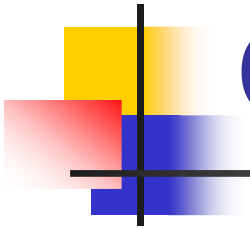
Geant4 Low Energy Electromagnetic Physics

Performance and Validation

Ziad Francis, IRSN, France

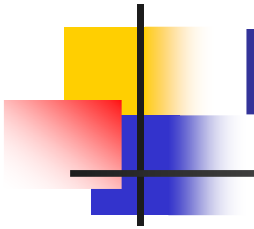
on behalf of the
EM working groups of the Geant4 collaboration

Geant4 14th collaboration workshop
Catania, Italy, October 15-22 2009



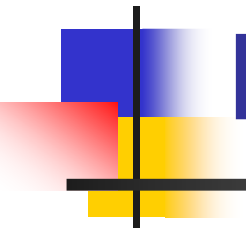
Content

- History
- Activity overview in 2009
  - Physics processes & models
  - Debugging
  - Computing performance
  - Testing
  - Validation
  - Documentation
- Workplan overview



History

- The Low energy EM working group has been entirely reoganized in May 2008
  - One coordinator
    - S. Incerti, CNRS/IN2P3, France
  - Two steering board representatives
    - G. Cuttone, INFN Catania, Italy
    - P. Guèye, Hampton Univ., USA (recently elected)
- 20 Geant4 collaborators are members of this working group
  - Open to new collaborators
- All developments take place in full coordination with the Standard EM working group
- 5 mini Working Groups
  - each being coordinated by a dedicated coordinator
  - report slides are presented in the following slides covering a one year duration since October 2008



Physics processes & models

From Geant4 9.3 BETA

Courtesy of L. Pandola

Integration of electromagnetic Physics models

- Convergence of software design between standard EM and low energy EM categories
- All low energy electromagnetic processes and models have been migrated to standard electromagnetic software design
  - including Livermore unpolarized and polarized, Penelope and Geant4-DNA physics lists
- In this design
  - a physical interaction or process is described by a process class (inherits from `G4VEmProcess` 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 take care to calculate:
    - total cross section and stopping power
    - final state (kinematics, production of secondaries…)
  - models can be alternative and/or complementary on certain energy ranges

Courtesy of L. Pandola

Migrated models

- Penelope ✓
  - Compton, Gamma Conversion, Rayleigh, Photoelectric (γ-rays)
  - Ionisation, Bremsstrahlung ($e^{\pm}$), Annihilation
- Livermore ✓
  - Compton, Gamma Conversion, Rayleigh, Photoelectric (γ-rays)
  - Ionisation, Bremsstrahlung (e^{-} only)
- Livermore Polarized ✓
  - Compton, Rayleigh (γ-rays)
- Ions
  - Ion parametrized loss ✓
  - G4hLowEnergyIonisation **not** migrated, buggy and *de facto* obsolete
- Geant4-DNA ✓
  - Ionisation, Excitation, Elastic, Charge Exchange

Courtesy of L. Pandola

Advantages of the common software design

- Easily retrieve Physics quantities
  - with the G4EmCalculator object
  - directly with the model's methods
    Eg. G4double xs1 = brem->CrossSectionPerVolume(material,electron,energy,tCut);
- Use Physics list builders in order to build a physics list
  - $G4INSTALL/source/physics_lists/builders
  - G4EmPenelopePhysics, G4EmLivermorePhysics, G4EmLivermorePolarizedPhysics, G4EmDNAPhysics
- These builders also explain to users how to combine low energy EM models with standard EM models
  - standard models below 1 GeV are replaced by low energy models – can be changed by the user
- Several bugs have been fixed automatically (see Debugging slides)
- Old non migrated models have been kept for compatibility but are not maintained anymore

From Geant4 9.3 BETA

Courtesy of A. Lechner

Ion parametrized model

- Describes the energy loss of ions heavier than Helium due to interaction with the atom shells of target atoms
- Developed in close collaboration with Standard EM group (V. Ivanchenko)
- First production version of model was included in Geant4 9.3.b01 (further iterations possible following the current validation)
- Model name: `G4IonParametrisedLossModel`
- Is designed to be used with the `G4ionIonisation` process (of the standard EM package):
  - The model is not activated by default when using `G4ionIonisation`
  - Users can employ model by utilizing `SetEmModel` method of `G4ionIonisation` process
  - Model is restricted to one Geant4 particle type: `G4GenericIon`

From Geant4 9.3 BETA

Courtesy of A. Lechner

Ion parametrized model

- Restricted stopping powers are calculated according to (T = kinetic energy per nucleon):
  - $T < T_L$: Free electron gas model
  - $T_L \leq T \leq T_H$: Interpolation of tables or parameterization approach
  - $T > T_H$: Bethe formula (using an effect. charge) + high corr.

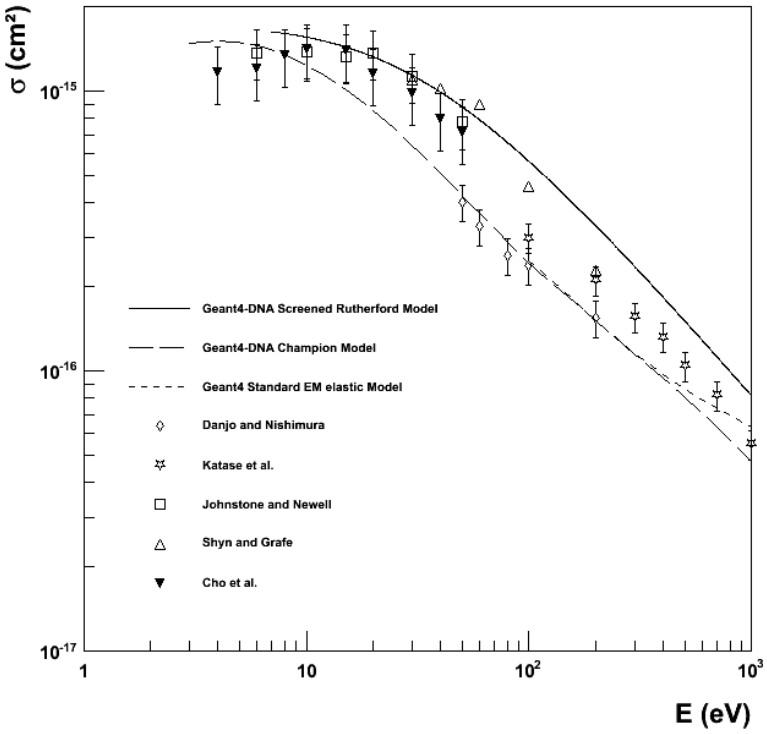
- Parameterization approach: model incorporates ICRU 73 stopping powers into Geant4
  - The ICRU 73 report covers a large range of ion-material pairs (Li to Ar ions, and Fe ions), stopping powers are based on binary theory
  - Special case **water**: **Revised ICRU 73** tables of P. Sigmund are used (since Geant4 9.3.b01), which imply a *I*-value of water of 78 eV
  - Current model parameters (Geant4 9.3 beta) for ICRU 73:
    - T_H = 10 MeV/nucleon (except Fe ions: T_H = 1 GeV/nucleon)
    - For ions heavier than Ar: Scaling of Fe ions based on effective charge approach

From Geant4 9.3

Courtesy of C. Champion, Z. Francis, S. Incerti

Geant4-DNA models

- Improvement of Physics models in liquid water
  - Electron ionisation models extended up to 1 MeV (i/o 30 keV)
  - Proton excitation and ionisation models up to 100 MeV
  - Electron elastic model by C. Champion extended up to 10 MeV
    - total cross section is close to alternative Screened Rutherford model and standard EM



From Geant4 9.3

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

Particle Induced X-ray Emission (PIXE)

- Problem fixing which were in the code for a long time
- New ionisation cross section models have been developed
  - K & L shells
  - for protons and alphas
  - based on ECPSSR theory
- Integration of models into processes
- Available from December 2009 release

Thanks to the constructively critical talk given by M.G. Pia at CHEP'09

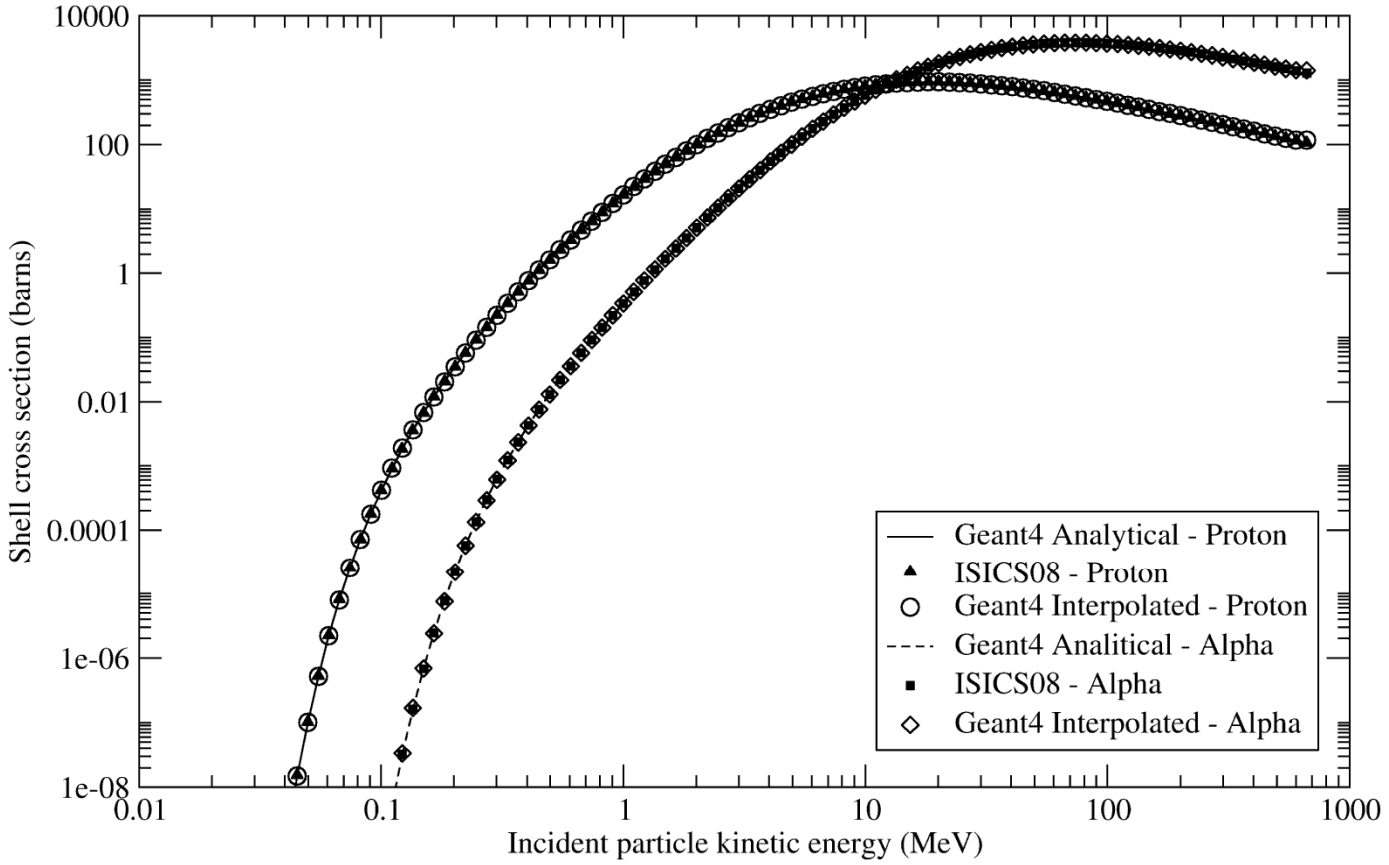
From Geant4 9.3

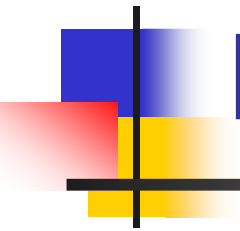
Courtesy of A. Mantero, H. Abdelouahed, V. Ivantchenko, S. Incerti

PIXE : what will be available in Geant4 9.3

- Ionisation cross section models
  - Empirical models :
    - Protons : Paul & Sacher (K), Orlic (L)
    - Alphas : Paul & Bolic (K)
  - Theoretical models based on ECPSSR theory
    - analytical
      - direct implementation of theory for K & L shells
    - interpolated tables created using the ISICS software
      - special version obtained from S. Cippola
- This is the first time that we can use PIXE with confidence in Geant4

Eg. ionization cross sections for Copper K shell (p, α)





Debugging

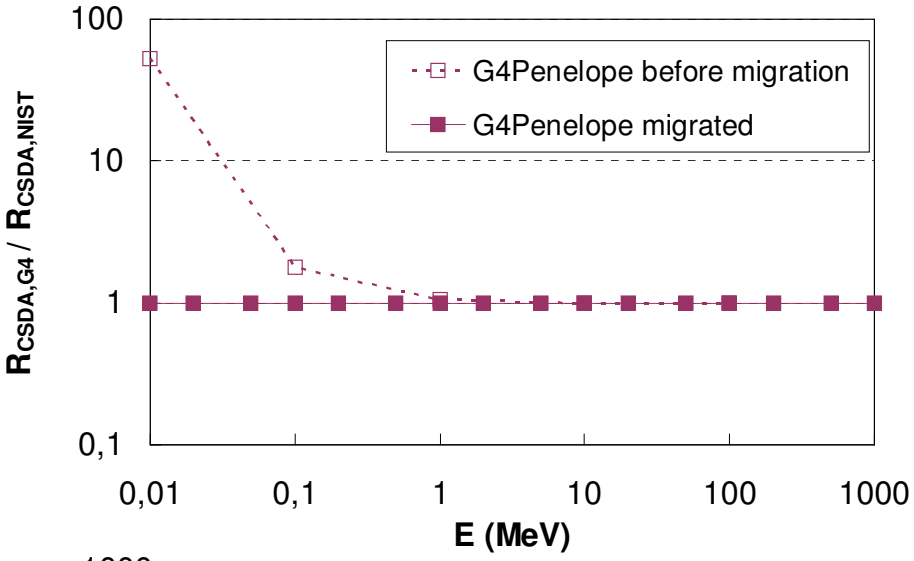
Debugging

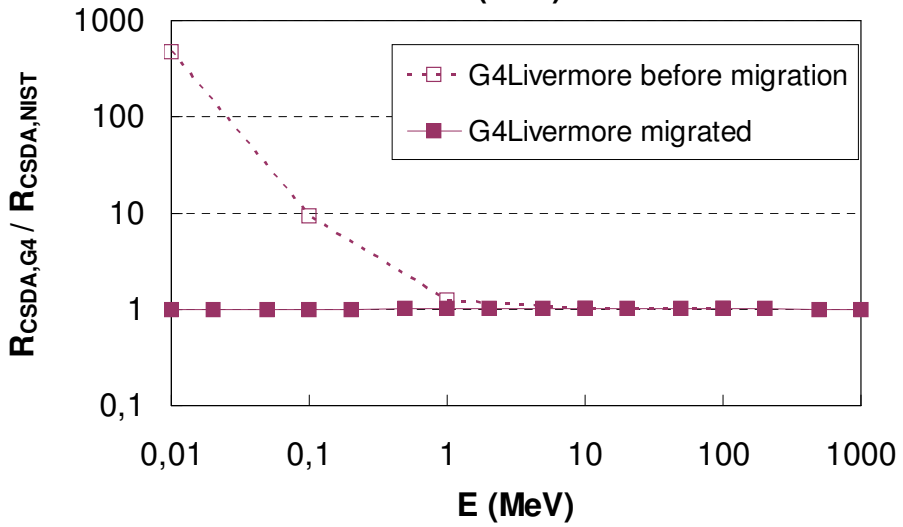
- Significative activity in solving long time accumulated bugs
- Several bugs have been fixed thanks to the new common software design of electromagnetic categories
  - Wrong electron ionization range below 1 MeV (see next slide)
  - Fixed angle sampling in Livermore Rayleigh scattering
  - Infinite loops in Livermore Rayleigh
  - Debuging of migrated Livermore, Penelope and Geant4-DNA models
  - Handling of materials with zero fraction elements (Bugzilla #1005)
  - Fixed corrupted files in G4LEDATA (from version 6.4) (Bugzilla #1042)
- On-going activity…

Low-energy models migration (Geant4 9.2 ref 4)

C. Zacharatou, V. Ivanchenko, M. Maire

Electron CSDA range G4/NIST:

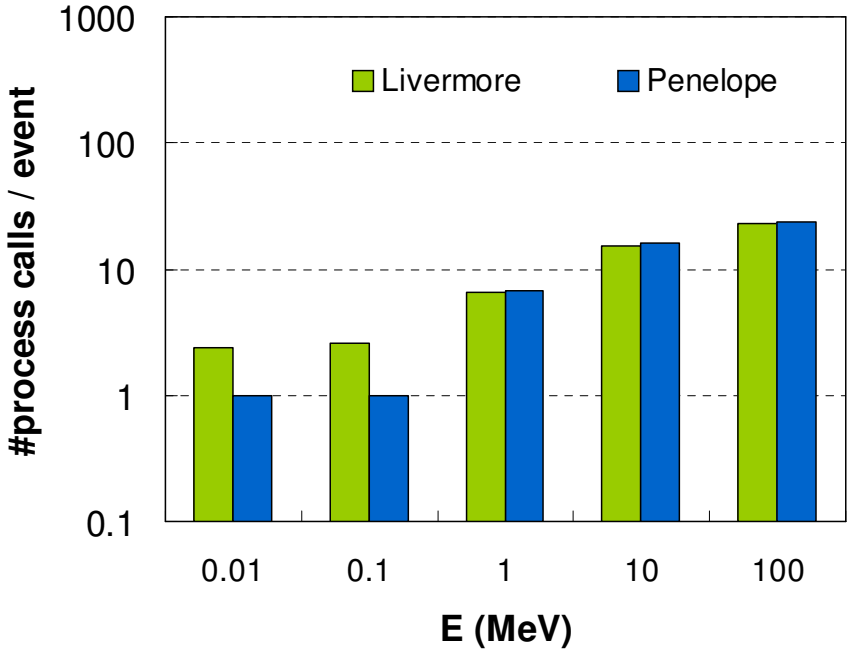


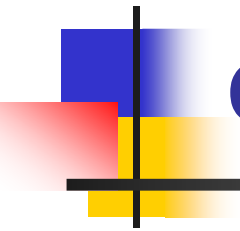


Non-migrated and migrated Penelope and Livermore ionisation in water

Geant4 9.2 ref 04

Number of process calls per event before the migration:





Improving low energy software computing performance

Courtesy of Nicolas A. Karakatsanis

Computing : efficiency optimization in low-EM Geant4 Log-Log interpolation class

- Geant4 low-energy electromagnetic physics processes
  - high performance cost compared with standard EM processes
- Profiling results on a GATE performance benchmark
  - G4LogLogInterpolation::Calculate method
    - at each iteration step, five log10 and one pow10 calculations are required
    - 61% of the total running time spent on this method
- Previous data handlers of Geant4 lowE EM processes
  - use LoadData methods to load tabulated G4LEDATA datasets to G4EMDataSets during initialization phase
  - perform log-log type of interpolation on G4EMDataSets to estimate the cross section values during simulation
- Revision #1 (validated and included in Geant4.9.2)
  - streamline G4LogLogInterpolation::Calculate math formula
    - Aim: reduce the number of required log10 calls required per iteration step down to four (from five)
  - Non-negligible speed up observed in profiling results
    - measured speed-up factor : 1.1 (10% faster)

Courtesy of Nicolas A. Karakatsanis

Computing next : efficiency optimization in low-EM Geant4 data handler classes

- Revision #3 (validated emlowen-V09-02-54 reference tag)
  - New LoadData methods
    - Logarithmic values of the original G4LEDATA data values are calculated once during initialization phase (negligible performance cost)
    - Both original and logarithmic values are loaded to G4EMDataSets during initialization phase
  - New G4LogLogInterpolation::Calculate methods
    - apply **linear-linear** type of interpolation (**fast**) over the already loaded pre-calculated logarithmic data during simulation
  - Old methods for data loading and interpolation are still implemented
    - Old LoadData method is renamed into LoadNonLogData
    - Old Calculate methods kept with the old list of (non-log) arguments
- New profiling results after revision #3
  - Total running time reduced by 33.5% (a speed-up factor of 1.5)
  - G4LogLogInterpolation::Calculate method
    - spends now 56% less amount of time
    - only one log10 and pow10 is required per iteration step

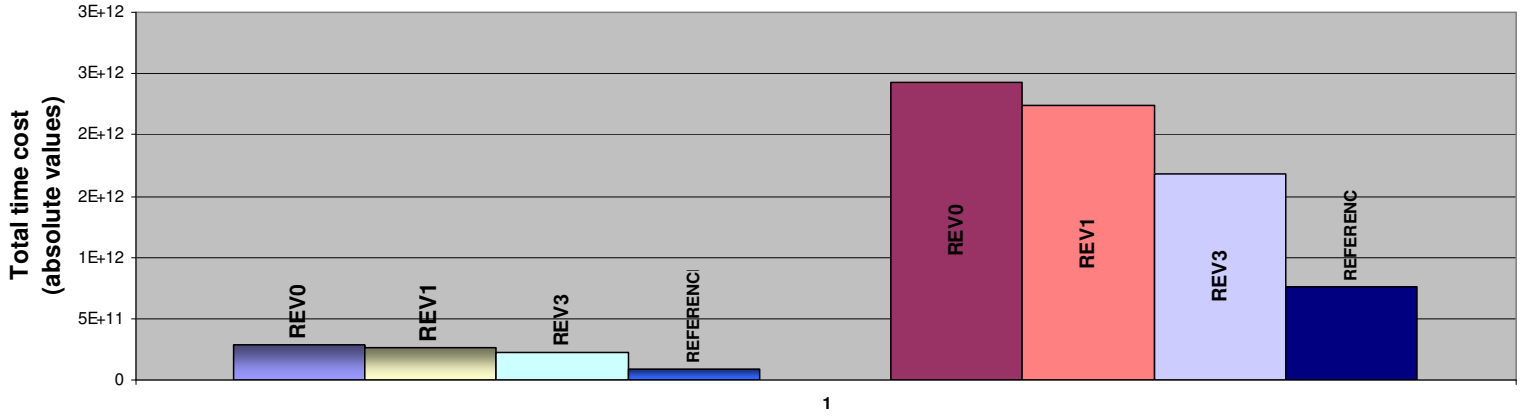
From Geant4 9.3

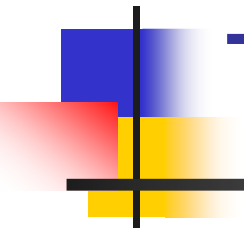
Courtesy of Nicolas A. Karakatsanis

Profiling results in GATE for each revision phase

- Total time performance cost of low-EM processes in GATE for each revision
  - rev0 → previous implementation
  - rev1 → streamlining of logarithmic interpolation (**geant4 9.2**)
  - rev3 → new data handling and interpolation methods (**geant4 9.3**)
  - reference case → performance cost when standard EM classes are employed
  - two cases of phantom geometries examined:
    - NEMA cylindrical phantom (left bars) and NCAT voxelized phantom (right bars)

Total time performance cost of G4 low-energy EM processes (migrated Livermore models) in GATE (NEMA cylindrical phantom vs. NCAT voxelized phantom)





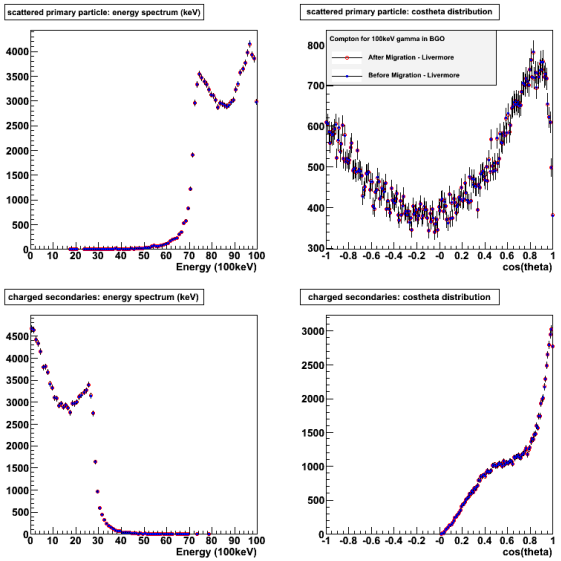
Testing of software

Testing of migrated design

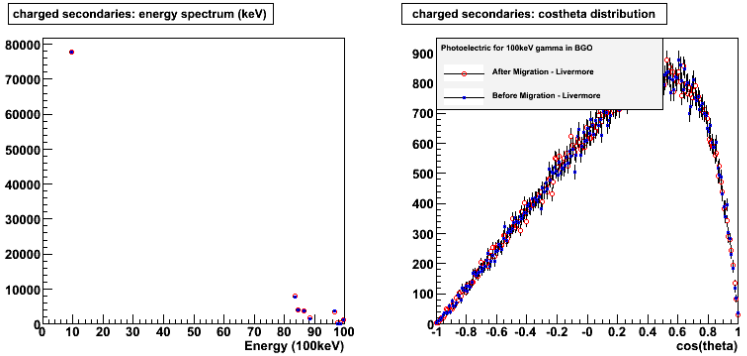
Z. El Bitar, P. Guèye, S. Incerti
Catania team

- Systematic testing of migrated Livermore, Penelope and Geant4-DNA models is performed on a regular monthly basis for electrons and gammas with energies from 100 eV to 1 TeV for several materials by independent teams (CENBG, INFN, IPHC, Hampton U.)
- Examples

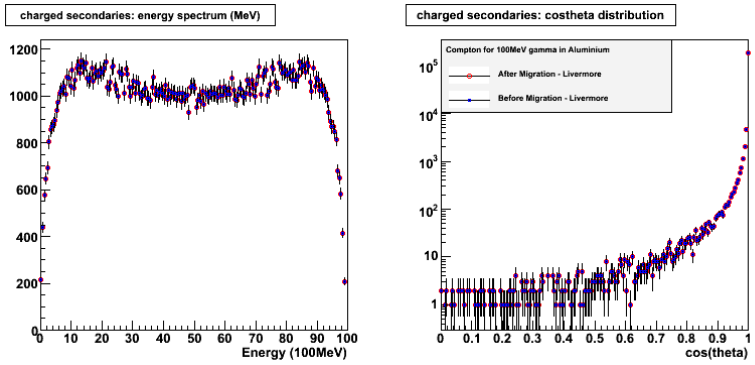
Compton 100 keV in BGO



PhotoElectric 100 keV in BGO



Conversion 100 MeV in Al

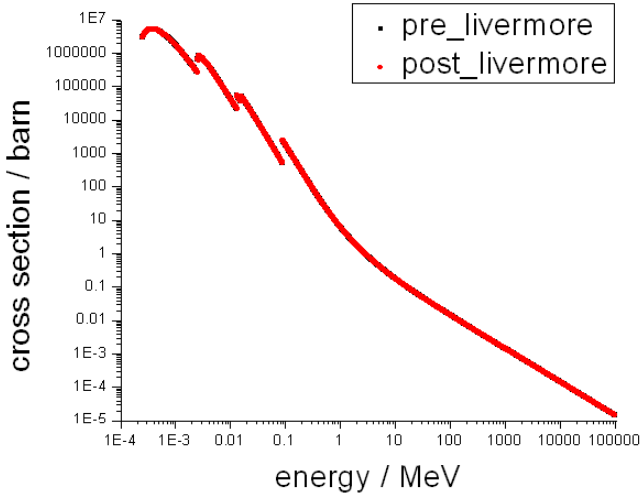


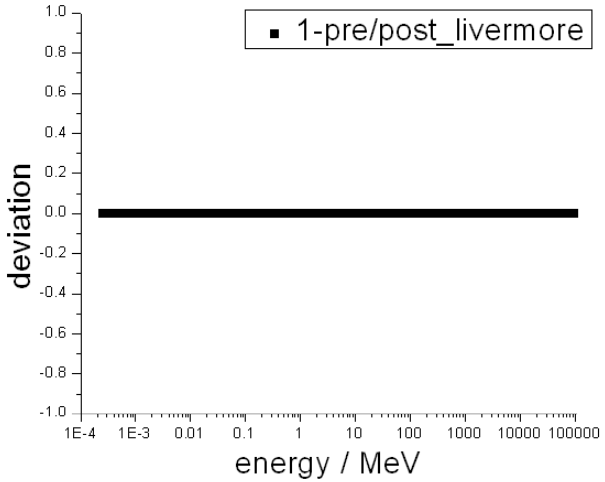
Testing of new interpolation

- Extensive testing performed by Catania team
- Comparison of pre-modified and post-modified cross setions using photon livermore and penelope models
- Elements: H O Ne Al Ca Fe Cu Se Nb Ag I Ba Eu W Pb
- Compounds: Air Water NaI

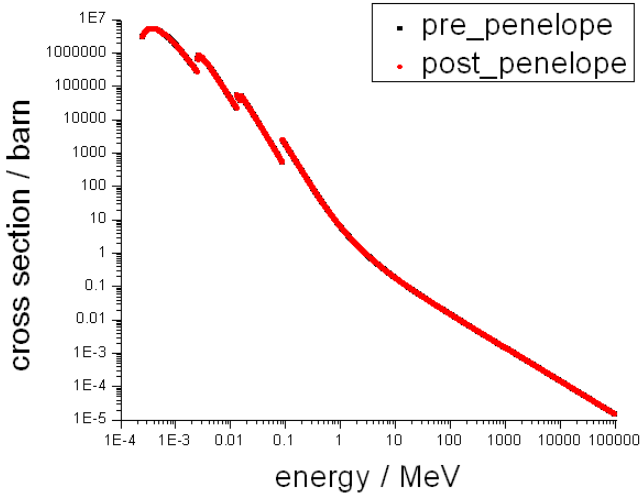
Eg: comparison of pre-modification and post-modification (Pb photoelectric)

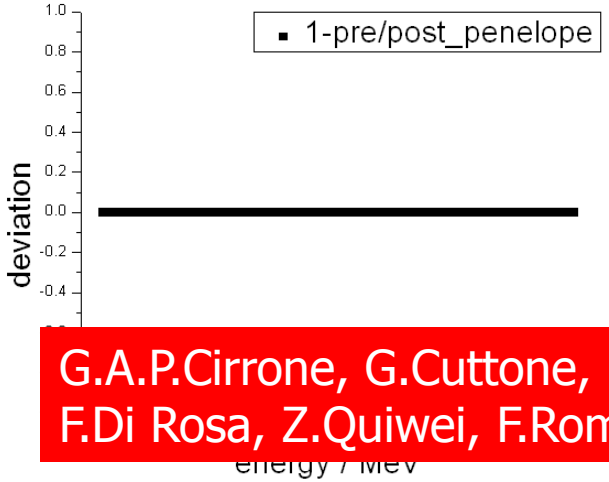
livermore



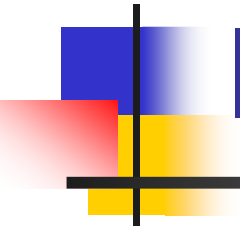


penelope





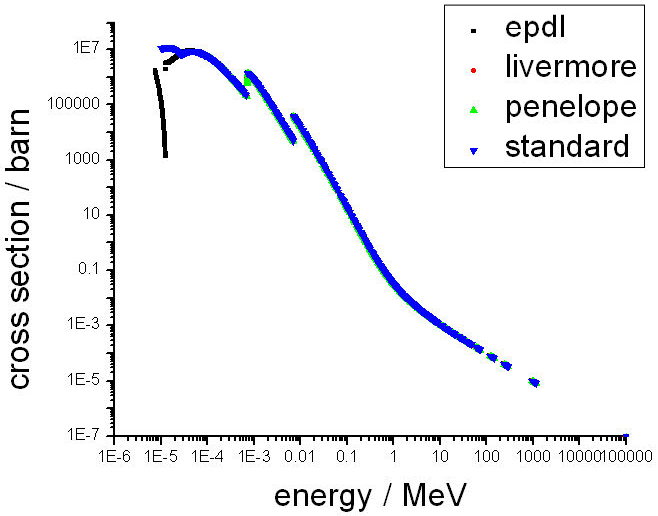
G.A.P.Cirrone, G.Cuttone, F.Di Rosa, Z.Quiwei, F.Romano



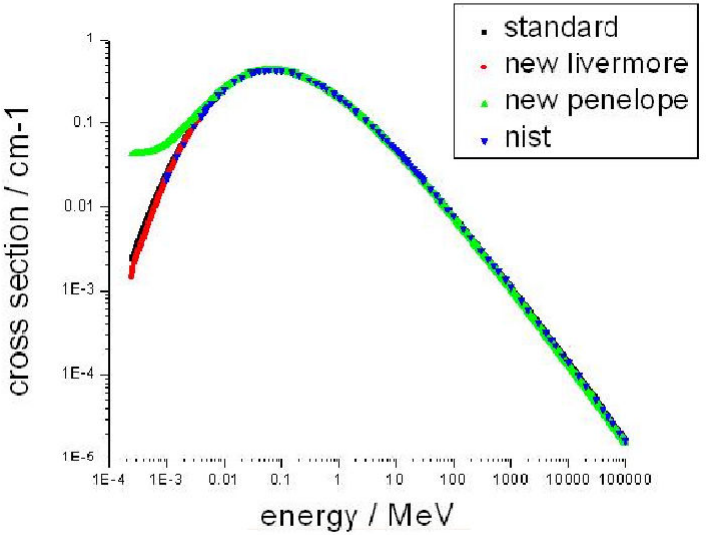
Validation of low energy models

Validation for migrated photon processes

- Verification for migrated Livermore & Penelope processes: migrated vs non migrated;
- Verification for migrated Livermore & Penelope processes: comparison with standard EM physics processes;
- Identification of data libraries for validation: SANDIA EPDL97 NIST;
- Validation of the Geant4 photon processes with respect to the libraries based on experimental data.



Comparison of XS per Atom between EPDL97 and Geant4 (Fe photoelectric)



Comparison of XS per Volume between NIST and Geant4 (Water compton)

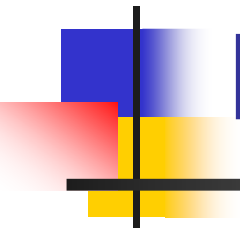
Elements: H O Ne Al Ca Fe Cu Se Nb Ag I Ba Eu W Pb
Compounds: Air Water NaI

More talks on validation

- Please refer to the following talks
  - Zhang QIWEI & Pablo CIRRONE talk
    - Validation of Geant4 EM physics for gamma rays against the SANDIA, EPDL97 and NIST databases
    - October 15
    - Parallel Session II - EM Physics: Validation and Applications
  - Christina Zacharatou *et al.* talk (collaboration restricted.)
    - Range validation for electrons, protons and alpha particles
    - October 21
    - Parallel Session XI - EM - new models and validation

Validation of Geant4-DNA Physics models

- large collection of experimental data for vapor water has been collected (Geant4-DNA models apply to liquid water)
- validation is performed systematically every month on reference tags with a dedicated suite
- agreement between Geant4-DNA models and experiental data is quantified using the statistical toolkit (B. Mascialino)
- Verification activity with PTB microdosimetry models is on-going showing overall good agreement : involved collaborators are M. U. Bug, E. Gargioni, S. Guatelli, S. Incerti, M. Reinhard, A. B. Rosenfeld and results have been presented at upcoming RADAM and NEUDOS 2009 conferences



Documentation

Courtesy of C. Zacharatou

Low Energy WG Web site

- Either from Geant4 web site
  - http://cern.ch/geant4
    - Who we are
      - Low energy Electromagnetic Physics
- or directly
  - http://geant4.web.cern.ch/geant4/collaboration/working_groups/LEelectromagnetic/
- There, links to :
  - Geant4 Low Energy Electromagnetic Physics working group Twiki pages
  - Geant4 Electromagnetic Physics TWiki pages
  - Geant4 Standard Electromagnetic Physics working group pages

Courtesy of C. Zacharatou

Low Energy WG CERN TWiki

https://twiki.cern.ch/twiki/bin/view/Geant4/LowEnergyElectromagneticPhysicsWorkingGroup

The Geant4 Low Energy Electromagnetic Physics Working Group

This web site is the official web site of the Geant4 collaboration Low Energy Electromagnetic Physics working group .

Purpose

The **Geant4 Low Energy Electromagnetic Physics Working Group** develops and maintains a set of models to describe the **electromagnetic interactions of photons, electrons, hadrons and ions with matter down to very low energies**, including the Geant4-DNA project (link). Applications of such models range from high energy physics experiments to space science and astrophysics to the medical and biological fields.

What's new ? NEW

- Overview of our most recent developments.
- This link shows the list of recent updates of this TWiki web site.

Physics UPDATED

- Processes is a link to the catalog of Geant4 Physics processes and to other useful information related to processes.
- Physics Lists describes Physics lists for specific applications involving low energy electromagnetic Physics processes.

Courtesy of C. Zacharatou

CERN Geant4 TWiki

https://twiki.cern.ch/twiki/bin/view/Geant4/WebHome

Welcome to the Geant4 web

Main topics

- Geant4PerformanceTips: Tips for creating faster simulations with Geant4
- Physics Lists: References to physics lists covering all energy domains

Working groups

- ElectromagneticPhysics: General resources for all electromagnetic physics models of Geant4
- Geant4MedicalPhysics: Resources for medical physics applications

Geant4 home pages

- Geant4 Home
- Electromagnetic Physics Home
- Low Energy Electromagnetic Working Group

Courtesy of C. Zacharatou

EM Physics CERN TWiki

https://twiki.cern.ch/twiki/bin/view/Geant4/ElectromagneticPhysics

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 and optical photons. This is central TWiki 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

Courtesy of C. Zacharatou

Medical physics CERN TWiki

https://twiki.cern.ch/twiki/bin/view/Geant4/Geant4MedicalPhysics

Resources for medical physics applications

The following links are to talks, publications and application web pages, including Geant4 Collaboration web pages, relating to medical physics. The links are, as much as possible, grouped by topic. The first section of links covers topics of common interest, such as physics, geometry, tracking and biasing. The next three sections refer to applications specific to radiology, radiotherapy and micro/nano-dosimetry. Lastly, we suggest some links to medical physics meetings and communities, including the Geant4 User Forum for medical applications.

These pages are maintained by the Geant4 Collaboration. Please contact us if you would like to present your talks and publications on these pages.

Physics, geometry and tracking

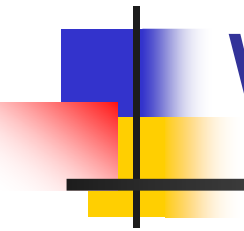
- Navigation and DICOM
- Physics
- Biasing
- CPU performance
- Reverse Monte Carlo
- Interfaces (phase spaces, anatomy/dose rendering)

Radiology

- CT
- Proton CT
- Geant4 Application for Emission Tomography (GATE) home page
- fGATE home page

Radiotherapy

- External electrons
- External photons
- Proton and heavy ion therapy



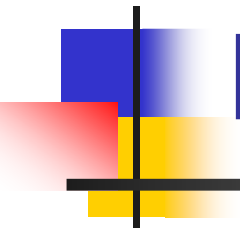
Workplan

Expected developments

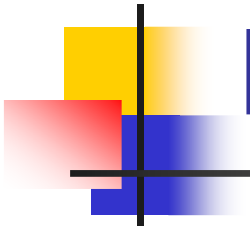
- deliver additional photon processes for space applications
  - polarized photoelectric
  - polarized gamma conversion
  - triple conversion (gamma ➠ e+e-e-)
- design iteration of atomic de-excitation package for integration in standard EM category
- Geant4-DNA
  - Deliver Physics builder for combination of Standard EM models and Geant4-DNA models (below energy threshold, in given G4Region's…)
  - Extensive workplan (ESA-AO6041 & ANR fundings till 2013)
- migration of anti-proton interaction model

Summary : Geant4 9.3

- Low energy Physics models (Livermore, Penelope, Geant4-DNA) have been migrated to the standard EM software design for a coherent approach of EM interaction modelling in Geant4
- PIXE fully integrated
- New interpolation method improves significantly CPU performance of models
- Extensive testing of migrated models and new interpolation method based models
- Several bug fixes, thanks to
  - new design
  - systemmatic testing
- Full documentation in web site

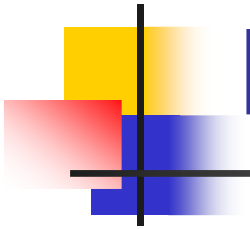


Backup



For full details…

- Please see
  Luciano Pandola's talk
  - October 21
  - Migration of low-energy physics to common EM design
  - Plenary Session V - EM Physics Validation and Development



For full details…

- Please see
  Anton Lechner's talk
  - October 21
  - ICRU'73 stopping powers
  - Parallel Session XI – EM – new models and validation