

# Negative improvements, relative validity and elusive goodness

*Food for thought for Monte Carlo simulation users and developers*

M. Batic<sup>1</sup>, G. Hoff<sup>2</sup>, S. H. Kim<sup>3</sup>, M. G. Pia<sup>4</sup>, P. Saracco<sup>4</sup>, G. Weidenspointner<sup>5</sup>

*<sup>1</sup>Sinergise, Ljubljana, Slovenia*

*<sup>2</sup>Pontificia Universidade Catolica do Rio Grande do Sul, Porto Alegre, Brazil*

*<sup>3</sup>Hanyang University, Seoul, Korea*

*<sup>4</sup>INFN Genova, Italy*

*<sup>5</sup>Halbleiterlabor, MPI-MPE, München, Germany*

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27 October – 2 November 2013

Seoul, Korea

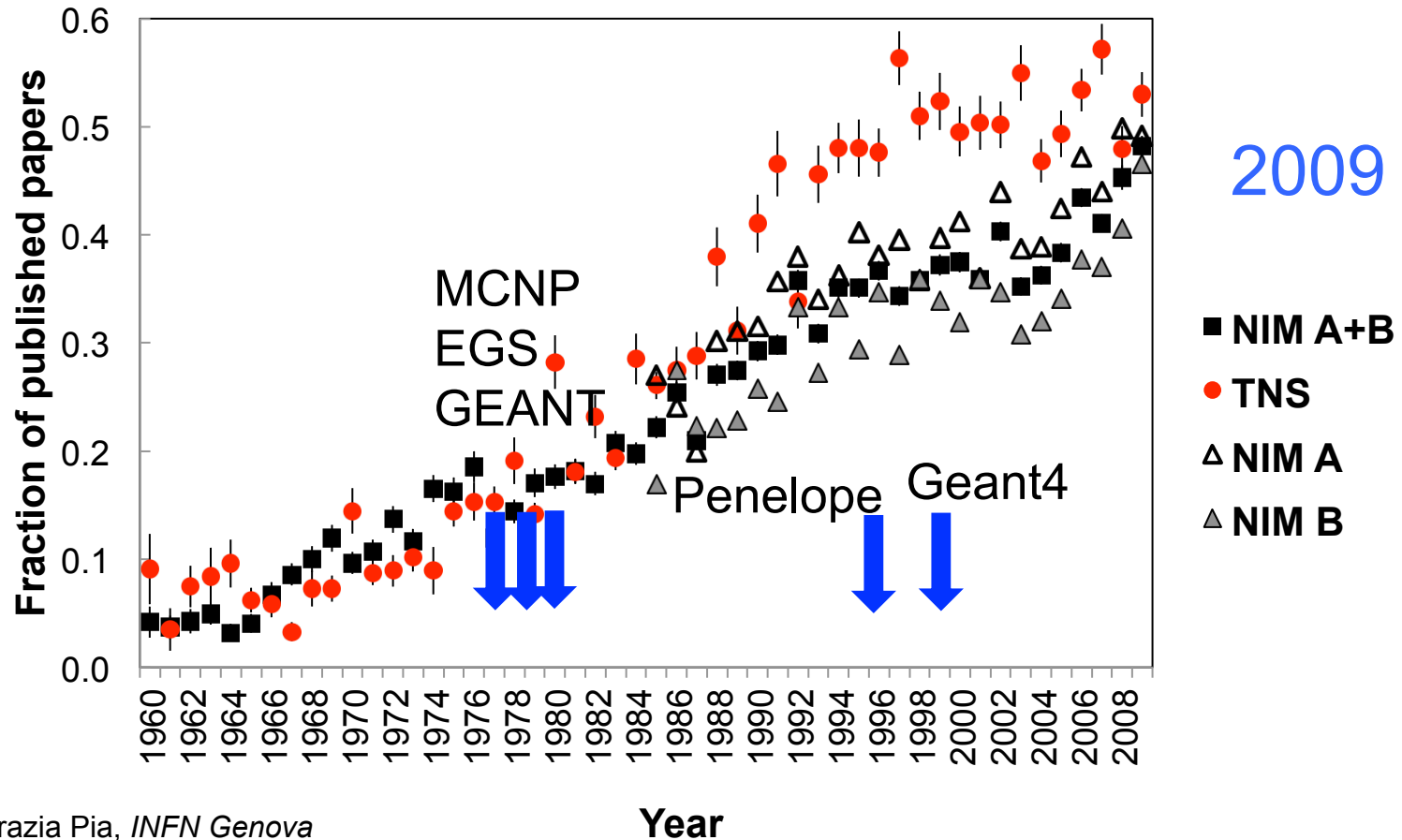


# Aging

- Our Monte Carlo codes are getting old
- (Monte Carlo) simulation gets more and more popular in experimental practice



## Monte Carlo OR simulation



# Revisiting old successes

2007 IEEE Nuclear Science Symposium Conference Record

N36-4

Best Student paper, IEEE NSS 2007

## Validation of Geant4 low energy physics models against electron energy deposition and backscattering data

Anton Lechner, *Student Member, IEEE*, Maria Grazia Pia and Manju Sudhakar



398 TNS, 2009

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 2, APRIL 2009

## Validation of Geant4 Low Energy Electromagnetic Processes Against Precision Measurements of Electron Energy Deposition

Anton Lechner, Maria Grazia Pia, and Manju Sudhakar

**How does it look like a few years later?**

V. Ivanchenko et al., Recent **Progress** of Geant4  
Electromagnetic Physics and Readiness for the LHC Start,  
*XII Advanced Computing and Analysis Techniques in  
Physics Research, Erice, Italy, 3-7 November 2008*

Progress in NUCLEAR SCIENCE and TECHNOLOGY, Vol. 2, pp.898-903 (2011)

REVIEW

SNA+Monte Carlo 2010

## Recent **Improvements** in Geant4 Electromagnetic Physics Models and Interfaces

Vladimir IVANCHENKO<sup>1,2,3\*</sup>, John APOSTOLAKIS<sup>1</sup>, Alexander BAGULYA<sup>4</sup>, Haifa Ben ABDELOUAHED<sup>5</sup>,  
Rachel BLACK<sup>6</sup>, Alexey BOGDANOV<sup>7</sup>, Helmut BURKHARD<sup>1</sup>, Stéphane CHAUVIE<sup>8</sup>, Pablo CIRRONE<sup>9</sup>,  
Giacomo CUTTONE<sup>9</sup>, Gerardo DEPAOLA<sup>10</sup>, Francesco Di ROSA<sup>9</sup>, Sabine ELLES<sup>11</sup>, Ziad FRANCIS<sup>12</sup>,  
Vladimir GRICHINE<sup>4</sup>, Peter GUMPLINGER<sup>13</sup>, Paul GUEYE<sup>6</sup>, Sebastien INCERTI<sup>14</sup>, Anton IVANCHENKO<sup>14</sup>,  
Jean JACQUEMIER<sup>11</sup>, Anton LECHNER<sup>1,15</sup>, Francesco LONGO<sup>16</sup>, Omrane KADRI<sup>5</sup>, Nicolas KARAKATSANIS<sup>17</sup>,  
Mathieu KARAMITROS<sup>14</sup>, Rostislav KOKOULIN<sup>7</sup>, Hisaya KURASHIGE<sup>18</sup>, Michel MAIRE<sup>11,19</sup>, Alfonso MANTERO<sup>20</sup>,  
Barbara MASCIALINO<sup>21</sup>, Jakub MOSCICKI<sup>1</sup>, Luciano PANDOLA<sup>22</sup>, Joseph PERL<sup>23</sup>, Ivan PETROVIC<sup>9</sup>,  
Aleksandra RISTIC-FIRA<sup>9</sup>, Francesco ROMANO<sup>9</sup>, Giorgio RUSSO<sup>9</sup>, Giovanni SANTIN<sup>24</sup>, Andreas SCHAELOCKE<sup>25</sup>,  
Toshiyuki TOSHITO<sup>26</sup>, Hoang TRAN<sup>14</sup>, Laszlo URBAN<sup>19</sup>, Tomohiro YAMASHITA<sup>27</sup> and Christina ZACHARATOU<sup>28</sup>

RADECS 2011 Proceedings - PA-19

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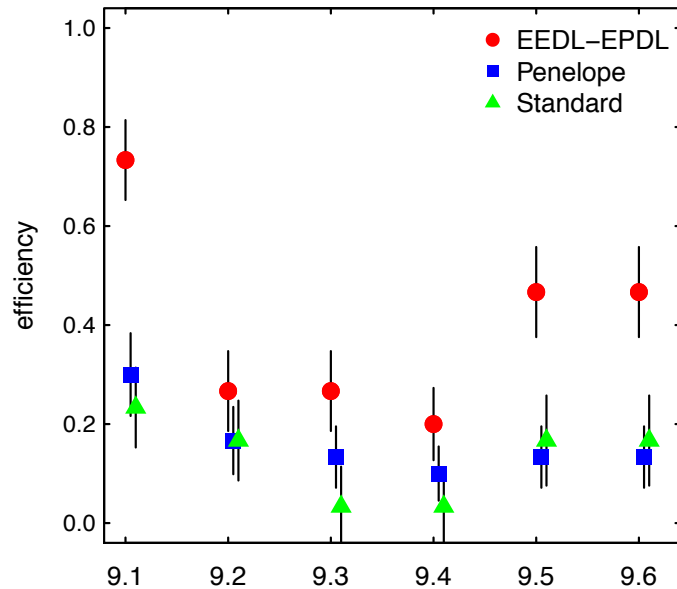
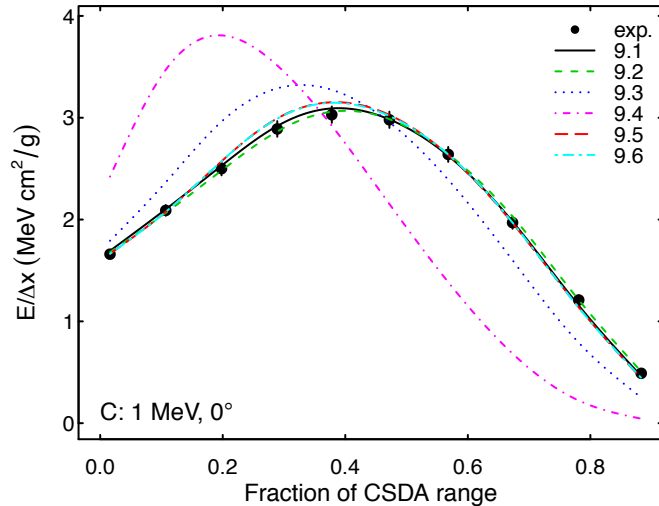
## New Geant4 Model and Interface Developments for **Improved** Space Electron Transport Simulations: First results

John Allison, Juan Cueto, Vladimir Grichine, Alexander Howard, Sergio Ibarria, Vladimir  
Ivanchenko, Michel Maire, Giovanni Santin and Laszlo Urban

Improvements



# Negative improvements



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

# How to facilitate negative improvements

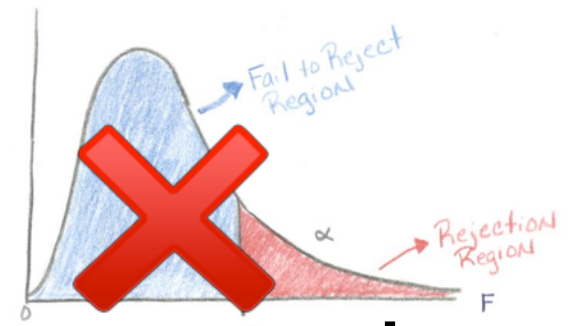
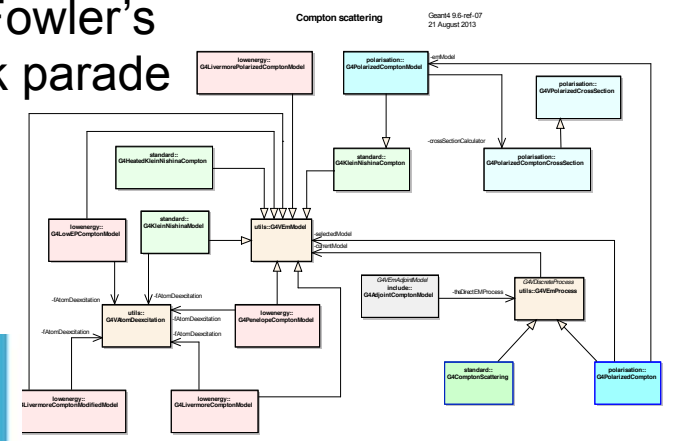


```
static const double hecorr[15] = {120.70, 117.50, 105.00, 92.92,
79.23, 74.510, 68.29, 57.39, 41.97, 36.14, 24.53, 10.21, -7.855,
-16.84, -22.30};

c1 = bg2lim*sig0[iZ]*(1.+hecorr[iZ]*(beta2-beta2lim))/bg2;
c2 = bg2lim*sig0[iZ+1]*(1.+hecorr[iZ+1]*(beta2-beta2lim))/bg2;
```

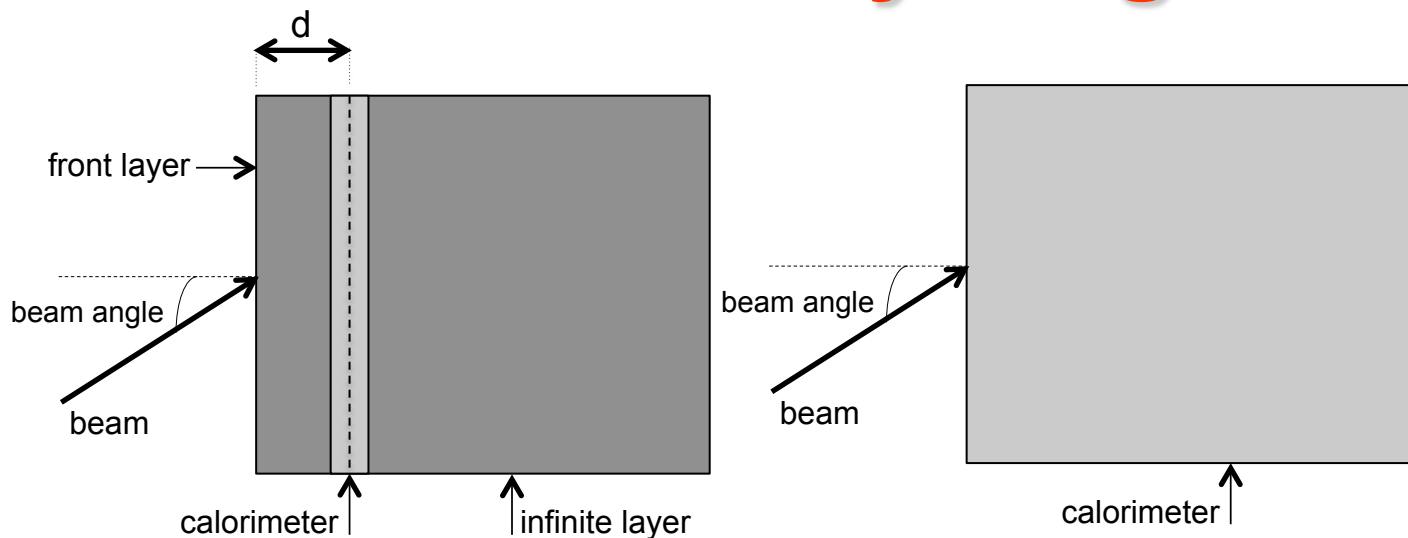


M. Fowler's  
stink parade



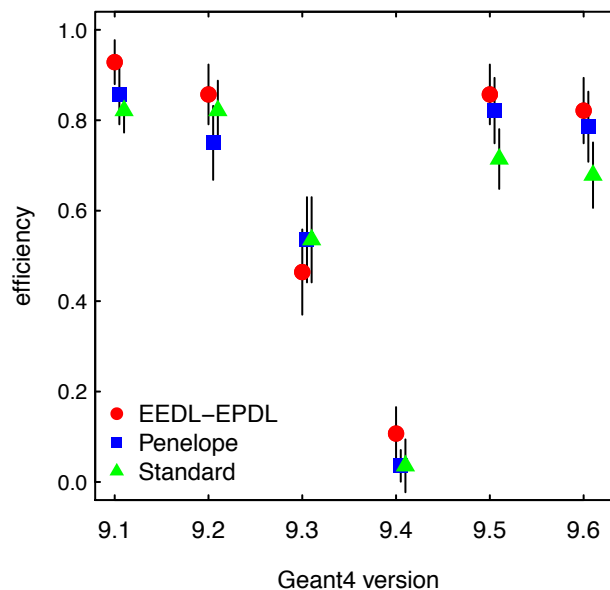
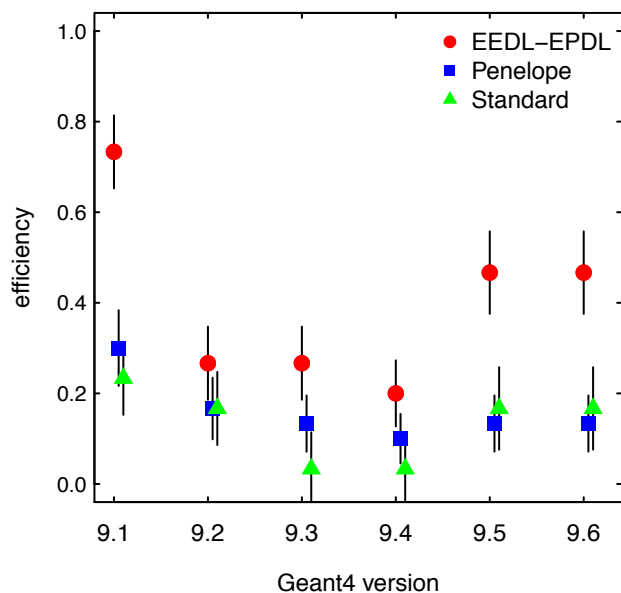
...and more!<sub>6</sub>

# What is bad may be good



## IEEE Standard 1012

**validation: (A)** [...] **(B)** The process of providing evidence that the system, software, or hardware and its associated products satisfy requirements allocated to it at the end of each life cycle activity, solve the right problem (e.g., correctly model physical laws, implement business rules, and use the proper system assumptions), and **satisfy intended use and user needs.**





# How good?

- Hardly any systematic, comprehensive, quantitative validation of the “**ingredients**” of Monte Carlo simulation codes is documented in the literature
- Comparison of simulation results and experimental data in **use cases** mainly rests on visual appraisal of figures or indicators (%) deprived of any statistical relevance



Agreement  
Good agreement  
Excellent agreement  
Satisfactory agreement



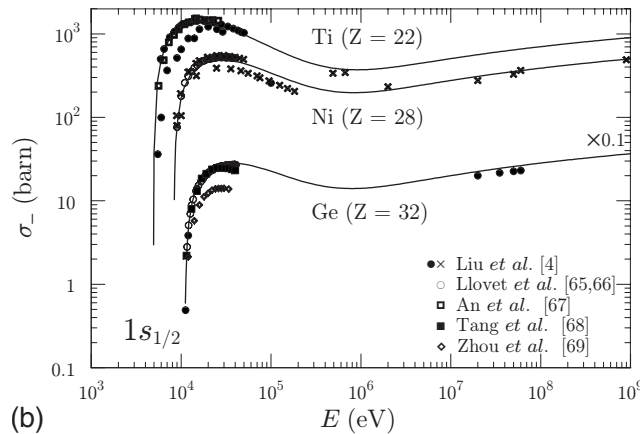


D. Bote and F. Salvat, Calculations of inner-shell ionization by electron impact with the distorted-wave and plane wave Born approximation, Phys. Rev. A 77, 042701, 2008

# Elusive goodness

Are these cross sections good?

Are they any better than existing calculations?



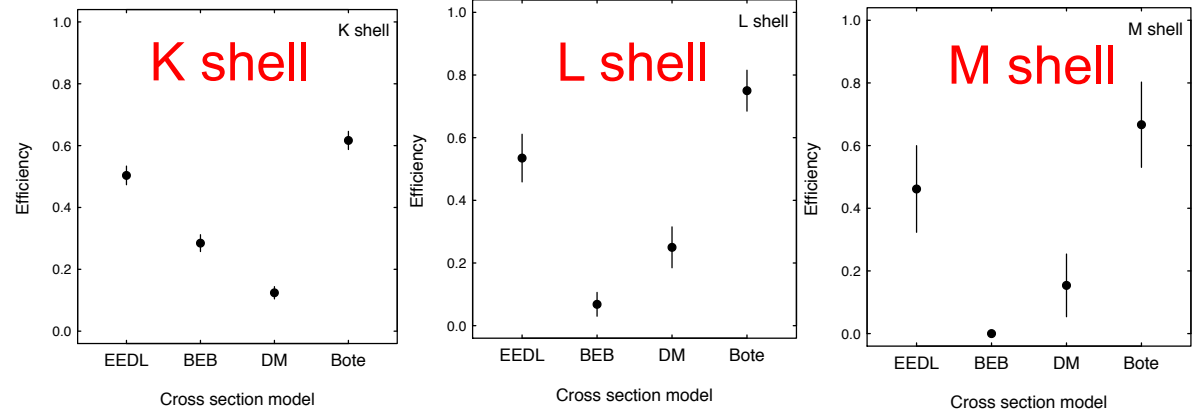
Fraction of test cases that “pass” the  $\chi^2$  test

$\chi^2$  test

Significance:  $\alpha=0.01$

p-value  $\geq \alpha \rightarrow$  Pass

p-value  $< \alpha \rightarrow$  Fail



**Categorical analysis**  
EEDL-B/S

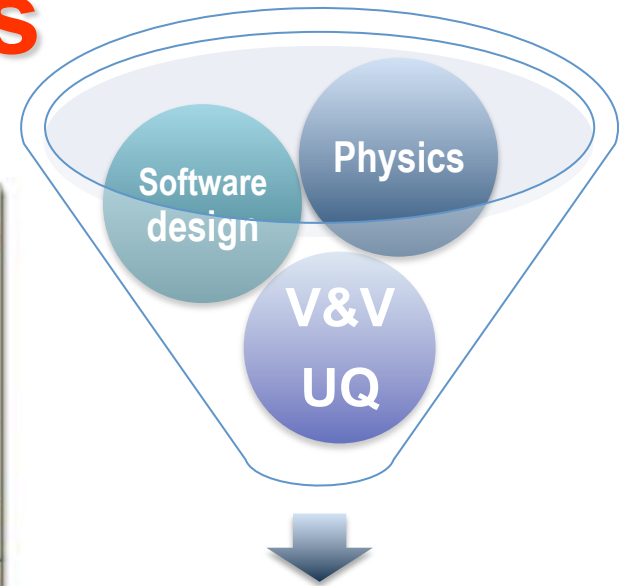
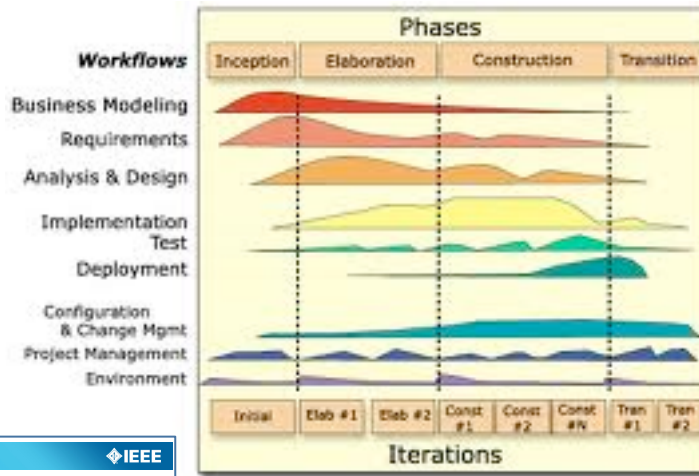
Test	preliminary	P-value	
Fisher	0.0098	0.0453	0.4283
Pearson $\chi^2$	0.0076	0.0362	
Barnard	0.0079	0.0383	0.3519

# Positive improvements

## Physics



## methods



State-of-the-art, quantified simulation

IEEE STANDARDS ASSOCIATION IEEE

**IEEE Standard for System and Software Verification and Validation**

IEEE Computer Society

Sponsored by the Software & Systems Engineering Standards Committee (C/S2ESC)

IEEE 3 Park Avenue New York, NY 10016-5997 USA

Statistical Inference  
Second Edition  
George Casella  
Roger L. Berger

**statistics**

DUXBURY ADVANCED SERIES

Electron impact ionisation cross sections

EEDL, Bate et al. (Penelope)

```

classDiagram
    class G4CsBEB {
        + CrossSection(int, double) :double
        + CrossSection(int, int, double) :double
    }
    class G4CsDM {
        + CrossSection(int, double) :double
        + CrossSection(int, int, double) :double
    }
    class G4CsTabula {
        + CrossSection(int, double) :double
        + CrossSection(int, int, double) :double
    }
    class G4Atom {
        + AtomicNumber() :int (query)
        + IonisationPotential() :double (query)
        + NShells() :int (query)
        + ShellByIndex(int) :G4Shell* (query)
        + Shell(int) :G4Shell* (query)
        + ShellByZ(int) :G4Shell* (query)
    }
    class G4AtomicProperties {
        + FindAtom(int) :G4Atom*
        + NAtoms() :int
    }
    class G4DataUI {
        + Interpolator() :G4String5 (query)
        + ApplicableRangeMin() :G4Double (query)
        + ApplicableRangeMax() :G4Double (query)
        + Zmin() :G4Double (query)
        + Zmax() :G4Double (query)
    }
    class G4Shell {
        + MyAtom() :int
        + Index() :int
        + Id() :int
        + BindingEnergy() :double
        + FiniteEnergy() :double
        + Occupancy() :double (query)
        + Radius() :double
        + Name() :G4String
    }
    class G4DataSet {
        + FindValue(G4Double, G4int, G4int) :G4Double (query)
    }
    class G4CompositeDataSet {
    }
    class G4DataVector {
        + global_management() :G4DataVector
    }

    G4CsBEB --> G4AtomicProperties
    G4CsDM --> G4AtomicProperties
    G4CsTabula --> G4AtomicProperties
    G4AtomicProperties --> G4Atom
    G4AtomicProperties --> G4Shell
    G4DataUI --> G4CompositeDataSet
    G4CompositeDataSet --> G4DataVector
    G4DataVector --> G4DataSet
    
```

Migration to STL vector foreshen

**technology**

ENTERPRISE ARCHITECT

SPARK SYSTEMS

st 2013 jhun Kim



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

Ongoing effort

# Validation of Geant4 Simulation of Electron Energy Deposition

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

3246

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

# Evaluation of Atomic Electron Binding Energies for Monte Carlo Particle Transport

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

1636

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

# Photon Elastic Scattering Simulation: Validation and Improvements to Geant4

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

2984

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

# Validation of Geant4-Based Radioactive Decay Simulation

Steffen Hauf, Markus Kuster, Matej Batič, Zane W. Bell, Dieter H. H. Hoffmann, Philipp M. Lang, Stephan Neff, Maria Grazia Pia, Georg Weidenspointner, and Andreas Zoglauer

3269

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

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

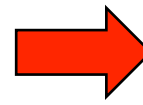
Matej Batič, Maria Grazia Pia, and Paolo Saracco

Publications



...and more! ■ Geant4 collaboration ■ Our team 1

# Supporting tools



Monte Carlo simulation  
as quantitative science

Enabling quantitative validation of Monte Carlo codes

2056

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 51, NO. 5, OCTOBER 2004

## A Goodness-of-Fit Statistical Toolkit

G. A. P. Cirrone, S. Donadio, S. Guatelli, A. Mantero, B. Mascialino, S. Parlati, M. G. Pia, A. Pfeiffer, A. Ribon, and P. Viarengo

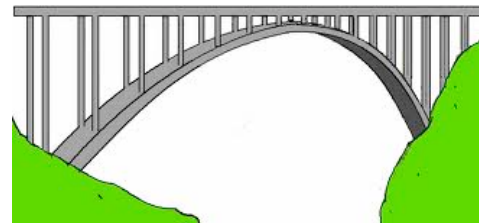
3834

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 53, NO. 6, DECEMBER 2006

## New Developments of the Goodness-of-Fit Statistical Toolkit

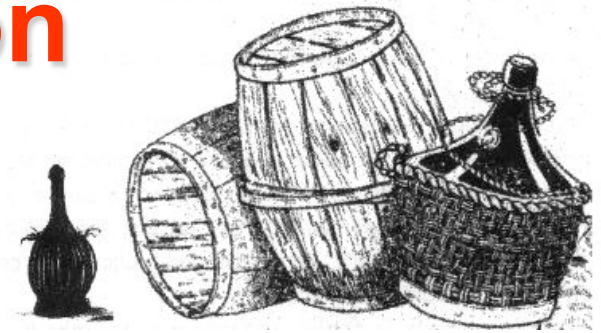
Barbara Mascialino, Andreas Pfeiffer, Maria Grazia Pia, Alberto Ribon, and Paolo Viarengo

The logo for AIDA (Advanced Instrumentation for Data Analysis) is displayed in a large, bold, orange, 3D-style font. Below it, the logo for iAIDA (integrated AIDA) is shown in a smaller, orange, 3D-style font.



**N45-8**, Data Analysis with R in an Experimental Physics Environment

# Monte Carlo simulation as a science



A collaborative effort across different Monte Carlo codes for the validation of the “bricks” would be beneficial to the experimental community

## A paradigm shift

The scientific community needs a paradigm shift with regard to validation experiments. Experimenters and funding agencies understand the value of experiments designed to explore new scientific phenomena, test theories, or examine the performance of design components. But few appreciate the value of experiments explicitly conducted for code validation. Even when experimenters are interested in validating a code, few mechanisms exist for funding such an experiment. It's essential that the scientific community provide support for code-validation experiments.

**Software  
for experiments  
Experiments  
for software**

## Computational Science Demands a New Paradigm

Douglass E. Post and Lawrence G. Votta

January 2005 Physics Today **35**