Uncertainty quantification and going beyond the independent-particle approximation

What's hot and new in a mature field
Monte Carlo for particle transport in particle/nuclear/astro/medical/etc. physics

Maria Grazia Pia
Paolo Saracco
INFN Genova, Italy

Implicit throughout this talk

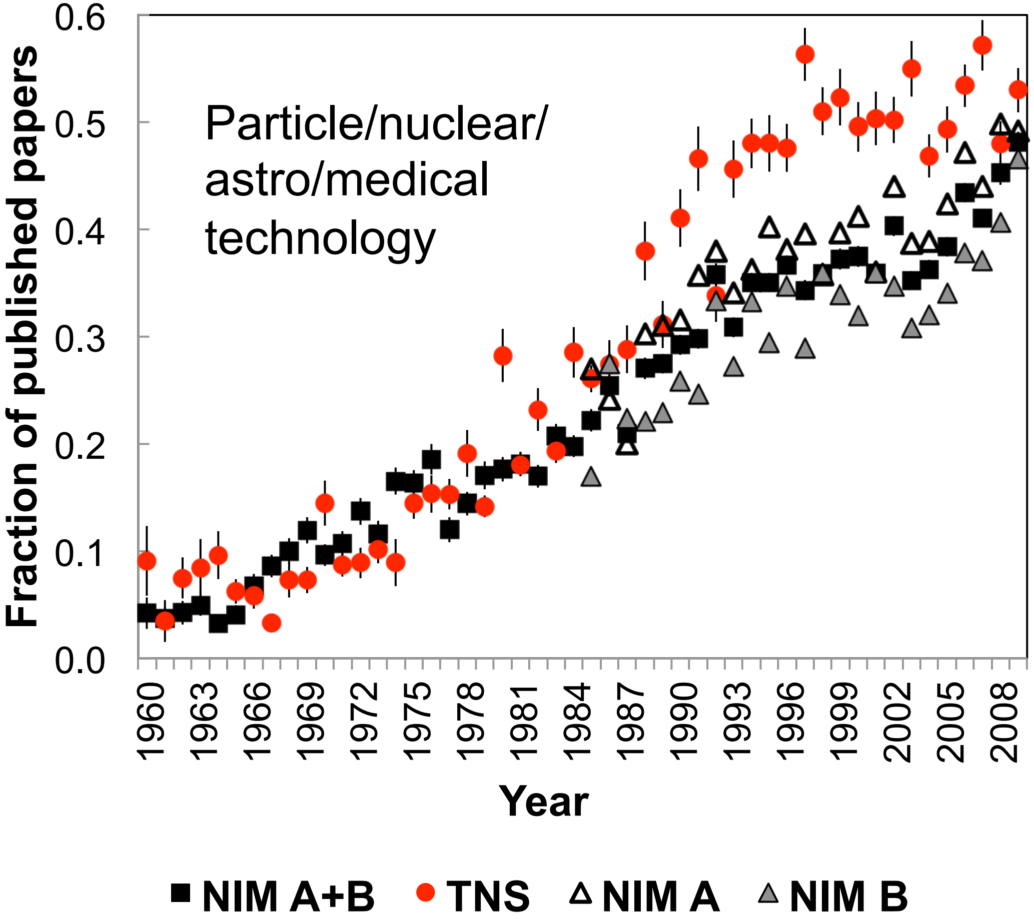
Monte Carlo

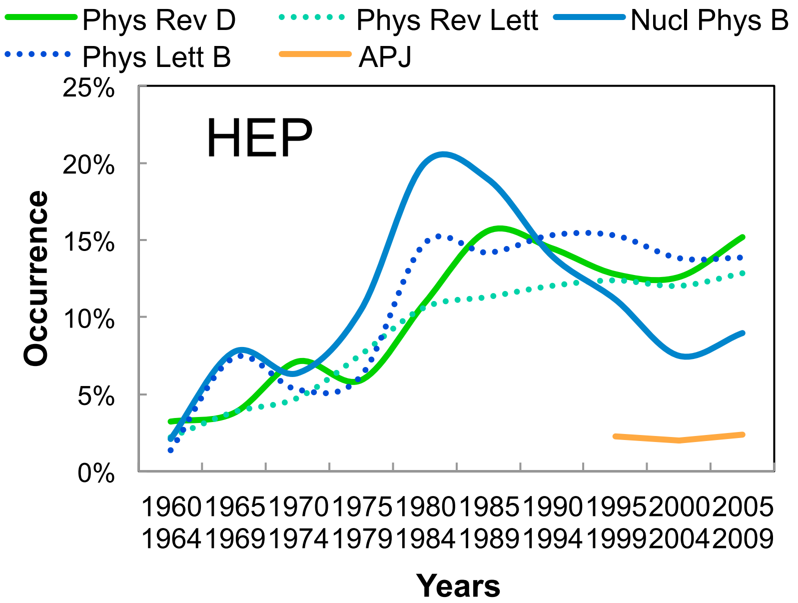
=

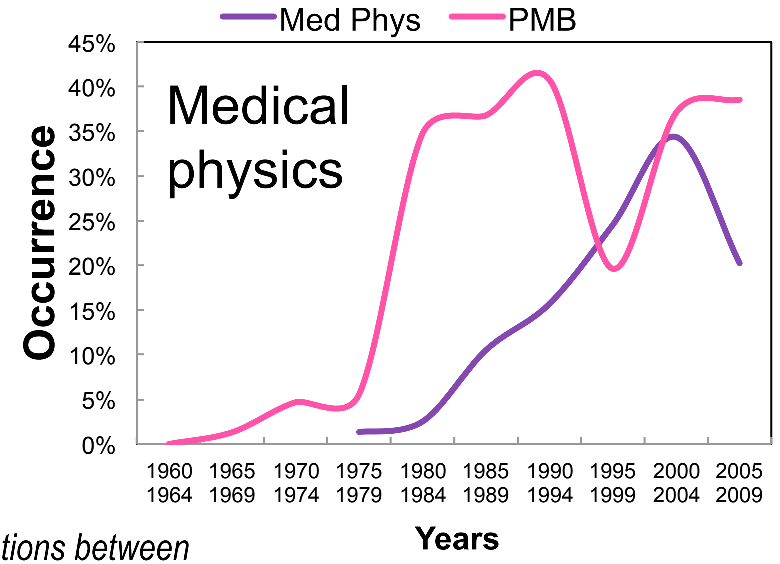
Monte Carlo for particle transport in matter

Monte Carlo in journals 1960-2009

Fraction of papers mentioning
Monte Carlo or **simulation**







M.G. Pia, T. Basaglia, Z.W. Bell, P.V. Dressendorfer, The butterfly effect: Correlations between modeling in nuclear-particle physics and socioeconomic factors, Proc. IEEE NSS 2010

Nuclear Science & Technology Instruments & Instrumentation

604059 publications

J. P. Biersack, L. L. Haggmark,
A Monte-Carlo computer-program for the transport of energetic ions in amorphous targets
NIM, vol. 174, no. 1-2, pp. 257-269, 1980
Times Cited: **3661**

S. Agostinelli et al.,
GEANT4 - a simulation toolkit
NIM A, vol. 506, no. 3, pp. 250-303, 2003
Times Cited: **3640**

L. R. Doolittle,
Algorithms for the rapid simulation of Rutherford backscattering spectra
NIM B, vol. 9, no. 3, pp. 344-351, 1985
Times Cited: **2095**

Thomson-Reuters, ISI Web of Science
Updated 15 February 2013

Physics, Particles & Fields

256905 publications

A. H. Guth,
Inflationary universe - a possible solution to the horizon and flatness problems
Phys. Rev. D, vol. 23, no. 2, pp. 347-356,1981
Times Cited: **4,157**

Particle Data Group
Review of particle physics
J. Phys. G, vol. 33, no. 1 Special Issue, 2006
Times Cited: **3,661**

S. Agostinelli et al.,
GEANT4 - a simulation toolkit
NIM A, vol. 506, no. 3, pp. 250-303, 2003
Times Cited: **3640**

Most cited CERN paper
(excluding Rev. Part. Phys.)

Thomson-Reuters, ISI Web of Science
Updated 15 February 2013

An international collaboration of ~ 100 physicists, engineers and computer scientists

Laboratories, national institutes and universities

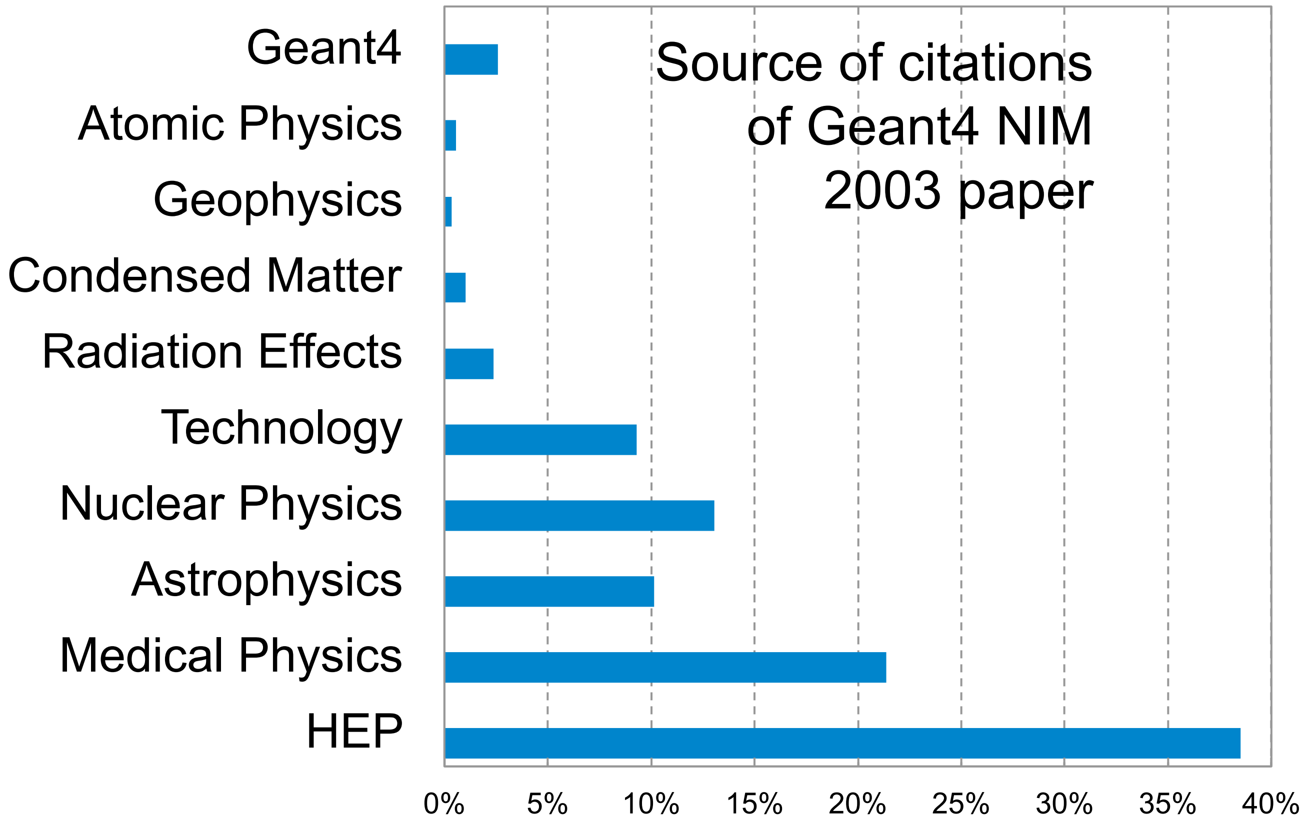
- 1994-1998 RD44 (CERN): R&D phase
- 1st public release: 15 December 1998
- 1-2 new versions/year

Open source
Freely downloadable
No limitations on use

Who uses Geant4?

Some degree of subjectivity in the classification:

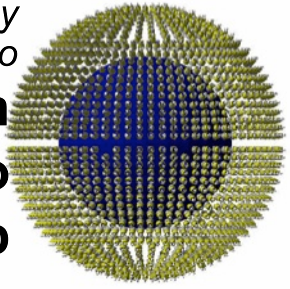
- journal scope
- manual inspection



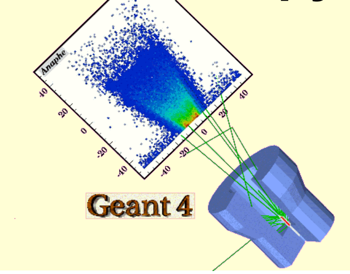
Update: end 2009 *Roughly similar distribution in recent scientometric data*

Courtesy Borexino

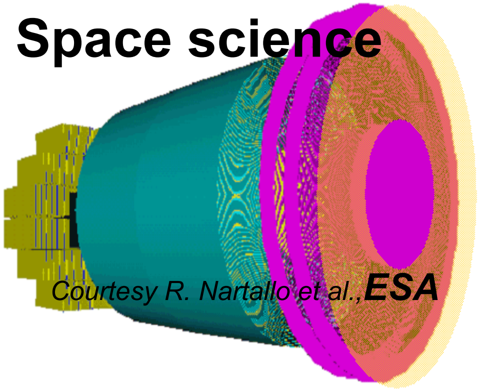
Gran Sasso lab



Oncological radiotherapy

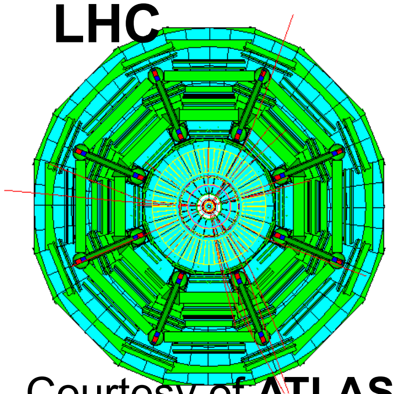


Space science



Courtesy R. Nartallo et al., ***ESA***

LHC



Courtesy of **ATLAS**

Simulation in HEP/nuclear/astro experiments

- Fundamental in various domains and phases of an experiment
  - design of the experimental set-up
  - evaluation and definition of the potential physics output of the project
  - evaluation of potential risks to the project
  - development and optimisation of reconstruction and physics analysis software
  - contribution to the calculation and validation of physics results
- **Simulation of the passage of particles through matter**
  - other kinds of simulation components, such as ***physics event generators***, ***electronics response*** generation, etc.
  - often the simulation of a complex experiment consists of several of these components interfaced to one another

Basic ingredients

- Modeling the experiment: **geometry** + **materials**
- **Tracking** particles through matter
- Interaction of particles with matter: **physics** models

- Modeling the detector response
- Run and event control
- Interface to primary event generators
- Accessory utilities *(random number generators, PDG particle data etc.)*
- Visualisation of the set-up, tracks and hits
- User interface
- Persistency

Monte Carlo codes at the MC200 Conference, Lisbon, October 2000

The zoo

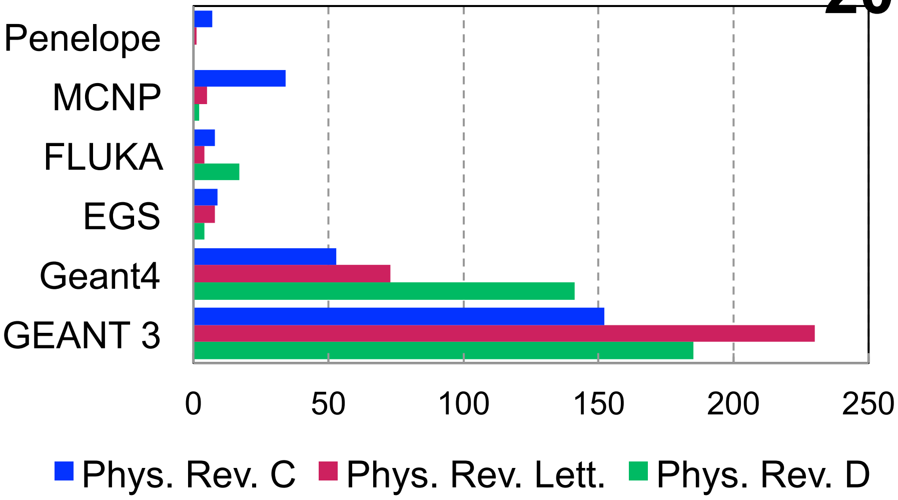
Many codes not publicly distributed

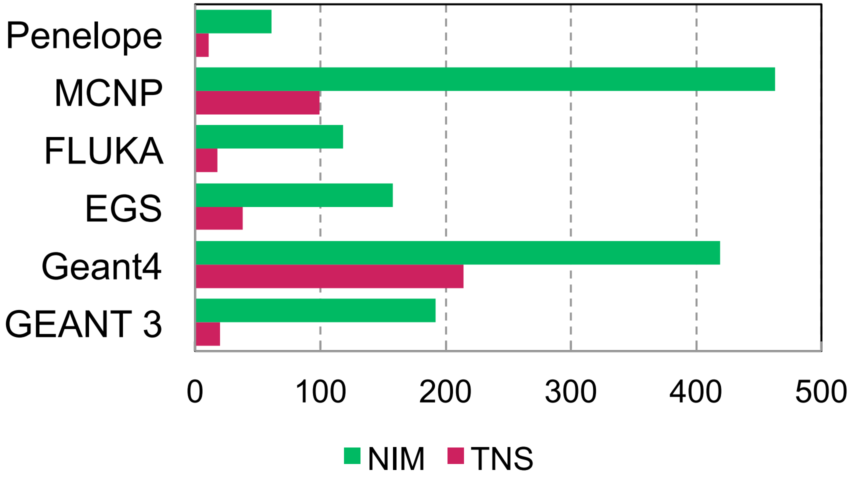
EGS4, EGS5, EGSnrc
GEANT 3, Geant4
MARS
MCNP, MCNPX, A3MCNP, MCNP-DSP, MCNP4B
MVP, MVP-BURN
Penelope
Peregrine
Tripoli-3, Tripoli-3 A, Tripoli-4

...and I probably forgot some more

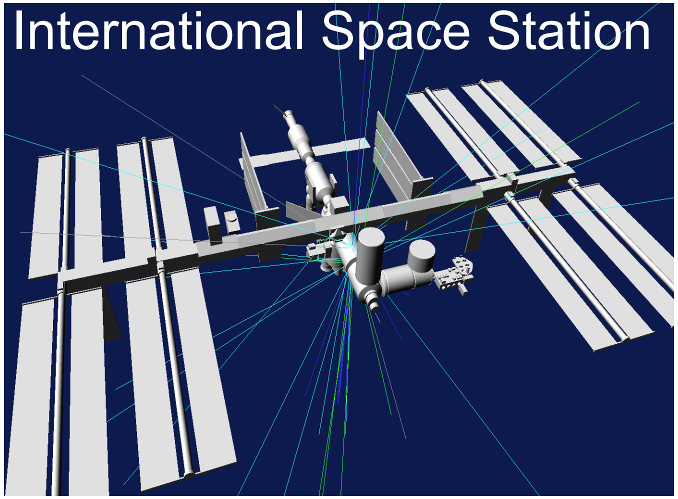
DPM
EA-MC
FLUKA
GEM
HERMES
LAHET
MCBEND MCU
MF3D
NMTC
MONK
MORSE
RTS&T-2000
SCALE
TRAX
VMC++

2004-2008



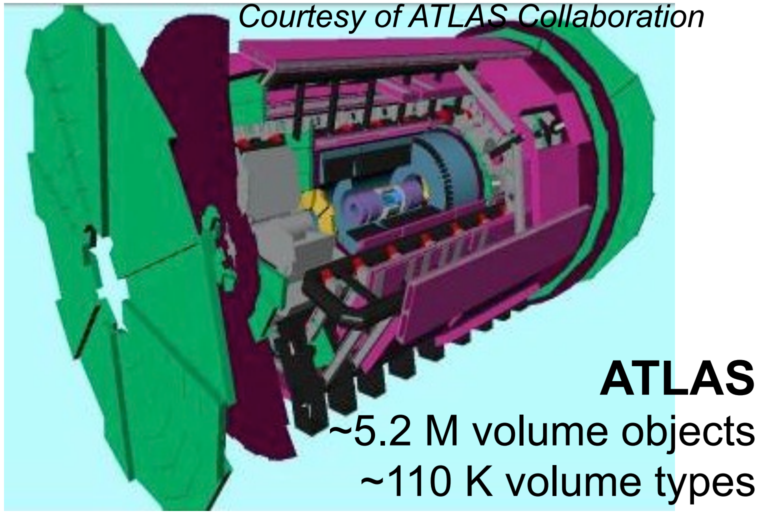


Geometry


International Space Station

Courtesy T. Ersmark, KTH Stockholm

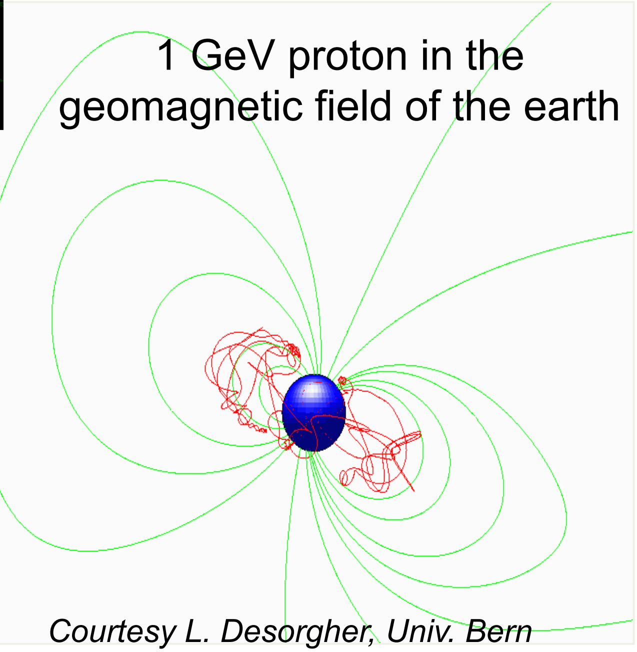

Courtesy HUREL, Hanyang Univ.


Courtesy of ATLAS Collaboration

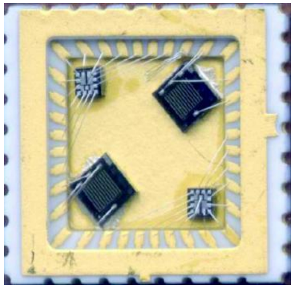
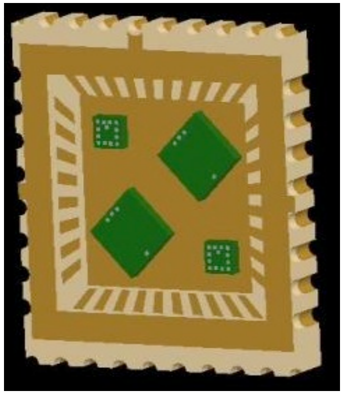
ATLAS
~5.2 M volume objects
~110 K volume types

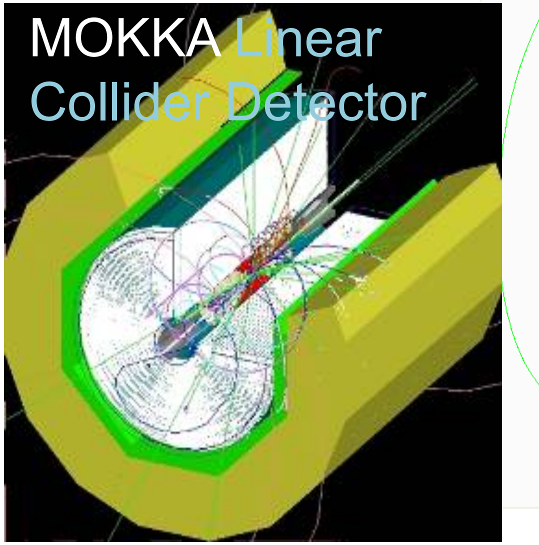
Intestine

Electric and magnetic fields


1 GeV proton in the geomagnetic field of the earth

Courtesy L. Desorgher, Univ. Bern



RADMON, CERN


MOKKA Linear Collider Detector

Geant4 electromagnetic physics

- electrons and positrons
- photons *(including optical photons)*
- muons
- charged hadrons
- ions

Multiple models for the same process:

- Standard
- Based on EADL-EEDL-EPDL data libraries
- Penelope-like
- + some variants, e.g. polarised photons

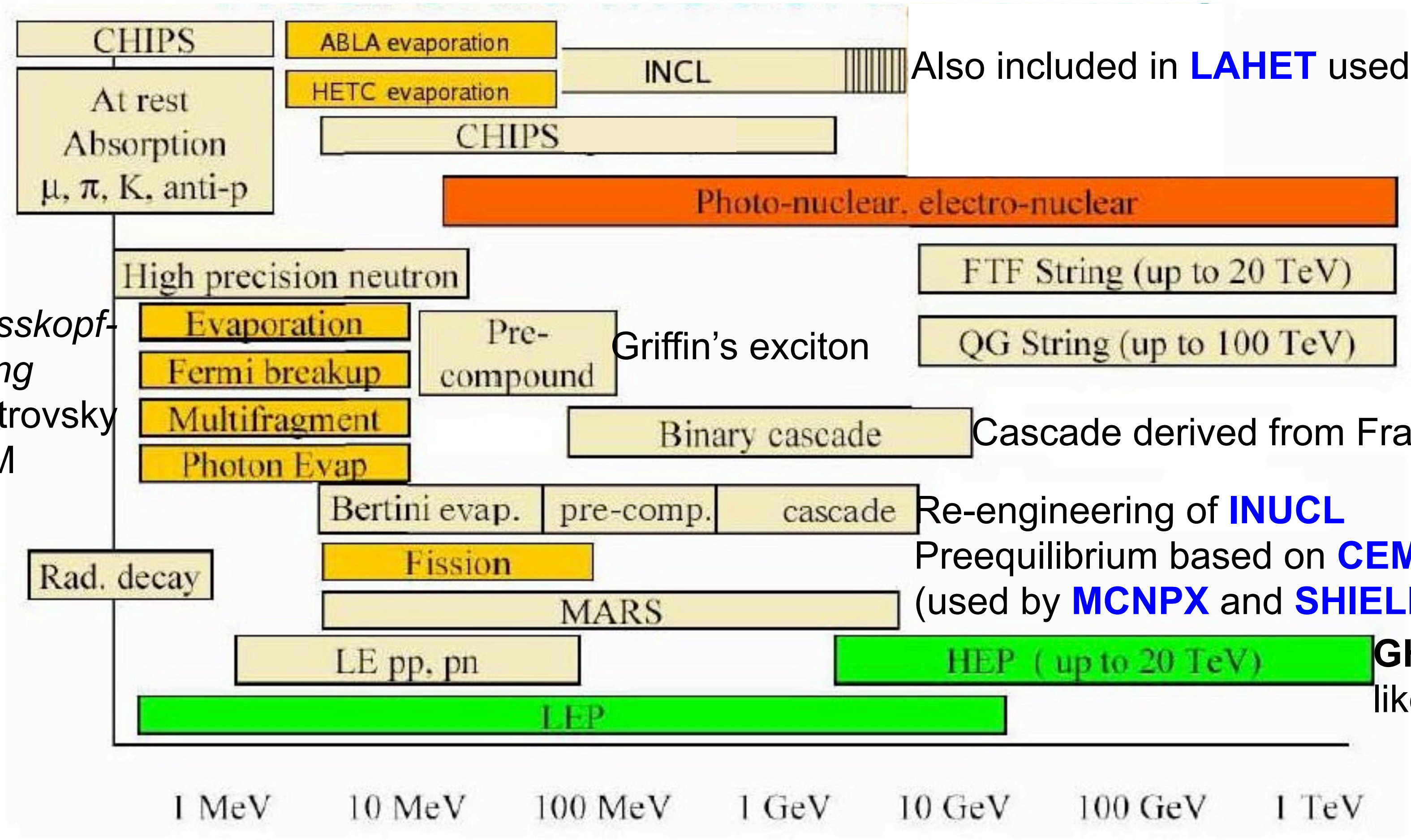
Multiple scattering
Bremsstrahlung
Ionisation
Annihilation
Photoelectric effect
Compton scattering
Rayleigh scattering
γ conversion
Synchrotron radiation
Transition radiation
Cherenkov
Refraction
Reflection
Absorption
Scintillation
Fluorescence
Auger electron emission

…sometimes nominally different models are actually identical

also across different Monte Carlo codes…

Geant4 hadronic inelastic model inventory

■ Data-driven ■ Parameterised ■ Theory-driven



Also included in **LAHET** used by **MCNPX**

FRITIOF

Weisskopf-Ewing
Dostrovsky
GEM

Griffin's exciton

Cascade derived from Frankfurt **QMD**

Re-engineering of **INUCL**
Preequilibrium based on **CEM**
(used by **MCNPX** and **SHIELD**)

GHEISHA-like

Many physics models are the same across different codes!

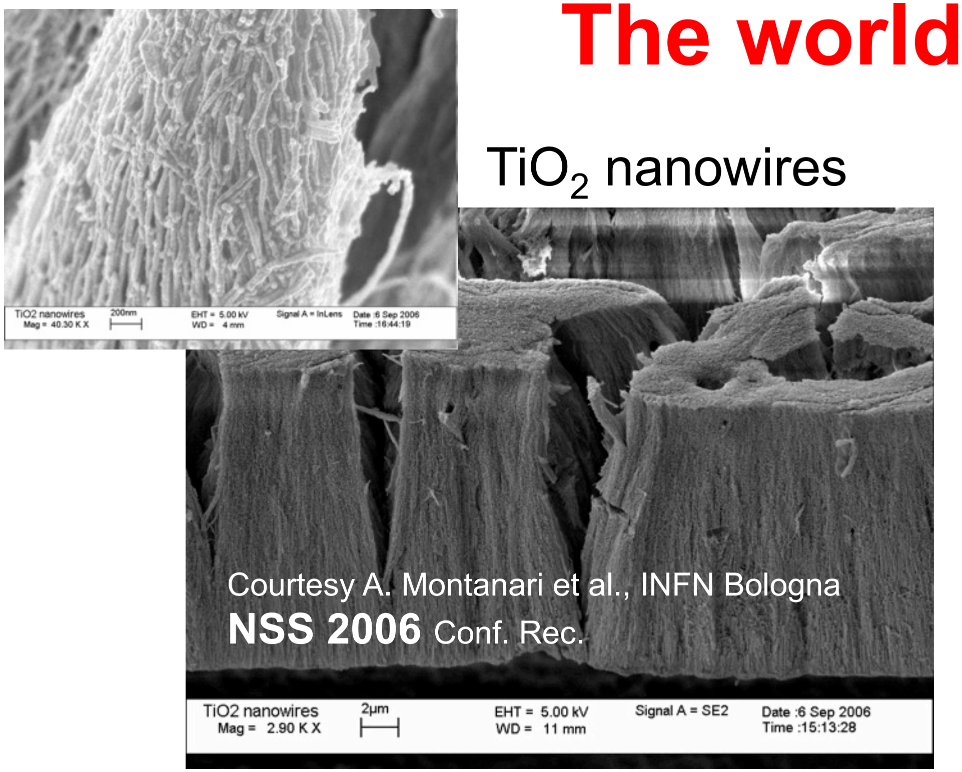
A mature Monte Carlo code

- Successfully used in many, multi-disciplinary experimental applications
- Cited by many relevant publications
  - e.g. Higgs boson discovery
- Ongoing improvements and refinements
  - Similar evolution also in other Monte Carlo codes
- Adaptation to evolving computing technologies
  - e.g. multithreading

Anything new and hot in the field?

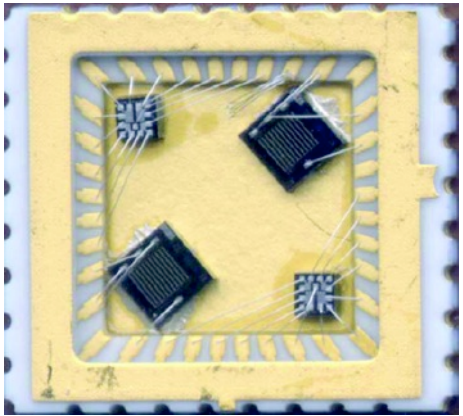
The world changes…

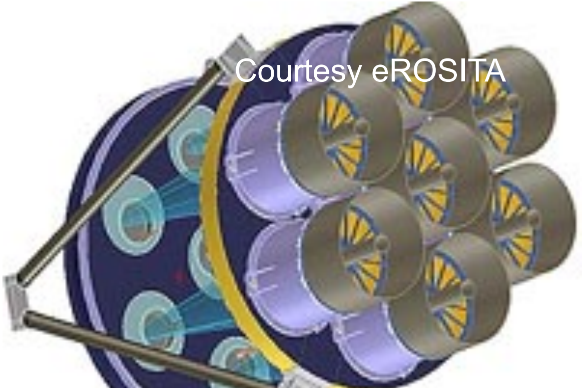
TiO$_2$ nanowires



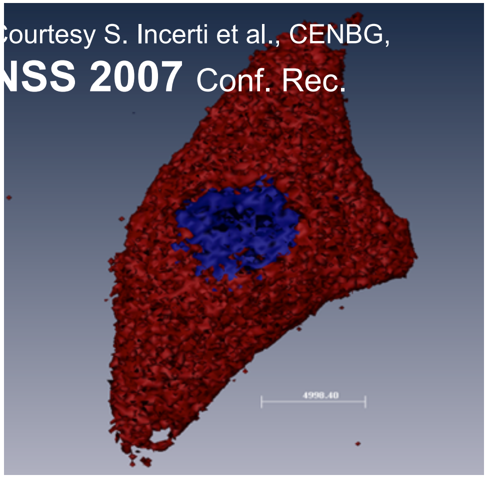
Courtesy A. Montanari et al., INFN Bologna
NSS 2006 Conf. Rec.

Courtesy RADMON (M. Moll et al.) Team, CERN,
NSS 2006 Conf. Rec.



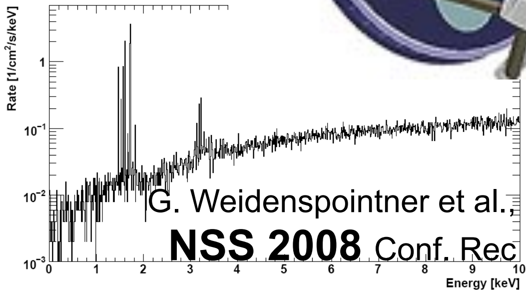


Courtesy eROSITA



ourtesy S. Incerti et al., CENBG,
NSS 2007 Conf. Rec.

S. Incerti et al., Monte Carlo dosimetry for targeted irradiation of individual cells using a microbeam facility, Radiat. Prot. Dosim., vol. 133, no. 1, pp. 2-11, 2009

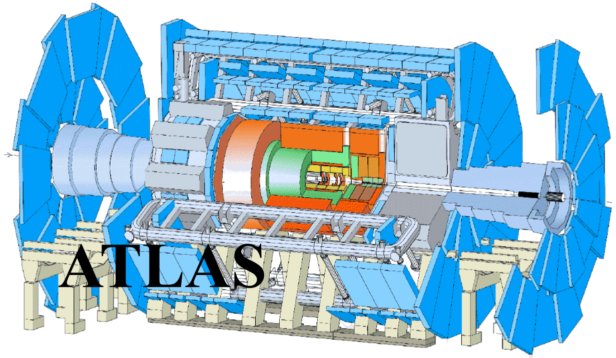


G. Weidenspointner et al.,
NSS 2008 Conf. Rec

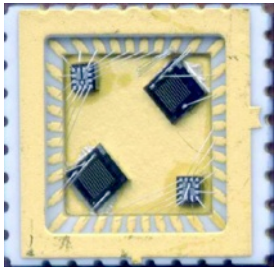
Two worlds…

Condensed-random-walk OR "discrete" régime

Characterizing choice in a Monte Carlo system



RADMON

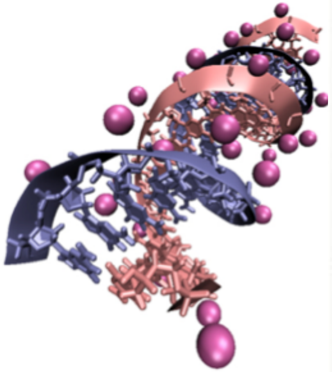


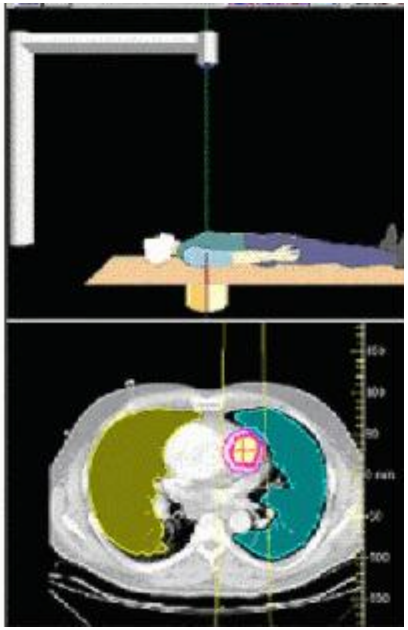
How does one estimate radiation effects on components exposed to LHC + detector environment?

And what about **nanotechnology**-based detectors for HEP?
And tracking in a **gaseous detector**?

*And **plasma** facing material in a fusion reactor?*

How does one relate **dosimetry** to **radiation biology**?





Simulation at small scale

Transport very low energy particles (~eV scale)

Physics models
Experimental data

- ➡ Drop the condensed history scheme
- ➡ Move beyond the independent particle approximation

Multi-scale simulation

Nano- and macro-scale in the same environment
Condensed and discrete schemes

…it is not just a matter of if-then-else
Source of inconsistency even in conventional scenarios (e.g. PIXE)

Independent particle approximation

Particles interact with atoms

Molecules?
Solids?

Each electron is considered to move **independently** in the **average field** of the Z - 1 other electrons plus the nucleus

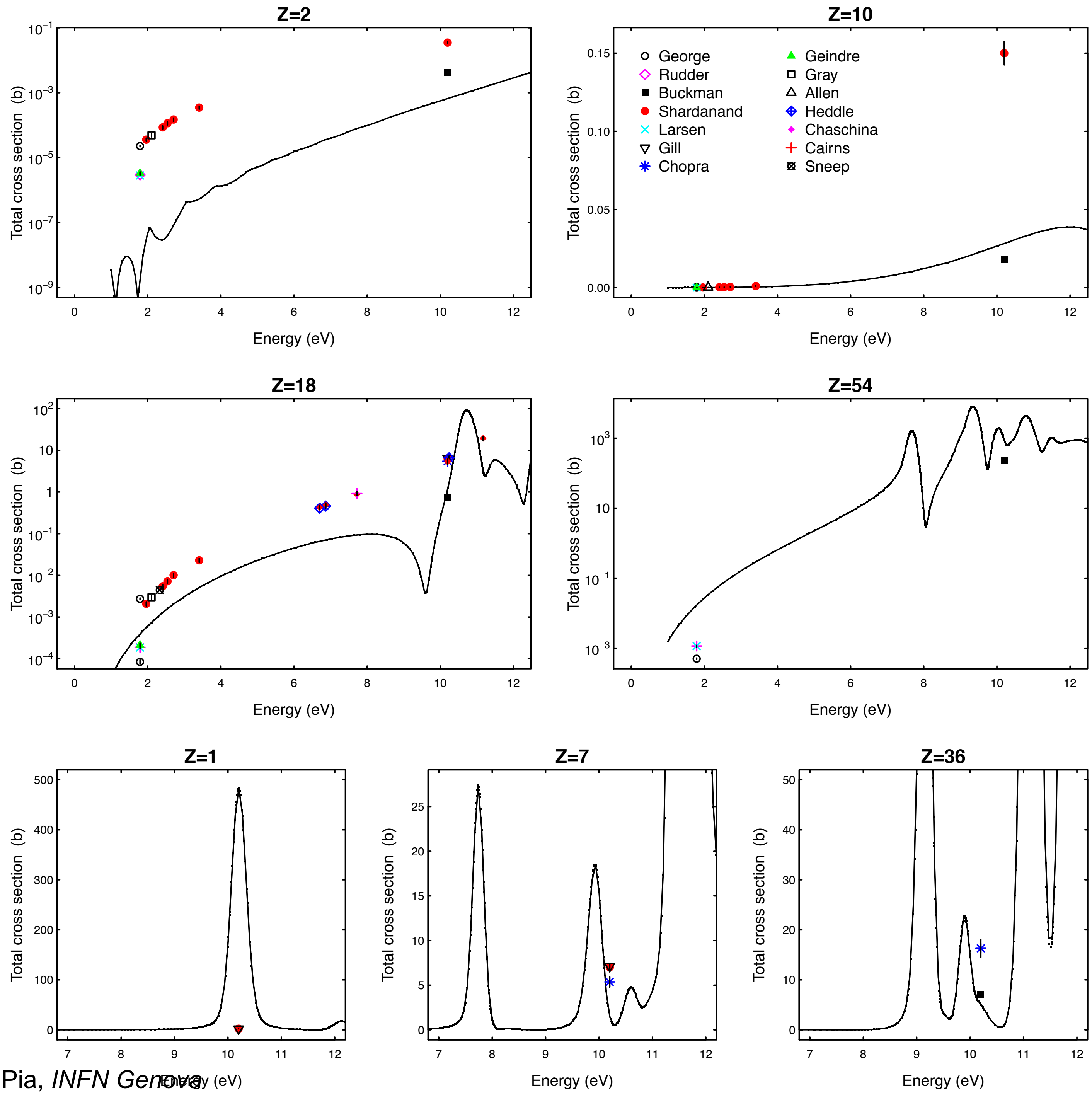
Central-field approximation

the distribution of the Z - 1 other electrons is spherically symmetric around the nucleus

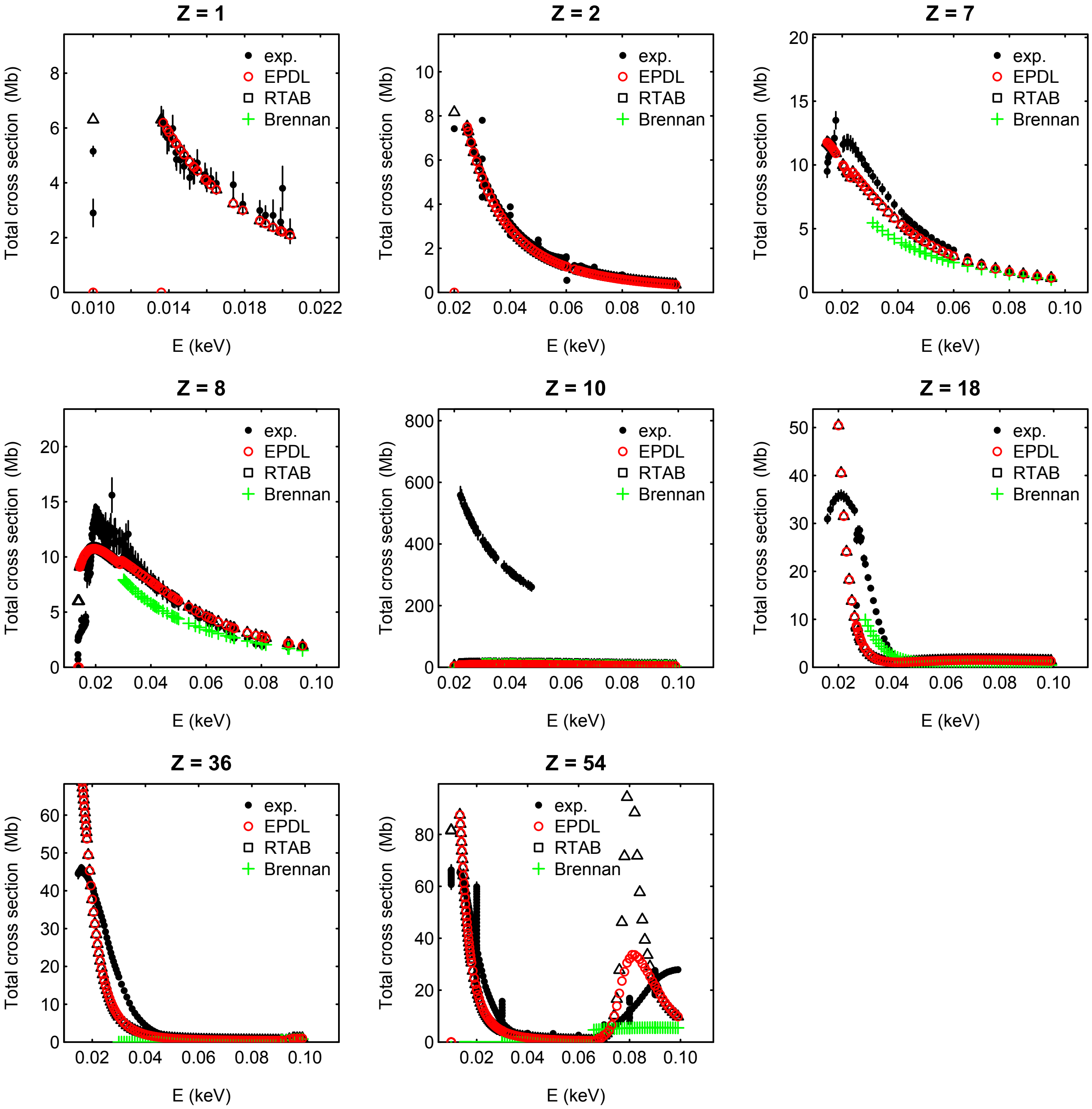
(Dirac) **Hartree-Fock calculations** are at the basis of the physics models used in Monte Carlo particle transport

When does it break?

Photon elastic scattering



Photoionization



Maria Grazia Pia, *INFN Genova*

PARTRAC, OREC, NOREC, LAPPA, MC4V, MC4L,TRION…

- M. Zaider, D. J. Brenner, W. E. Wilson, "The application of track calculations to radiobiology: I. Monte Carlo simulation of proton tracks", *Radiat. Res.*, vol. 95, pp. 231-247, 1983.
- H. G. Paretzke, "Radiation track structure theory", in *Kinetics of Non- homogeneous Processes*, Ed. New York: Wiley, 1987, pp. 89-170.
- W. E. Wilson and H. G. Paretzke, "Calculation of distribution of energy imparted and ionisations by fast protons in nanometer sites", *Radiat. Res.*, vol. 81, pp. 521-537, 1981.
- A. Ito, "Electron track simulation for microdosimetry", in *Monte Carlo Transport of Electrons and Photons*, Ed. Plenum, 1988, pp. 361-382.
- S. Uehara, H. Nikjoo, and D. T. Goodhead, "Cross-sections for water vapor for the Monte Carlo electron track structure code from 10 eV to the MeV region", *Phys. Med. Biol.*, vol. 37, pp. 1841-1858, 1992.
- A. V. Lappa, E. A. Bigildeev, D. S. Burmistrov, and O. N. Vasilyev, "Trion code for radiation action calculations and its application in microdosimetry and radiobiology", *Radiat. Environ. Biophys.*, vol. 32, pp. 1-19, 1993.
- C. Champion, "Multiple ionization of water by heavy ions: a Monte Carlo approach", *Nucl. Instrum. Meth. B*, vol. 205, pp. 671-676, 2003
- W. E. Wilson and H. Nikjoo, "A Monte Carlo code for positive ion track simulation", *Radiat. Environ. Biophys.*, vol. 38, pp. 97-104, 1999.
- S. Uehara, L. H. Toburen, and H. Nikjoo, "Development of a Monte Carlo track structure code for low-energy protons in water", *Int. J. Radiat. Biol.*, vol. 77, pp. 138-154, 2001.
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- D. Emfietzoglou, G. Papamichael, K. Kostarelos, and M. Moscovitch, "A Monte Carlo track structure code for electrons (10 eV-10 keV) and protons (0.3-10 MeV) in water: partitioning of energy and collision events", *Phys. Med. Biol.*, vol. 45, pp. 3171-3194, 2000.
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- M. Terrissol and A. Beaudre, "Simulation of space and time evolution of radiolytic species induced by electrons in water", *Radiat. Prot. Dosim.*, vol. 31, pp. 171-175, 1990.
- S. M. Pimblott, J. A. LaVerne, A. Mozumder, N. J. B Green, "Structure of electron tracks in water. 1. Distribution of energy deposition events", *J. Phys. Chem.*, vol. 94, pp. 488-495, 1990.
- R. H. Ritchie et al., "Radiation Interactions and Energy Transport in the Condensed Phase", in *Physical and Chemical Mechanisms in Molecular Radiation Biology*, Ed. Plenum Press, 1991, pp. 99-136.
- M. Zaider, M. G. Vracko, A. Y. C. Fung, J. L. Fry, "Electron transport in condensed water", *Radiat. Prot. Dosim.*, vol. 52, pp. 139-146, 1994.
- M.A. Hill, F. A. Smith, "Calculation of initial and primary yields in the radiolysis of water", *Int. J. Appl. Radiat. Isot.*, 43, pp. 265-280, 1994.
- V. Cobut, Y. Frongillo, J. P. Patau, T. Goulet, M. J. Fraser, and J. P. Jay-Gerin, "Monte Carlo simulation of fast electron and proton tracks in liquid water I. Physical and physicochemical aspects", *Radiat. Phys. Chem.*, vol. 51, pp. 229-243, 1998.
- V. A. Semenenko et al., "NOREC, a Monte Carlo code for simulating electron tracks in liquid water", *Radiat. Environ. Biophys.*, vol. 42, pp. 213-217, 2003.

Very-low energy models

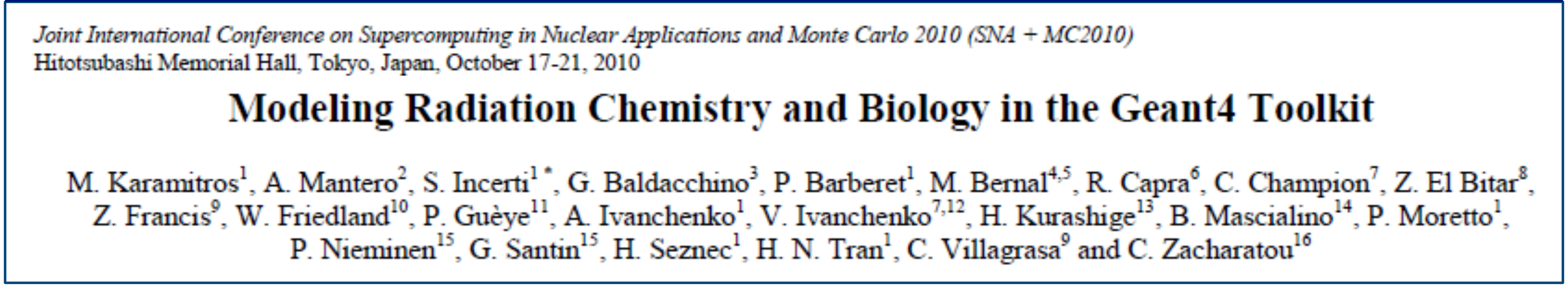
1st development cycle:
Physics of interactions in water down to the eV scale

IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 54, NO. 6, DECEMBER 2007 2619

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. Karamitros[1], A. Mantero[2], S. Incerti[1*], G. Baldacchino[3], P. Barberet[1], M. Bernal[4,5], R. Capra[6], C. Champion[7], Z. El Bitar[8], Z. Francis[9], W. Friedland[10], P. Guèye[11], A. Ivanchenko[1], V. Ivanchenko[7,12], H. Kurashige[13], B. Mascialino[14], P. Moretto[1], P. Nieminen[15], G. Santin[15], H. Seznec[1], H. N. Tran[1], C. Villagrasa[9] and C. Zacharatou[16]

Physics mostly derived from other "track structure" codes

Incerti S, Ivanchenko A, Karamitros M, Mantero A, Moretto P, Tran HN, Mascialino B, Champion C, Ivanchenko VN, Bernal MA, Francis Z, Villagrasa C, Baldacchin G, Guèye P, Capra R, Nieminen P, Zacharatou C.

Comparison of GEANT4 very low energy cross section models with experimental data in water

Med. Phys., vol. 37, no. 9, pp. 4692-4708, 2010

Software
Good software
Validated software

1012™

IEEE Standard for Software Verification and Validation

Best Student Award Monte Carlo 2010

Ionization cross sections for low energy electron transport

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

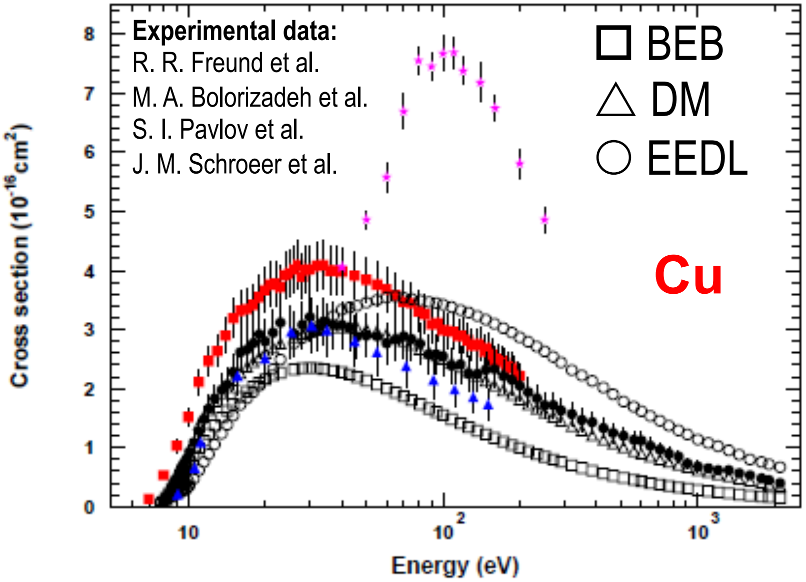
IEEE Trans. Nucl. Sci., vol. 58, no. 6, pp. 3219–3245, 2011

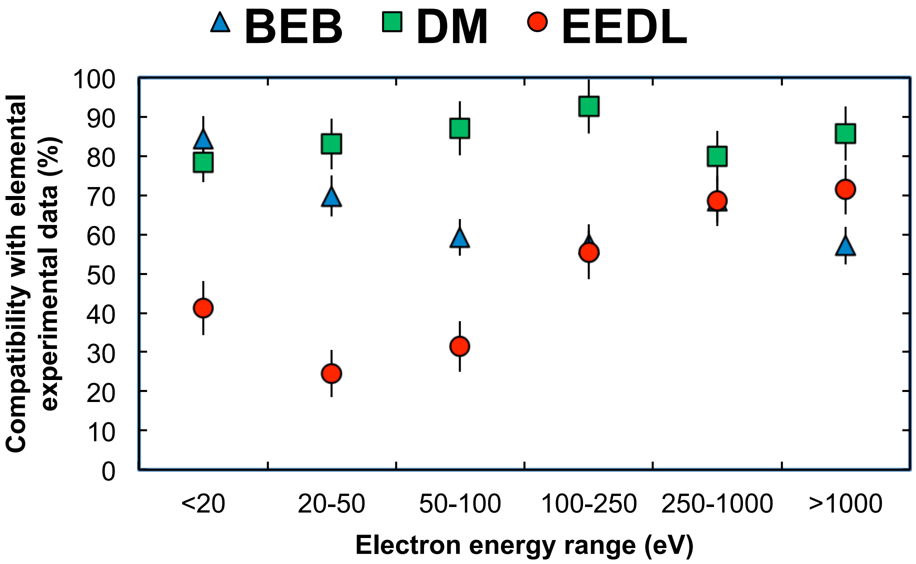
Cross section models

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

Validation

- 57 elements
- **181** experimental data sets
- statistical data analysis





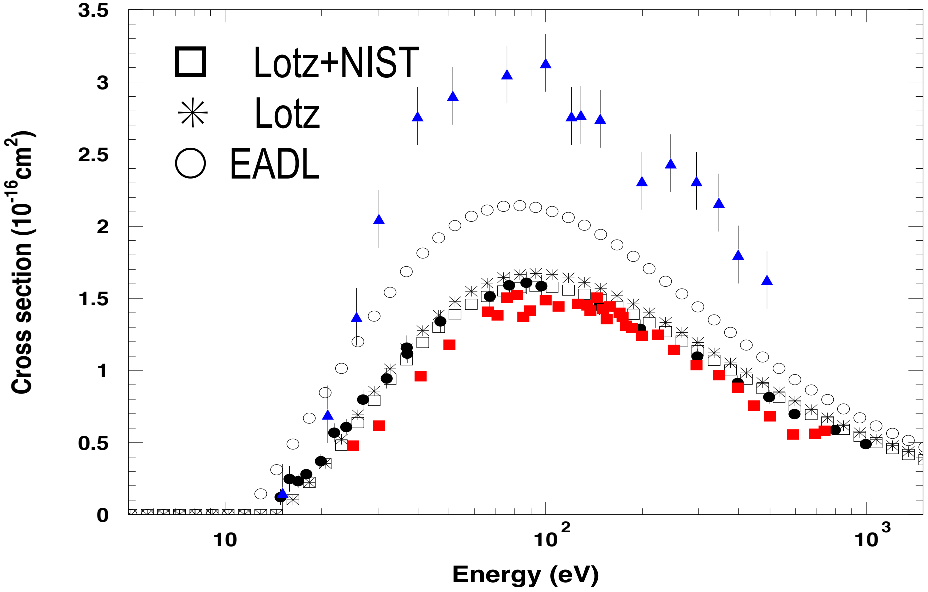
Percentage of elements for which a model is compatible with experimental data at **95% CL**

A fresh look at atomic parameters

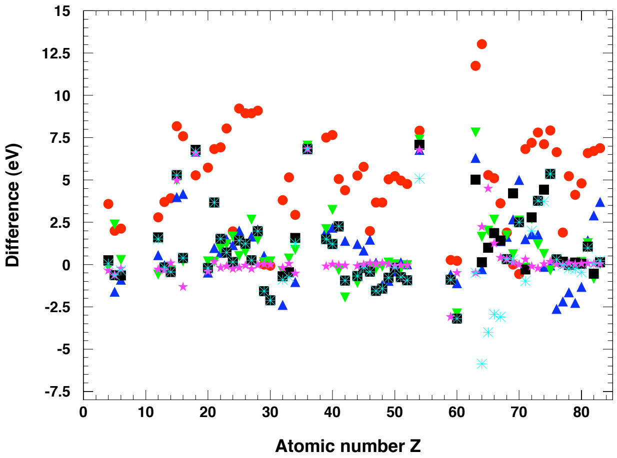
3246 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 58, NO. 6, DECEMBER 2011

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

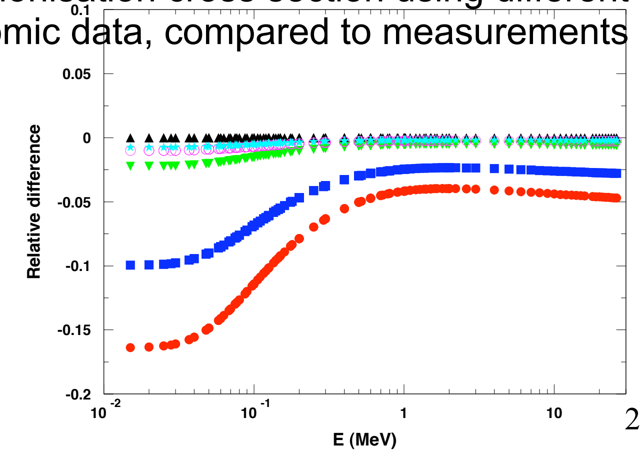


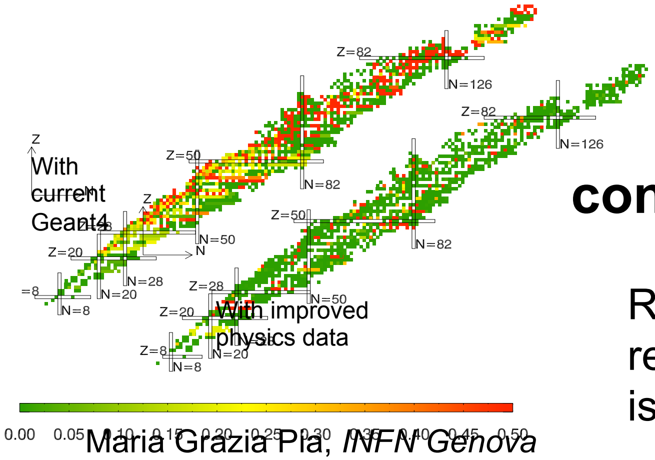
C, K shell



Atomic binding energies from various sources compared to experimental data

Proton ionisation cross section using different atomic data, compared to measurements





With current Geant4

With improved physics data

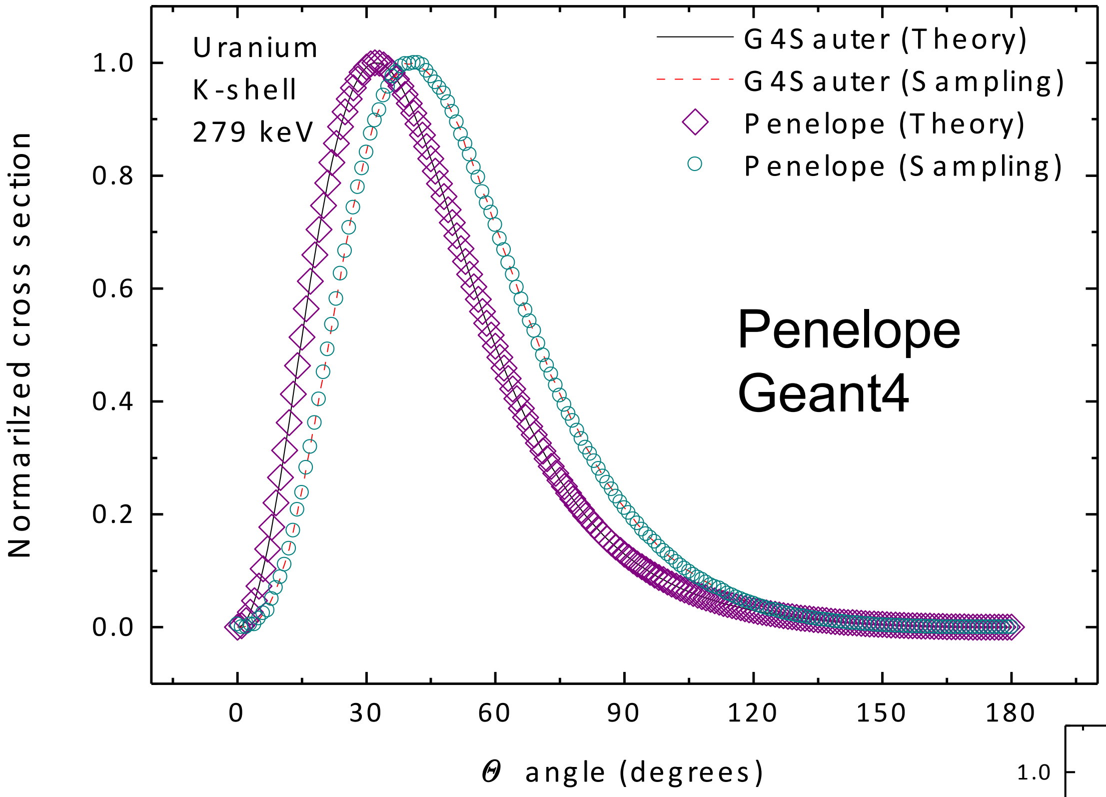
Benefits also in **conventional simulations**

Radioactive decay: Median relative intensity deviation per isotope for X-ray emission

How good are Monte Carlo codes?

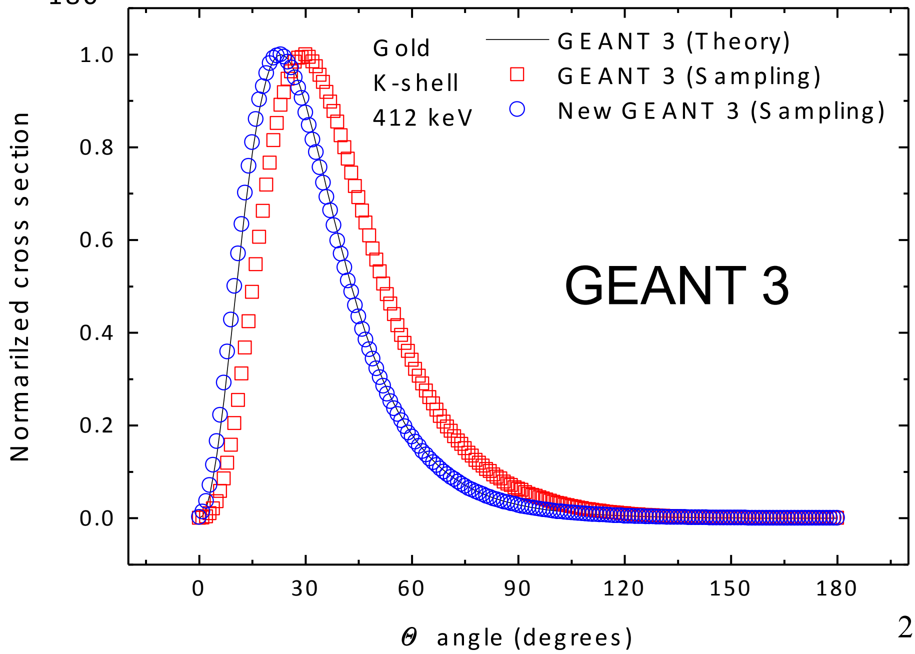
Hardly any systematic, quantitative validation of the physics models in Monte Carlo codes for particle transport is documented in the literature

Photoelectron angular distribution



Error aged for ~30 years and propagated across different Monte Carlo codes

New, correct sampling algorithm reproduces the expected theoretical distribution



Monte Carlo as a predictive instrument

If we know the uncertainties of the “ingredients” of our Monte Carlo code, can we calculate the uncertainties of the observables resulting from the simulation?

Quantify the uncertainties of the “ingredients”

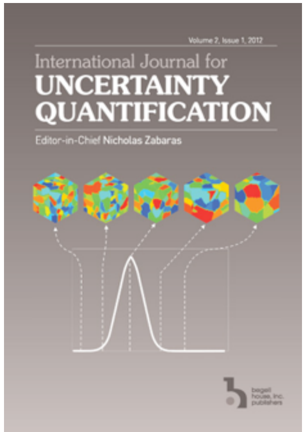
Validation of physics models and parameters

Epistemic uncertainties

Induced **systematic effects**

Propagation of uncertainties into observables

Uncertainty Quantification

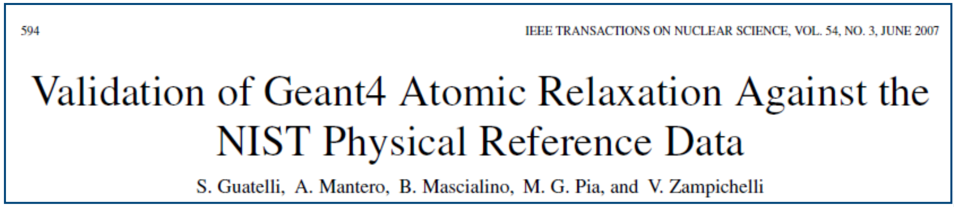


Volume 2, Issue 1, 2012
International Journal for
UNCERTAINTY QUANTIFICATION
Editor-in-Chief Nicholas Zabaras

begell house, inc. publishers

Hot topic in deterministic simulation,
still in its infancy in Monte Carlo simulation

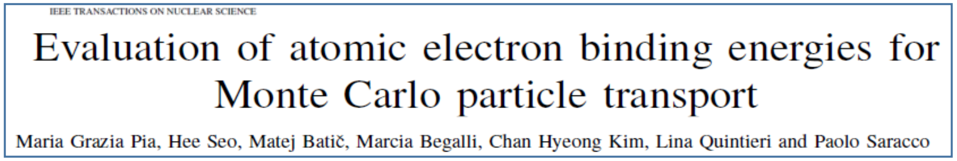
Validation of the “ingredients”



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

Validation of Geant4 Atomic Relaxation Against the NIST Physical Reference Data

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



IEEE TRANSACTIONS ON NUCLEAR SCIENCE

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

IEEE TRANSACTIONS ON NUCLEAR SCIENCE

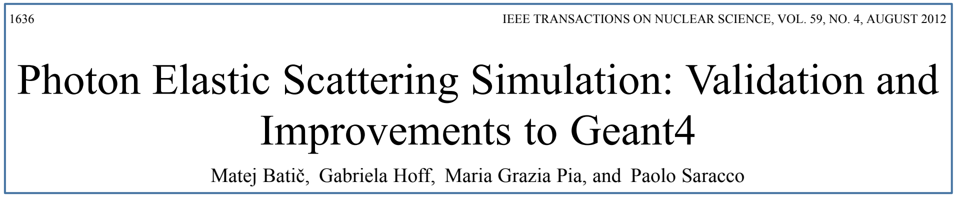
Validation of Proton Ionization Cross Section Generators for Monte Carlo Particle Transport

Matej Batič, Maria Grazia Pia, and Paolo Saracco

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

Ionization Cross Sections for Low Energy Electron Transport

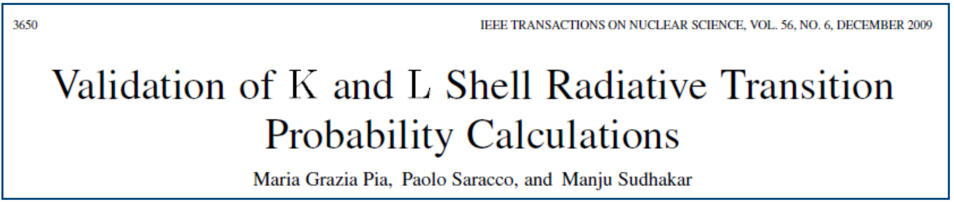
Hee Seo, Maria Grazia Pia, Paolo Saracco, and Chan Hyeong Kim



1636 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 59, NO. 4, AUGUST 2012

Photon Elastic Scattering Simulation: Validation and Improvements to Geant4

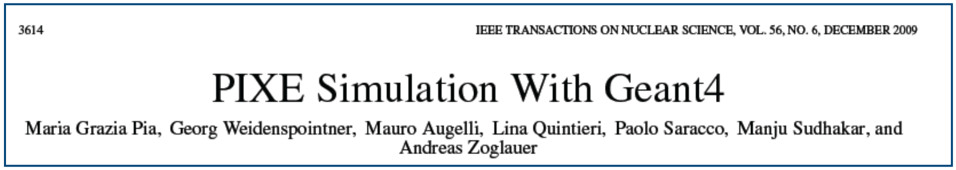
Matej Batič, Gabriela Hoff, Maria Grazia Pia, and Paolo Saracco



3650 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

Validation of K and L Shell Radiative Transition Probability Calculations

Maria Grazia Pia, Paolo Saracco, and Manju Sudhakar



3614 IEEE TRANSACTIONS ON NUCLEAR SCIENCE, VOL. 56, NO. 6, DECEMBER 2009

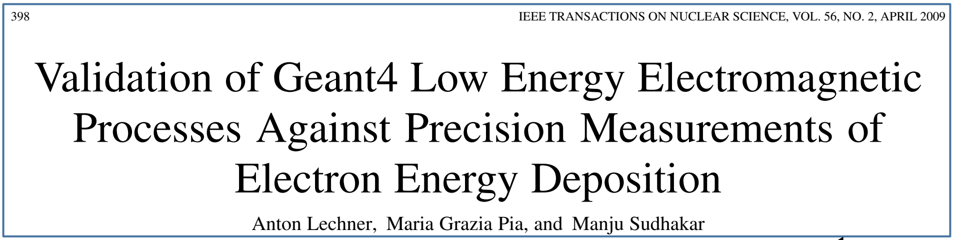
PIXE Simulation With Geant4

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

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

Geant4 Model for the Stopping Power of Low Energy Negatively Charged Hadrons

Stéphane Chauvie, Petteri Nieminen, and Maria Grazia Pia



398 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

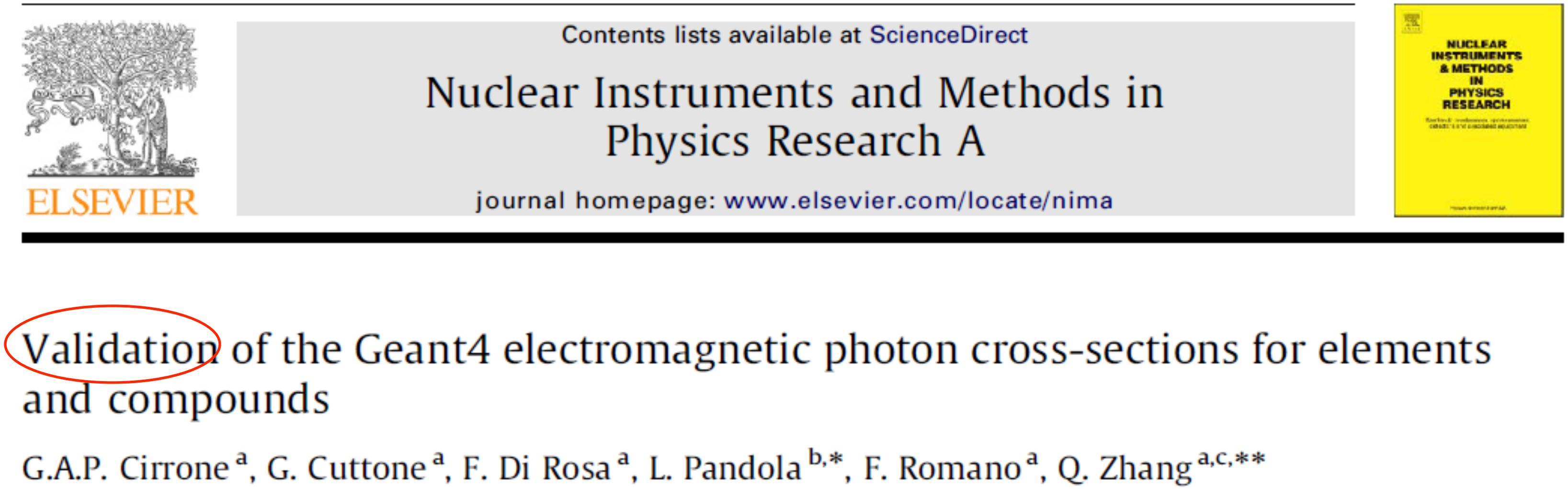
Anton Lechner, Maria Grazia Pia, and Manju Sudhakar

etc.

Computational Science Demands a New Paradigm

Douglass E. Post and Lawrence G. Votta

Physics Today, vol. 58, no. 1, 2005



Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

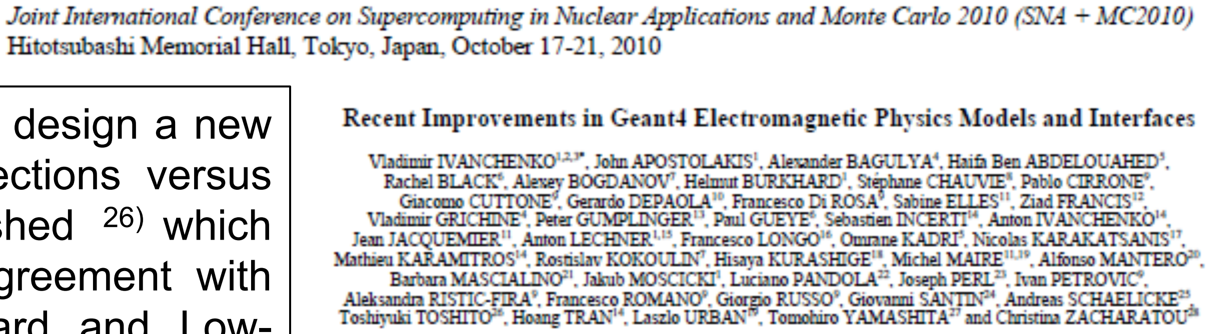
journal homepage: www.elsevier.com/locate/nima

ELSEVIER

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

Recent Improvements in Geant4 Electromagnetic Physics Models and Interfaces

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

"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."

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


Source:NASA

The launch of STS-107 on January 16,2003

Columbia Space Shuttle accident, 2003

Epistemic uncertainties

Epistemic uncertainties originate from **lack of knowledge**

Relatively scarce attention so far in Monte Carlo simulation
Studies in deterministic simulation *(especially for critical applications)*

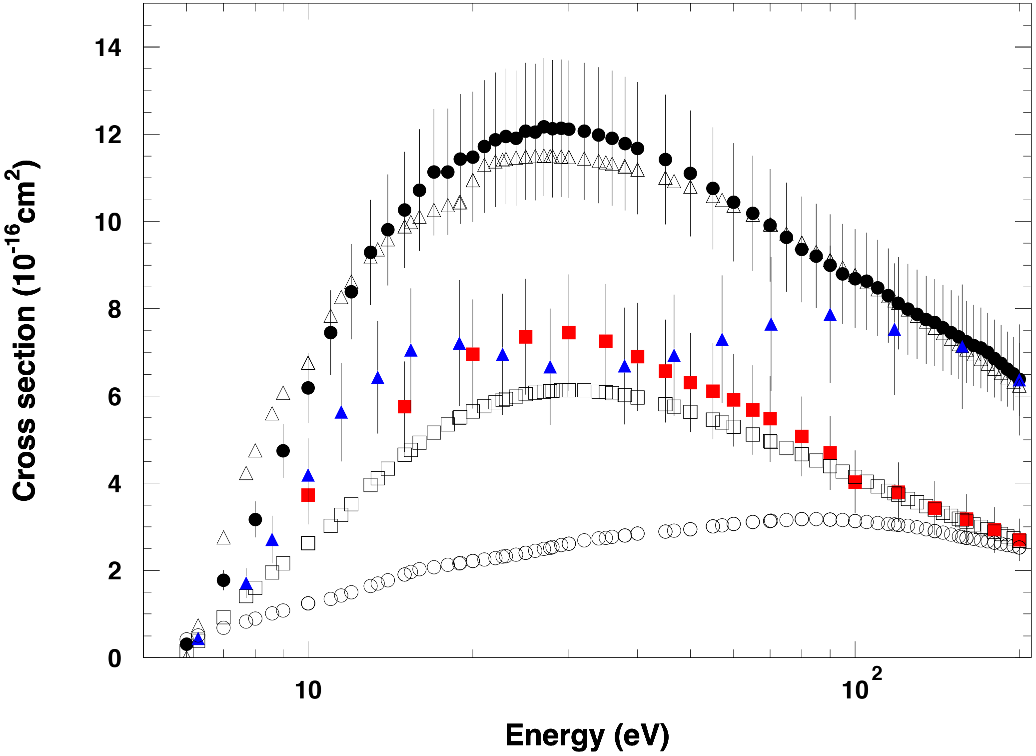
Possible sources in Monte Carlo simulation

- incomplete understanding of fundamental (physics) processes, or practical inability to treat them thoroughly
- non-existent or conflicting experimental data for a (physical) parameter or model
- applying a (physics) model beyond the experimental conditions in which its validity has been demonstrated

Epistemic uncertainties affect the **reliability** of simulation results

Can we quantify them?

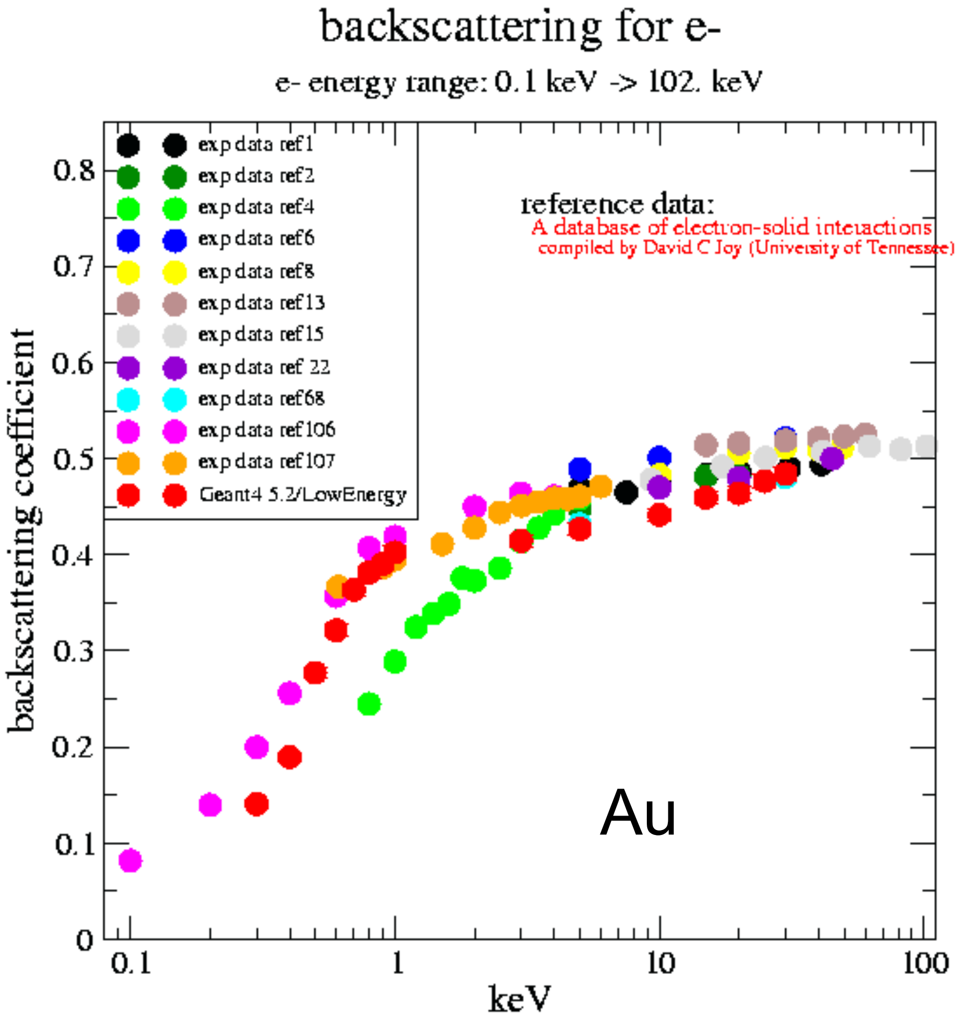
Which one is right?

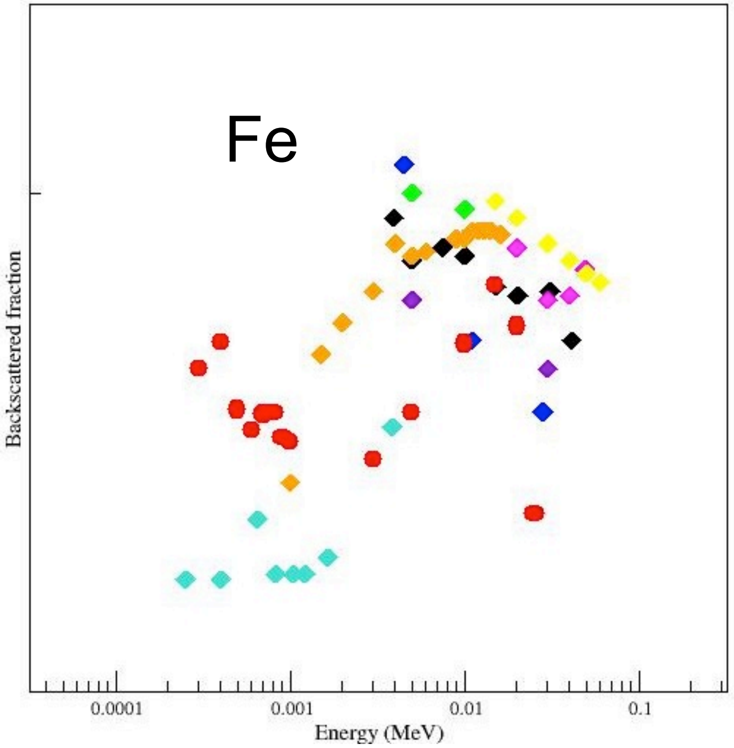


Often an answer can be found only through a **statistical analysis** over a **large sample** of simulated and experimental data *(and would be a result with a given CL, rather than black & white)*

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

The main problem of validation: experimental data!

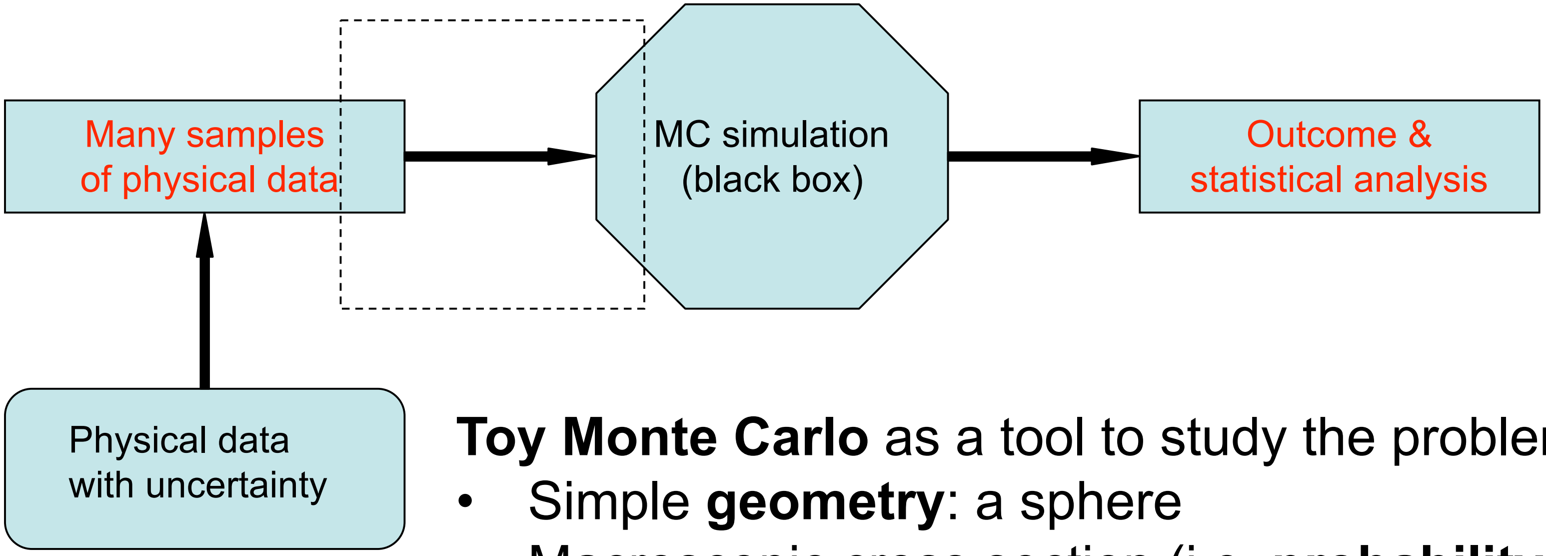




Experimental data often exhibit large differences!

First steps to establish a

theoretical ground of Uncertainty Quantification


Many samples of physical data

MC simulation (black box)

Outcome & statistical analysis

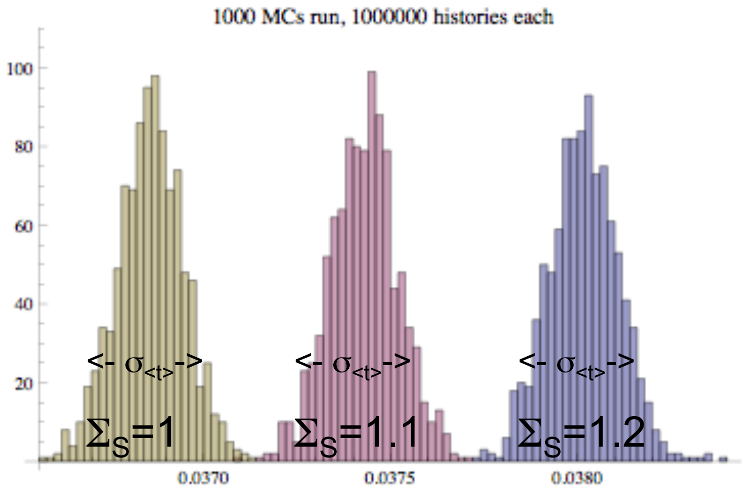
Physical data with uncertainty

Toy Monte Carlo as a tool to study the problem

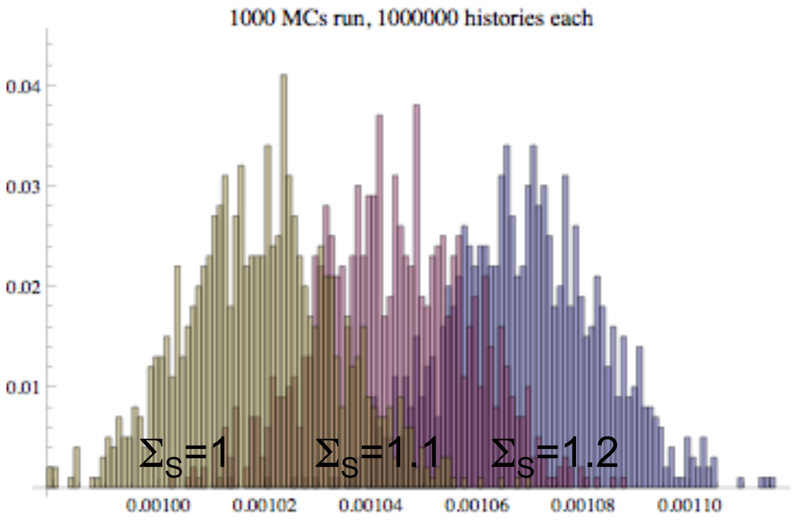
- Simple **geometry**: a sphere
- Macroscopic cross section (i.e. **probability**) for each process: scattering, absorption…
- **Tallies** (e.g. particle flux) in various positions

How do uncertainties in the cross section affect the tally?

We vary the “ingredients”, e.g. the scattering cross section Σ_S We observe the effect on the tally



Tally near the source:
higher statistics



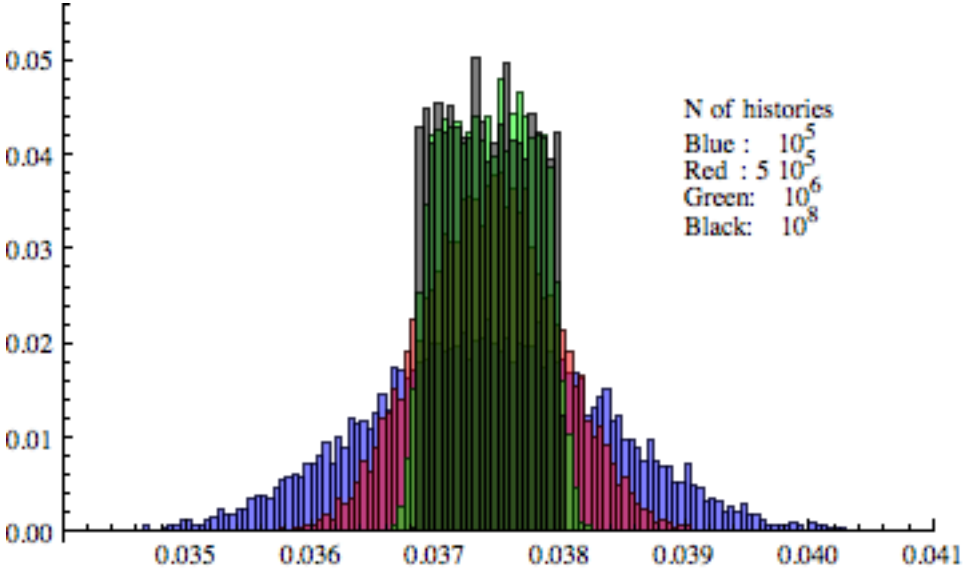
Tally far from source:
lower statistics

The Central Limit Theorem ensures that we can reduce the widths by increasing the number of histories in each Monte Carlo run:

$$\sigma_{<t>} \cong \sigma_t / \sqrt{N}$$

For instance, here Σ_S varies continuously with a flat distribution in a given interval $1.0 < \Sigma_S < 1.2$

We observe the effect on the tally



If the number of histories N is “small”, the outcome may be confused with a gaussian distribution

As the number of histories in each MC increases, the outcome becomes closer and closer to a flat distribution *(the same form we assumed for the variability of the ingredient)*

MC simulation transfers the original form of the uncertainty into the final outcome, adding some statistical “noise”

This stems from the identity:

$$\lim_{\sigma \to 0} \sqrt{\frac{1}{2\pi\sigma^2}} \int_{-\infty}^{\infty} p(x_0) \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right] dx_0 = p(x)$$

The statistical “noise” can be reduced in principle arbitrarily by increasing the number of histories

If we run many N-histories MCs varying the parameter(s) Σ_S in some interval with probability $f(\Sigma_S)$, the final distribution of the tally will be

$$G(x) = \int_{-\infty}^{+\infty} f(\Sigma_S) \exp\left[-\frac{(x - x_0(\Sigma_S))^2}{2\sigma^2_{x_0}/N}\right]\sqrt{\frac{N}{2\pi\sigma^2_{x_0}}}\, d\Sigma_S$$

exact mean value of the tally

(invertible) function $x_0(\Sigma_S)$

original value of the “ingredient”

This assumption relies on the interpretation of the simulation as a surrogate for the solution of **Boltzman transport equation**

In the limit of infinite histories

$$G(x) = K\left|\frac{d\Sigma_S(x)}{dx}\right| f(\Sigma_S^{-1}(x))$$

If the range of variability of Σ_S is sufficiently small, $x(\Sigma_S)$ can be approximated by a linear relation

$\Downarrow$

the final distribution of tallies has the same form of the original uncertainty

$\Sigma_{min} \leq \Sigma_S \leq \Sigma_{max}$ $\Rightarrow$ $x_{min} \leq x \leq x_{max}$

Maria Grazia Pia, *INFN Genova*

Ongoing activity

Further work in progress

two papers in preparation

Deal with {
- many ingredients
- many observables

Define **best practices**
to quantify uncertainties of a simulation

Experimental application use cases

…along with Geant4 physics validation

Acknowledments

- Tullio Basaglia
- Matej Batic
- Marcia Begalli
- Zane W. Bell
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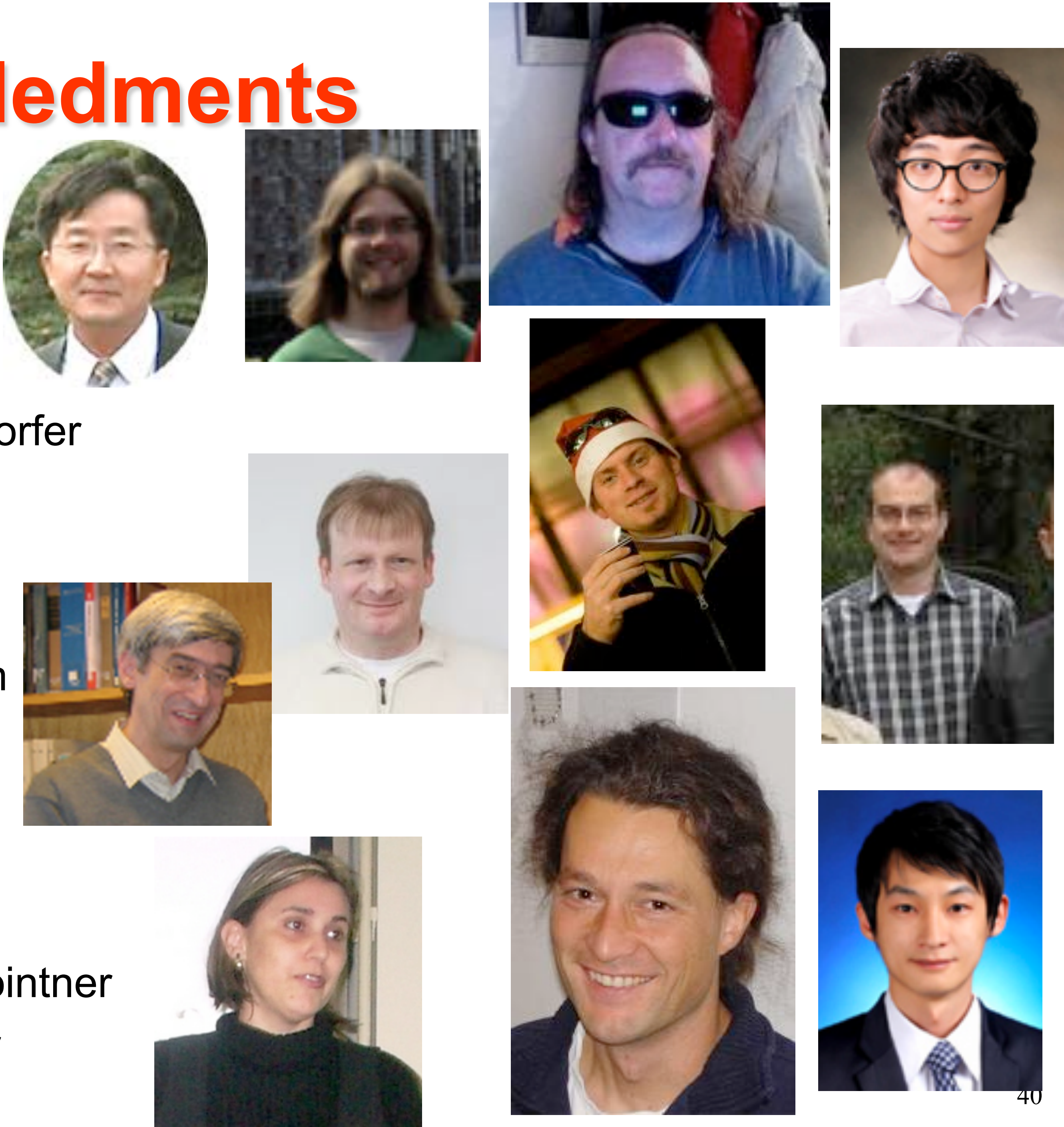
- Steffen Hauf
- Gabriela Hoff
- Chan Hyeong Kim
- Han Sung Kim
- Markus Kuster
- Paolo Saracco
- Hee Seo
- Georg Weidenspointner
- Andreas Zoglauer



Thank you, Thomas!

post workshop…

Commonality across different disciplines

Uncertainty Quantification
Epistemic uncertainties

Beyond the IPA
Physics calculations

Cross-disciplinary cooperation?

Maria.Grazia.Pia@cern.ch
MariaGrazia.Pia@ge.infn.it

http://www.nss-mic.org/2013/

Seoul, 27 October – 2 November 2013
Abstracts: 13 May 2013

IEEE Nuclear Science Symposium

Contributions concerning Monte Carlo methods are welcome!

IEEE Transactions on Nuclear Science

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space science, medical physics,
photon science etc.

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