

Courtesy T. Ersmark, KTH Stockholm

R. Taschereau, R. Roy, J. Pouliot





Courtesy of ATLAS Collaboration

not GEANT

Physics Modeling Capabilities



INFN Genova, Italy







Food for thought at IEEE NSS-MIC 2010

Thursday, 4 November 2010 Knoxville, TN





FAQ

Geant4 users

- What is the difference between Standard and low energy?
- What is the difference between Geant4 and FLUKA?

(mostly CERN-INFN question)

 Which PhysicsList should I use?

TNS editor

- Could you please document the validation of your simulation?
 Either through your own experimental measurements of through references to pertinent literature
- Could you please
 quantify the accuracy of your simulation?
- Why did you use model
 X in your simulation?



Courtesy ATLAS Collaboration









Born from the requirements of large scale HEP experiments

Widely used also in

- Space science and astrophysics
- Medical physics, nuclear medicine
- Radiation protection
- Accelerator physics
- Pest control, food irradiation
- Humanitarian projects, security
- etc.
- Technology transfer to industry, hospitals.



Most cited "Nuclear Science and Technology" publication Thomson-Reuters, ISI Web of Science, 1970-October 2010





IST and INFN Genova





"It was noted that experiments have requirements for **independent**, **alternative physics models**. In Geant4 these models, *differently from the concept of packages*, allow the user to **understand** how the results are produced, and hence improve the **physics validation**. Geant4 is developed with a modular architecture and is the ideal framework where existing components are integrated and new models continue to be developed."

Minutes of LCB (LHCC Computing Board) meeting, 21/10/1997

Physics: general features

- Ample variety of physics functionality
- Abstract interface to physics processes
 - Tracking independent from physics
- Open system
 - Users can easily create and use their own models
- Distinction between processes and models
 - often multiple models for the same physics process
 - complementary/alternative

Electromagnetic physics

- electrons and positrons
- photons (including optical photons)
- muons
- charged hadrons
- ions
- Comparable to GEANT 3 already in α release 1997
- Further extensions (facilitated by OO technology)
- High energy extensions
 - Motivated by LHC experiments, cosmic ray experiments...
- Low energy extensions
 - motivated by space and medical applications, dark matter and v experiments, antimatter spectroscopy, radiation effects on components etc.
- Alternative models for the same process

- Multiple scattering
- Bremsstrahlung
- Ionisation
- Annihilation
- Photoelectric effect
- Compton scattering
- Rayleigh effect
- γ conversion
- e⁺e⁻ pair production
- Synchrotron radiation
- Transition radiation
- Cherenkov
- Refraction
- Reflection
- Absorption
- Scintillation
- Fluorescence
- Auger emission

Hadronic physics

• Completely different approach w.r.t. the past (GEANT 3)

- native
- transparent (in the original design)
- no longer interface to external packages
- clear separation between data and their use in algorithms

Cross section data sets

- Transparent and interchangeable

Final state calculation

- Models by particle, energy, material

Ample variety of models

- Alternative/complementary
- It is possible to mix-and-match, with fine granularity
- Data-driven, parameterised and theory-driven models

Outline

Geant4 physics in one hour...

A little bit of software

- Basic concepts of Geant4 use: application, PhysicsList

Overview of Geant4 physics functionality

Electromagnetic and hadronic physics

Validation

- Concepts and a few results

Outlook

Toolkit + User application

Geant4 is a toolkit

- i.e. one cannot "run" Geant4 out of the box
- One must write an application, which uses Geant4 tools

Consequences

- There is no such concept as "Geant4 defaults"
- One must provide the necessary information to configure one's simulation
- The user must deliberately **choose** which Geant4 tools to use
- Guidance: many **examples** are distributed with Geant4

Basic actions

- What a user **must** do:
 - Describe the **experimental set-up**
 - Provide the **primary particles** input to the simulation
 - Decide which particles and physics models one wants to use out of those available in Geant4 and the desired precision of the simulation (*cuts to produce and track secondary particles*)
- One may also want
 - To interact with Geant4 kernel to **control** the simulation
 - To **visualise** the simulation configuration or results
- To produce **objects encoding simulation results** to be further analysed Maria Grazia Pia, INFN Genova

Interaction with Geant4 kernel

- Geant4 design provides tools for a user application
 - To tell the kernel about one's simulation configuration
 - To interact with Geant4 kernel itself
- Geant4 tools for user interaction are base classes
 - One creates **one's own concrete class** derived from the base classes
 - Geant4 kernel handles derived classes transparently through their base class interface (polymorphism)

Abstract base classes for user interaction

- User derived concrete classes are **mandatory**
- Concrete base classes (with *virtual* dummy methods) for user interaction
 - User derived classes are **optional**

User classes

Initialisation classes

Invoked at initialization

- G4VUserDetectorConstruction
- G4VUserPhysicsList

Mandatory classes:

Action classes

Invoked during the execution

- G4VUserPrimaryGeneratorAction
- G4UserRunAction
- G4UserEventAction
- G4UserTrackingAction
- G4UserStackingAction
- G4UserSteppingAction
- G4VUserDetectorConstruction describe the experimental set-up
- G4VUserPhysicsList

select the physics one wants to activate

- G4VUserPrimaryGeneratorAction
 - generate primary events

G4VUserPhysicsList

- It is one of the mandatory user classes (abstract class)
- It is the way one interacts with Geant4 kernel to tell it
 - which **particles** one intends to track in the simulation
 - which **processes** and models one decides to activate
 - the **thresholds** to produce secondary particles
- Pure virtual methods
 - ConstructParticles()
 - ConstructProcesses()
 - SetCuts()

to be implemented by the user in his/her concrete derived class



What is tracked

G4ParticleDefinition G4DynamicParticle G4Track

Process interface

G4VProcess Processes interacting with tracking

Production cuts

Why production cuts are needed The cuts scheme in Geant4

How the user interacts with Geant4 kernel

G4VUserPhysicsList Concrete physics lists



G4DynamicParticle

- Describes the purely dynamic part of the particle state:
 - momentum, energy, polarization
- Holds a G4ParticleDefinition pointer
- Retains eventual pre-assigned decay information
 - decay products, lifetime

G4Track

- Defines the class of objects propagated by Geant4 tracking
- Represents a snapshot of the particle state
- Aggregates
 - a G4ParticleDefinition
 - a G4DynamicParticle
 - geometrical information: *position, current volume etc.*
 - track ID, parent ID
 - process which created it
 - weight, used for event biasing



The classes involved in implementing a **PhysicsList** are:

- G4ParticleDefinition concrete classes
- G4ProcessManager
- the processes

Processes

- Processes describe how particles interact with material or with a volume
- Three basic types
 - At rest process
 (eg. decay at rest)
 - **Continuous** process *(eg. ionisation)*
 - Discrete process
 (eg. Compton scattering)



- Transportation is a process
 - interacting with volume boundary
- A process which requires the shortest interaction length limits the step

G4VProcess

Abstract class defining the common interface of all processes in Geant4

- Defines three kinds of actions:
- AtRest actions: decay, annihilation ...
- AlongStep actions: continuous interactions occuring along the path, like ionisation
- **PostStep** actions: point-like interactions, like decay in flight, hard radiation...
- A process can implement any combination of the three actions
- Each action defines two methods:
 - GetPhysicalInteractionLength
 - used to limit the step size
 - Dolt
 - implements the actual action to be applied to the track
 - implements the related production of secondaries

Geant4 stepping treats processes generically

- it does not know which process it is handling
- Geant4 stepping lets the processes
 - cooperate for AlongStep actions
 - compete for PostStep and AtRest actions

PostStep

AlongStep

Cuts in Geant4

• In Geant4 there are **no tracking cuts**

- particles are tracked down to a zero range/kinetic energy
- Only **production cuts** exist
 - i.e. thresholds allowing a particle to be born or not

Why are production cuts needed ?

- Some electromagnetic processes involve infrared divergences
 - This leads to an infinity [huge number] of smaller and smaller energy photons/electrons (such as in Bremsstrahlung, δ-ray production)
 - Production cuts limit this production to particles above a threshold
 - The remaining, divergent part is treated as a continuous effect (*AlongStep* action)
- Secondary production thresholds are defined in terms of range
 - The production of a secondary particle is relevant if it can generate visible effects in the detector, otherwise *"local energy deposit"*
 - A range cut allows one to easily define such visibility: "I want to produce particles able to travel at least 1 mm"
 - criterion which can be applied uniformly across the detector (whole or "region")

Electromagnetic packages in Geant4

- Standard
- Low energy
- High energy
- Optical
- Muons

Recent software design evolutions Improvements and drawbacks documented in conference proceedings (e.g. CHEP 2009, NSS 2009, Monte Carlo 2010)

- X-rays (but most X-ray physics is elsewhere)
- Polarisation (but some polarised processes are elsewhere)
- Different modeling approach
- Specialized according to particle type, energy scope

Standard electromagnetic physics

Package	Description
Standard	Gamma, Electrons up to 100 TeV, Hadrons, lons up to 100 TeV
Muons	Muons up to 1PeV, Energy loss propagator
X-rays	X-ray and optical photon production processes
Optical	Optical photon interactions
High-energy	Processes at high energy (E > 10 GeV), Physics for exotic particles
Polarization	Simulation of polarized beams

Processes: electrons and photons

Particle	Processes	
Photons	Gamma conversion into e⁺e⁻ pair Compton scattering Photoelectric effect	
Electrons, Positrons	Ionization Coulomb scattering Bremsstrahlung	
Positrons	Annihilation	
	Example: Electron energy deposition	

Processes: hadrons



Optical photons

Production of optical photons in detectors is mainly due to Cherenkov effect and scintillation

Processes in Geant4:

- in-flight absorption
- Rayleigh scattering
- medium-boundary interactions (reflection, refraction)



Muons

- simulation of ultra-high energy and cosmic ray physics
- High energy extensions based on theoretical models



End point deviation (mm)

Photo Absorption Ionisation (PAI) Model

Ionisation energy loss produced by charged particles in thin layers of absorbers



Ionisation energy loss distribution produced by pions, PAI model

Documentation of **validation** in the literature (V. Grichine)

Multiple scattering

- Original Geant4 (Urban) model based on Lewis theory
 - Uses phenomenological functions to sample angular and spatial distributions after a step in particle transport
 - The function parameters are chosen, in order that the moments of the distribution are the same as given by the Lewis theory
- Recent development of other models
 - Goudsmit-Sanderson
 - WentzelVI
 - Single scattering
 - Urban in various flavours (Urban90, Urban92, Urban93...)
 - Specialized by particle type (beware of design tricks!)
 - etc.
- See Geant4 Physics Reference Manual and various conference proceedings for details

Low energy electrons and photons

- Two "flavours" of models:
 - based on the **Livermore Library**
 - à la Penelope
- Nominally down
 - to 250 eV
 - based on the Livermore library
 - to a few hundreds eV
 - Penelope-like

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)

- 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

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



- -Chemical effect for compounds
- Nuclear stopping power
- PIXE included





Ziegler and ICRU, Si

-Spin dependent term - Barkas and Bloch terms



Positive charged ions

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

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

Scaling:

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- Nuclear stopping power





Recent implementation of ICRU73-based model and comparison with experimental data (A. Lechner et al.)



Comparison of simulated and measured ¹²C depthdose profiles in water (0.997 g/cm³). Simulations were performed with Geant4 9.3, using revised ICRU 73 stopping power tables and the QMD nuclear reaction model. Experimental data derive from Sihver et al. (triangles) and Haettner et al. (circles), where profiles of Haettner et al. were shifted to match more precise measurements of the peak position by D. Schardt et al. All experimental data by courtesy of D. Schardt.

A. Lechner et al., NIM B 268-14 (2010) 2343-2354

Models for antiprotons

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Geant4 Model for the Stopping Power of Low Energy Negatively Charged Hadrons Stéphane Chauvie, Petteri Nieminen, and Maria Grazia Pia

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

Bethe-Bloch formula

Quantum harmonic oscillator model

Free electron gas mode



Geant4 Atomic Relaxation 9 pages

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

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

Validation of Geant4 Atomic Relaxation Against the NIST Physical Reference Data 10 pages

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

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IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

Validation of K and L Shell Radiative Transition Probability Calculations 12 pages

Maria Grazia Pia, Paolo Saracco, and Manju Sudhakar

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

PIXE Simulation With Geant4 36 pages

Maria Grazia Pia, Georg Weidenspointner, Mauro Augelli, Lina Quintieri, Paolo Saracco, Manju Sudhakar, and Andreas Zoglauer

+ further ongoing activity and results

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Recent validation results

Geant4 Atomic Relaxation: X-ray fluorescence + Auger electron emission **Data-driven** Based on **EADL** (Evaluated Atomic Data Library)

Geant4 X-ray fluorescence simulation is as good as EADL



calculations compared to experiments Maria Grazia Pia, INFN Genova

1st development cycle



Correctly implemented empirical (Paul&Bolik) cross sections for α particles incorrectly documented as Paul&Sacher cross sections for protons

Mishaps of Geant4 PIXE...

Current low energy group's development

Nuclear Instruments and Methods in Physics Research B 267 (2009) 37-44



New Geant4 cross section models for PIXE simulation

H. Ben Abdelouahed a,*, S. Incerti^b, A. Mantero^c

Released in Geant4 9.2 Several flaws documented in *Pia et al., TNS 56(6), 3614-3649, 2003*

Recent progress

Hopefully, Geant4 collaboration will authorize the authors to release this code in Geant4, as requested by users, in December 2010

> 10 12



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Very-low energy extensions

1st development cycle: **Physics** of interactions in water down to the eV scale

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 6, DECEMBER 2007

Geant4 Physics Processes for Microdosimetry Simulation: Design Foundation and Implementation of the First Set of Models

S. Chauvie, Z. Francis, S. Guatelli, S. Incerti, B. Mascialino, P. Moretto, P. Nieminen, and M. G. Pia

Further developments

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

Modeling Radiation Chemistry and Biology in the Geant4 Toolkit

M. Karamitros¹, A. Mantero², S. Incerti^{1*}, G. Baldacchino³, P. Barberet¹, M. Bernal^{4,5}, R. Capra⁶, C. Champion⁷, Z. El Bitar⁸, Z. Francis⁹, W. Friedland¹⁰, P. Guèye¹¹, A. Ivanchenko¹, V. Ivanchenko^{7,12}, H. Kurashige¹³, B. Mascialino¹⁴, P. Moretto¹, P. Nieminen¹⁵, G. Santin¹⁵, H. Seznec¹, H. N. Tran¹, C. Villagrasa⁹ and C. Zacharatou¹⁶

Still consistent with transport assumptions?

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Ionisation models for nano-scale simulation

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

Design, development and validation of electron ionisation models for nano-scale simulation

Hee SEO¹, Maria Grazia PIA^{2*}, Paolo SARACCO², Chan-Hyeung KIM¹

Student Paper Award Monte Carlo 2010

¹ Hanyang University, 133-791 Seoul, Korea
² INFN Sezione di Genova, 16146 Genova, Italy

Cross section models:

- Binary-Encounter-Bethe (BEB)
- Deutsch-Märk (DM)

EEDL



Energy (eV)





Percentage of elements for which a model is compatible with experimental data at 95% **GL**

Hadronic physics challenge

- Even though there is an underlying theory (QCD), applying it is much more difficult than applying QED for simulating electromagnetic interactions
- Energy régimes:
 - Chiral perturbation theory (< 100 MeV)
 - Resonance and cascade region (100 MeV a few GeV)
 - QCD strings (> 20 GeV)
- Within each régime several models are available
 - Many of these are phenomenological

Hadronic framework



Maria Grazia Pia, INFN Genova

Hadronic process

At rest

- Stopped muon, pion, kaon, anti-proton
- Radioactive decay
- Particle decay (decay-in-flight is PostStep)

Elastic

- Multiple models available

Inelastic

- Different processes for each hadron (with multiple models)
- Photo-nuclear, electro-nuclear, μ -nuclear

Capture

– Pion- and kaon- in flight, neutron

Fission

Cross sections

- Default cross section data sets are provided for each type of hadronic process:
 - Fission, capture, elastic, inelastic
- Can be overridden
- Cross section data sets
 - Some contain only a few numbers
 - Some represent large databases

Alternative cross sections

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

• Low energy neutrons

- elastic, inelastic, fission and capture
 (< 20 MeV)
- **n** and **p 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

Parameterised and data-driven hadronic models

Au(* 10)

c) negatives

Based on experimental data

- Some models originally from GHEISHA
 - reengineered into OO design
 - refined physics parameterisations

New parameterisations

- pp, elastic differential cross section
- nN, total cross section
- pN, total cross section
- np, elastic differential cross section
- $-\pi N$, total cross section
- $-\pi N$, coherent elastic scattering







Transport of low-energy neutrons

- The energy coverage is from **thermal energies** to **20 MeV**
- Geant4 database deriving from evaluation of other databases
 - ENDFB/VI, JEFF, JENDL, CENDL...
 - 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

Nuclear elastic scattering

G4HadronElasticDataSet

G4LElastic

G4ElasticCascadeInterface

Not to be confused with G4CascadeElasticInterface

G4HadronElastic

G4UHadronElasticProcess

G4HadronElasticProcess

G4WHadronElasticProcess

Meant to treat elastic models similarly to inelastic ones

G4DiffuseElastic

G4QElasticProcess AKA "CHIPS elastic" V. Grichine, "GEANT4 hadron elastic diffuse model," *Comp. Phys. Comm.*, vol. 181, pp. 921–927, 2010

G4QElasticCrossSection

Maria Grazia Pia, INFN Genova

Theory-driven hadronic non-elastic models

- Complementary and alternative models
 - Evaporation phase
 - Low energy range, O(100 MeV): **pre-equilibrium**
 - Intermediate energy, O(100 MeV -5 GeV): intranuclear transport
 - High energy range: hadronic generator régime

Deexcitation

- Dostrovsky, GEM, Fermi break-up, ABLA, multifragmentation...

Preequilibrium

- Precompound, Bertini-embedded

Cascade

– Binary, Bertini-like, INCL (*Liège*)

High energy

- Quark-gluon-string, FTF (*FRITIOF*)
- CHIPS (Chiral Invariant Phase Space)

Hadronic inelastic model inventory Data-driven Parameterised Theory-driven models



Ion inelastic interactions

- Several cross section formulations for N-N collisions are available in Geant4
 - Tripathi, Shen, Kox, Sihver
- Final state according to models:
 G4BinaryLightIonCascade (variant of Binary cascade),
 G4WilsonAbrasion, G4EMDissociation

Radioactive decay

- To simulate the decay of radioactive nuclei
- α , β^+ , β^- decay and electron capture are implemented
- Data derived from Evaluated Nuclear Structure Data File (ENSDF)

Hadronic simulation validation

- Intensive activity since Geant4 early days
- Far from easy
 - Complex physics
 - Complex experimental data (e.g. LHC teast beam set-ups)
 - Lack of, or conflicting experimental data, large uncertainties etc.

• Validation or calibration?

- Often not documented
- "*Tuning*" (hand-made in most cases)

Recent improvements

Low energy range: **Preequilibrium** and **deexcitation**



Calibration or validation?

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

Recent Developments In Pre-Equilibrium And De-Excitation Models In Geant4

José Manuel QUESADA^{1,*}, Vladimir IVANCHENKO^{2,3,4}, Anton IVANCHENKO^{2,5}, Miguel Antonio CORTÉS-GIRALDO¹, Gunter FOLGER², Alex HOWARD⁶, Dennis WRIGHT⁷ on behalf of the Geant4 Hadronic Working Group

Maria Grazia Pia, INFN G....

Experimental comparisons



Lorentz invariant cross section for **inclusive proton production** at 59° (top row) and 119° (bottom row) in **p-Carbon** interactions at 1.4 GeV/c (left column) and 7.5 GeV/c (right column) as a function of proton kinetic energy, being compared with predictions of GEANT4 hadronic models

Bertini cascade Binary cascade LEP QGS+Precompound CHIPS

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

Validation of GEANT4 Hadronic Generators versus Thin Target Data

Banerjee¹, G. Folger², A. Ivanchenko^{2,3}, V. N. Ivanchenko^{2,4,5}, M. Kossov², J. M. Quesada⁶, A. Schalelicke⁷, V. Uzhinsky², H. Wenzel¹, D. H. Wright⁸ and J. Yarba¹

More in

Experimental comparisons: QGS

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

Experimental comparisons - FRITIOF



Experimental data: E. Bracci et al., CERN/HERA 73-1 (1973)

More in

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

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Development of the Fritiof Model in Geant4

Vladimir UZHINSKY^{1,2*} On behalf of the Geant4 Hadronics Working Group

> ¹ CERN, CH-1211, Geneva 23, Switzerland ² LIT, JINR, 141980 Dubna, Russia

HP neutron models



Geant4 simulation of γ-rays from 14 MeV neutron capture on uranium

Recent improvements



Shower shapes



180 GeV protons incident at 90° on the ATLAS TileCal wedge



Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

An Overview of Geant4 Hadronic Physics Improvements

Maria Grazia Pia, INFN Genova

Dennis H. WRIGHT¹, on behalf of the Geant4 Hadronic Working Group ⁵



Recognized as an American National Standard (ANSI) IEEE Std 1012[™]-2004 (Revision of IEEE Std 1012-1998)

IEEE Standard for Software Verification and Validation

The **validation** process provides **evidence** whether the software and its associated products and processes

1) **Satisfy system requirements** allocated to software at the end of each life cycle activity

2) Solve the right problem (e.g., correctly model physical laws, implement business rules, use the proper system assumptions)
3) Satisfy intended use and user needs

The main problem of validation: experimental data!

backscattering for e-

e-energy range: 0.1 keV -> 102. keV





- Empty symbols: simulation models
- Filled symbols: experimental data

To be documented in a forthcoming paper

Often and answer can be found only through a statistical analysis over a large sample of simulated and experimental data (and would be a result within a given *CL*, *rather than black* & *white*)

What to compare?



Are the data correct? Are the uncertainties correct? Are systematic effects under control?



Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Validation of the Geant4 electromagnetic photon cross-sections for elements and compounds

G.A.P. Cirrone^a, G. Cuttone^a, F. Di Rosa^a, L. Pandola^{b,*}, F. Romano^a, Q. Zhang^{a,c,**}

Comparison to theoretical data libraries NOT validation!

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010

"After the migration to common design a new **validation** of photon cross sections versus various databases was published ²⁶⁾ which demonstrated general good agreement with the data for both the Standard and Low-energy models."

Recent Improvements in Geant4 Electromagnetic Physics Models and Interfaces

NUCLEAR INSTRUMENTS & METHODS

RESEARCI

Vladimir IVANCHENKO^{1,2,3*}, John APOSTOLAKIS¹, Alexander BAGULYA⁴, Haifa Ben ABDELOUAHED⁵, Rachel BLACK⁶, Alexey BOGDANOV⁷, Helmut BURKHARD⁵, Stephane CHAUVIE⁸, Pablo CIRRONE⁹, Giacomo CUTTONE⁹, Gerardo DEPAOLA¹⁰, Francesco Di ROSA⁹, Sabine ELLES¹¹, Ziad FRANCIS¹², Vladimir GRICHINE¹, Peter GUMPLINGER¹³, Paul GUEYE⁹, Sebastien INCERTI¹⁴, Anton IVANCHENKO¹⁴, Jean JACQUEMIER¹¹, Anton LECHNER^{1,13}, Francesco LONGO¹⁶, Omrane KADRI⁵, Nicolas KARAKATSANIS¹⁷, Mathieu KARAMITROS¹⁴, Rostislav KOKOULIN⁷, Hisaya KURASHIGE¹⁴, Michel MAIRE^{11,19}, Alfonso MANTERO²⁰, Barbara MASCIALINO²¹, Jakub MOSCICK¹¹, Luciano PANDOLA²², Joseph PERL²³, Ivan PETROVIC⁶, Aleksandra RISTIC-FIRA⁹, Francesco ROMANO⁶, Giorgio RUSSO⁶, Giovanni SANTIN²⁴, Andreas SCHAELICKE²³, Toshiyuki TOSHITO²⁶, Hoang TRAN¹⁴, Laszlo URBAN¹⁶, Tomohiro YAMASHITA²⁷ and Christina ZACHARATOU³⁸

Validation or calibration?

Calibration is the process of **improving the agreement of a code** calculation with respect to a chosen set of benchmarks through the *adjustment of parameters* implemented in the code

Validation is the process of confirming that the predictions of a code adequately represent measured physical phenomena

T.G. Trucano et al., Calibration, validation, and sensitivity analysis: What's what, *Reliability Eng. & System Safety*, vol. 91, no. 10-11, *Maria Grazia Pia, INFN Genova* pp. 1331-1357, 2006



Validation is holistic

One must validate the entire calculation system

Including:

- User
- Computer system
- Problem setup
- Running
- Results analysis



An inexperienced user can easily get wrong answers out of a good code in a valid régime



Columbia Space Shuttle accident, 2003

Can we quantify our ignorance?

Simulation codes usually contain parameters or model assumptions, which are not validated (because of lack of experimental data, or conflicting data)

Or we may not have a complete understanding of some physics processes

Or we may use a simulation model outside the range where it has been validated (energy, material etc.)

These are sources of **epistemic uncertainties**, which in turn can be sources of **systematic effects**

Can we quantify them?

No generally accepted method of measuring epistemic uncertainties

Interval analysis

Dempster-Shafer theory of evidence

Fresh from the oven...

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Warm-up exercise: epistemic uncertainties quantification in proton Bragg peak simulation Physics-Related Epistemic Uncertainties in Proton Depth Dose Simulation

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Precompound model activated through **Binary Cascade** w.r.t. standalone Precompound model



Geant4 pre-assembled physics lists

- Initially a set of example PhysicsLists suitable to address specific use cases
 - "educated guess" in most cases
 - Not necessarily validated
- Now: combinatorial assembly of processes and models
 - Not necessarily validated
- Can be a starting point for a user application
- Not necessarily the end
- Can you build your own PhysicsList from scratch?

Summary

- Transparency and modularity were key characteristics of Geant4 original physics design in its RD44 phase
- Ample variety of processes and models
 - Open to extension and evolution thanks to the OO technology
- Geant4 design exposes, deliberately, the user to the choice of physics (*particles* + *processes*) relevant to his/her application
 - This is a critical task
 - Examples can be used as starting point
 - Not a "push the button" system, the user is invested of the responsibility of selecting the physics for his/her simulation
- Documentation in Geant4 Physics Reference Manual
- Growing set of Geant4 physics references in the literature
 - Conference proceedings and **refereed journals**
 - User application results

Conclusion

- Geant4 is a rich and powerful tool for experimental research
- ...but it invests the user with responsibility of making choices
- Validation is ongoing
- Check what is documented in the literature, that may be relevant to your experimental problem
 - **Refereed journals** (conference papers)
 - But some slips also in refereed journals

Trust what you can document quantitatively Document what you cannot trust [yet]

Slides available at http://www.ge.infn.it/geant4/training

Collection of physics references http://www.ge.infn.it/geant4/papers

General information: http://cern.ch/geant4

Acknowledgment: Geant4 developers and users