Overview of Geant4 Electromagnetic Physics Developments

Sébastien Incerti
CNRS/IN2P3/Bordeaux U., France

Vladimir Ivantchenko
CERN, Ecoanalytica MSU, G4AI Ltd., Met U.

on behalf of the Geant4 collaboration
« Electromagnetic Physics » working groups

7th Geant4 Space Users' Workshop
Seattle, WA, USA, 18-20 August 2010

Outline

- Overview of Geant4 EM Physics
  - EM Physics coverage & sub-libraries
  - Unified software design (since Geant4 9.3 BETA – June 2009)

- Recent results on EM Physics
  - EM “standard” sub-library update
  - EM “low energy” sub-library bug fixing
  - Electron, Proton & alpha transport
  - Ion transport
  - Validation of photon models
  - PIXE
  - Geant4-DNA models for microdosimetry

Geant4 Electromagnetic Physics

Geant4 EM Physics category sub-libraries

- Standard
  - γ, e+/- up to 100 TeV
  - hadrons up to 100 TeV
  - ions up to 100 TeV
- Muons
  - Up to 1 PeV
  - Energy loss propagator
- X-rays
  - X-ray and optical photon production processes
- High-energy
  - Processes at high energy (E>10 GeV)
  - Physics for exotic particles
- Polarisation
  - Simulation of polarized beams
- Optical
  - Optical photon interactions
- Low energy
  - Livermore: LPDL and EEDL data, γ, e- from 250 eV up to 1 GeV
  - Livermore LPDL data based polarized processes
  - PENELOPE code rewritten in C++, γ, e+/- from 100 eV up to 1 GeV
  - Ions up to 1 GeV
  - Microdosimetry (Geant4-DNA) from 7 eV to 100 MeV
  - Atomic de-excitation
- Adjoint
  - New sub-library for reverse Monte Carlo simulation from detector of interest back to source of radiation
- Utils
  - General EM interfaces

Recent developments in Geant4 EM physics

- For many years the Geant4 EM "low-energy" sub-library was developed separately
  - Focused on medical and space science requirements
  - Many unresolved software bugs & flaws have been accumulated over the years

- Instead, in 2008 we decided to reorganize fully the EM "low energy" working group and in particular to migrate EM "low energy" to common design with EM "standard" Physics
  - First public release with Geant4 9.3 BETA – June 2009
  - Geant4 EM Physics developers collaborate all together

- Significant benefits from the unification of EM interfaces:
  - Now possible to combine low-energy and high-energy models
  - Large number of long-standing unresolved issues of the EM low-energy sub-library are now fixed
  - CPU performance has been improved, including speed-up factor of 1.5
  - Easy access to cross sections and stopping powers

- New EM model development greatly facilitated

Common software design

- Convergence of software design between « standard » EM and « low energy » EM sub-libraries for a coherent approach of EM interactions

- In this design
  - a physical interaction or process is described by a process class
    - inherits from **G4VEmProcess, G4VMultipleScattering or G4VEnergyLossProcess**
  - a physical process can be simulated according to several models, each model being described by a model class
    - inherits from **G4VEmModel**
  - model classes calculate
    - total cross section and stopping power
    - final state (kinematics, production of secondaries…)
  - models can be alternative and/or complementary on certain energy ranges

EM Physics constructors (available since Geant4 9.3)

- G4EmStandardPhysics – default
- G4EmStandardPhysics_option1 – HEP fast but not precise
- G4EmStandardPhysics_option2 – Experimental
- G4EmStandardPhysics_option3 – medical, space
- G4EmLivermorePhysics
- G4EmLivermorePolarizedPhysics
- G4EmPenelopePhysics
- G4EmDNAPhysics

Combined Physics
Standard > 1 GeV
LowEnergy < 1 GeV
(changeable by the user)

- Located in $G4INSTALL/source/physics_list/builders

- Advantage of using of these classes : they are tested on regular basis and are used for regular validation

EM-utils sub-library update

- Improved initilisation: G4EmConfigurator can be used to add models per particle type and detector region to any PhysicsList

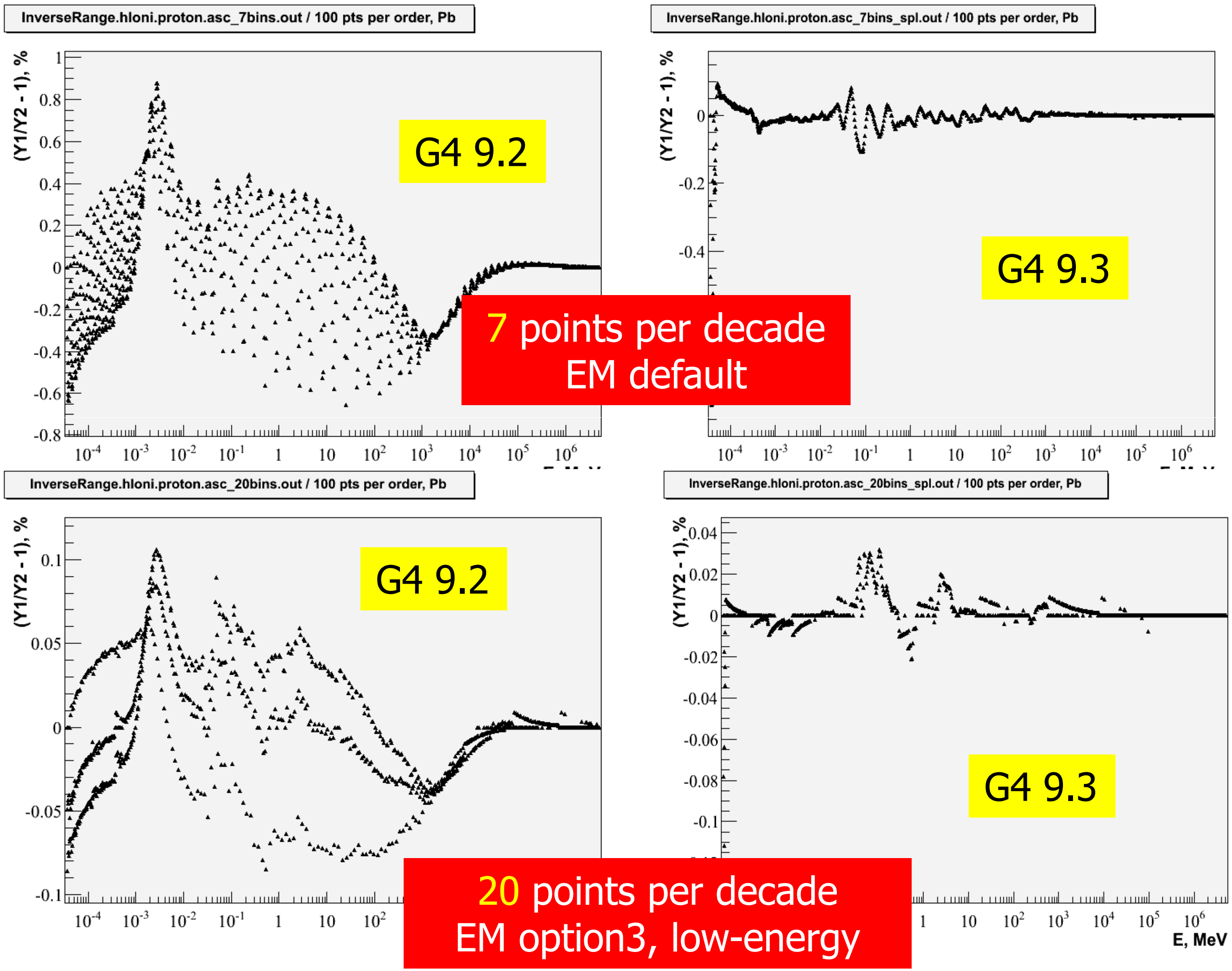
- G4EmCorrections: added protection/limit on value of Barkas and Bloch corrections
  - ATLAS reported on negative dedx of an object M=100 GeV, Q = -150e

- Fixed number of problems:
  - ion single scattering
  - Skin=1 (msc parameter)
  - Fixes inline methods
  - Added more comments to the code

EM-utils sub-library update

- MinCutEnergy computation is disabled
- Limit of energy threshold is defined only in PhysicsList and not anymore by the model itself
  - Delta-electron production is affected
- User may set any low limit for production thresholds on his/her own risk

Spline method for interpolation of stopping powers and ranges improving accuracy of proton transport in Lead



Materials sub-library*
(* not located in EM category)

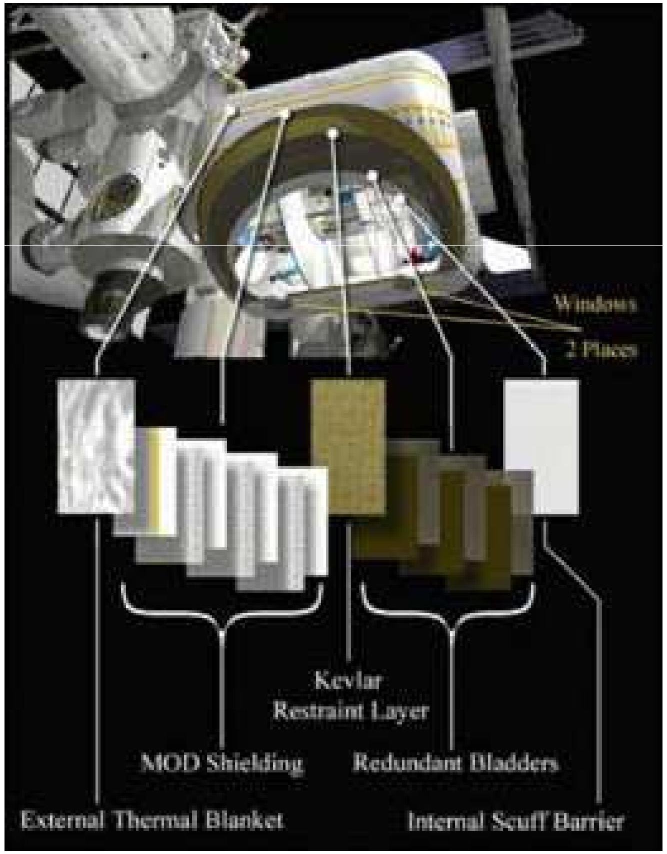
- Mean ionisation energy of atoms is now taken directly from NIST data (3-digit values) and not from ICRU'37 anymore (2-digit values)

- Parameterization of density effect for simple materials is taken from new class G4DensityEffectData independently on material name (state is controlled)

- PSTAR and ASTAR data have been re-verified
  - Data for 6 materials were fixed
  - G4PhysicsVector with spline instead of old interpolation

- G4AtomicShell class was updated
  - optimized computation of binding energy (introduction of extra array)

Materials sub-library*
(* not located in EM category)



- Development context of ESA AO6041
- New method added to G4NistMaterialBuilder class: G4SpaceMaterials()
- New materials added:
  - **G4_KEVLAR**
  - **G4_NEOPRENE**
  - **G4_DACRON**

EM-standard sub-library update of models

EM-standard sub-library update of models

- G4eBremsstrahlungModel – bug in element selection (Bug#1115)
- G4GoudsmitSaundersonMscModel – upgraded, now it is the most precise model for electrons
- G4WentzelVIModel – recently upgraded, intended for msc of muons, hadrons, and ions
- G4eCoulombScatteringModel, G4CoulombScatteringModel – fixed ion scattering
- G4UrbanMscModel93
  – scattering in low-Z media improved (9.3)
  – randomization of step limit is added for 9.4beta

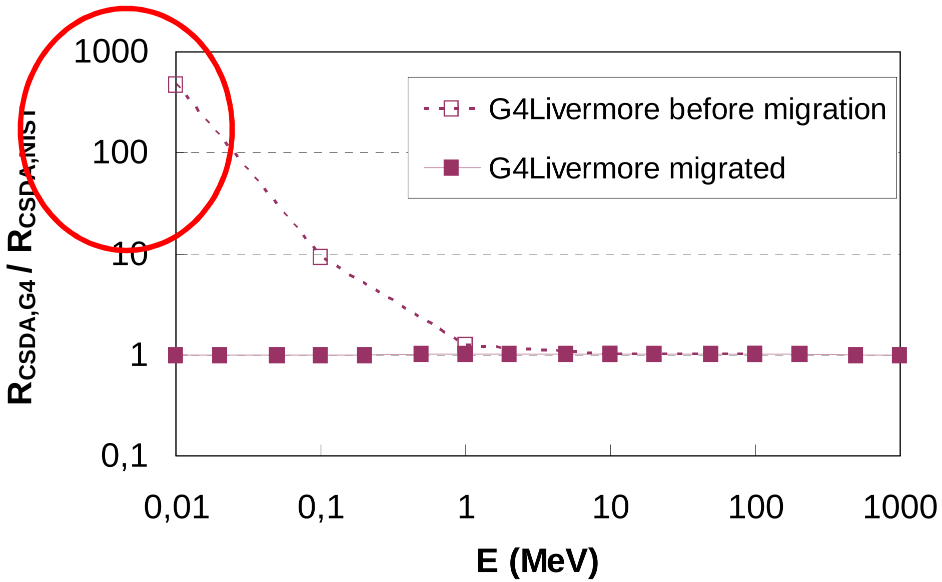
Fixes of the EM
« low energy » sub-library

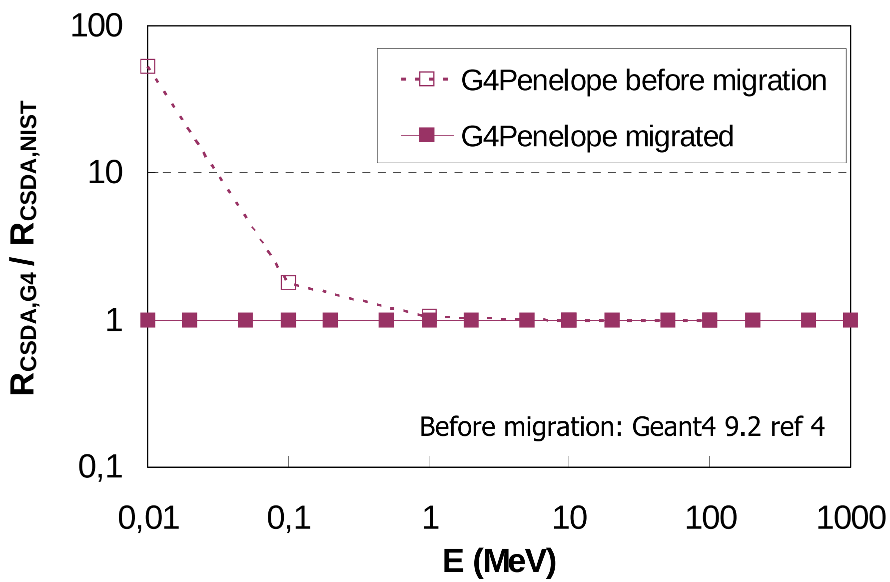
Software flaws till Geant4 9.3

- Many bugs & software flaws have been accumulated over the past years in the Geant4 EM « low energy » sub-category and have been left unfixed for a long time
- The Geant4 9.3 (December 2009) release includes many fixes in the EM « low energy » sub-category
- Verification / validation activity is on-going
  - We try to correct all bugs
- As an illustration, a selection of software flaws is shown hereafter

Electron « low energy » ionisation models in water

- Electron CSDA range vs NIST
- Ionisation in liquid water
- Non-migrated and migrated Livermore and Penelope alternatives
- Wrong computation below 1 MeV

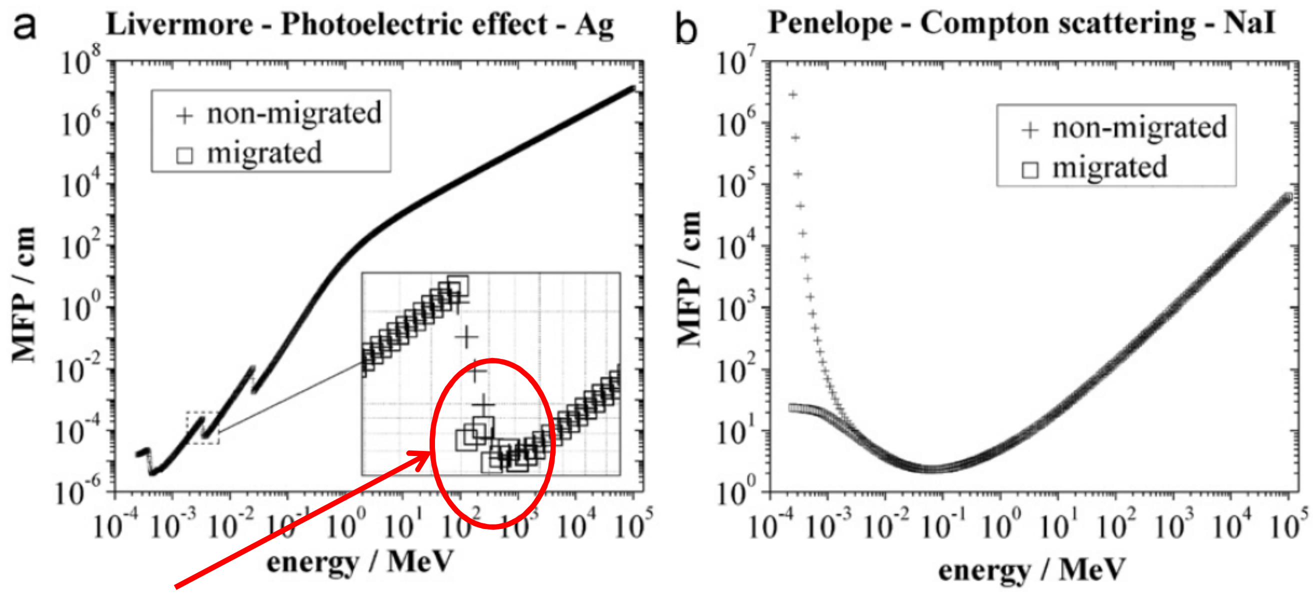




Courtesy of C. Zacharatou, V. Ivanchenko, M. Maire

Photon « low energy » models

- Missing shell structure from old Geant4 Livermore photoelectric models
  - due to a non-accurate interpolation table
- Bug in old low energy region of Penelope Compton scattering model



Mean free path (MFP) for the original EM processes vs. the new migrated models.
(a) Livermore photoelectric effect in Silver; (b) Penelope Compton scattering in NaI.

From TestEm5

And many more…

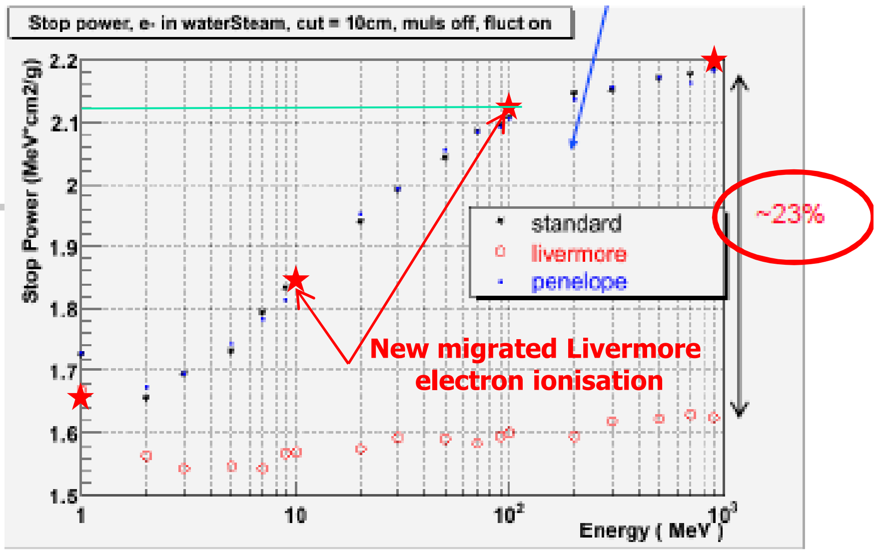
- Livermore ionisation for electrons
  - restricted stopping power of electron in gases is off by ~20%

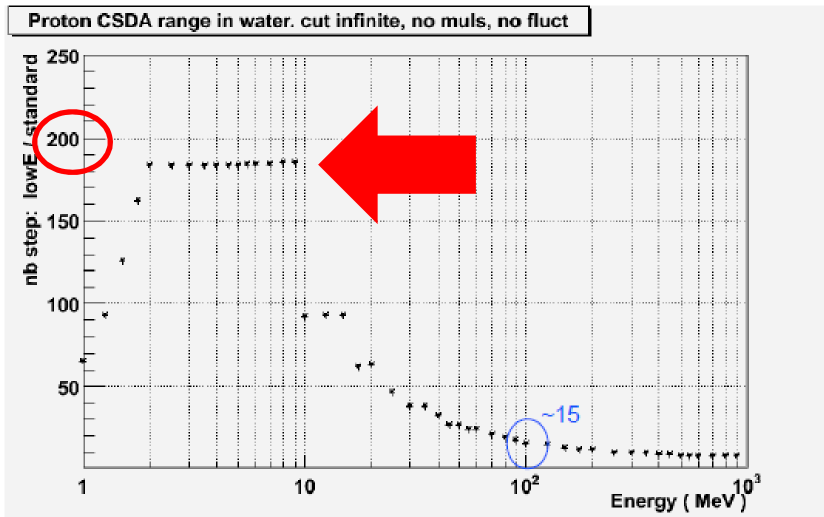
- Proton transport much slower than EM "standard" , due to excessive step limitation, CSDA proton range systematically off by at least 1% from NIST,…

- Wrong energy deposition in thin layer (Si, 50 um) by 2 GeV pion

- FPE exceptions, corrupted files in G4LEDATA data archive, etc…

- G4hLowEnergyIonisation was **not** migrated, buggy and *de facto* obsolete





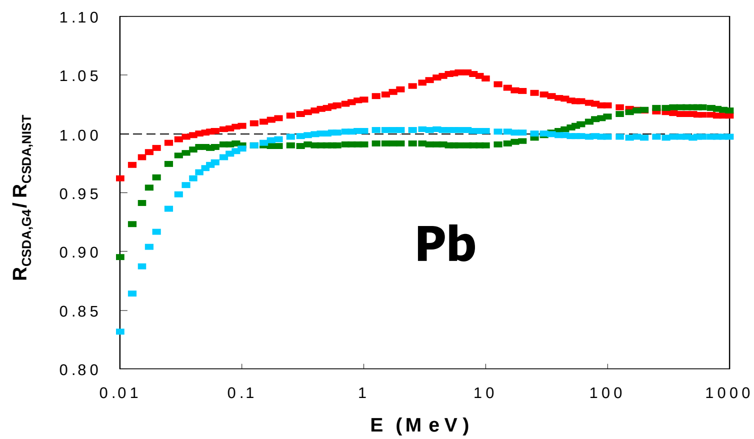
Plots courtesy of M. Maire, L. Urban, J. Jacquemier (since Lisbon - 2006 !)

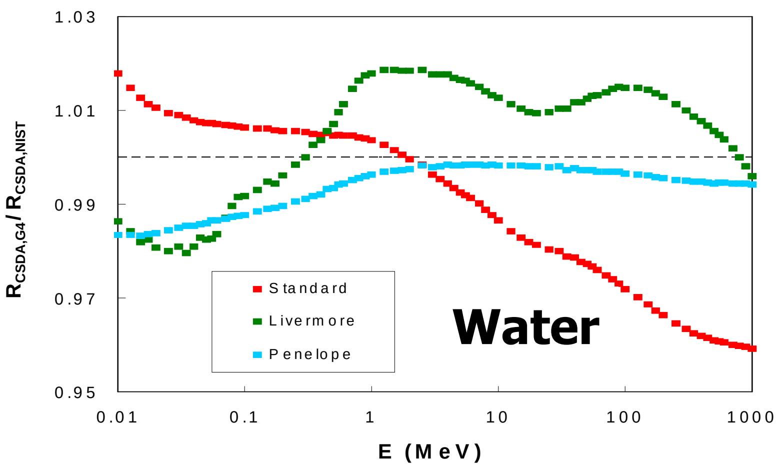
Electron, proton, alpha transport

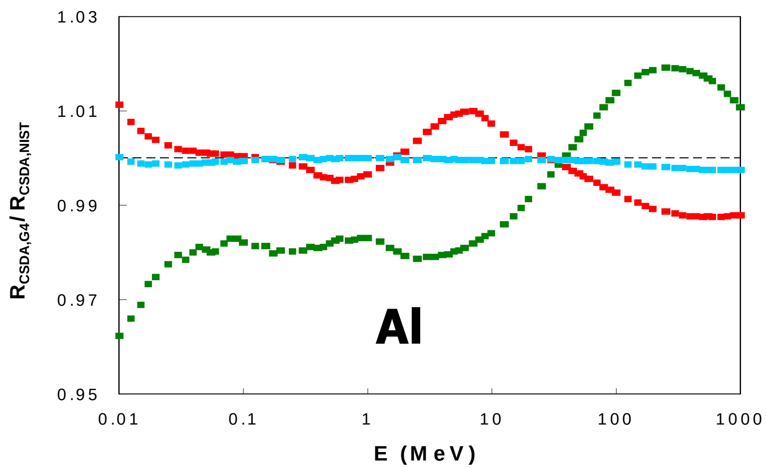
Courtesy of C. Zacharatou, V. Ivanchenko, M. Maire

Electron ranges Geant4 (9.3beta) versus NIST ESTAR data

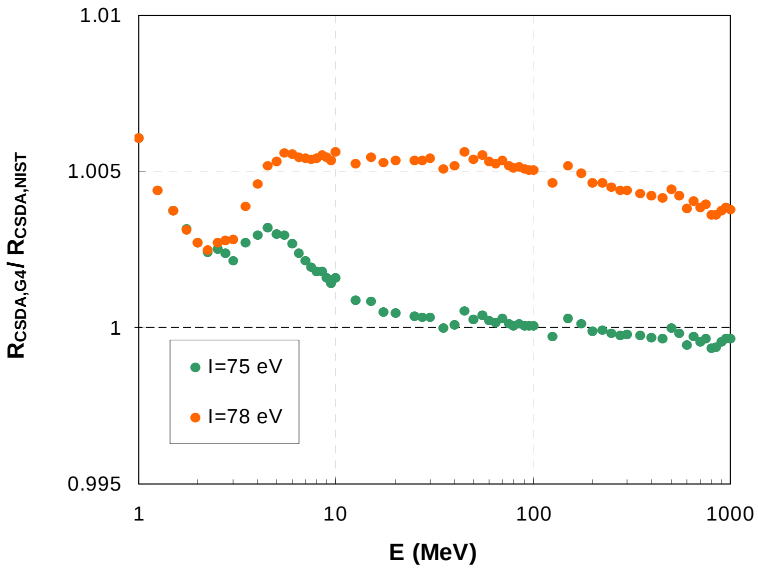
- Penelope results are more close to NIST
  - the difference <5% in the energy range 0.1 MeV – 1000 MeV
  - except for Pb below 0.1 MeV, where EM standard is best

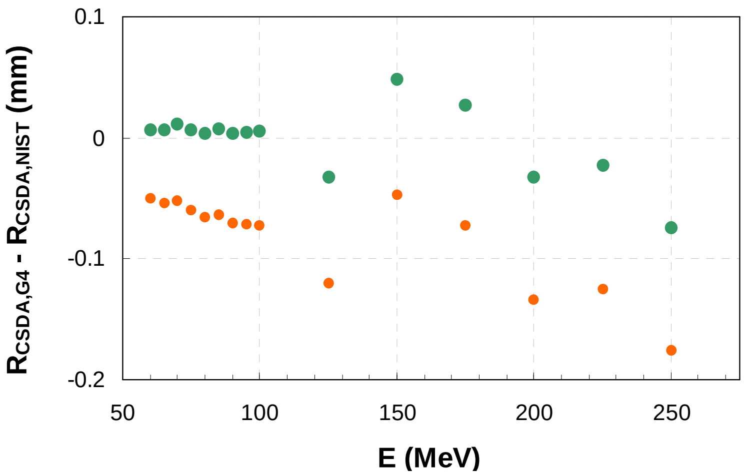






Proton ranges Geant4 (9.3beta) versus NIST PSTAR data for water

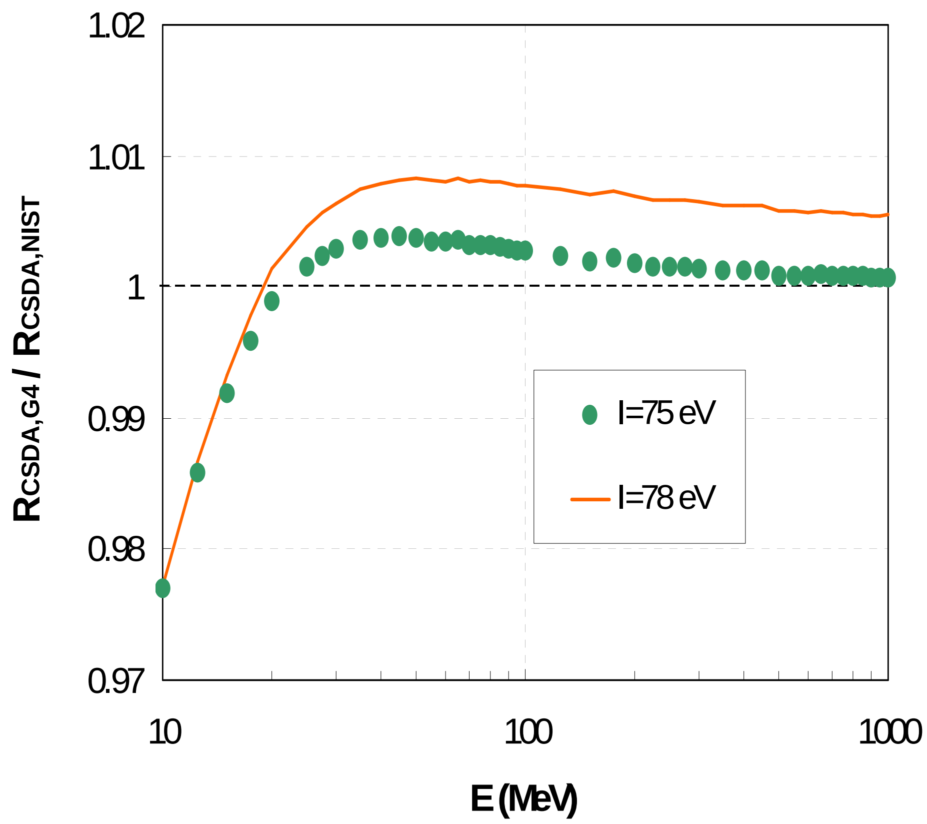




- Spline interpolation improve stability of ranges for cut and step limit modification
- Carbon ion Bragg peak results support change of the mean ionisation potential for water from 75 eV to 78 eV
- This leads to a 0.5% difference between Geant4 and NIST for protons in water
  - 0.1 mm shift of the Bragg peak

Alpha ranges Geant4 (9.3beta) versus NIST ASTAR data for water

- Similar difference due to mean ionisation potential change
- Geant4 Standard process for protons
  - G4hIonisation
- Geant4 Standard process for He ions
  - G4ionIonisation



Ion transport

ICRU 73 stopping powers in a new Geant4 model

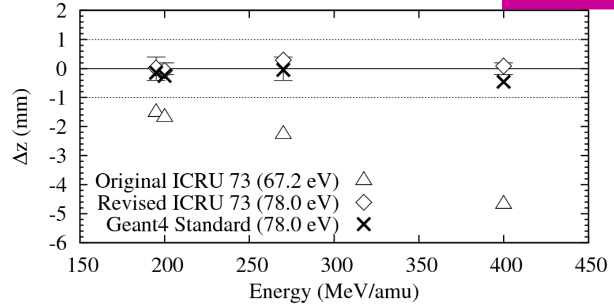
- ICRU 73 report
  - presents tabulated stopping powers of ions heavier than He for many elemental media and compounds.
  - energy range: up to 1 GeV/nucleon
  - stopping power calculations are based on the PASS code and binary theory
    - P. Sigmund and A. Schinner, Nucl. Instr. and Meth. B 195 (2002) 64
    - P. Sigmund and A. Schinner, Eur. Phys. J. D 12 (2000) 425
- ICRU 7 (PASS) stopping powers in Geant4
  - Since release 9.3, all ICRU 73 tables are available for ion transport simulations in Geant4
    - tables incorporated in the EM low-energy sub-library
  - For a few materials revised tables were included, which replace original ICRU 73 tables (tables provided by P. Sigmund)
    - P. Sigmund, A. Schinner and H. Paul, Errata and Addenda: ICRU Report 73, 2009
  - In addition PASS tables for Fe ions in water, which are not included in ICRU 73 report, were incorporated in Gean4 (tables provided by P. Sigmund)

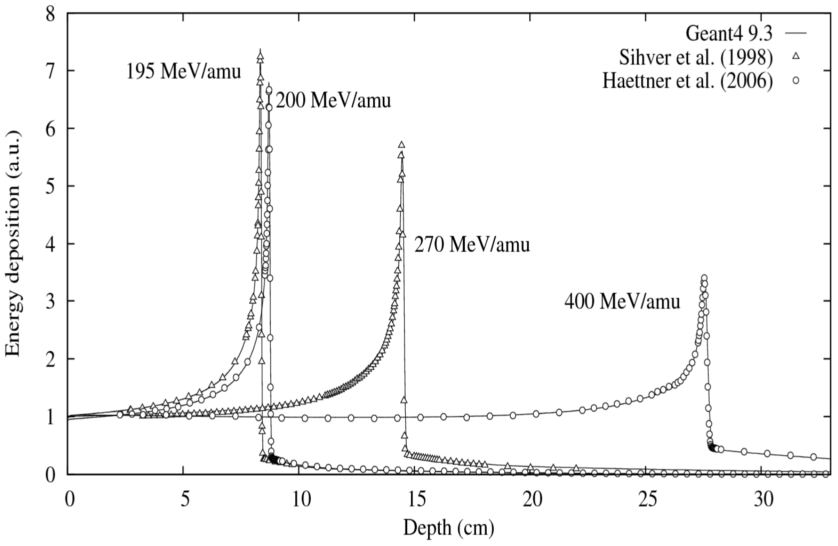
See : A. Lechner et al., NIM B268 (2010) 2343

Validation of ICRU 73-based ion model in Geant4

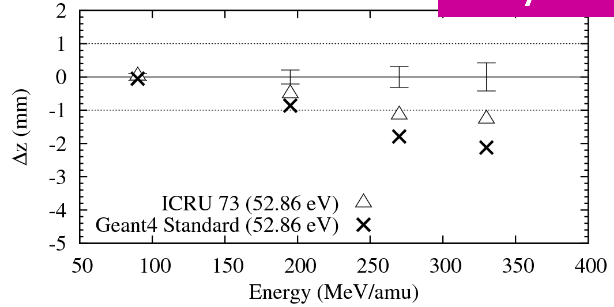
- Validation of ^{12}C Bragg peak simulation in water and polyethylene (90-400 MeV/amu) for G4ionIonisation process
- Experimental Bragg peak position can be reproduced
  - within 0.2% of ion range in case of water
  - within 0.9% in case of polyethylene

Water





Polyethylene



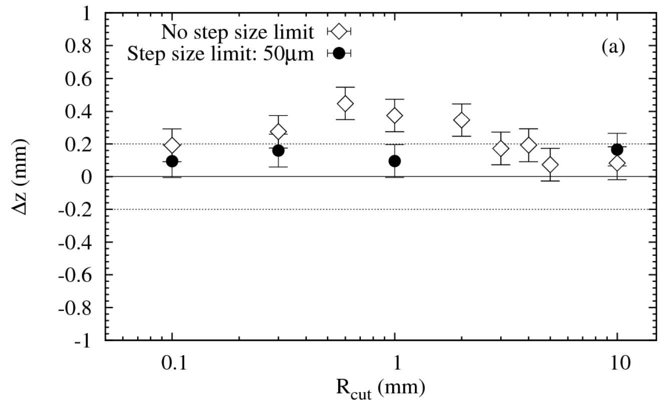
Experimental data courtesy of D. Schardt and U. Weber

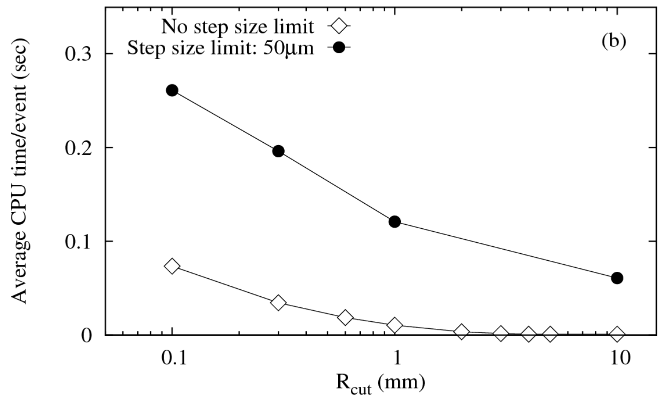
Range stability in Geant4 9.3

- Stability of ^{12}C Bragg peak position with respect to simulation parameters was investigated: production cut, step size limiter.
- Ionization step function: same parameters used as in LowE builders (dRoverRange=0.1, finalRange=100 µm)

  - **Figure (a)** shows the difference between simulated and measured Bragg peak position of a 400 MeV/u ^{12}C beam in water as a function of the δ-production cut.
  - **Figure (b)** presents the average CPU time per event of corresponding simulation runs.

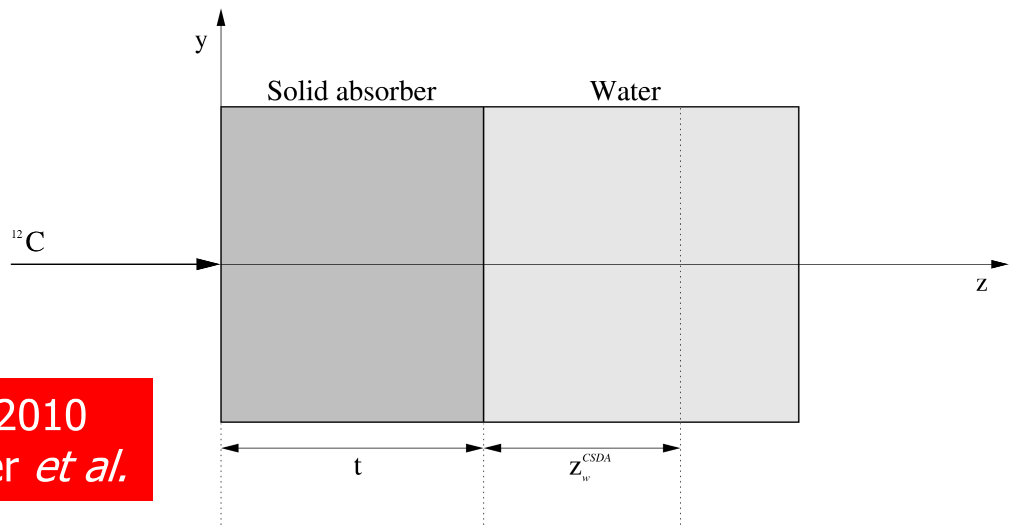
  - Geant4 results were obtained using the low-energy ICRU 73-based parametrization model. For simplicity, no hadronic processes were activated.
  - Simulations without user-defined step size limitation (diamonds) are compared against calculations with a maximum step size of 50 µm (circles).
  - Experimental data by courtesy of D. Schardt/GSI (personal communication).
  - The dashed lines indicate the experimental uncertainty. Error bars account for the uncertainty of simulated peak positions.





Validation of ^{12}C CSDA ranges in elemental media and compounds

- Range validation
  - Comparison of Geant4 (9.3) ranges, computed with ICRU 73-based model, against experimental data from the literature
    - Bichsel et al., Radiat. Res. 153 (2000), 208
  - Bichsel et al. report residual CSDA range of ≈275 MeV/u ^{12}C ions in water after traversing a solid absorber of thickness t
  - Beam energy in simulation was calibrated (275.5 MeV/u) aiming to reproduce the experimental range in water for the case t=0



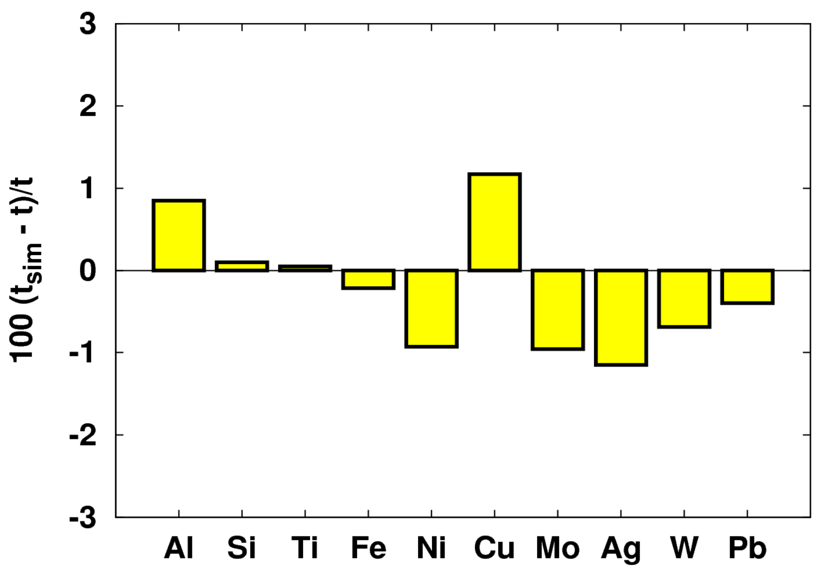
Presented at COSPAR2010
Courtesy of A. Lechner *et al.*

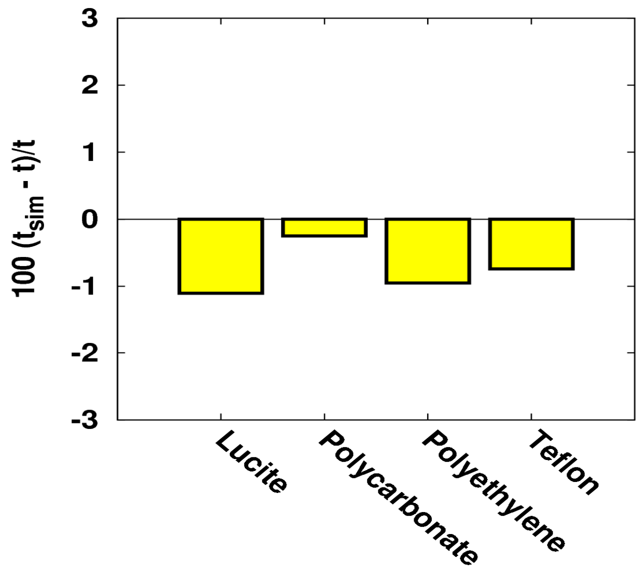
Validation of ^{12}C CSDA ranges in elemental media and compounds

- Calculation of absorber thickness (tsim) required in the simulation to achieve the same residual CSDA range in water as in the experiment.

- Figures: percentage difference of tsim and t
  - in elemental (left) targets
  - in compound (right) targets

Presented at COSPAR2010
Courtesy of A. Lechner *et al.*

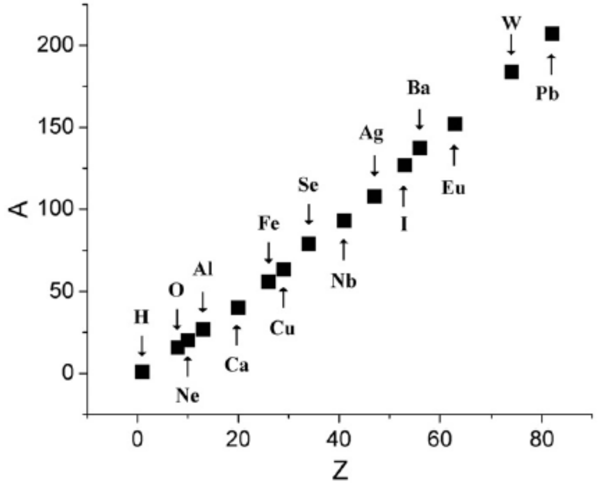


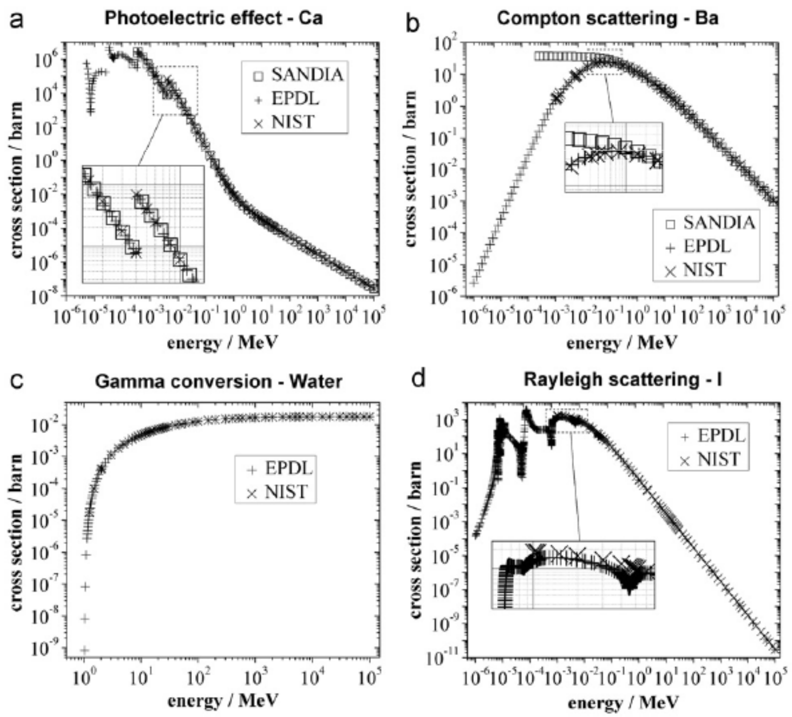


Validation of EM photon models

Geant4 EM photon models validation

- Systematic validation of cross-sections for electromagnetic photon models
  - for the 3 EM packages : standard, low-energy : Livermore & Penelope
  - Photoelectirc, Compton, gamma conversion, Rayleigh scattering
- Against the SANDIA, EPDL97 and NIST data libraries
- For several elements and compounds
  - 15 elements Z=1 to 82
  - 3 compounds: air, water, NaI
- 250 eV – 10^5 MeV





See full details in:
Validation of the Geant4 electromagnetic photon cross-sections for elements and compounds
G.A.P. Cirrone et al., NIMA 618 (2010) 315–322

Geant4 EM photon models validation

- All the Geant4 photon models are in statistical agreement with the NIST data sets, with the exception of Rayleigh scattering
  - Disagreement for G4LivermoreRayleighModel is due to the fact that the NIST and the EPDL97 libraries are mutually inconsistent at low energy
- The Livermore cross section models use interpolated EPDL97 cross section data
  - the deviation between EPDL97 data and the Livermore cross sections is below 0.2% for all models and materials, in consistence with the accuracy of the interpolation algorithms

PIXE

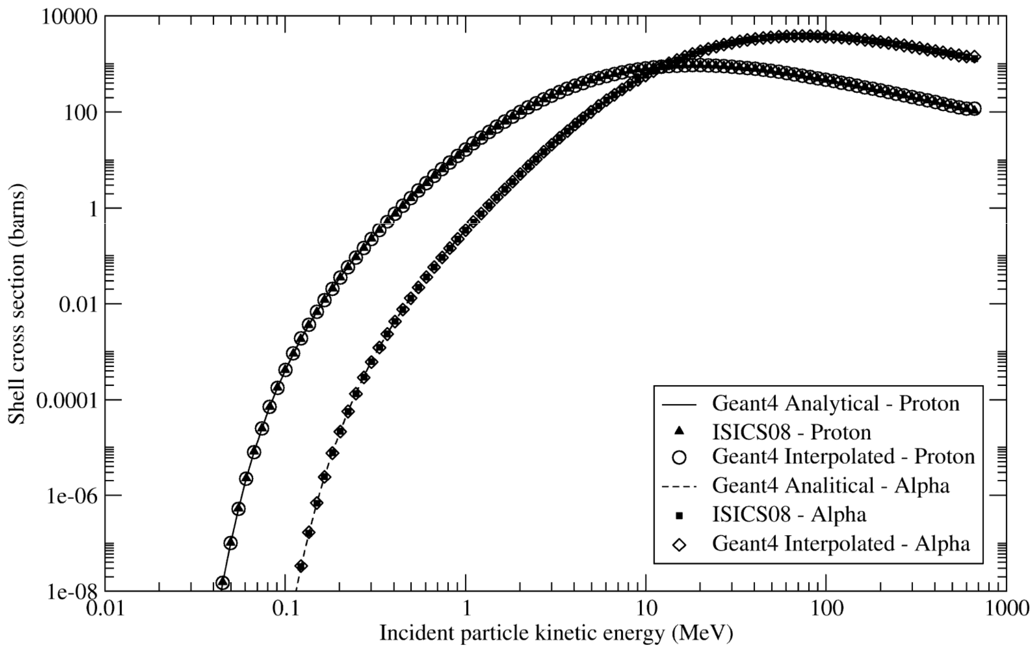
Particle Induced X-ray Emission (PIXE)

- Part of the Geant4 EM « low energy » sub-library
- Was not accurately simulated for many years
- First prototype software for low energy region was delivered into Geant4 9.2
  - see "New Geant4 cross section models for PIXE simulation", H. Ben Abdelouahed et al. Nucl. Instrum. and Meth. B 267 (2009) 37-44
  - for protons and alphas
- New updated ionisation cross section models have been released with Geant4 9.4 BETA
  - now in compliance with the common software EM design, models are integrated into processes
  - extended to higher energies, based on the ECPSSR theory
  - K, L shells
  - Full release in Geant4 9.4

Courtesy of A. Mantero, H. Abdelouahed, V. Ivantchenko, S. Incerti

What is available in Geant4 9.4 BETA

- Ionisation cross section models
  - Empirical models :
    - Protons : Paul & Sacher (K), Orlic (L)
    - Alphas : Paul & Bolic (K)
  - Theoretical analytical models based on the ECPSSR theory



Ionization cross sections for Copper K shell (p, α)

Geant4-DNA

How can Geant4-DNA model radiation biology ?

See ESA AO6041 talk

Physics stage
step-by-step modelling of **physical interactions** of incoming & secondary ionising radiation with biological medium (liquid water)

- Excited **water molecules**
- Ionised **water molecules**
- Solvated **electrons**

Physico-chemistry/chemistry stage
- **Radical** species production
- Diffusion
- Mutual interactions

Geometry stage
DNA strands, chromatine fibers, chromosomes, whole cell nucleus, individual cells…
for the prediction of damages resulting from direct and indirect hits

Biology stage
DIRECT DNA damages

Biology stage
INDIRECT DNA damages (~70%)

t=0 | t=10^{-15}s | t=10^{-6}s

Physics stage : Physics models available in Geant4-DNA release 9.4 BETA (June 2010)

- Applicable to liquid water, the main component of biological matter

- Can reach the very low energy domain (sub-eV limit)
  - 8.23 eV lower energy limit for excitation
  - Compatible with molecular description of interactions

- Purely discrete
  - Simulate all elementary interactions on an event-by-event basis
  - No condensed history approximation

- Models can be purely analytical and/or use interpolated data tables
  - eg. cross sections
  - Computing speed increase in e- elastic scattering by C. Champion model (gain 4)

- Since December 2009, they use the same software design as all electromagnetic models available in Geant4 (standard EM and low energy EM)

- Extensive validation of Physics models : comparison to experimental data & international recommendations on stopping powers in progress

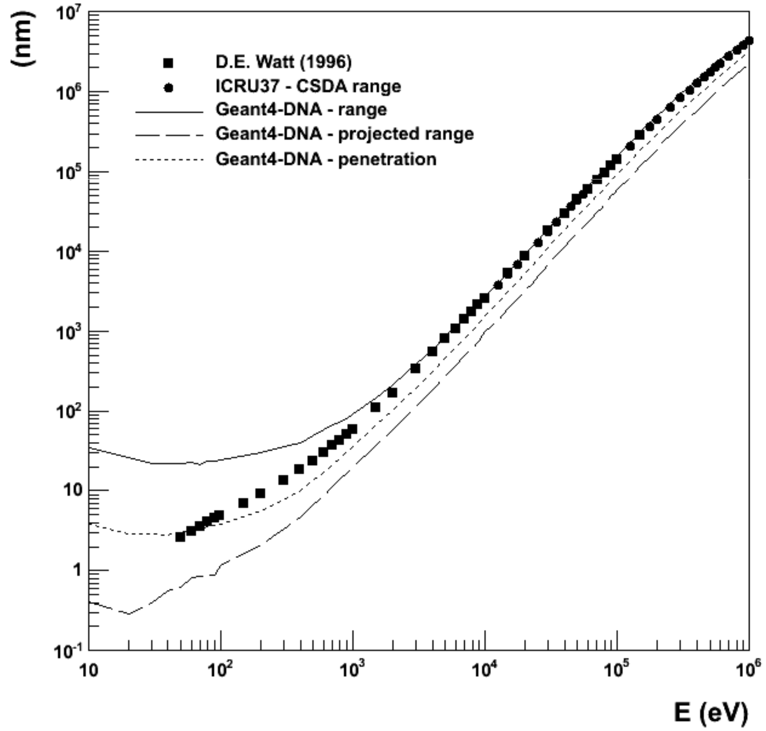
Physics stage :
status of Physics models in 9.4 BETA

	e	p	H	α, He+, He
Elastic scattering	> 8.23 eV Screened Rutherford > 8.23 eV Champion	-	-	-
Excitation A_1B_1, B_1A_1, Ryd A+B, Ryd C+D, diffuse bands	8.23 eV – 10 MeV Emfietzoglou	10 eV – 500 keV Miller Green 500 keV – 100 MeV Born	-	Effective charge scaling from same models as for proton 1 keV – 10 MeV
Charge Change	-	100 eV – 10 MeV Dingfelder	100 eV – 10 MeV Dingfelder	
Ionisation $1b_1$, $3a_1$, $1b_2$, $2a_1$ + $1a_1$	11 eV – 1 MeV Born	100 eV – 500 keV Rudd 500 keV – 100 MeV Born	100 eV – 100 MeV Rudd	

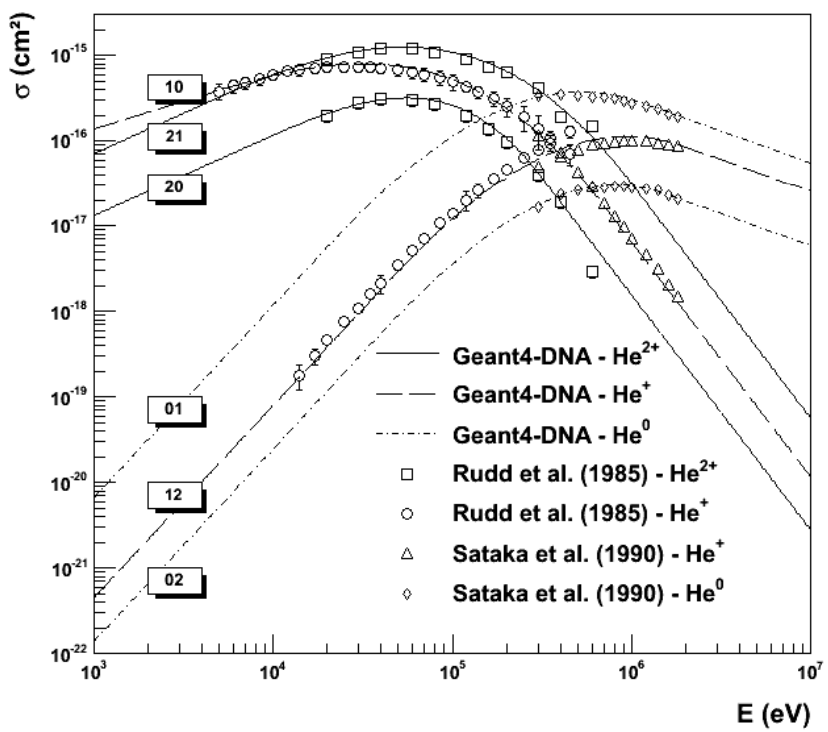
More will be released in 9.4

Example of validation

Electron range



Helium charge exchange XS



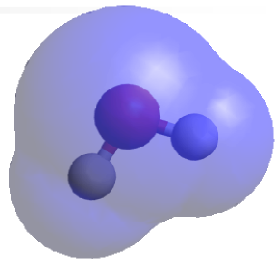
G4TRAP: Geant4-DNA Physics TRacking vAlidation Project

Paul Gueye
Hampton University, Physics Department, Hampton VA USA
gueye@jlab.org

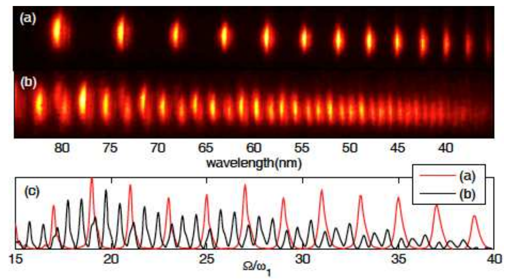
On Behalf of the G4TRAP Collaboration

G4TRAP: Geant4-DNA Physics TRacking vAlidation Project

G4TRAP Goals - 1



(1) **Probing electrons in molecular bonds** to identify the (dominant) physical processes associated with a given incident particle type and energy. Such information can be obtained by measurements of x-rays emitted during high harmonic generation initiated by an ultrafast, low power laser beam with polarization capability (to gain information on the quantum numbers);

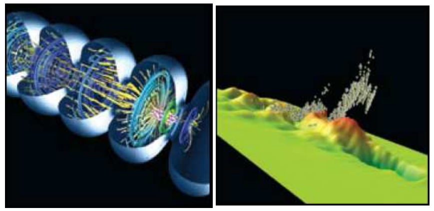


(2) **Image particles tracks within cells** using a dedicated ultrafast laser (having femtosecond and attosecond time resolution) with a large tunable wavelength so as to optimize the matching of the wave functions between the probe laser, the incident particle and cell molecules of interest. The capability to monitor the trajectories of particulate radiation while they traverse biological targets will provide key information regarding their average angular distribution and energy loss in order to identify dominant physical processes involved during particle-matter interaction;

G4TRAP: Geant4-DNA Physics TRacking vAlidation Project

G4TRAP Goals - 2

(1) **Couple Geant4 with Particle In Cell (PIC) simulation tool** to develop a dedicate simulation tool for the G4TRAP experiments. PIC simulations are the basis for modeling fluid dynamics processes, at the core of ultrafast laser technology and for wakefield acceleration scheme (to be used in this research). Geant4 is needed for both the G4DNA component and basic scattering physics associated experiments;



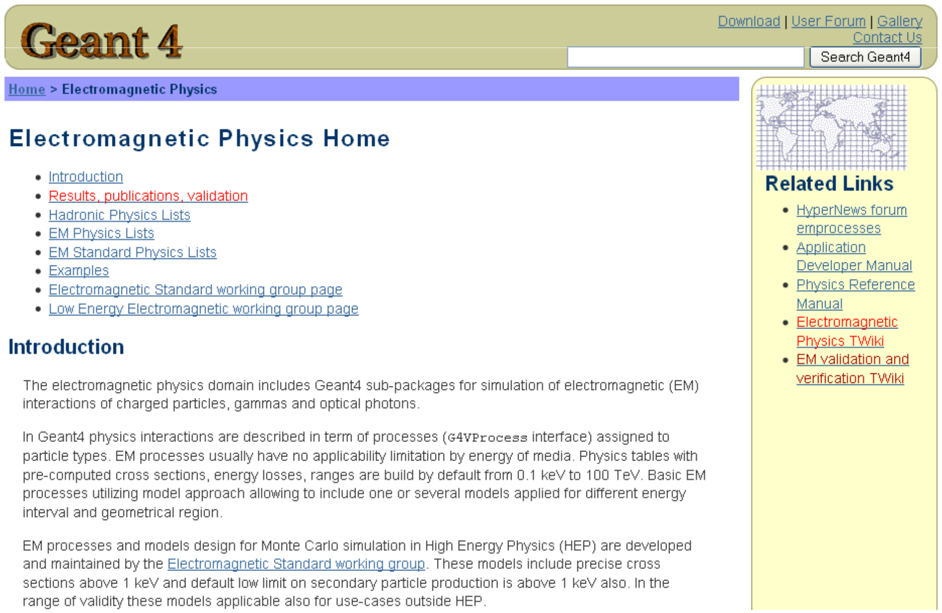
(2) **Use of space and earth based radiation biology experiments** from low and high energy experimental data using electromagnetic and hadronic probes beyond the G4DNA currently available database to assess the accuracy of this tool;

(3) **New educational component** will be implemented at various institutions (Hampton University, UCAD …) with new MS and PhD tracks, along with establishing joint thesis programs between several US, European and African institutions that will extend to other fields such as materials sciences.

Documentation

Documentation

- Geant4 Home Page → Who we are
- http://www.geant4.org/geant4/collaboration/EMindex.shtml
- From there, you can access our Twiki pages too



Geant 4

Download | User Forum | Gallery
Contact Us
Search Geant4

Home > Electromagnetic Physics

Electromagnetic Physics Home

- Introduction
- Results, publications, validation
- Hadronic Physics Lists
- EM Physics Lists
- EM Standard Physics Lists
- Examples
- Electromagnetic Standard working group page
- Low Energy Electromagnetic working group page

Introduction

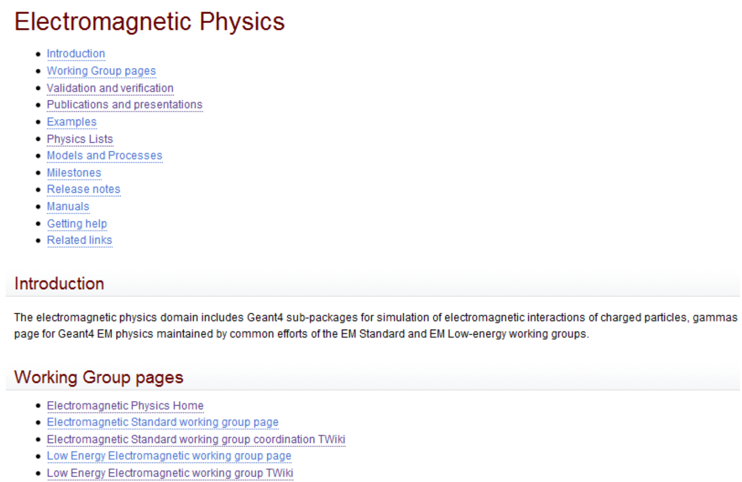
The electromagnetic physics domain includes Geant4 sub-packages for simulation of electromagnetic (EM) interactions of charged particles, gammas and optical photons.

In Geant4 physics interactions are described in term of processes (G4VProcess interface) assigned to particle types. EM processes usually have no applicability limitation by energy of media. Physics tables with pre-computed cross sections, energy losses, ranges are build by default from 0.1 keV to 100 TeV. Basic EM processes utilizing model approach allowing to include one or several models applied for different energy interval and geometrical region.

EM processes and models design for Monte Carlo simulation in High Energy Physics (HEP) are developed and maintained by the Electromagnetic Standard working group. These models include precise cross sections above 1 keV and default low limit on secondary particle production is above 1 keV also. In the range of validity these models applicable also for use-cases outside HEP.

Related Links

- HyperNews forum emprocesses
- Application Developer Manual
- Physics Reference Manual
- Electromagnetic Physics TWiki
- EM validation and verification TWiki



Electromagnetic Physics

- Introduction
- Working Group pages
- Validation and verification
- Publications and presentations
- Examples
- Physics Lists
- Models and Processes
- Milestones
- Release notes
- Manuals
- Getting help
- Related links

Introduction

The electromagnetic physics domain includes Geant4 sub-packages for simulation of electromagnetic interactions of charged particles, gammas page for Geant4 EM physics maintained by common efforts of the EM Standard and EM Low-energy working groups.

Working Group pages

- Electromagnetic Physics Home
- Electromagnetic Standard working group page
- Electromagnetic Standard working group coordination TWiki
- Low Energy Electromagnetic working group page
- Low Energy Electromagnetic working group TWiki

In summary

- Unification of Geant4 EM « standard » and « low energy » Physics was achieved with Geant4 9.3 in December 2009
- Combined Physics constructors with standard and low-energy models are available in Physics List library of Geant4
- Many bugs and software flaws affecting the « low energy » sub-library and which were left un-fixed for years have been fixed. More are still probably there.
- Electron, proton and ^{4}He ranges are in good agreement with NIST data
- New model for ion ionisation based on ICRU73 report is available
  - Accuracy of 1% is achieved for range of Carbon ions
- All photon EM models are in agreement with NIST
- PIXE models have extended to higher energies for Geant4 9.4 BETA
- Geant4-DNA microdosimetry models have been validated against data in water

Work presented on behalf of all Geant4 electromagnetic Physics developers

Standard EM Physics WG collaborators

A. Bagulya, A. Bogdanov, H. Burkhardt, S. Elles, V. Grichine, P. Gumplinger, V. Ivanchenko, J. Jacquemier, O. Kadri, R. Kokoulin, M. Maire, A. Schaelicke, T. Toshito, L. Urban, T. Yamashita

Low-energy EM Physics WG collaborators

H. Abdelaouhed, R. Black, S. Chauvie, G.A.P. Cirrone, G. Cuttone, G. Depaola, F. Di Rosa, Z. Francis, P. Guèye, S. Incerti, A. Ivanchenko, V. Ivanchenko, N. Karakatsanis, M. Karamitros, A. Lechner, F. Longo, A. Mantero, B. Mascialino, J. Moscicki, L. Pandola, I. Petrovic, A. Ristic-Fira, G. Russo, G. Santin, H. Tran, C. Zacharatou

One last slide: reminder

- If you encounter difficulties/problems with your Geant4 simulations:
  - Please migrate to the most recent Geant4 release
    - eg. G4 9.2 is almost 2 years old and many bugs have been affecting the « low energy » EM category for years
  - Go to the Geant4 User Forum
    - Someone else may have the same difficulties and solutions can be proposed
  - Contact the WG coordinators from the Geant4 contact web page
    - We will be happy to provide guidance and to put you in contact with Geant4 developers if needed

Most useful & appropriate way to interact with the Geant4 collaboration

- Please keep in mind that Geant4 is a ~large collaboration where current and future developments are exclusively driven by a steering board (25 members, including all WG coordinators)

Thank you for your attention