInelasticProcess process for = new G4ProtonInelasticProcess(); inelastic scattering **G4LEProtonInelastic*** protonLEInelasticModel = new G4LEProtonInelastic(); LEP **model** up protonLEInelasticModel-> to 20 GeV **SetMaxEnergy**(20.0*GeV); protonInelasticProcess-> register LEP model to **RegisterMe**(protonLEInelasticModel); the process **G4HEProtonInelastic*** protonHEInelasticModel = new G4HEProtonInelastic(); HFP model protonHEInelasticModel->SetMinEnergy(20.0*GeV); from 20 GeV protonInelasticProcess ->**RegisterMe**(protonHEInelasticModel); registers HEP model to the process

Code example

G4NeutronInelasticProcess*

theNeutronInelasticProcess = new
G4NeutronInelasticProcess();

G4NeutronHPInelastic* theHPInelastic

= new G4NeutronHPInelastic();

theNeutronInelasticProcess

->**RegisterMe**(theHPInelastic);

create the **process** for neutron inelastic scattering register the data-

driven HP model for neutron inelastic

G4NeutronHPInelasticData* theHPInData

= new G4NeutronHPInelasticData();

theNeutronInelasticProcess->

AddDataSet(theHPInData);

HP cross section table (data-driven)

attach the cross section to the process

Code example

table of ions and defined particles

const G4IonTable *theIonTable =
 G4ParticleTable::GetParticleTable()->GetIonTable();

G4RadioactiveDecay* theRadioactiveDecay = creates the process new G4RadioactiveDecay();

Validation of hadronic physics models



Hadronic validation

- A website is available to collect relevant information for validation of Geant4 hadronic models
 - plots, tables, references to data and to models, etc.
 - http://geant4.fnal.gov/hadronic_validation/validation_plots.htm
- Several physics lists and several use-cases have been considered
 - e.g. thick target, stopped particles, low-energy
- Includes final states and cross sections



Gean3.21based Geant4 LEP model: pion production from 730 MeV protons on Carbon \rightarrow fast, but not working very well for this purpose

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Bertini cascade model: pion production from 730 MeV proton on Carbon \rightarrow more appropriate than the previous one, for this application

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Nuclear fragmentation



Bertini and Binary cascade models: neutron production vs. angle from 1.5 GeV protons on Lead

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Neutron production by protons



Binary cascade model: double differential crosssection for neutrons produced by 256 MeV protons impinging on different targets Scattering off Mg (Whitmore et al, Z.P. C62, p.199ff, 1994)



Comparison of differential pion yields for positive and negative pions in pion-Mg reactions at 320 GeV lab momentum. The dots are data and the open circles are Monte Carlo predictions by G4QGSModel



Geant4 simulation (HP neutron models) of γ-rays from 14 MeV neutron capture on uranium

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Spectrum of secondary particles from G4NeutronHPInelastic

¹⁵⁴Gd(n,2n) channel



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G4EMDissociationModel for ion-ion inelastic interactions

Projectile	Energy [GeV/nuc]	Product from ED	G4EM Dissociation [mbarn]	Experiment [mbarn]
²⁴ Mg	3.7	Na-23 + p	124 ± 2	154 ± 31
²⁸ Si	3.7	Al-27 + p	107 ± 1	186 ± 56
²⁸ Si	14.5	Al-27 + p	216 ± 2	$165 \pm 24 \\ 128 \pm 33$
¹⁶ O	200	N-15 + p	331 ± 2	$\begin{array}{c} 293 \pm 39 \\ 342 \pm 22 \end{array}$

Summary

- Geant4 hadronic physics allows the user to choose models for a process
 - cross sections (\rightarrow interaction length)
 - models (\rightarrow final state)
- Many models and cross sections available to choose from
 - appropriate for specific particles and energy range
 - hadronic framework makes it easier to add more
- Parameterized models (LEP, HEP) handle most particle types over the largest energy range
 - based on *fits to data* and some theory
 - not very detailed, but fast
- Cascade models (Bertini, Binary, Liège) are valid for fewer particles over a smaller energy range
 - more *theory-based*
 - more detailed, but slower
- The user should find the best trade-off
 - One size does NOT fit all