

# Simulation Validation Epistemics in a Geant4 Case Study

 food for thought in 15'

Maria Grazia Pia, *INFN Genova, Italy*

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# Lessons learned from...

>3 years with Geant4 electron backscattering

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 62, NO. 2, APRIL 2015

451

## Validation Test of Geant4 Simulation of Electron Backscattering

Sung Hun Kim, Maria Grazia Pia, Tullio Basaglia, Min Cheol Han, Gabriela Hoff, Chan Hyeong Kim, and  
Paolo Saracco

29 pages

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 62, NO. 4, AUGUST 2015

1805

## Investigation of Geant4 Simulation of Electron Backscattering

Tullio Basaglia, Min Cheol Han, Gabriela Hoff, Chan Hyeong Kim, Sung Hun Kim, Maria Grazia Pia, and  
Paolo Saracco

8 pages

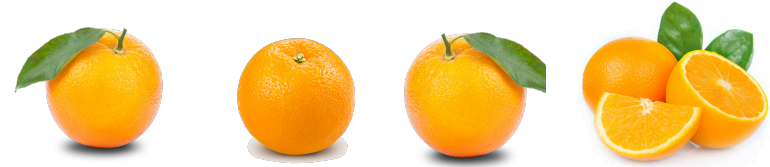
This article has been accepted for publication in a future issue of this journal, but has not been fully edited. Content may change prior to final publication. Citation information: DOI 10.1109/TNS.2016.2617834, IEEE  
Transactions on Nuclear Science

1

## Quantitative Test of the Evolution of Geant4 Electron Backscattering Simulation

Tullio Basaglia, Min Cheol Han, Gabriela Hoff, Chan Hyeong Kim, Sung Hun Kim, Maria Grazia Pia, and Paolo  
Saracco

18 pages



## Simulation ingredients

- Cross sections
- Angular distributions
- Secondary particle spectra
- Atomic parameters
- Nuclear parameters
- ...

### Unit test

**Validating Geant4** (*MCMP, EGS, Penelope, FLUKA etc.*)  
**cross sections, ...**

*Maria Grazia Pia, INFN Genova*

## Simulation use case

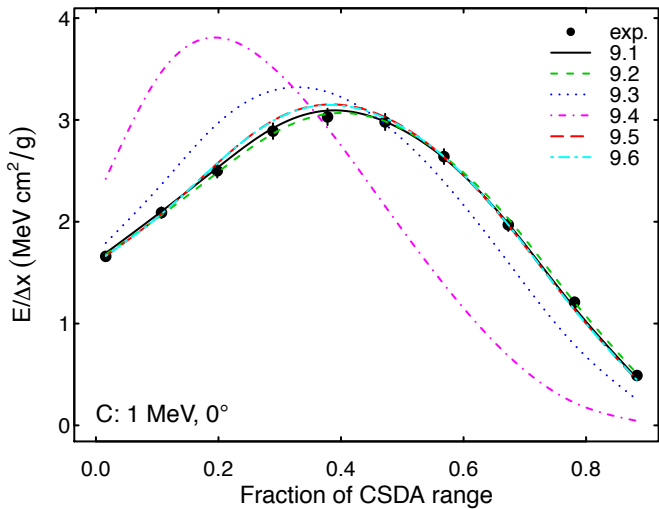
- A simulated model of an experimental scenario
  - Geometry
  - Materials
  - Detector response
  - ...
  - Monte Carlo transport code
- Simulated observable

### Full simulation

dependencies

~~**Validating Geant4**~~ (*MCMP, EGS, Penelope, FLUKA etc.*)

# The background: 2007-2013



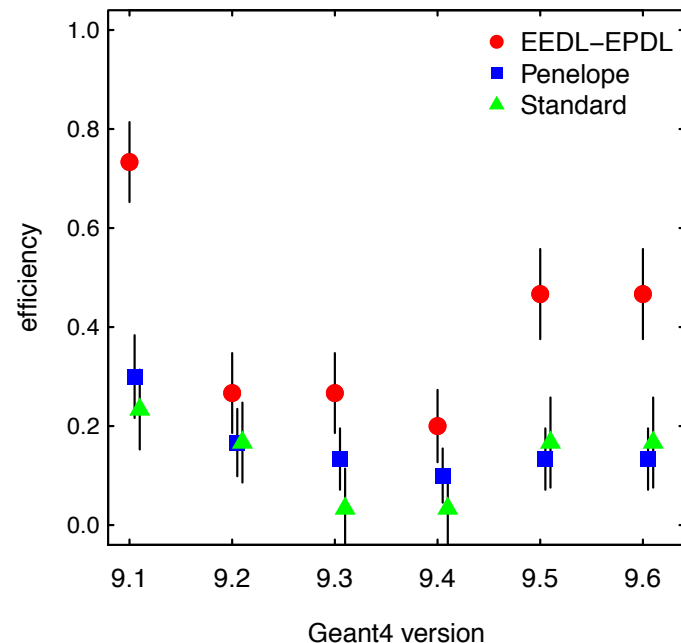
2934

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 60, NO. 4, AUGUST 2013

## Validation of Geant4 Simulation of Electron Energy Deposition

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

Target	Z	E (keV)	angle (degrees)	Geant4 version					
				9.1	9.2	9.3	9.4	9.5	9.6
Be	4	58	0	0.071	0.014	0.124	0.311	0.149	0.156
Be	4	109	0	0.021	< 0.001	< 0.001	< 0.001	0.015	0.013
Be	4	314	0	0.015	0.764	< 0.001	< 0.001	0.013	0.014
Be	4	521	0	0.092	0.967	< 0.001	< 0.001	0.832	0.793
Be	4	1033	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
C	6	1000	0	0.917	0.994	< 0.001	< 0.001	0.290	0.346
Al	13	314	0	0.182	< 0.001	< 0.001	< 0.001	0.004	0.007
Al	13	521	0	0.574	< 0.001	< 0.001	< 0.001	0.091	0.089
Al	13	1033	0	0.484	0.123	< 0.001	< 0.001	< 0.001	< 0.001
Al	13	314	60	0.396	0.596	< 0.001	< 0.001	0.001	0.002
Al	13	521	60	0.137	0.011	0.001	< 0.001	0.056	0.086
Al	13	1033	60	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Fe	26	300	0	0.832	< 0.001	0.351	0.741	0.787	0.742
Fe	26	500	0	0.055	< 0.001	0.314	0.003	0.814	0.808
Fe	26	1000	0	< 0.001	< 0.001	0.169	0.003	< 0.001	< 0.001
Cu	29	300	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Cu	29	500	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	100	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	300	0	0.062	< 0.001	0.001	< 0.001	0.008	0.002
Mo	42	500	0	0.020	< 0.001	< 0.001	0.001	0.128	0.115
Mo	42	1000	0	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Mo	42	300	60	0.023	0.002	0.049	0.043	0.029	0.022
Mo	42	500	60	0.022	< 0.001	0.011	0.006	0.003	0.007
Mo	42	1000	60	0.037	< 0.001	0.010	0.028	0.001	0.002
Ta	73	300	0	0.043	0.511	0.242	0.272	0.364	0.294
Ta	73	500	0	0.025	0.003	< 0.001	< 0.001	0.012	0.019
Ta	73	1000	0	0.030	< 0.001	< 0.001	< 0.001	0.002	0.001
Ta	73	500	60	0.011	0.003	0.040	0.042	0.010	0.007
Ta	73	1000	60	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
Ta	73	500	30	0.034	0.005	0.004	0.006	0.020	0.017



Hint at effects of multiple scattering simulation

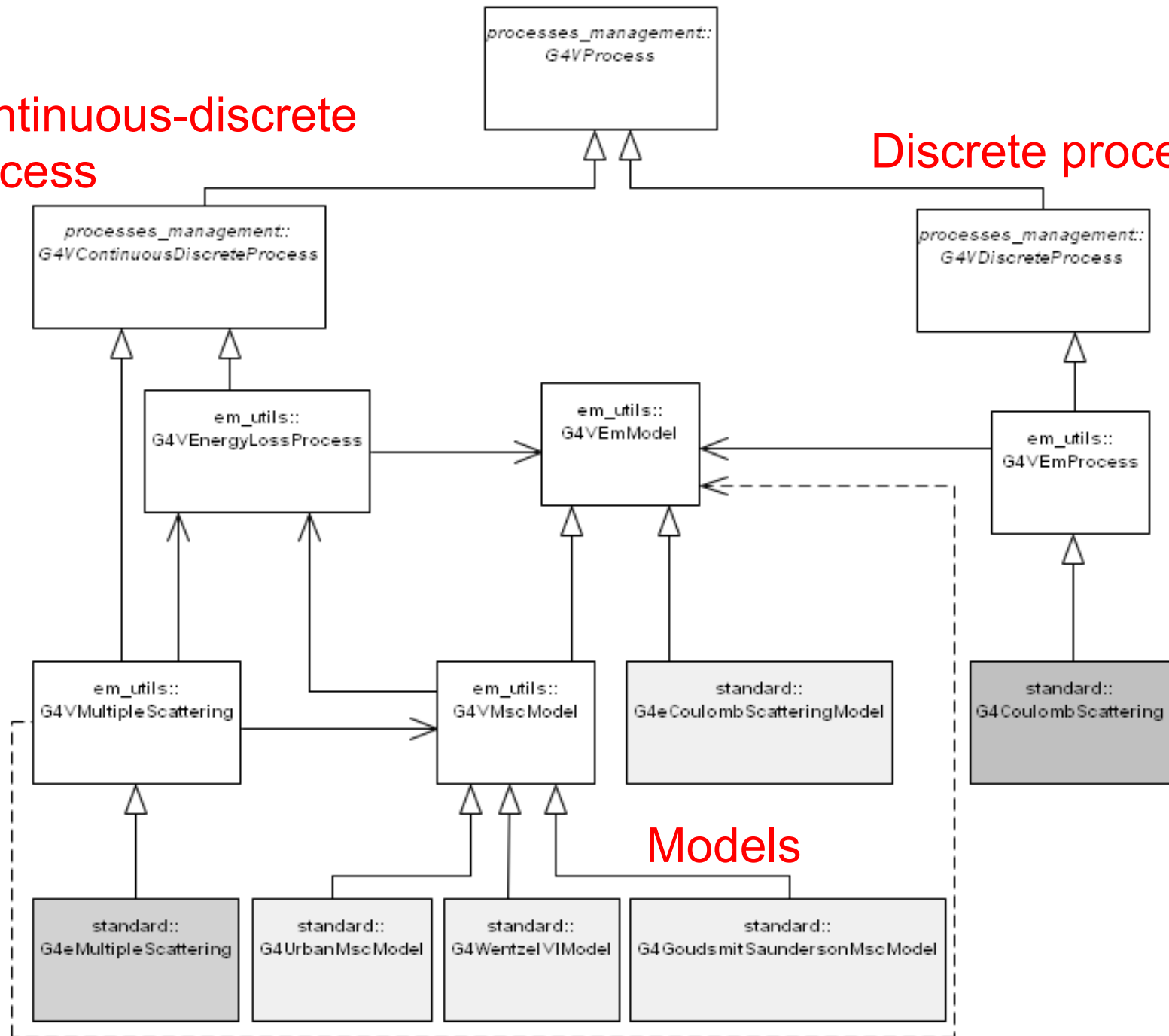


Continuous-discrete process

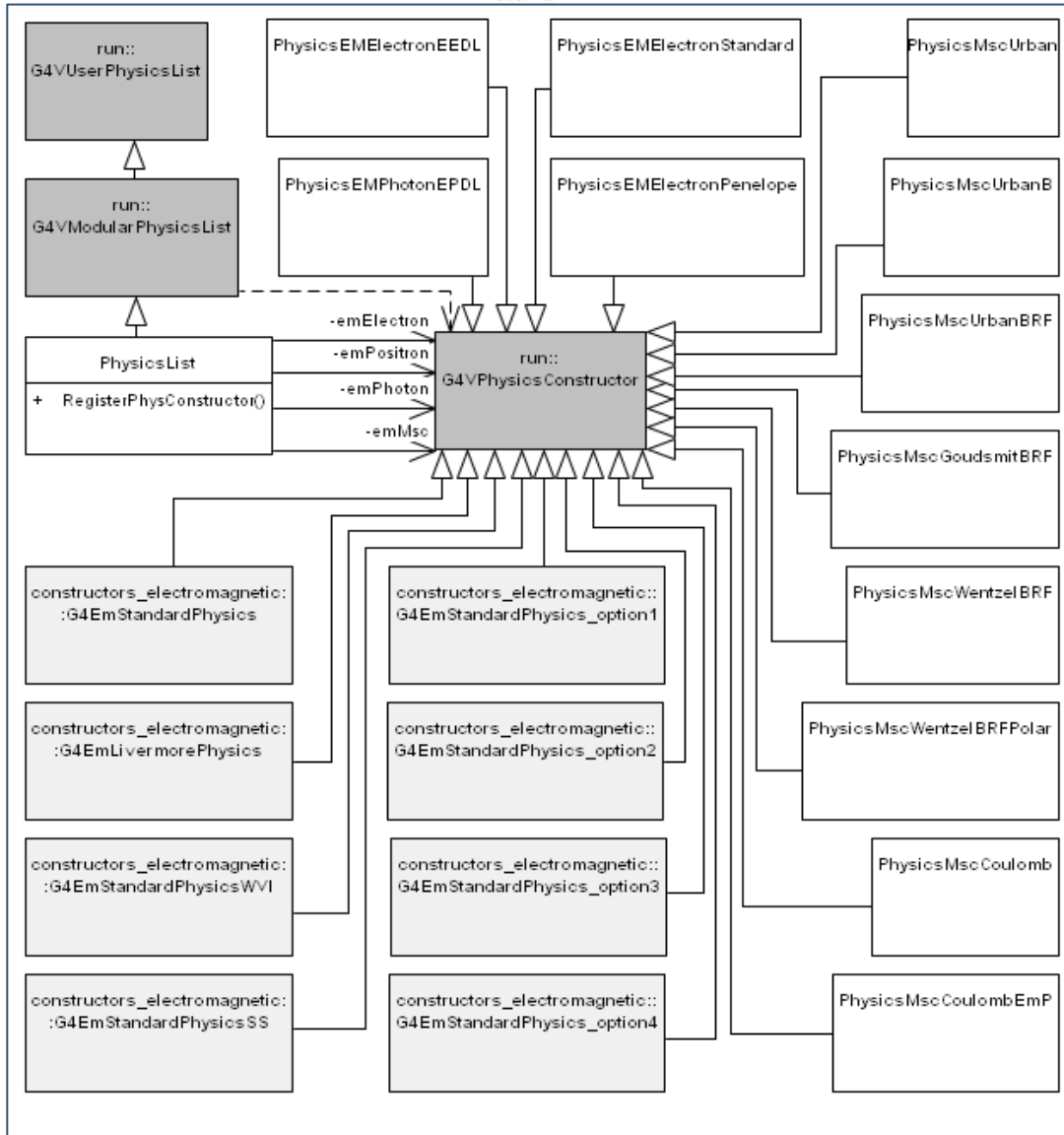
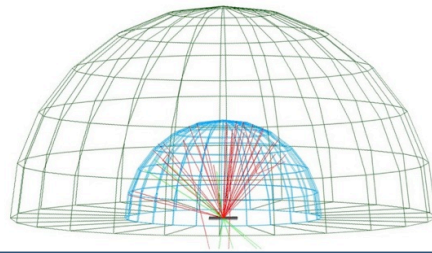
Discrete process

Multiple scattering

Single scattering



Models



Geant4 electron multiple and single electron scattering **processes**

Urban  
Goudsmit-Saunderson  
WentzelVI  
eCoulombScattering  
eSingleCoulombScattering  
**models**

EmStandard  
EmLivermore  
EmStandard\_option1  
EmStandard\_option2  
EmStandard\_option3  
EmStandard\_option4  
EmStandard\_WVI  
EmStandard\_SS  
EmStandard\_GS  
**PhysicsConstructors**

9.1-10.2 (except 9.5)  
**Geant4 versions**

# Experimental data

- Collected from the literature: 1947-2008
  - >3000 measurements
  - $Z = 4-92$
  - Electron energy: 78 eV – 22.2 MeV
- Many experimental papers do not report errors at all
- Many papers only report statistical uncertainties, neglecting sources of systematic errors
- Risk of underestimated experimental errors
  - Uncertainties differ even by an order of magnitude among measurements performed with similar techniques by different groups
- Inconsistencies in the experimental data (*systematics*)
  - Rely on statistical analysis of a large data sample to infer conclusions regarding Geant4 validation

Validation



Comparison  
with  
experiment

*not with another Monte Carlo code,  
with analytical calculations*

# Quantitative, objective

# Statistics

## Hypothesis testing

### Goodness-of-Fit testing

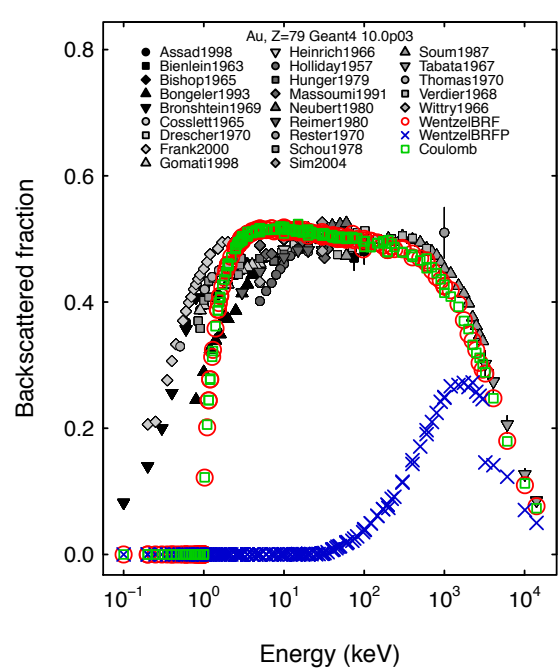
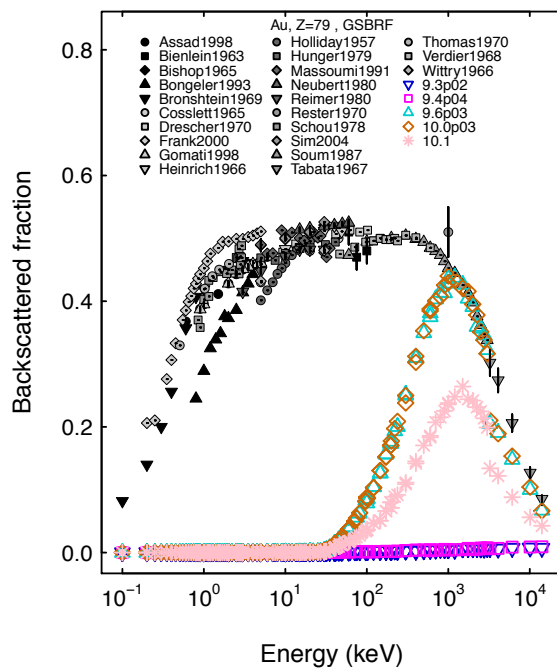
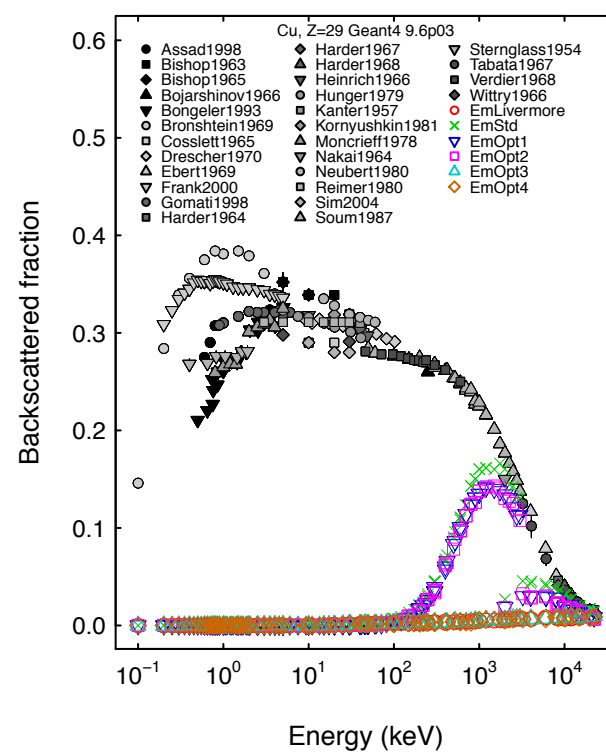
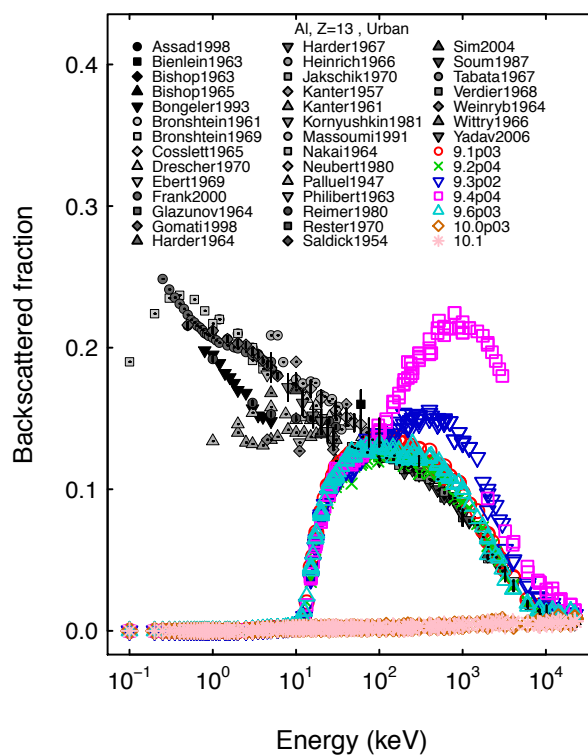
Simulation compatible with experiment?

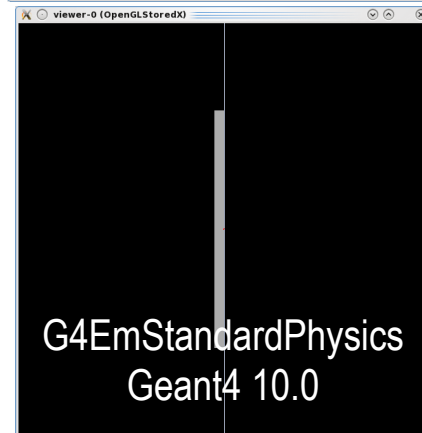
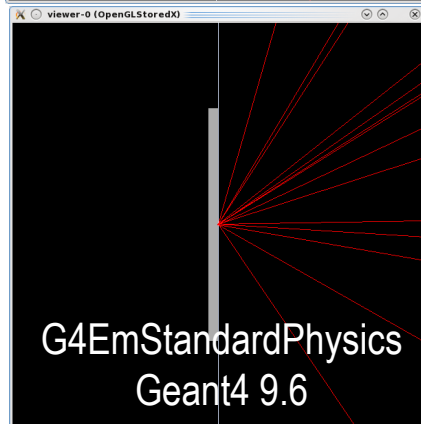
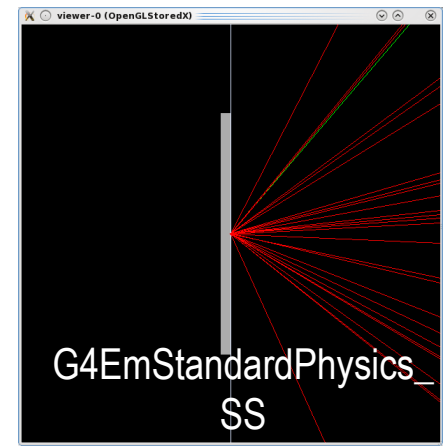
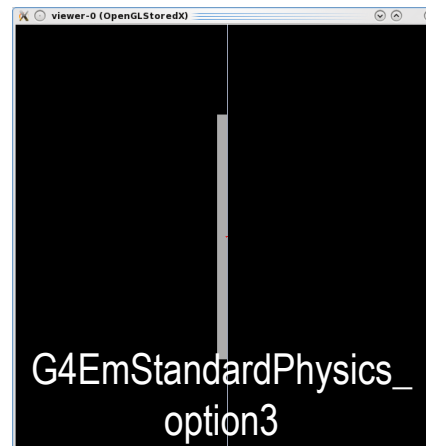
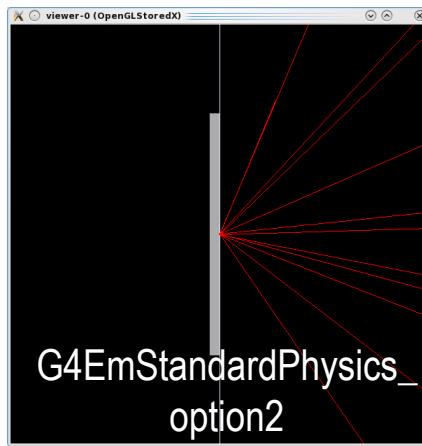
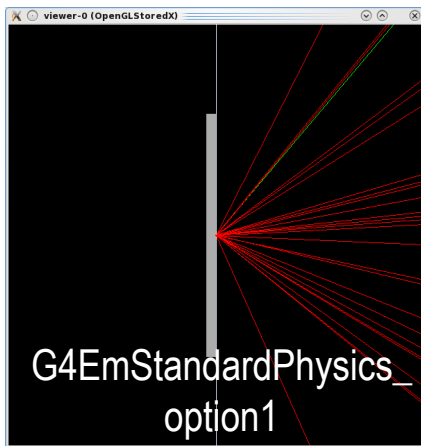


### Categorical data testing

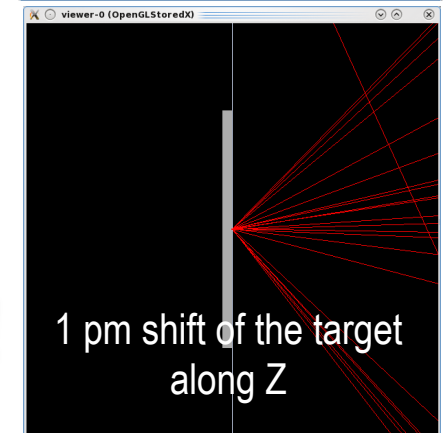
Equivalent compatibility with experiment?

- %
- good agreement
- excellent agreement
- satisfactory agreement
- ...





**1 pm  
makes a  
difference!**



**Beware:**

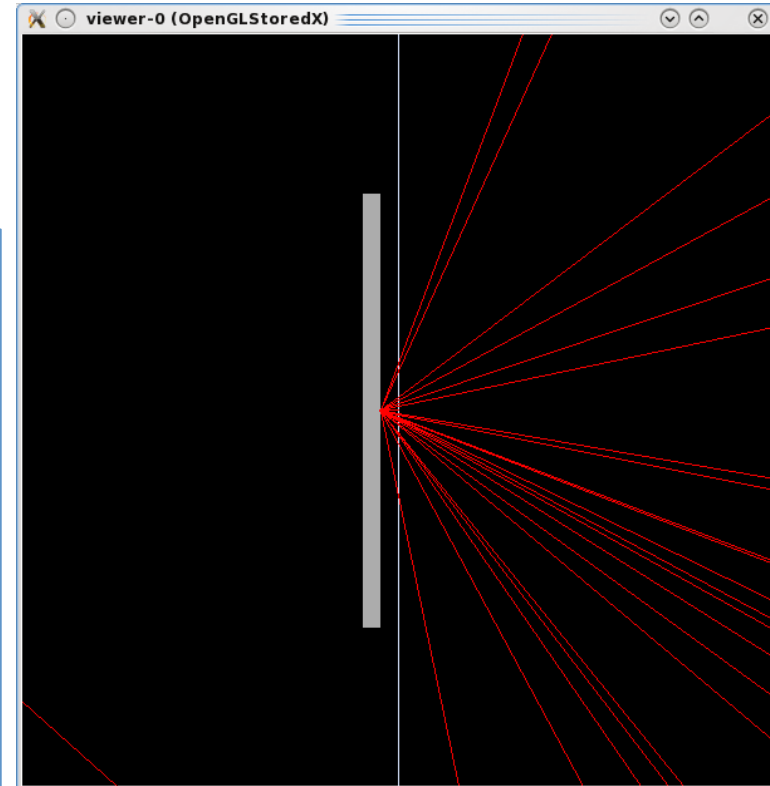
In an experimental use case we test the physics of the simulation along with **all its dependencies**



# Partly fixed, fixed

Target displaced by 1 pm / 1 μm / 1 mm →

```
----- WWWWW ----- G4Exception-START ----- WWWWW -----  
*** G4Exception : GeomNav1002  
    issued by : G4Navigator::ComputeStep()  
Track stuck or not moving.  
    Track stuck, not moving for 10 steps  
    in volume -Inside- at point (0,0,0)  
    direction: (-0,0,1).  
    Potential geometry or navigation problem !  
    Trying pushing it of 1e-07 mm ...Potential overlap in geometry!  
  
*** This is just a warning message. ***  
----- WWWWW ----- G4Exception-END ----- WWWWW -----
```



**Geant4**

**10.1p02**



**10.2**



**10.1p03**

# Laundry detergents, swans and PhysicsLists

## Geant4 User's Guide for Application Developers

Version: *geant4 10.1*

Publication date 5 December 2014

Geant4 Collaboration

**How you can prove that Persil washes whiter than any other washing powder!**

TAKE TWO white things, equally soiled—say a couple of towels, or handkerchiefs, or pillow-slips. Follow the instructions on the packets and wash one article in Persil, the other in any other washing powder you choose. One article will come up whiter than the other—much whiter! *WE SAY IT WILL BE THE PERSIL*

*ONE.* Yes, Persil washes whiter than any other washing powder! Because it washes *cleaner!* The Persil laboratories make sure that Persil is always one step ahead of any other washing powder!

And Persil is kind to *all* your wash—whites, woollens, coloureds, fine things.

The BIGGEST-SELLING washing powder in the country

**BOIL OR NO BOIL. PERSIL BEATS THE LOT!**

**DO TAKE CARE OF YOUR HANDS**  
Women are now thinking twice about using detergents that are harsh to their hands. The blessing of Persil is that it is always kind to your hands—you can *feel* it is!

**PERSIL washes whiter!**  
— and that means **CLEANER!**

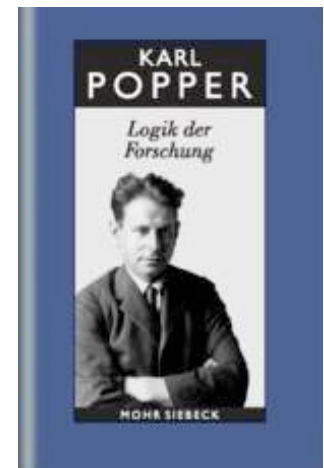
## 5.2.1.1. Electromagnetic Processes

- Combination of **best** EM models for simulation with high accuracy

# Swans



**modus tollens**



## 5.2.1.1. Electromagnetic Processes

- Combination of **best** EM models for simulation with high accuracy  
(class name G4EmStandardPhysics\_option4)

<b>Efficiency</b> ( $\alpha=0.01$ )	
Coulomb	0.81±0.05
G4EmStandardPhysicsWVI	0.82±0.05
G4EmStandardPhysicsSS	0.82±0.05
<b>G4EmStandardPhysics_option4</b>	<b>0.74±0.06</b>
GSBRF	0.95±0.03
WentzelBRF	0.79±0.05

p-value<sub>Boschloo</sub> = **0.003**

# Which is the best prepackaged PhysicsList in this experimental scenario?

## Efficiency

*evolution with Geant4 version*

Configuration	1-20 keV				20-100 keV				≥100 keV			
	10.1p03	10.2	10.2p01	10.2p02	10.1p03	10.2	10.2p01	10.2p02	10.1p03	10.2	10.2p01	10.2p02
EmLivermore	0.13±0.03	0.11±0.03	0.11±0.03	0.11±0.03	0.29±0.04	0.24±0.04	0.24±0.04	0.25±0.04	0.61±0.06	0.61±0.06	0.61±0.06	0.61±0.06
EmStd	0.13±0.03	0.08±0.03	0.08±0.03	0.08±0.03	0.19±0.04	0.16±0.03	0.16±0.03	0.16±0.03	0.71±0.06	0.86±0.05	0.86±0.05	0.86±0.05
EmOpt1	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	0.41±0.06	0.39±0.06	0.39±0.06	0.39±0.06
EmOpt2	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	0.41±0.06	0.39±0.06	0.39±0.06	0.39±0.06
EmOpt3	0.21±0.03	0.17±0.03	0.17±0.03	0.17±0.03	0.14±0.03	0.19±0.04	0.19±0.04	0.19±0.04	0.68±0.06	0.75±0.06	0.75±0.06	0.75±0.06
EmOpt4	0.23±0.03	0.10±0.03	0.10±0.03	0.10±0.03	0.21±0.04	0.24±0.04	0.24±0.04	0.24±0.04	0.73±0.06	0.66±0.06	0.66±0.06	0.68±0.06
EmWVI	0.45±0.04	0.36±0.04	0.36±0.04	0.36±0.04	0.46±0.05	0.47±0.05	0.47±0.05	0.47±0.05	0.82±0.05	0.82±0.05	0.82±0.05	0.82±0.05
EmSS	0.46±0.04	0.35±0.04	0.35±0.04	0.35±0.04	0.51±0.05	0.53±0.05	0.53±0.05	0.53±0.05	0.82±0.05	0.82±0.05	0.82±0.05	0.82±0.05
EmGS		0.58±0.04	0.58±0.04	0.58±0.04		0.18±0.04	0.19±0.04	0.19±0.04		0.54±0.06	0.50±0.06	0.50±0.06

## Model equivalence

*dependence on energy*

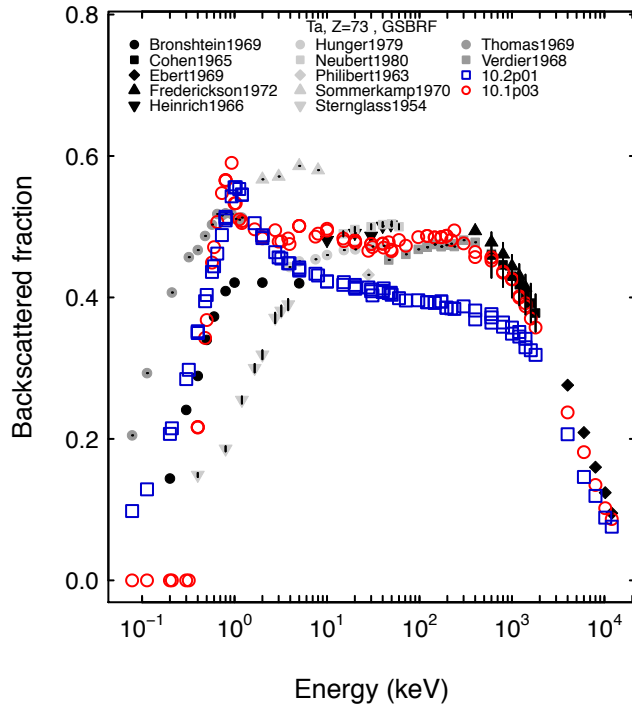
Configuration	EmGS <20 keV				EmSS 20-100 keV					EmStd ≥100 keV					
	Fisher	$\chi^2$	Z-pooled	Boschloo	CSM	Fisher	$\chi^2$	Z-pooled	Boschloo	CSM	Fisher	$\chi^2$	Z-pooled	Boschloo	CSM
EmLivermore	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.005	0.003	0.003	0.003	0.003
EmStd	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001					
EmOpt1	< 0.001		< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
EmOpt2	< 0.001		< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001
EmOpt3	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.234	0.154	0.209	0.176	0.274
EmOpt4	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.043	0.025	0.029	0.029	0.038
EmWVI	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	0.504	0.423	0.532	0.462	1.000	0.798	0.607	0.681	0.653	1.000
EmSS	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001						0.798	0.607	0.681	0.653	1.000
EmGS						< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001	< 0.001



Better the devil you know than the one you don't know

# Devils and Goudsmit-Saunderson

## Efficiency



	Geant4 10.1p03	Geant4 10.2p02
GS	$0.77 \pm 0.06$	$0.55 \pm 0.06$
GS <sub>BRF</sub>	$0.95 \pm 0.03$	$0.55 \pm 0.06$
GS <sub>PWA</sub>		$0.61 \pm 0.06$

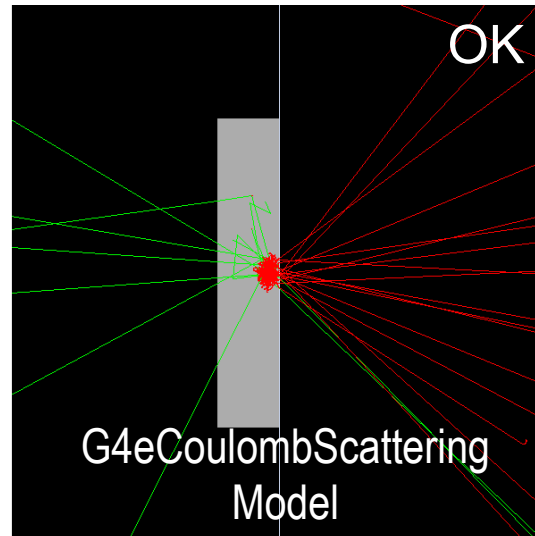
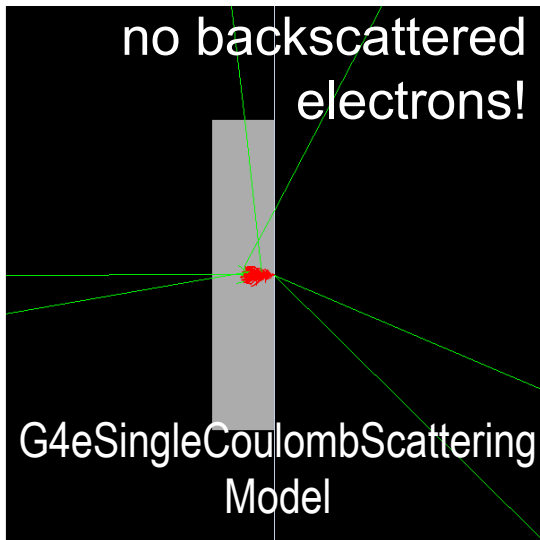
Compatibility with experiment  
 model<sub>old</sub> vs. model<sub>new</sub>:  **$p < 0.001$**   
 (Fisher, Boschloo, Z-pooled, Barnard,  $\chi^2$ )

Configuration	1-20 keV				20-100 keV				$\geq 100$ keV			
	10.1p03	10.2	10.2p01	10.2p02	10.1p03	10.2	10.2p01	10.2p02	10.1p03	10.2	10.2p01	10.2p02
GS	$0.51 \pm 0.04$	$0.57 \pm 0.04$	$0.56 \pm 0.04$	$0.56 \pm 0.04$	$0.32 \pm 0.04$	$0.18 \pm 0.04$	$0.16 \pm 0.04$	$0.16 \pm 0.04$	$0.77 \pm 0.06$	$0.52 \pm 0.07$	$0.55 \pm 0.06$	$0.55 \pm 0.06$
GSBRF	$0.37 \pm 0.04$	$0.38 \pm 0.04$	$0.57 \pm 0.04$	$0.57 \pm 0.04$	$0.51 \pm 0.05$	$0.46 \pm 0.05$	$0.14 \pm 0.05$	$0.14 \pm 0.05$	$0.95 \pm 0.03$	$0.61 \pm 0.06$	$0.55 \pm 0.06$	$0.55 \pm 0.06$
GSBRF1		$0.35 \pm 0.04$	$0.42 \pm 0.04$	$0.42 \pm 0.04$		$0.45 \pm 0.05$	$0.44 \pm 0.05$	$0.45 \pm 0.05$		$0.61 \pm 0.06$	$0.59 \pm 0.06$	$0.57 \pm 0.06$
GSERF		$0.32 \pm 0.04$	$0.31 \pm 0.04$	$0.32 \pm 0.04$		$0.49 \pm 0.05$	$0.43 \pm 0.05$	$0.46 \pm 0.05$		$0.63 \pm 0.06$	$0.61 \pm 0.06$	$0.59 \pm 0.06$
GSPWA		$0.15 \pm 0.03$	$0.15 \pm 0.03$	$0.15 \pm 0.03$		$0.17 \pm 0.04$	$0.15 \pm 0.04$	$0.15 \pm 0.04$		$0.61 \pm 0.06$	$0.61 \pm 0.06$	$0.61 \pm 0.06$
GSPWABRF		$0.39 \pm 0.04$	$0.16 \pm 0.04$	$0.16 \pm 0.04$		$0.44 \pm 0.05$	$0.11 \pm 0.05$	$0.11 \pm 0.05$		$0.57 \pm 0.06$	$0.55 \pm 0.06$	$0.55 \pm 0.06$
GSPWAERF		$0.44 \pm 0.04$	$0.44 \pm 0.04$	$0.44 \pm 0.04$		$0.51 \pm 0.04$	$0.46 \pm 0.04$	$0.47 \pm 0.04$		$0.52 \pm 0.07$	$0.55 \pm 0.07$	$0.55 \pm 0.07$

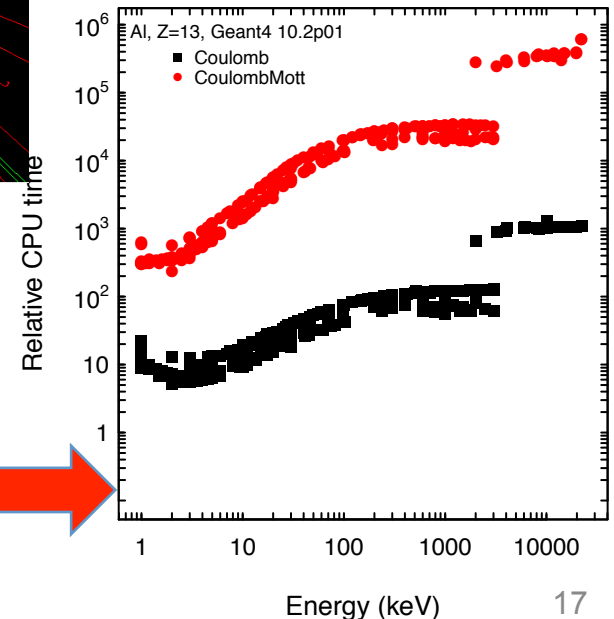


# Incorrect OR slow?

**G4eSingleCoulombScatteringModel** based on *Mott cross section*



**Geant4 10.2**



The model with the highest compatibility with experiment in **Geant4 10.2p02**, but...



# Distilled wisdom

detailed results → papers

- Understand your **experimental context**
- Master the simulation **problem domain**
- Beware of **dependencies** in your simulation
- Trust **objective, quantitative** validation references
  - Do not trust laundry detergent advertisement
- Sometimes **new** is better than **old**, sometimes it is not
- Collect and evaluate pertinent **experimental data**
  - Many, from different experiments, if possible
  - All what shines (*is published*) is not gold...
- Use **statistics** to compare simulation and experiment

## Measure, measure, measure...

Epistemology of science

Statistical data analysis