

New software technologies brains and hands

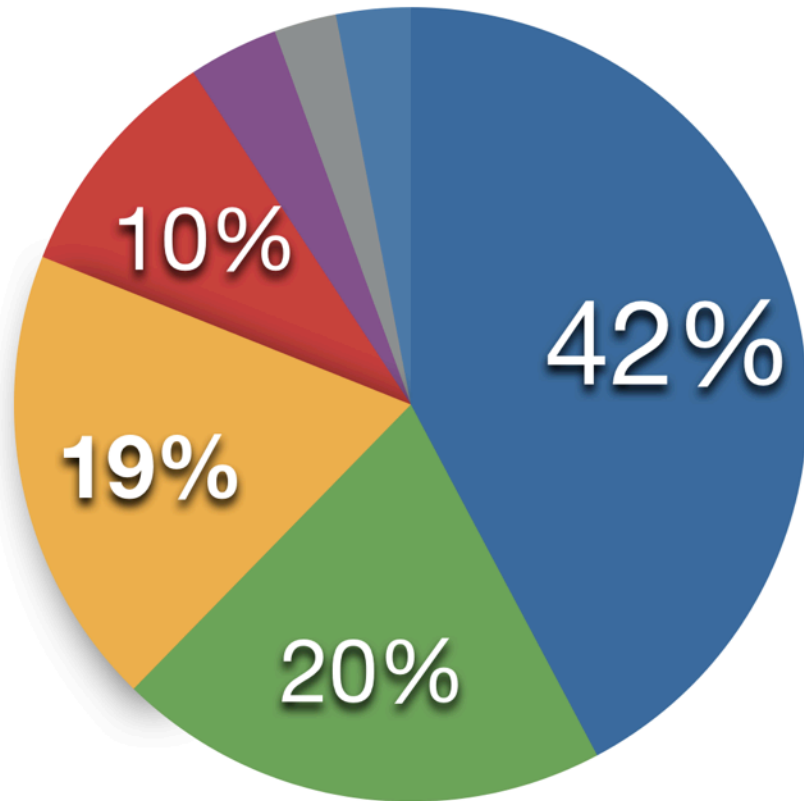


Maria Grazia Pia
INFN Genova, Italy

Workshop CCR INFN
Frascati, 28 maggio 2015



GRID CPU Consumption



- MC Simulation
- MC Reconstruction
- Final Analysis
- Group Production
- Group Analysis
- Data Reconstruction
- Others

ATLAS, Run 1

Courtesy of Graeme Stewart for the ATLAS Collaboration

Geant 4

S. Agostinelli et al.

Geant4: a simulation toolkit

NIM A, vol. 506, no. 3, pp. 250-303, 2003

5743 citations

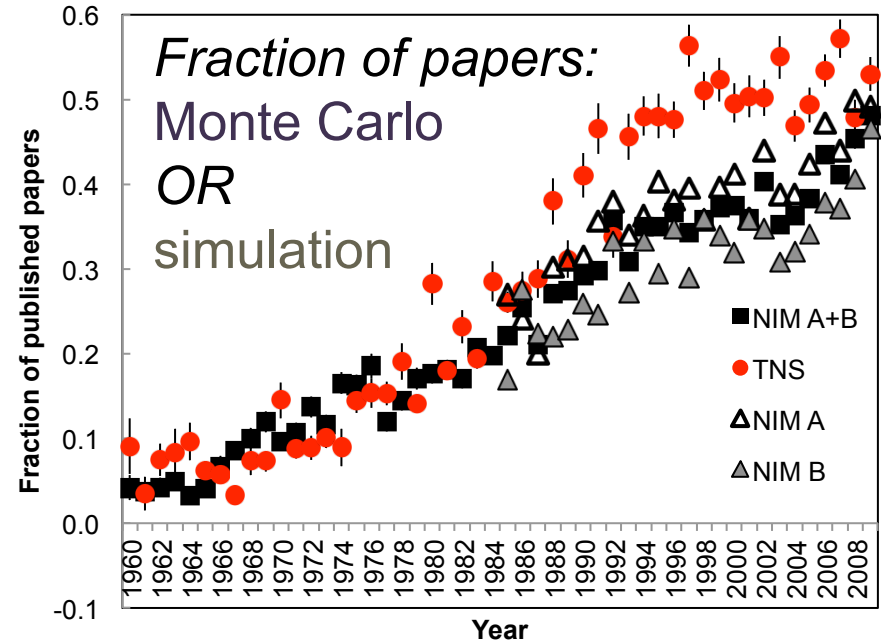
Most cited publication in

- **Nuclear Science and Technology**
 - **Instruments and Instrumentation**
 - **Particle and Fields Physics**
- (656886 papers)
- (282766 papers)

Most cited **INFN** publication
Most cited **CERN** publication

*Citation analysis: Thomson-Reuters' WoS, 22 May 2015
Database since 1970*

Instruments and Instrumentation Nuclear Science and Technology



Top cited papers

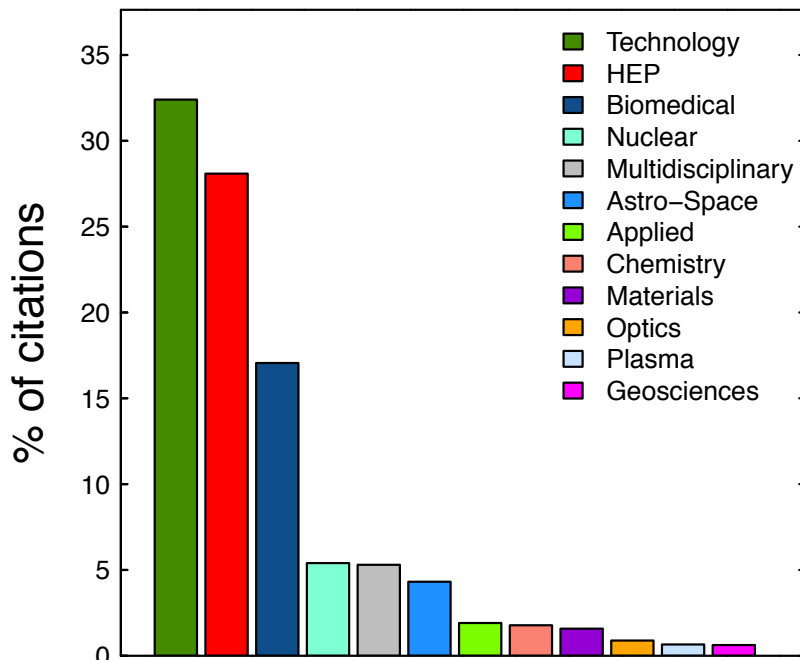
dominated by software!

1.	GEANT4-a simulation toolkit By: Agostinelli, S; Allison, J; Amako, K; et al. NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT Volume: 506 Issue: 3 Pages: 250-303 Published: JUL 1 2003	5743
2.	A MONTE-CARLO COMPUTER-PROGRAM FOR THE TRANSPORT OF ENERGETIC IONS IN AMORPHOUS TARGETS By: BIERSACK, JP; HAGGMARK, LG NUCLEAR INSTRUMENTS & METHODS Volume: 174 Issue: 1-2 Pages: 257-269 Published: 1980	3771
3.	ATHENA, ARTEMIS, HEPHAESTUS: data analysis for X-ray absorption spectroscopy using IFFFIT By: Ravel, B; Newville, M JOURNAL OF SYNCHROTRON RADIATION Volume: 12 Pages: 537-541 Part: 4 Published: JUL 2005	3033
4.	WSXM: A software for scanning probe microscopy and a tool for nanotechnology By: Horcas, I.; Fernandez, R.; Gomez-Rodriguez, J. M.; et al. REVIEW OF SCIENTIFIC INSTRUMENTS Volume: 78 Issue: 1 Article Number: 013705 Published: JAN 2007	2660

Geant 4

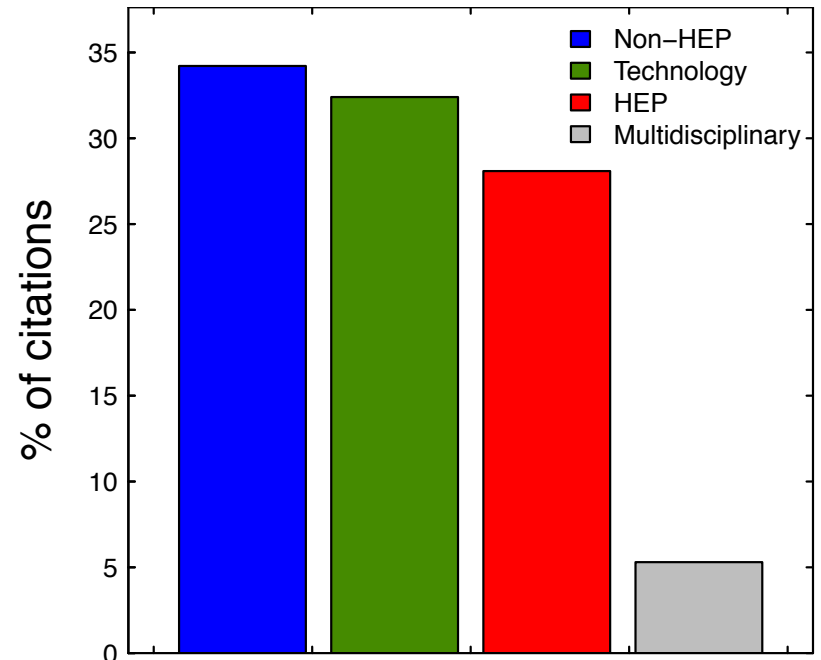
Born from LHC experimental requirements
Multidisciplinary sources of citations

Geant4 citations



Source of citations

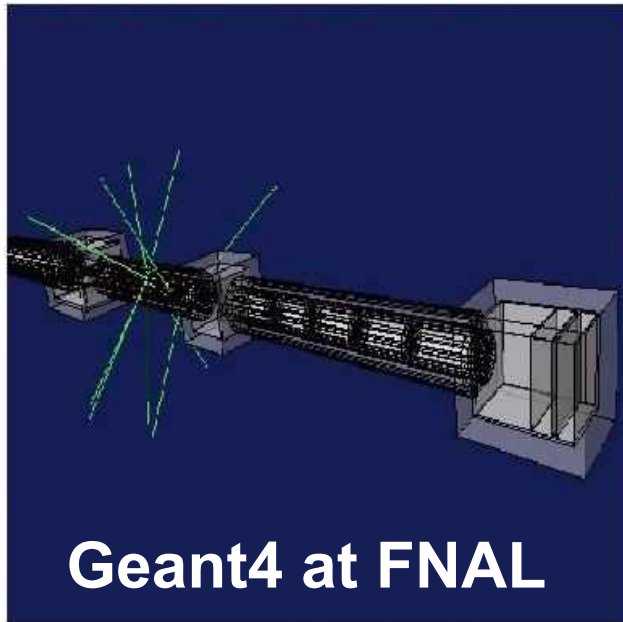
Geant4 citations



Source of citations

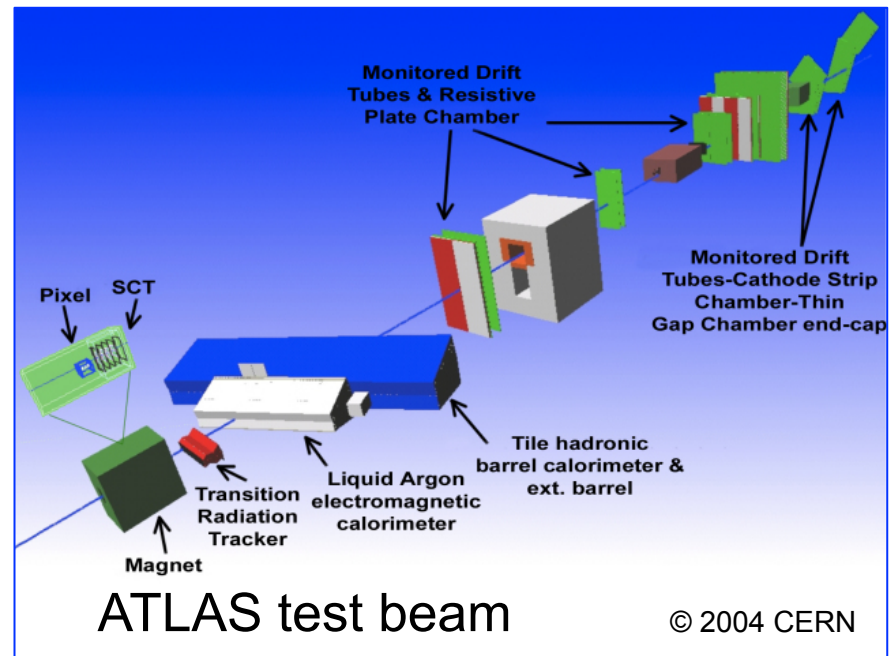
Based on Thomson-Reuters' Web of Science data

Beam lines



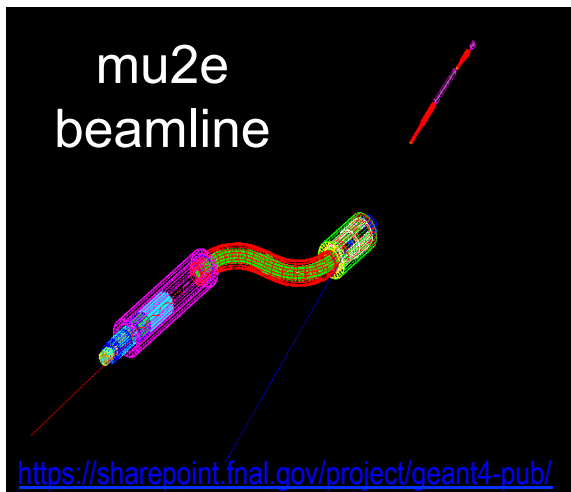
Geant4 at FNAL

Picture of the MiniBooNE beamline (image:Panagiotis Spentzouris)



BDSIM - Accelerator Beamline simulation tool

BDSIM is a Geant4 extension toolkit for simulation of particle transport in accelerator beamlines.





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➤ Projects
G4beamline

Simulation tools based on Geant4

Future accelerator facilities

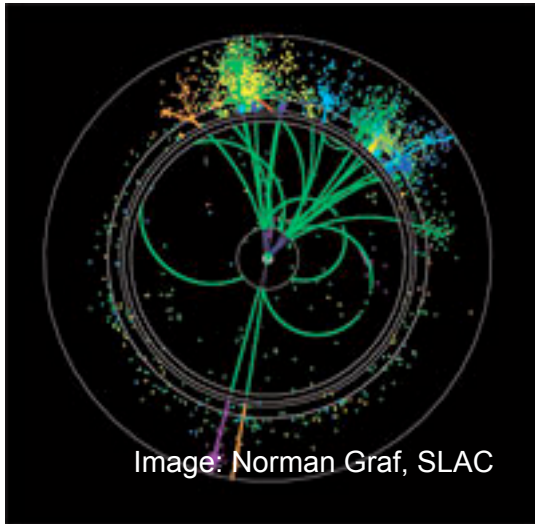


Image: Norman Graf, SLAC

ILC International Linear Collider
simulated response to
 $e^+e^- \rightarrow Z(\rightarrow \mu^+\mu^-) + \text{higgs} (\rightarrow bb)$

Proceedings of IPAC'10, Kyoto, Japan

POSITRON SOURCE SIMULATIONS USING GEANT4

A. Ushakov*, S. Riemann, A. Schälicke
DESY, Zeuthen, Germany

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Physics Procedia 37 (2012) 2114 – 2122

Physics

Procedia

TIPP 2011 – Technology and Instrumentation in Particle Physics 2011

Accelerator Backgrounds in a Muon Collider

Mary Anne Cummings a*, Stephen Kahn

Proceedings of 2011 Particle Accelerator Conference, New York, NY, USA

MOP019

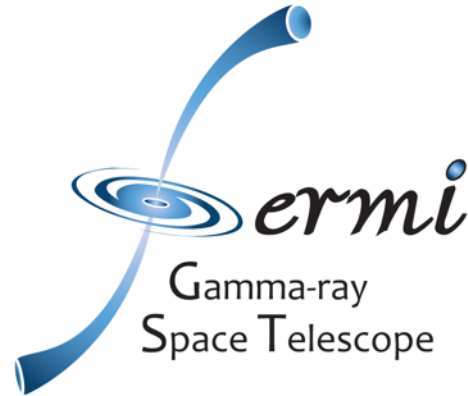
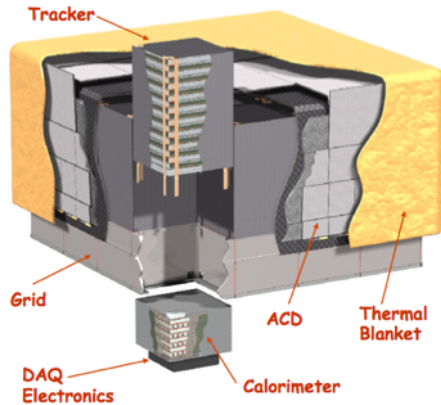
PERFORMANCE OF THE BUCKED COILS MUON-COOLING LATTICE FOR THE NEUTRINO FACTORY*

A. Alekou[#], Imperial College London, London, U.K
J. Pasternak, Imperial College London, London/STFC-RAL ISIS, Chilton, Didcot, UK
C.Rogers, RAL ASTeC, Chilton, Didcot, UK

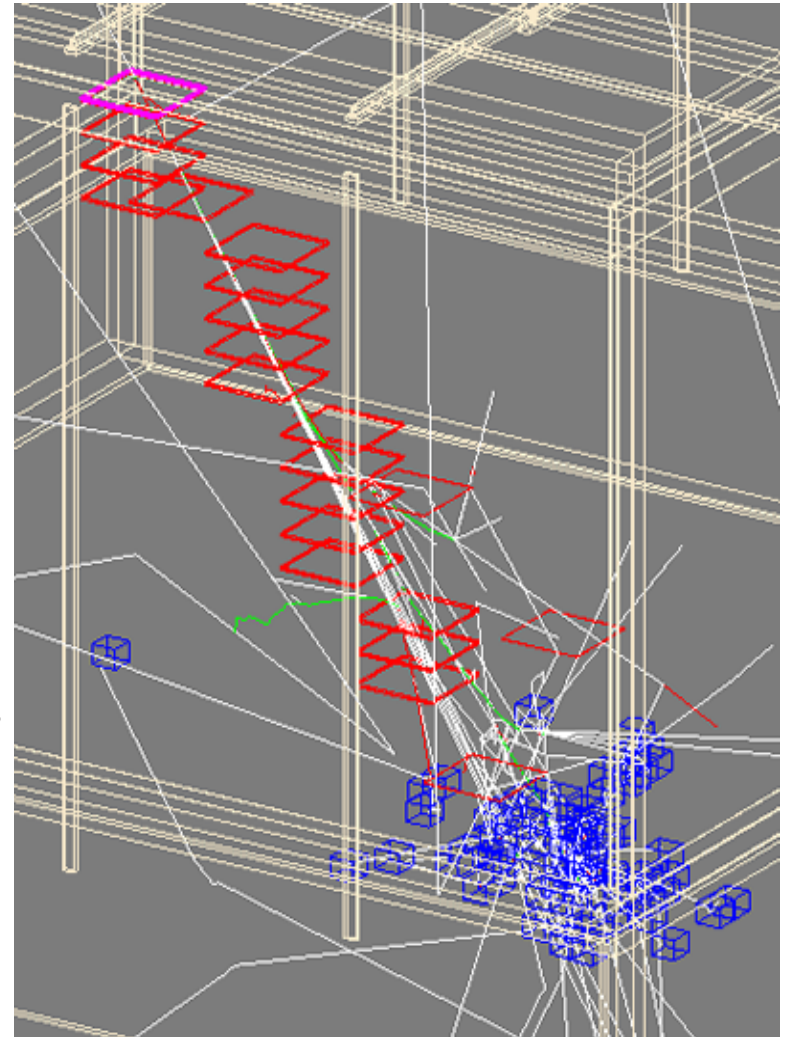
...and more

G4 Simulation for Fermi Large Area Telescope

Courtesy of Francesco Longo for the Fermi Collaboration



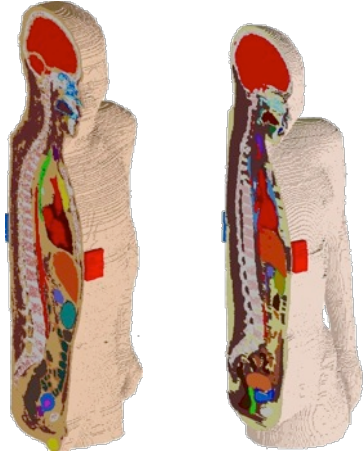
- Fermi Large Area Telescope: (<http://www-glast.stanford.edu>)
- Geant4 for MC particle interactions within the Fermi LAT simulation framework since 2004
 - Stored for further processing
 - ▷ McParticles – particles produced during tracking
 - ▷ McPositionHits – positions and energy deposited in Silicon and ACD
 - ▷ McIntegratingHits – energy deposited in CsI crystals
- Still using Geant4 version 9.4.p01
- Generated at least 200e9 events
- So far stored MC triggered events
 - Gamma-rays (4.12e9 evts)
 - Protons (1.32e9)
 - HE electrons (5.14e8)
 - AllBackground (5.43e9)



Example of gamma-ray event

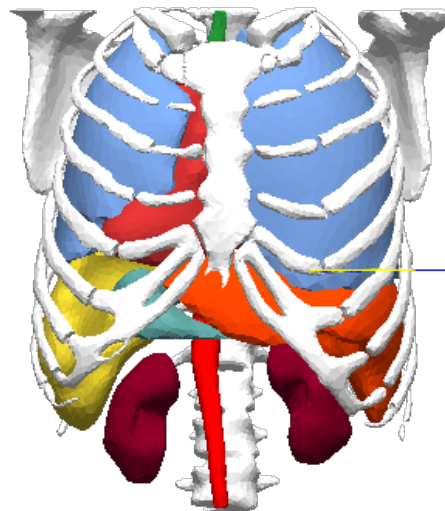
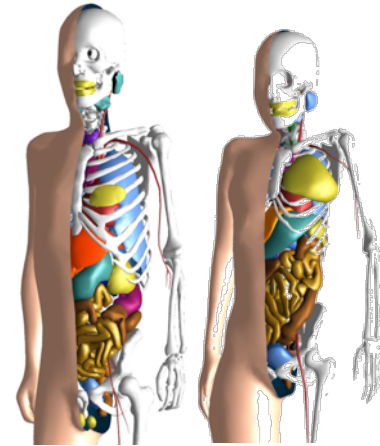
Computational Human Phantom

Voxel Phantom It can be implemented in Geant4, MCNP6, EGS, FLUKA...



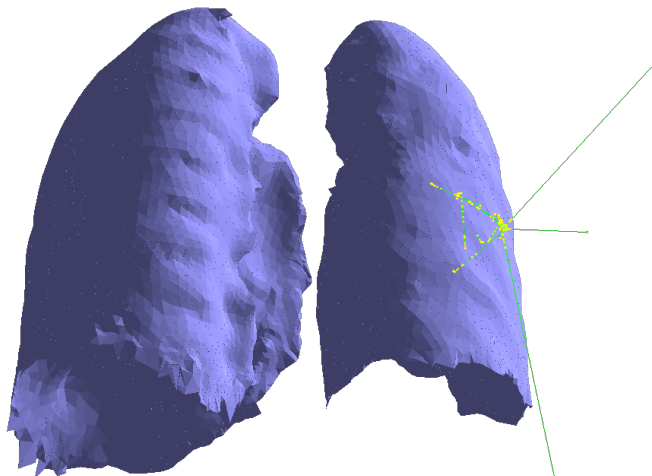
Polygonal Phantom

It can be implemented in Geant4 and MCNP6, but in MCNP6 electrons cannot be transported in an *unstructured mesh geometry*



4D Phantom

It can be implemented only in Geant4 at the present time



Nuclear power

GEANT4 STUDIES OF THE THORIUM FUEL CYCLE

Cristian Bungau, Roger Barlow, University of Manchester, UK
Adriana Bungau, Robert Cywinski, University of Huddersfield, UK

Annals of Nuclear Energy 71 (2014) 451–461



ELSEVIER

Contents lists available at ScienceDirect

Annals of Nuclear Energy

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



G4-STORK: A Geant4-based Monte Carlo reactor kinetics simulation code



Liam Russell^{a,1}, Adriaan Buijs^{a,*}, Guy Jonkmans^b

^aDepartment of Engineering Physics, McMaster University, Hamilton, Ontario, Canada

^bChalk River Laboratories, AECL, Chalk River, Ontario, Canada

PRL 109, 152501 (2012)

PHYSICAL REVIEW LETTERS

week ending
12 OCTOBER 2012



Cosmic Ray Radiography of the Damaged Cores of the Fukushima Reactors

Konstantin Borozdin,¹ Steven Greene,¹ Zarija Lukić,² Edward Milner,¹ Haruo Miyadera,¹
Christopher Morris,^{1,*} and John Perry¹

¹Los Alamos National Laboratory, Los Alamos, New Mexico 87544, USA

²Computational Cosmology Center, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

(Received 9 August 2012; published 11 October 2012)

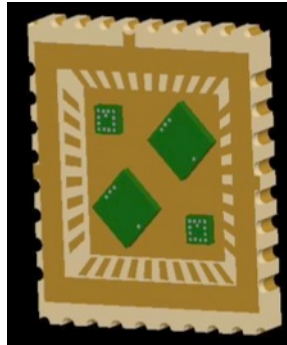
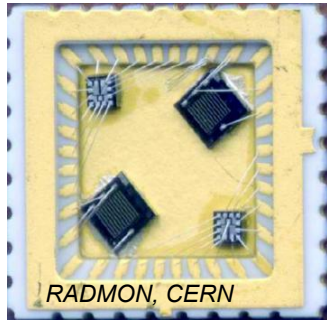
18th World Conference on Nondestructive Testing, 16-20 April 2012, Durban, South Africa

Design of New Neutron Imaging Facility at Triga Reactor in Morocco

Afaf OUARDI¹, Rachad ALAMI¹, Abdeslam BENSITEL¹

...and more

Radiation effects



Impact of the Radial Ionization Profile on SEE Prediction for SOI Transistors and SRAMs Beyond the 32-nm Technological Node

Mélanie Raine, *Student Member, IEEE*, Guillaume Hubert, Marc Gaillardin, *Member, IEEE*, Laurent Artola, Philippe Paillet, *Senior Member, IEEE*, Sylvain Girard, *Member, IEEE*, Jean-Etienne Sauvestre, *Member, IEEE*, and Arnaud Bournel

Packaging Effects on RadFET Sensors for High Energy Physics Experiments

Julien Mekki, Laurent Dusseau, *Senior Member, IEEE*, Maurice Glaser, Susanna Guatelli, *Member, IEEE*, Michael Moll, Maria Grazia Pia, and Federico Ravotti, *Member, IEEE*

Operational SER Calculations on the SAC-C Orbit Using the Multi-Scales Single Event Phenomena Predictive Platform (MUSCA SEP³)

Guillaume Hubert, Sophie Duzellier, Christophe Inguibert, César Boatella-Polo, Françoise Bezerra, and Robert Ecoffet

第46卷增刊
2012年9月

原子能科学技术
Atomic Energy Science and Technology

Vol. 46, Suppl.
Sep. 2012

Geant4 在中子辐射效应中的应用

金晓明, 王园明, 杨善潮, 马强, 刘岩, 林东生, 陈伟

(西北核技术研究所, 陕西 西安 710024)

摘要: 中子辐射效应是半导体器件在辐射环境中损伤的重要因素。本文建立了中子在半导体材料中的电离和非电离能量沉积、原子空位密度的 Geant4 模拟方法。电离能量沉积可用于分析电离总剂量效应, 非电离能量沉积可用于分析位移损伤效应。电离 kerma 因子的模拟结果定量解释了中子辐照在 CMOS 工艺单片机组成的电离增强效应。通过原子空位密度计算了中子引入的附加陷阱密度, 分析了位移损伤对电离效应的增强作用。实验和模拟结果表明, 中子的电离能量沉积加剧了 CMOS 工艺单片机的退化。

关键词: 中子辐射效应; 电离能量沉积; 非电离能量沉积; 原子空位

中图分类号: TN431; TN792 **文献标志码:** A **文章编号:** 1000-6931(2012)S0-0607-04

Geant4 Application in Neutron Radiation Effects

JIN Xiao-ming, WANG Yuan-ming, YANG Shan-chao, MA Qiang,

LIU Yan, LIN Dong-sheng, CHEN Wei

(Northwest Institute of Nuclear Technology, Xi'an 710024, China)

ARTICLE

GEANT4 Micro Geometry Study of Ionising Radiation Effects in Digital ASIC's

Miguel A. CORTES-GIRALDO^{1,*}, Francisco R. PALOMO²,
Esther GARCIA-SANJUAN² and José M. QUESADA¹

¹Departamento de Física Atómica, Molecular y Nuclear, Universidad de Sevilla, 41080-Sevilla, Spain

²Departamento de Ingeniería Electrónica, Escuela Superior de Ingenieros Industriales, Sevilla, 41092-Sevilla, Spain



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Nuclear Instruments and Methods in Physics Research B 261 (2007) 1133–1136

NIM B
Beam Interactions
with Materials & Atoms

www.elsevier.com/locate/nimb

Physical mechanisms of single-event effects in advanced microelectronics

Ronald D. Schrimpf^{a,*}, Robert A. Weller^a, Marcus H. Mendenhall^b, Robert A. Reed^a,
Lloyd W. Massengill^a

^aElectrical Engineering and Computer Science, Vanderbilt University, 5635 Stevenson Center, Nashville, TN 37235, United States

^bFree Electron Laser Center, Vanderbilt University, Station B 351816, Nashville, TN 37235, United States

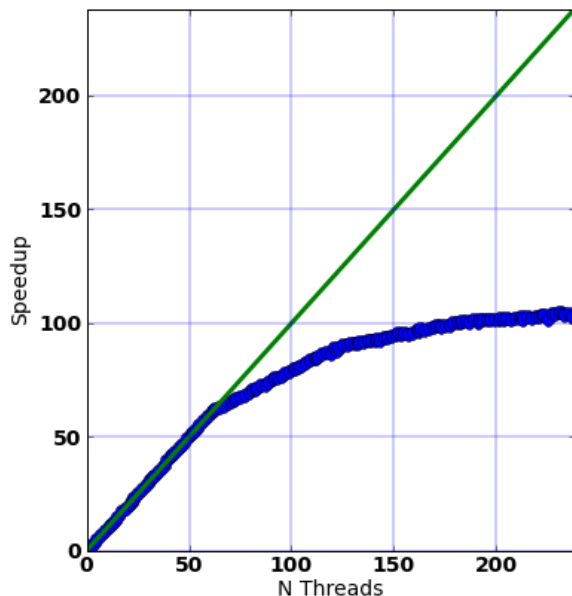
Speed



Today's hype

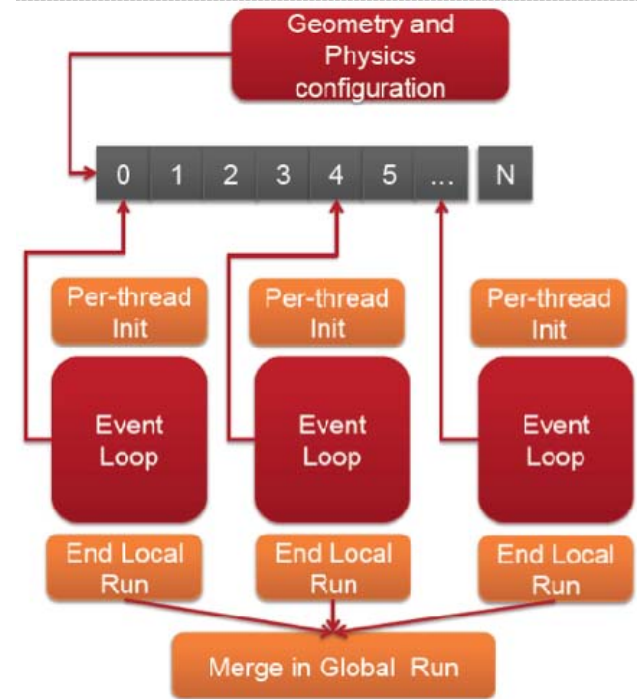
Geant4-MultiThreaded

- Adopt the same event-level parallelism as the prior distributed memory parallelization has done
- Replace k independent copies of the Geant4 process with an equivalent single process with k threads
- Uses the many-core machine in a memory-efficient scalable manner



Speedup obtained by running a HEP simulation (50 GeV pions with B-field) on the Intel® Xeon Phi™ (7110P, 1.238 GHz, 61 cores) co-processor, up to the maximum number of threads

Released in Geant4 10.0





Geant

The best Geant ever

[Home](#)[About](#)[Development Tools](#)[Installation](#)[Documentation](#)[Download](#)[Forum](#)

Detector simulation is one of the most CPU intensive tasks in modern High Energy Physics.

While its importance for the design of the detector and the estimation of the efficiency is ever increasing, the amount of events that can be simulated is often constrained by the available computing resources.

Various kind of "fast simulations" have been developed to alleviate this problem, however, while successful, these are mostly "ad hoc" solutions which do not replace completely the need for detailed simulations.

One of the common features of both detailed and fast simulation is the inability of the codes to exploit fully the parallelism which is increasingly offered by the new generations of CPUs.

In the next years it is reasonable to expect an increase on one side of the needs for detector simulation, and on the other in the parallelism of the hardware, widening the gap between the needs and the available means. In the past years, and indeed since the beginning of simulation programs, several unsuccessful efforts have been made to exploit the "embarrassing parallelism" of simulation programmes.

GeantV News

[Discussion on April 24, 2013](#)

Here is the [file](#) summarising our discussions.

And what there is to conquer
By strength and submission, has already been discovered
Once or twice, or several times...

T. S. Eliot

Four Quartets - East Coker

CERN 90-06
29 May 1990

ORGANISATION EUROPÉENNE POUR LA RECHERCHE NUCLÉAIRE
CERN EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

EXPERIENCE WITH VECTOR PROCESSORS IN HEP

Federico Carminati

CERN, Geneva, Switzerland

“In studying the vectorization opportunities offered by the GEANT code, it has been realized that the fundamental strategy should be to handle more than one particle at a time in the tracking process. This means that the program should now answer questions like *is a given particle in a given volume?* or *which is the next interaction point for the given particle?* and so on, not any more for a single particle at a time, but for the maximum number of eligible particles in any given moment.”

1989 CERN SCHOOL OF COMPUTING

Bad Herrenalb, Federal Republic of Germany
20 August-2 September 1989

Algorithms

Popular belief

Physics model X is intrinsically slow

Baroque methods to combine it with “faster” lower precision models and limit its use to cases where one is willing to pay for higher precision

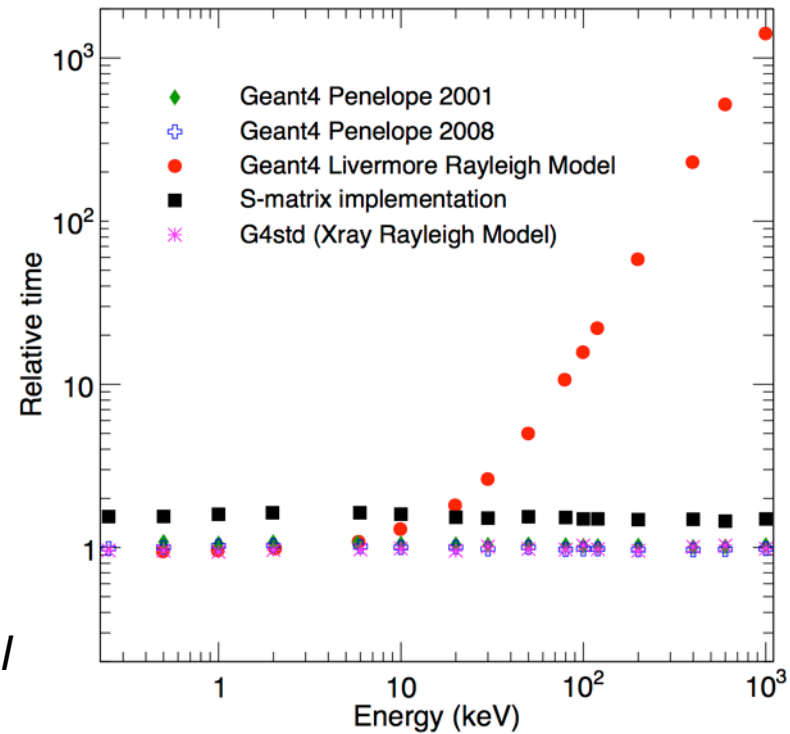
This design introduces an additional computational burden due to the effects of inheritance and the combination algorithms themselves

Truth

Physics model X is intrinsically fast

But its computationally fast physics functionality is spoiled by an inefficient sampling algorithm

Change the sampling algorithm!



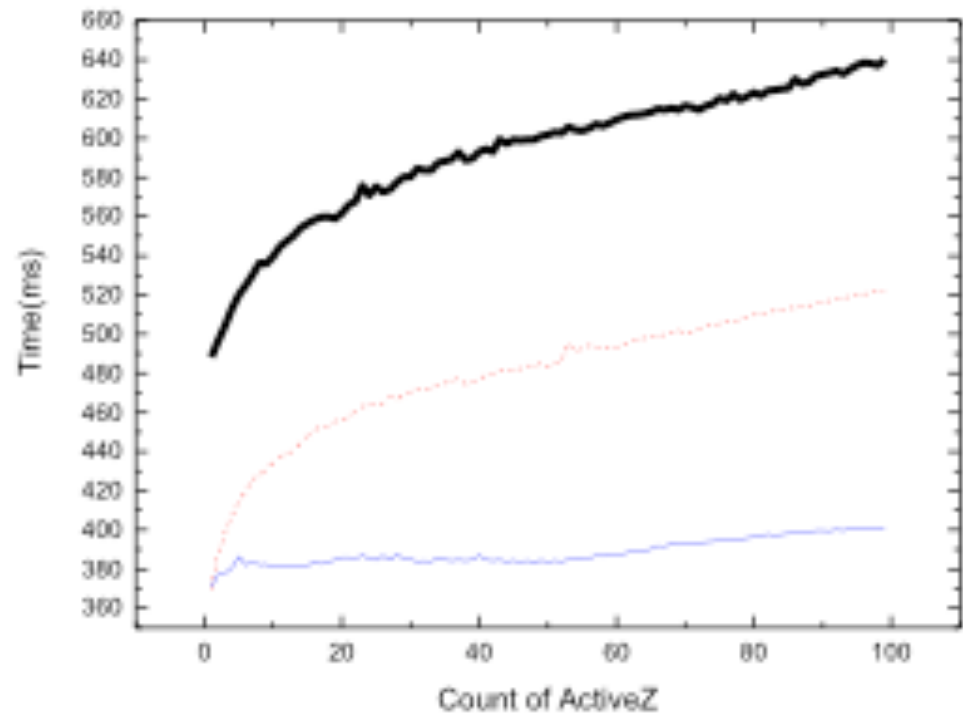
- ▶ No code smell
- ▶ Spotted through in-depth **code review** in the course of **software validation**

Refactoring data management

- Today's technology
 - ...keeping an eye on the new C++ Standard

- Optimal container
- Pruning data
- Splitting files
- Software design

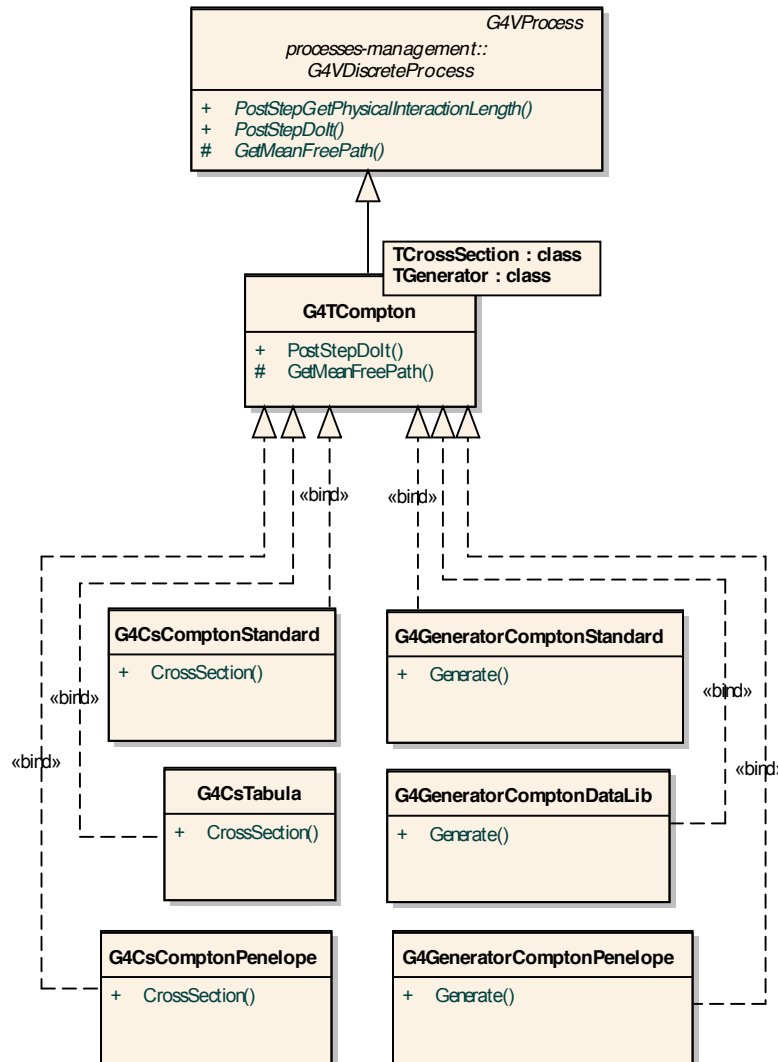
Min Cheol Han
Hanyang Univ., Seoul



Policy-based class design

Same functionality
refactored into new design

No attempt to do any
performance optimisation



~30% speed gain in
electromagnetic physics
processes
(preliminary)

The fastest algorithm

no algorithm at all

Shift modeling from algorithms to data

Merging models



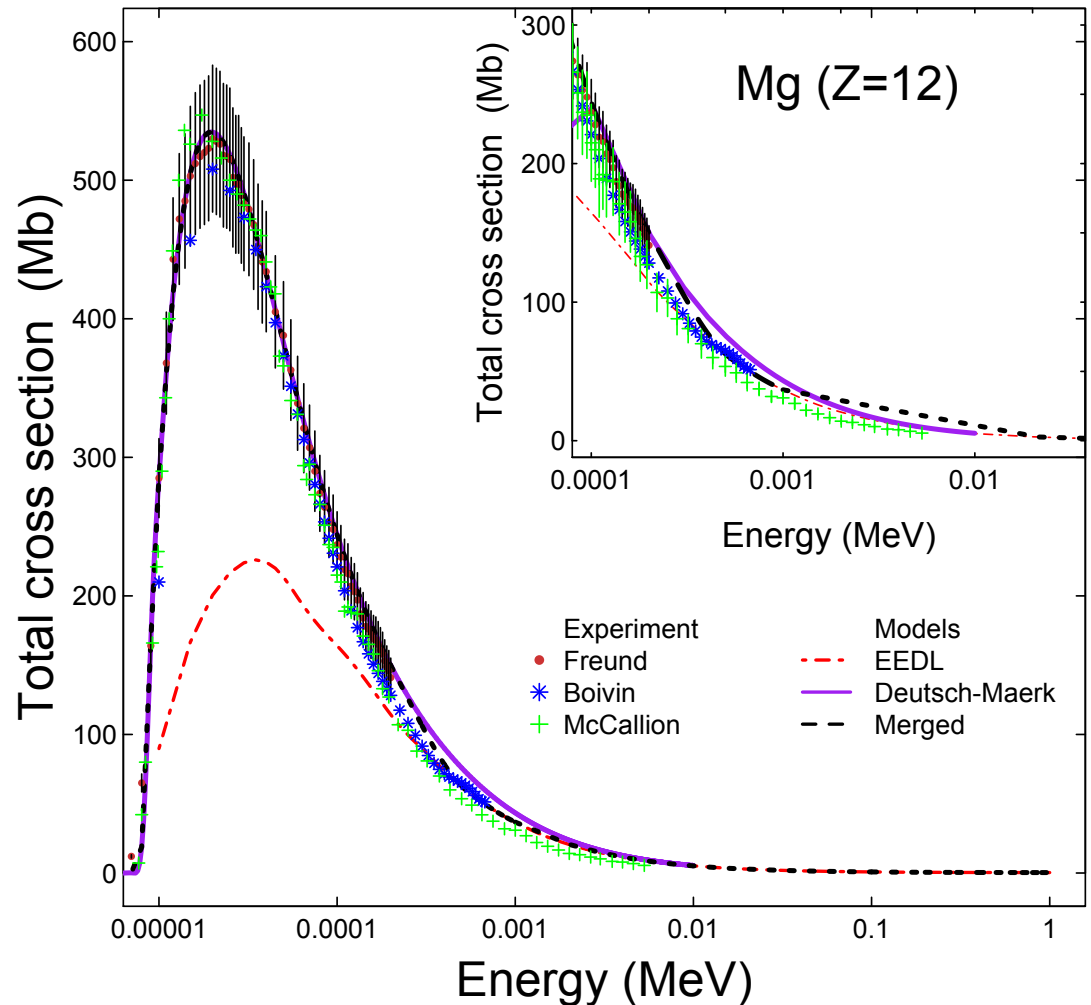
Smoothing data

Guidance from
experimental data
(when available)

Data libraries

Need mathematical expertise
(smoothing algorithms)

Electron impact ionisation cross sections



Example: LOESS local polynomial regression fitting
Beware: not optimized!

Prune

Number one in the stink parade is duplicated ~~code~~

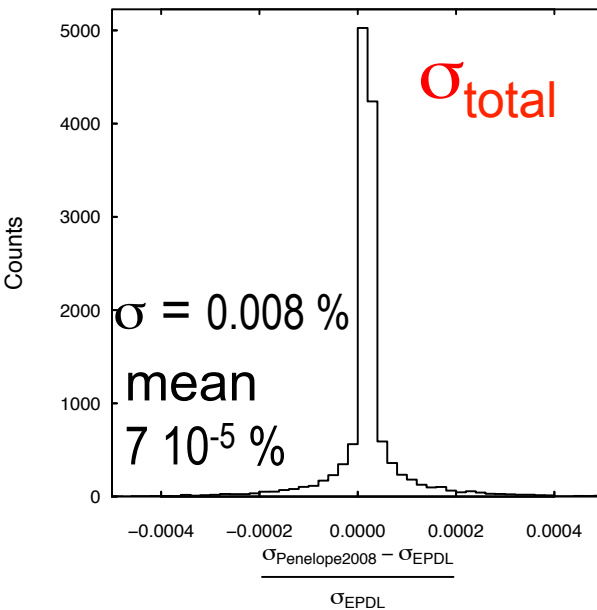
M. Fowler,
Refactoring

physics

Two Geant4 models, identical underlying physics content (*it used to be different*)

Efficiency w.r.t. experiment

"Livermore"	Penelope
EPDL97	EPDL97
0.38±0.06	0.38±0.06



Code bloat

Burden on

- Software design
- Maintenance
- User support

Unnecessary complexity

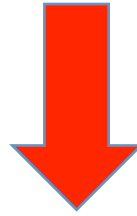
Content

- Physics
- Reliability
 - Validation
 - Testability
- Maintainability
- Predictivity



Physics

The physics of Monte Carlo codes is still intended for the detectors of the '80s



IA assumption
IPA

*Is this physics validated?
Does it reflect the state of the art?*

New frontiers in detector R&D

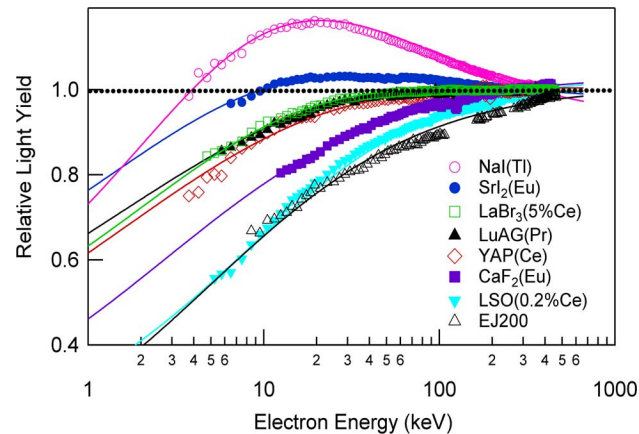
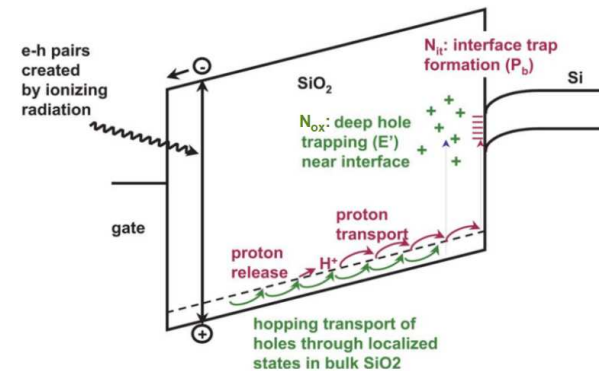


Fig. 1. Electron response (relative scintillation efficiency versus electron energy) of eight scintillators. Reprinted with permission from [17].

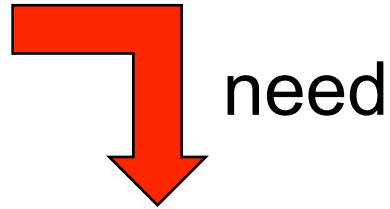


Incorporating materials science knowledge
Understanding underlying phenomena that contribute to making the signal in detectors

Ionization Cross Sections for Low Energy Electron Transport

Hee Seo, Maria Grazia Pia, Paolo Saracco, and Chan Hyeong Kim

Reliability



documented, objective, quantitative
validation



Testable physics

Validation

- Limited documentation of **simulation validation**

- Mostly in the form of specific use cases compared to measurements in the same experimental scenario
 - ▷ Do they apply to similar/different use cases?
 - ▷ How to extrapolate the results to different scenarios?

- Hardly any ^(quantitative) **validation of the basic physics models** implemented in Monte Carlo codes

- Why?

- Oenology and Mozart opera

- Widely applied in experimental practice





Establishing validity

Agreement
Good agreement
Excellent agreement
Satisfactory agreement
...

Comparison of simulation results and experimental data in the literature mainly rests on

- qualitative visual appraisal of figures
- indicators (%) deprived of any statistical meaning

Statistical methods and tools

R&D needed

Epistemological mistakes

- Comparison of different Monte Carlo codes
- Comparison of different physics models
- Comparison of simulation with theory

You need an experiment to test a cross section

Testing total cross sections calculated by *G4PEEffectFluoModel*

You can find the photoelectric cross section *G4PEEffectFluoModel* class in `$G4INSTALL/source/processes/electromagnetic/standard/include` (*G4PEEffectFluoModel.hh* header file) and `$G4INSTALL/source/processes/electromagnetic/standard/src/` (*G4PEEffectFluoModel.cc* implementation). *G4PEEffectFluoModel* has a *ComputeCrossSectionPerAtom* public member function, which returns the total photoelectric cross section for a given element corresponding to a given photon energy:

```
G4double ComputeCrossSectionPerAtom(const G4ParticleDefinition*,
                                   G4double kinEnergy,
                                   G4double Z,
                                   G4double A,
                                   G4double, G4double)
```

Geant4 photoelectric cross section

This is what we need indeed!

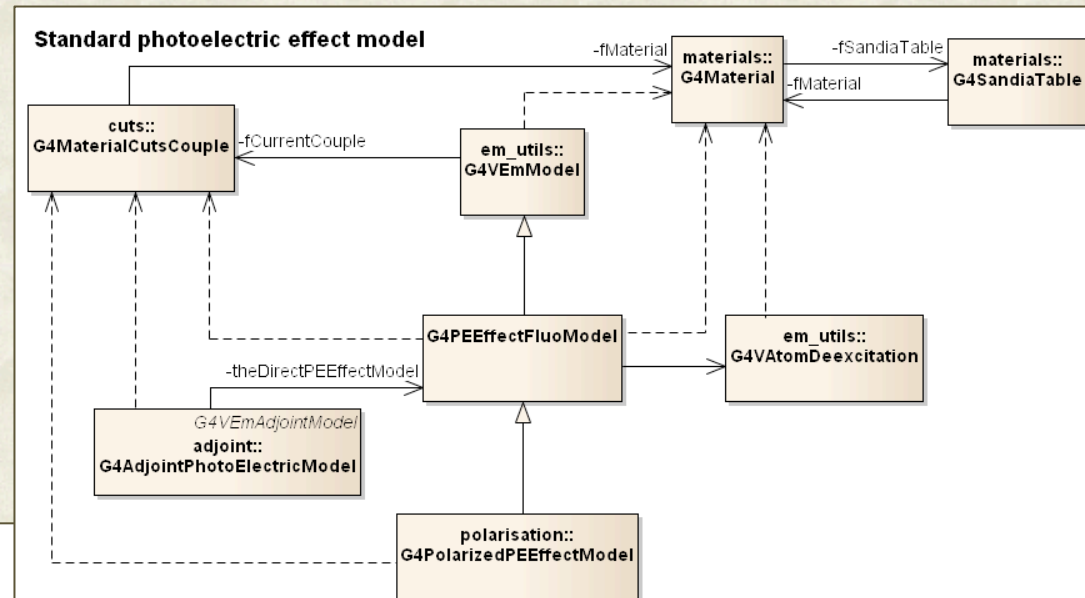
We create a simple [unit test](#) *G4PEEffectFluoModelTest.cc*, which instantiates a *G4PEEffectFluoModel* object and invokes *ComputeCrossSectionPerAtom* in pre-defined configurations of photon energy and target element. We place the unit test in `$APCDIR/test`.

We build the test:

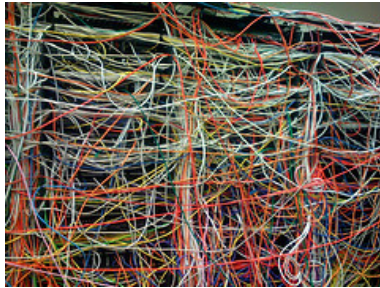
```
cd $APCDIR/test
setenv TESTTARGET G4PEEffectFluoModelTest
gmake
```

Then we run the test:

```
$G4WORKDIR/bin/Linux-g++/G4PEEffectFluoModelTest
```



Post-RD44 Geant4 electromagnetic software design



Hidden dependencies

on other parts of the software

One needs a geometry
(and a full scale application)
to test any photon cross section

Difficult to test → no testing
often

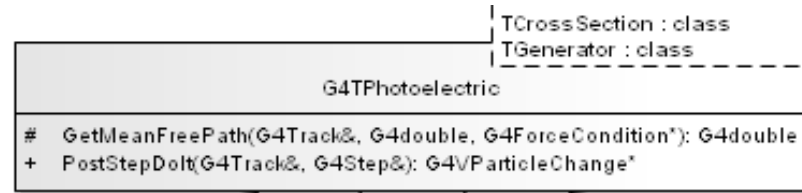


Detangling

Photoionisation

Testable
Open - closed

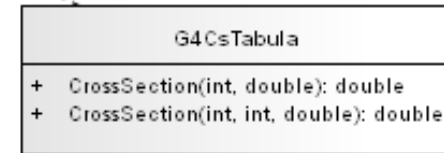
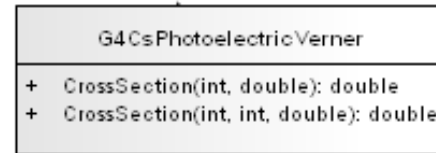
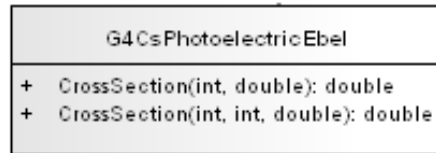
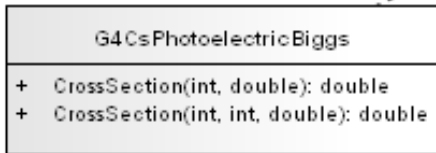
Can be validated
in a unit test



Cross section models can
be compared with
statistical categorical tests

Handles any tabulated
cross section

New models



Sweeping
under the
carpet?

Refactoring Geant4 physics into “clean code”

Refactoring → preserve functionality

Was the original code **verified**?
Was the original code **validated**?
What was the test coverage?

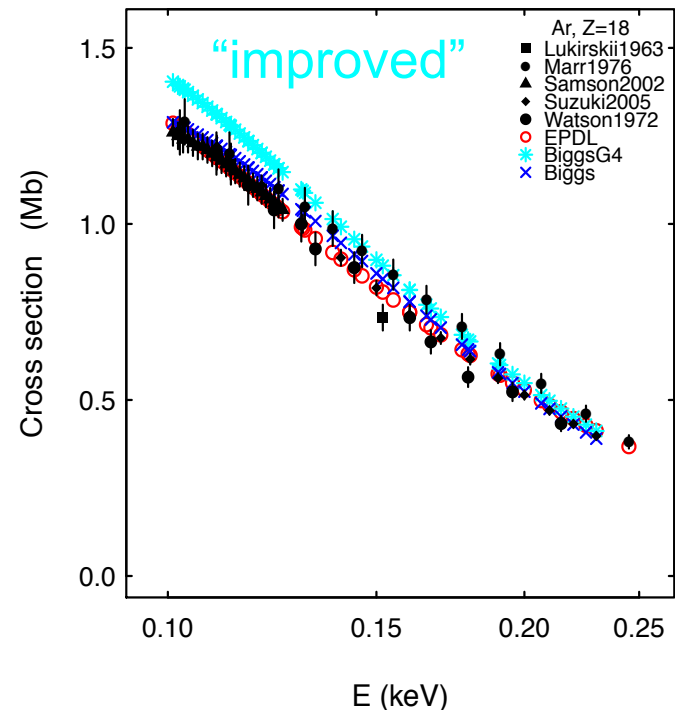
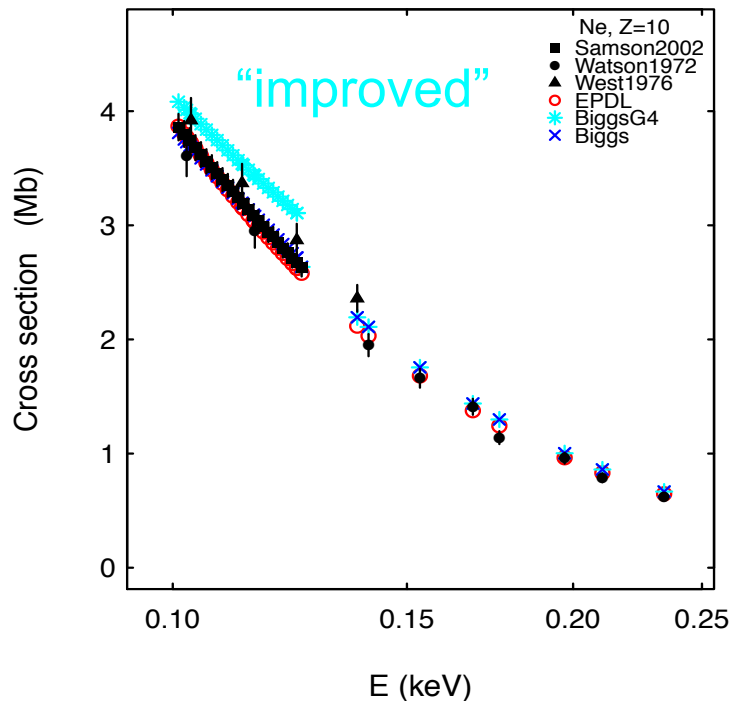
Were the test process and the test results documented?

Photoionisation cross section

Cross sections in Geant4 “standard” photoelectric model are based on “improved”

Biggs-Lighthill parameterisation

F. Biggs and R. Lighthill, Analytical Approximation for X-ray Cross Sections III, Sandia Lab. Report SAND-0070, 1988



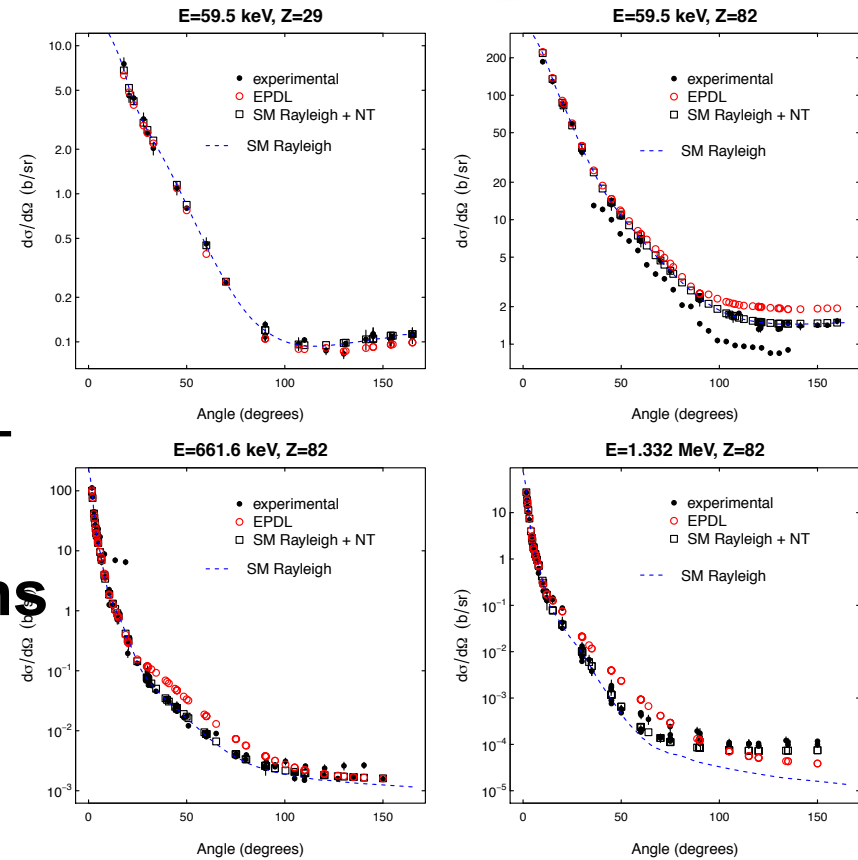
Photon elastic scattering

Differential cross section

- relativistic form factors (*EGS*)
- non-relativistic form factors (*Geant4, MCNP, Penelope, FLUKA...*): Hubbell et al., EPDL

New

- numerical **S-matrix calculations**
- modified relativistic form factors,
- modified relativistic form factors with anomalous scattering factors

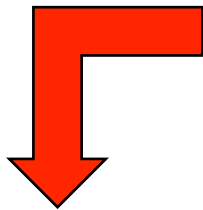


	Penelope 2001	Penelope 2008	EPDL	Relativ. FF	Non-Rel. FF	Modified FF	MFF ASF	RFF ASF	SM NT
ϵ	0.27	0.38	0.38	0.25	0.35	0.49	0.52	0.48	0.77
error	± 0.05	± 0.06	± 0.06	± 0.05	± 0.06	± 0.06	± 0.06	± 0.06	± 0.05

ϵ = fraction of test cases compatible with experiment, 0.01 significance

Maintainability

The time scale of HEP, astroparticle and astrophysics experiments extends over decades



Maintainability is a major concern

See Elisabetta Ronchieri's talk

(maintainability implies testability: verify that functionality is preserved)

Lehman laws

M. M. Lehman,
Programs, Life Cycles, and Laws of Software Evolution,
Proc. IEEE, vol. 68, no. 9, Sep. 1980

1. Continuing Change

- A program that is used and that as an implementation of its specification reflects some other reality, **undergoes continual change** or **becomes progressively less useful**. The change or decay process continues until it is judged more cost effective to replace the system with a recreated version.

2. Increasing Complexity

- As an evolving program is continually changed, **its complexity, reflecting deteriorating structure, increases unless work is done to maintain or reduce it.**

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Answer to the Ultimate Question of Life, the Universe, and Everything
Douglas Adams, The Hitchhiker's Guide to the Galaxy

```
// G4HadronElastic  
// 29 June 2009 (redesign old elastic model)
```

```
G4double dd = 10.;  
G4Pow* g4pow = G4Pow::GetInstance();  
if (A <= 62) {  
  bb = 14.5*g4pow->Z23(A);  
  aa = g4pow->powZ(A, 1.63)/bb;  
  cc = 1.4*g4pow->Z13(A)/dd;  
} else {  
  bb = 60.*g4pow->Z13(A);  
  aa = g4pow->powZ(A, 1.33)/bb;  
  cc = 0.4*g4pow->powZ(A, 0.4)/dd;  
}
```

Epistemology!

```
G4UrbanMscModel
```

```
coeffc1 = 2.3785 - Z13*(4.1981e-1 - Z13*6.3100e-2);
```

Testable?
Calibrated?

Epistemic uncertainties?

```
G4ChipsAntiBaryonElasticXS
```

```
lastPAR[43]=920.+03*a8*a3;  
lastPAR[44]=93.+0023*a12;
```

```
G4GoudsmitSaundersonMscModel
```

```
if(i>=19)ws=cos(sqrtA);
```

```
G4EmCorrections
```

```
if(15 >= iz) {  
  if(3 > j) { tet = 0.25*Z2*(1.0 + 5*Z2*alpha2/16.); }  
  else { tet = 0.25*Z2*(1.0 + Z2*alpha2/16.); }  
}
```

A new paradigm

simulation **result \pm error**

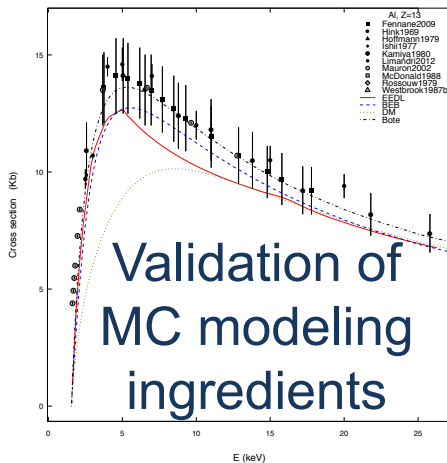
Today's hype in many research domains

Uncertainty Quantification

Theoretical Grounds for the Propagation of
Uncertainties in Monte Carlo Particle Transport

Paolo Saracco, Maria Grazia Pia, and Matej Batic

input
with uncertainties

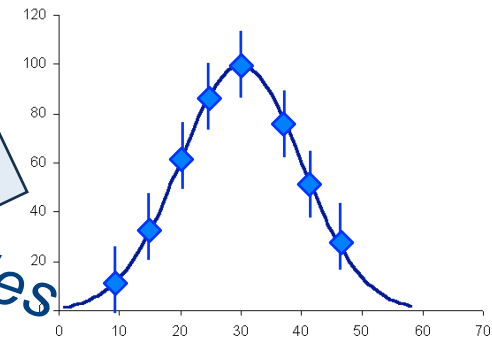


Beware: input uncertainties
can be hidden in models and
algorithms in the code



Monte Carlo method

observable
with uncertainties



Uncertainties deriving from

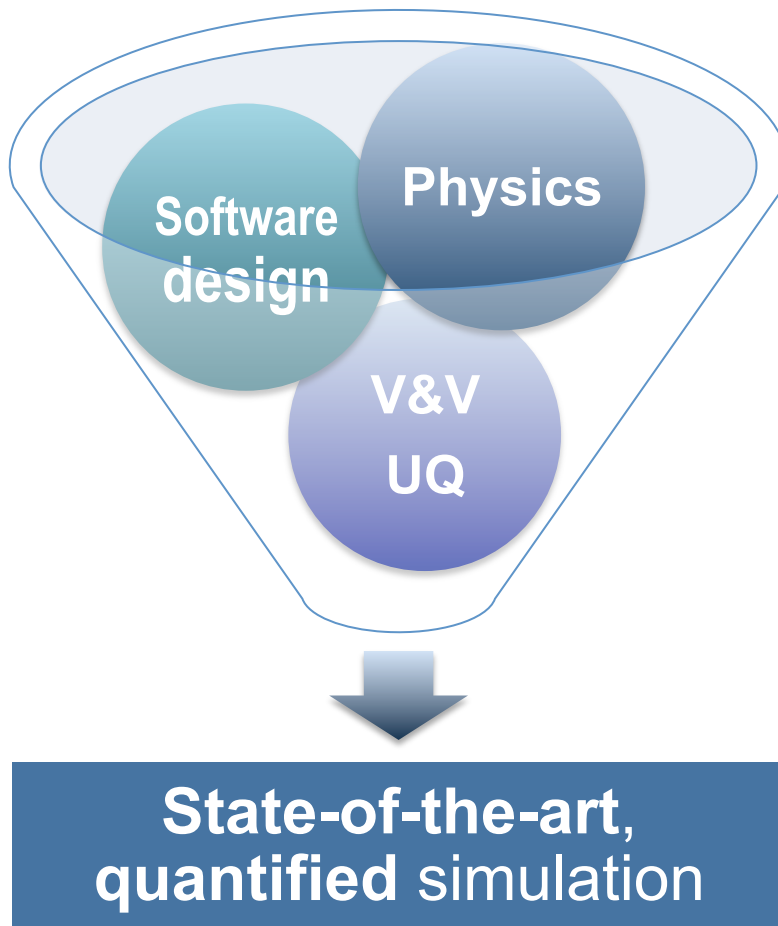
- input uncertainties
- Monte Carlo algorithm
- simulation model

Uncertainty quantification is the ground for
predictive Monte Carlo simulation

Conclusions



Vision supporting our research



- **State-of-the-art physics**
- Quantitative **validation** applying statistical methods
- Exploration of modern **software design** methods
- Computational performance measurements
- R&D for simulation as a **predictive instrument**

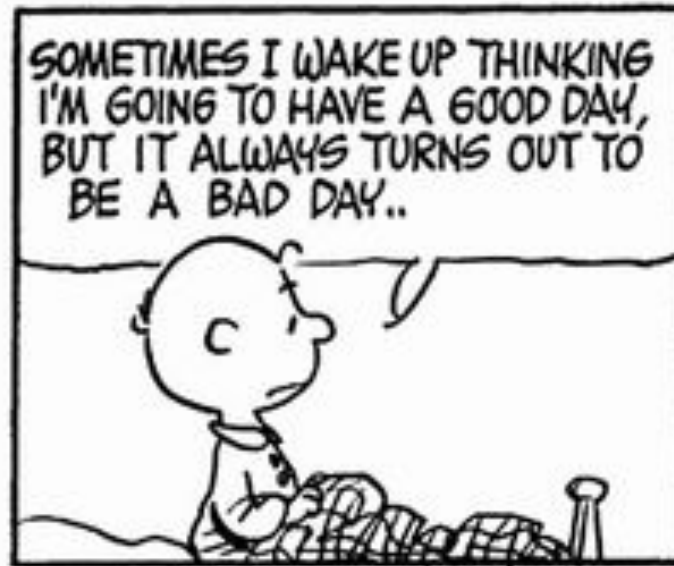
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<http://www.ge.infn.it/geant4/papers>



Ein unnütz Leben ist ein früher Tod.

(Johann Wolfgang von Goethe)