

Courtesy T. Ersmark, KTH Stockholm

R. Taschereau, R. Roy, J. Pouliot





Courtesy of ATLAS Collaboration

Refresher Course

(mostly about Geant4 physics)





INFN Genova, Italy



Lunch break at IEEE NSS-MIC 2012

Wednesday, 1 November 2012 Disneyland, CA, USA



















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...



> 3000 citations

Thomson-Reuters, ISI Web of Science, 1970-October 2012





IST and INFN Genova



Outline

Geant4 in one hour...

A little bit of software

Geant4 users

- What is the difference between Standard and low energy?
- What is the difference between Geant4 and MCNP? (Geant4 and EGS, Geant4 and FLUKA...)
- Which PhysicsList should I use?
- Basic concepts of Geant4 use: application, PhysicsList

Overview of Geant4 physics functionality

Electromagnetic and hadronic physics

Validation

Concepts and a few results

Outlook

TNS editor

- Could you please document the validation of your simulation?
- Could you please quantify the accuracy of your simulation?
- Why did you use model X in your simulation?

What is **Geant 4**?

OO Toolkit for the simulation of next generation HEP detectors

...of the current generation ...not only of HEP detectors

Born from **RD44**, 1994 – 1998 (R&D phase) 1st release: 15 December 1998 1-2 new releases/year since then



RD44 was also an experiment of

■distributed software production and management

application of rigorous software engineering methodologies

introduction of the object oriented technology in the HEP environment

OO technology

Open to extension and evolution
 new implementations can be added w/o changing existing code
 Robustness and ease of maintenance
 protocols and well defined dependencies minimize coupling

Strategic vision

Toolk

A set of **compatible components**

- each component is **specialised** for specific functionality
- each component can be refined independently
- components can cooperate at any degree of complexity
- it is easy to provide (and use) alternative components
- the user application can be customised as needed



Geant4 kernel: Run and Event

- Conceptually, a run is a collection of events that share the same detector conditions
 - Detector and physics settings are frozen in a run
- An event initially contains the primary particles; they are pushed into a stack and further processed
 - When the stack becomes empty, processing of an event is over

Multiple events

possibility to handle pile-up

• Multiple runs in the same job

- with different geometries, materials etc.
- Powerful stacking mechanism
 - three levels by default: handle trigger studies, loopers etc.

Geant4 kernel: Tracking

- Decoupled from physics
 - all processes handled through the same abstract interface
- Independent from particle type
- New physics processes can be added to the toolkit without affecting tracking
- Geant4 has only secondary production thresholds, no tracking cuts
 - all particles are tracked down to zero range
 - energy, TOF ... cuts can be defined by the user

Materials

- Different kinds of materials can be defined
 - isotopes
 - elements
 - molecules
 - compounds and mixtures
- Associated attributes:
 - temperature
 - pressure
 - state
 - density

```
G4double density = 1.390*g/cm3;
G4double a = 39.95*g/mole;
G4Material* lAr =
new G4Material("liquidArgon",z=18.,a,density);
```



Geometry

- Role
 - detailed detector description
 - efficient navigation
- Three conceptual layers
 - Solid: shape, size
 - LogicalVolume: material, sensitivity, daughter volumes, etc.
 - PhysicalVolume: position, rotation
- One can do fancy things with geometry...

Boolean operations





Transparent solids





Solids

Multiple representations Same **abstract interface**





CSG (Constructed Solid Geometries

simple solids

STEP extensions

- polyhedra, spheres, cylinders, cones, toroids, etc.
- BREPS (Boundary REPresented Solids
 - volumes defined by boundary surfaces

CAD exchange



urtesy of LHCb Collaboration

Courtesy of CMS

Physical Volumes



Electric and magnetic fields



MOKKA Linear Collider Detector



of variable non-uniformity and differentiability





Not only large scale, complex detectors...





Geant4 anthropomorphic phantoms

Maria Grazia Pia, INFN Genova





One may also do it wrong...



Tools to detect badly defined geometries



(including: info about translation, rotation, solid specs)

Other features

Particles

- all PDG data and more for specific Geant4 use, like ions

Hits & Digitization

to describe detector response

Primary event generation

- some general purpose tools provided in the toolkit
- Event biasing
- Fast simulation
- Persistency
- Parallelisation
- No time to review them in detail
 - Geant4 user documentation



The user is free to choose the concrete system he/ she prefers for each component



User Interface

File r Lo

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tor pc

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_ 🗆 X

nmı 👻

Delete a Row

ordDefault

Each if clause corresponds to a row in the Physic sTable

pmanager->AddProcess(new G4eIonisation(),ordInActive, 2, 2);

pmanager->AddProcess(new G4Mulonisation(),ordInActive, 2, 2);

Multiplescatt

Mulonisation

IMulonisation

Cerenkov

LECompton

LEIonisation

hL Flonisation

kterm

& Particles

pmanager->AddProcess(new G4eBremsstrahlung(),ordInActive,ordInActive,3);

pmanager->AddProcess(new G4MuBremsstrahlung(),ordInActive,ordInActive,3);

PostStep

pmanager->AddProcess(new G4ComptonScattering(),ordInActive.ordInActive.ordDefault);

pmanager->AddProcess(new G4SynchrotronRadiation(),ordInActive.ordInActive.ordDefault);

MuBrems

IMuBrems

Scintillation

I FGammaCons

LEBrems

kterm

& EMProce...

MuPairProd

IMuPairProd

LEPhotoElec

& Geant4 P.

kterm

& C++ Sour.

- Several implementations, all handled through abstract interfaces
- Command-line (batch and terminal)
- **GUIs**

Geant4 Physics Editor

Open Tables =>

Open Tables =>

Particles Table

all to sons

all leptons

all mesons

all barvons

all ions

all shortlived

Particle(s) == :

Particle

Enter PhysicsClassName MyPhysicsList

Particles

AtRest

ordInActive

ordInActive

ordInActive

ordInActive

ordInActive

ordInActive

Particle EMProc

Defa

Standar

Muon EM

X Rays

Low energy EM

Append

geantino

#-

#+

Π-

K-

D-

B--

п

 $\Sigma +$

anti $-\Sigma$ +

ΣC++

anti-ΣC++

d

Process

Compton

elonisation eBrems

SynchrotronRad

Mulonisation MuBrems

Null

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Null

Null Null

Null

e

e+

π+

K+

D+

B+

p

Δ

anti-A

ΔC+

anti-Ac-

File Make

reanting

anti-v e

anti-v "a

anti-v 7

chargedgeantino

X11/Motif, GAG, MOMO, OPACS, Java

EM Processes

ordInActive

Hle Edit

C++ Source Code Editor

if (particleName == "gamma") {

if (particleName == "e-") {

if (particleName == "e-") {

if (particleName == "e-") {

if (particleName == "mu-") {

if (particleName == "mu_") {

nni-/mui+

integral

all charged

photon

e-/e+

hadron/ion

Enter defaultCutValue 1.0

Along Step

маке	source							
gical Vo	lume ———			ر VisAttrib		ÌåГ	Physical Volume ——	
Appen	d Ins	ert	Delete	Create	Del	100000		
ect a sol	id PolyConeSe	egment	•	lightblue		Sectors.		
Name	Solid	Material	VisAtb	ered		0000	Single P	lacement
(Вох	Air	lightblue	violet		1000		
р	SymTrapezoid	AI	skyblue	• indigo		0000		
IS	TubeSegment	Si	red	😑 grass		ana a	Deveted Discovery	
s	ConeSegment	Mylar	violet	orange			Kepeted Placement	
e	SphereSegm	Plexiglas	indigo	🟓 purple		0000		
a	Parallelepiped	BGO	grass	🟓 brow n				
JS	TorusSegment	BaF2	orange	gray		1000	Translation	AxialSymmetric
ne	PolyConeSeg	Fe	purple			0000		
n	PolyGonSeg	Pt	brown			0000		
te	Box	U	gray			2005		
						10000	Slicing	
							Translation	AxialSymmetric
	sed M	aterials					Paramet	risation

- - - -

Automatic code generation for geometry and physics through a GUI

GGE (Geant4 Geometry Editor) GPE (Geant4 Physics Editor)

Visualisation

- Control of several kinds of visualisation
 - detector geometry
 - particle trajectories
 - hits in detectors

• Various drivers

- OpenGL
- OpenInventor
- X11
- Postscript
- DAWN
- OPACS
- HepRep
- VRML...
- all handled through abstract interfaces





Distribution

- Geant4 is open-source
- Freely available
 - Source code, libraries, associated data files and documentation can be downloaded from <u>http://cern.ch/geant4</u>
- User support provided on a best effort basis
 - User Forum: mutual support within the user community

🕙 Geant4: A toolkit for the simulation of the passage of particles through matter - Mozilla Firefox											
Eile Edit View History Bookmarks Tools Help											
😮 🕞 C 🗙 🏠 🚰 🗋 http://geant4.web.cern.ch/geant4/		☆ 🔹 Google	P								
🖻 Most Visited 🏶 Getting Started 🔊 Latest Headlines 🔧 Google											
🖓 CERN Users' pages 💿 📑 Geant4: A toolkit for the simulati 🛛 🎽 McCarran Flight Information - Departures 🖾 🌘 CernVM Software Appliance	× +		-								
Geant 4		Download Use	r Forum Gallery Contact Us Search Geant4								

Geant4 is a toolkit for the simulation of the passage of particles through matter. Its areas of application include high energy, nuclear and accelerator physics, as well as studies in medical and space science. The two main reference papers for Geant4 are published in Nuclear Instruments and Methods in Physics Research A 506 (2003) 250-303, and IEEE Transactions on Nuclear Science 53 No. 1 (2006) 270-278.

Applications



A <u>sampling of applications</u>, technology transfer and other uses of Geant4





<u>Getting started, guides</u> and information for users and developers

Results & Publications



<u>Validation of Geant4,</u> results from experiments and publications

Collaboration



<u>Who we are</u>: collaborating institutions, <u>members</u>, organization and legal information

News

- 24 September 2010 -Patch-02 to release 9.3 is available from the download area.
- 24 September 2010 -Patch-04 to release 9.2 is available from the archive download area.
- 25 June 2010 -
- Release 9.4 BETA is available from the <u>Beta download</u> area.
- 16 March 2010 -2010 planned developments



"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 scattering
- 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

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

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**

A simple Geant4-based application



User classes

Initialisation classes

Invoked at initialization

- G4VUserDetectorConstruction
- G4VUserPhysicsList

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

Mandatory classes:

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")
 Maria Grazia Pia, INFN Genova

Electromagnetic packages in Geant4

- High energy
- Low energy
- Standard
- Muons
- Optical
- Pii
- Polarisation (but some polarised processes are elsewhere)
- X-rays (but most X-ray physics is 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

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)



Cherenkov

Milagro is a Water-Cherenkov detector located in a 60m x 80m x 8m covered pond near Los Alamos, NM





LHCb

Aerogel Thickness		Yield	Cherenkov
		Per Event	Angle mrad
4 cm	DATA	6.3 ± 0.7	247.1+-5.0
	MC	7.4 ± 0.8	246.8+-3.1
8 cm	DATA	9.4 ± 1.0	245.4+-4.8
	MC	10.1 ±1.1	243.7+-3.0

prompt scintillation



ZEPLIN III Dark Matter Detector

signal in PMT

Scintillation

GEANT4 Scintillation Event in BOREXINO, INFN Gran Sasso National Laboratory



Courtesy of Borexino

termoluminescense



Courtesy of H, Araujo, Imperial College London



Muons

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



End point deviation (mm)

Deviation of 45 GeV muons in L3

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

- 5 parameterisation models, E < 2 MeV ٩
 - based on Ziegler and ICRU reviews
- **3 models of energy loss fluctuations** ٩
- Density correction for high energy - Shell 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





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 < β < 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

3650

3614

594

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



3614



PIXE Simulation With Geant4

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

- Critical evaluation of conceptual challenges
- Wide collection of ionisation cross section models
- Validation and comparative evaluation of theoretical and empirical cross sections





Fig. 12. A comparison of the fluorescence background due to ionization by cosmic-ray protons in an L2 orbit for three different graded Z shield designs for the eROSITA X-ray detectors. (a) Cu shield; (b) Cu-Al shield; (c) Cu - Al - B_4C shield.

Other implementation released in Geant4 9.2: several flaws



Validation of Proton Ionization Cross Section Generators for Monte Carlo Particle Transport

Matej Batič, Maria Grazia Pia, and Paolo Saracco



Contents lists available at SciVerse ScienceDirect

Computer Physics Communications

www.elsevier.com/locate/cpc

ISICSoo: A class for the calculation of ionization cross sections from ECPSSR and PWBA theory $^{\bigstar}$

Matej Batič^{a,b,*}, Maria Grazia Pia^a, Sam J. Cipolla^c

IEEE TRANSACTIONS ON NUCLEAR SCIENCE

IEEE Trans. Nucl. Sci., vol. 58, no. 6, December 2011

IEEE Trans. Nucl. Sci., vol. 58, no. 6, December 2011

Evaluation of atomic electron binding energies for Monte Carlo particle transport

Maria Grazia Pia, Hee Seo, Matej Batič, Marcia Begalli, Chan Hyeong Kim, Lina Quintieri and Paolo Saracco

COMPUTER PHYSICS

Atomic parameters

Geant4 Atomic Relaxation: X-ray fluorescence + Auger electron emission **Data-driven** \implies 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

Difference w.r.t. DesLattes et al., experimental review

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?

Maria Grazia Pia, INFN Genova

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Ionisation models for nano-scale simulation

Joint International Conference on Supercomputing in Nuclear Applications and Monte Carlo 2010 (SNA + MC2010) IEEE TRANSACTIONS ON NUCLEAR SCIENCE Hitotsubashi Memorial Hall, Tokyo, Japan, October 17-21, 2010 Design, development and validation of electron ionisation models for nano-scale simulation Ionization cross sections for low energy electron Hee SEO1, Maria Grazia PIA2*, Paolo SARACCO2, Chan-Hyeung KIM1 transport ¹ Hanyang University, 133-791 Seoul, Korea ² INFN Sezione di Genova, 16146 Genova, Italy Hee Seo, Maria Grazia Pia, Paolo Saracco and Chan Hyeong Kim IEEE Trans. Nucl. Sci., vol. 58, no. 6, December 2011

Best Student Award Monte Carlo 2010

Cross section models

- Binary-Encounter-Bethe (**BEB**)
- Deutsch-Märk (DM)
- EEDL (Geant4 Low Energy)



Validation

- 57 elements
- 181 experimental data sets



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

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

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

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



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
- πN , total cross section
- πN , coherent elastic scattering







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)

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



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

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

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

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)



Experimental data: Z.W. Bell, ORNL



New, more accurate and computationally faster model

Maria Grazia Pia, INFN Genova

See talks N28-6/7 at NSS 2012

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

 $\begin{array}{c} \widehat{\mathbf{q}}\\ \widehat{\mathbf{q}}\\ \widehat{\mathbf{p}}\\ \widehat{\mathbf{q}}\\ \widehat{\mathbf{$

Maria Grazia Pia, INFN Genova

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

Data-driven models

Recent improvements



Shower shapes



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

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

An Overview of Geant4 Hadronic Physics Improvements

Maria Grazia Pia, INFN Genova

Dennis H. WRIGHT¹, on behalf of the Geant4 Hadronic Working Group 4

Validation

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



Which one is right?



Often an 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*)

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



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

RESEARC

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 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 59, NO. 4, AUGUST 2012

Photon Elastic Scattering Simulation: Validation and Improvements to Geant4 29 pages

Matej Batič, Gabriela Hoff, Maria Grazia Pia, and Paolo Saracco







Angle (degrees)

Test		Penelope	Penelope	EPDL	EPDL	SM	RF	NF	MF	MF	RF
		2001	2008-2011		ASF					ASF	ASF
all	Test cases	71	71	71	71	71	71	71	71	71	71
	Pass	19	27	27	18	55	18	25	35	37	34
	Fail	52	44	44	53	16	53	46	36	34	37
	Efficiency	0.27	0.38	0.38	0.25	0.77	0.25	0.35	0.49	0.52	0.48
	Error	± 0.05	± 0.06	± 0.06	± 0.05	± 0.06	± 0.05	± 0.06	± 0.06	± 0.06	± 0.06
$ heta \leq 90^\circ$	Test cases	67	67	67	67	67	67	67	67	67	67
	Pass	19	27	27	18	55	18	25	35	36	32
	Fail	48	40	40	49	12	49	42	32	31	35
	Efficiency	0.28	0.40	0.40	0.27	0.82	0.27	0.37	0.52	0.54	0.48
	Error	± 0.05	± 0.06	± 0.06	± 0.05	± 0.05	± 0.05	± 0.06	± 0.06	± 0.06	± 0.06
$\theta > 90^{\circ}$	Test cases	17	17	17	17	17	17	17	17	17	17
	Pass	1	1	1	1	10	1	1	0	2	4
	Fail	16	16	16	16	7	16	16	17	15	13
	Efficiency	0.06	0.06	0.06	0.06	0.59	0.06	0.06	< 0.06	0.12	0.24
	Error	+0.06	+0.06	± 0.06	± 0.06	± 0.12	+0.06	± 0.06		+0.08	+0.10

 v^2 Test Outcome: Test Cases Compatible With Experiment at 0.01 Significance Level



Photolectric effect: total

cross section



Validation of Geant4 photon interactions, see N7-4 talk at NSS 2012



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

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



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?

Through the narrow gate

Think

Learn

- Master the technology
- Search the literature
- Read Geant4 documentation

Work

- You do not run Geant4, you run your own application
- Understand what you are doing
- Understand what Geant4 does



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)

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