Geant4 Electromagnetic Physics

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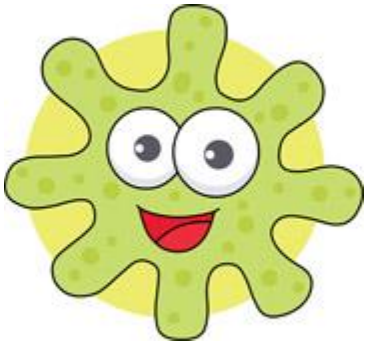
ENSAR2 Workshop: Geant4 in Nuclear Physics

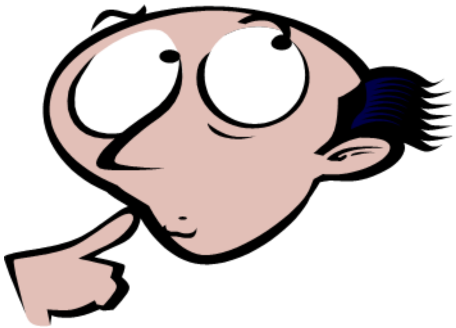
CIEMAT, Madrid, Spain - April 24-26, 2019

Outline



- Electromagnetic (EM) physics libraries
- Gean4 EM for HEP
- Recent developments
- Selected results
- Ion ionisation
- EM Physics configurations
- Geant4-DNA
- Summary

Geant4 EM libraries



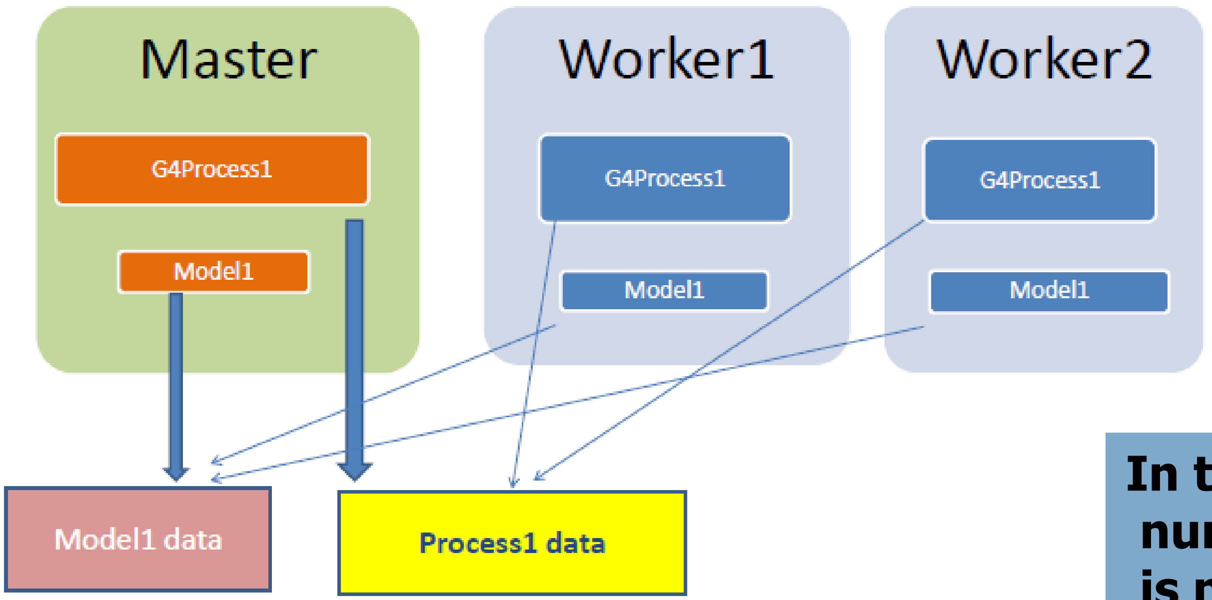
- Low-energy
  - Livermore library γ, e- from 10 eV up to 1 GeV
  - Livermore library based polarized processes
  - PENELOPE code rewrite , γ, e- , e+ from 100 eV up to 1 GeV (2008 version)
  - hadrons and ions up to 1 GeV
  - atomic de-excitation (fluorescence + Auger)
- Geant4-DNA
  - micro dosimetry models for radiobiology (Geant4-DNA project) from 0.025 eV to 10 MeV
- Adjoint
  - Reverse Monte Carlo processes and models to track from the volume of interest back to source of radiation
- Utils
  - general EM interfaces
- 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>10GeV)
  - physics for exotic particles
- Polarisation
  - simulation of circular polarized beam transport
- Optical
  - optical photon interactions

Software Design of EM Physics

- The uniform coherent approach for all EM packages
  - low energy and high energy models may work together
- A physical interaction or process is described by a process class
  - For example: G4ComptonScattering
    - Assigned to Geant4 particle types in Physics List
  - Three EM base processes:
    - G4VEmProcess
    - G4VEnergyLossProcess
    - G4VMultipleScattering
- A physical process can be simulated according to several models
  - each model being described by a model class
  - Naming scheme : « G4ModelNameProcessNameModel »
    - For example: G4LivermoreComptonModel
  - Models can be assigned to certain energy ranges and G4Regions
  - Inherit from G4VEmModel base class
- Model classes provide the computation of
  - Cross section and stopping power
  - Sample selection of atom in compound
  - Final state (kinematics, production of secondaries…)

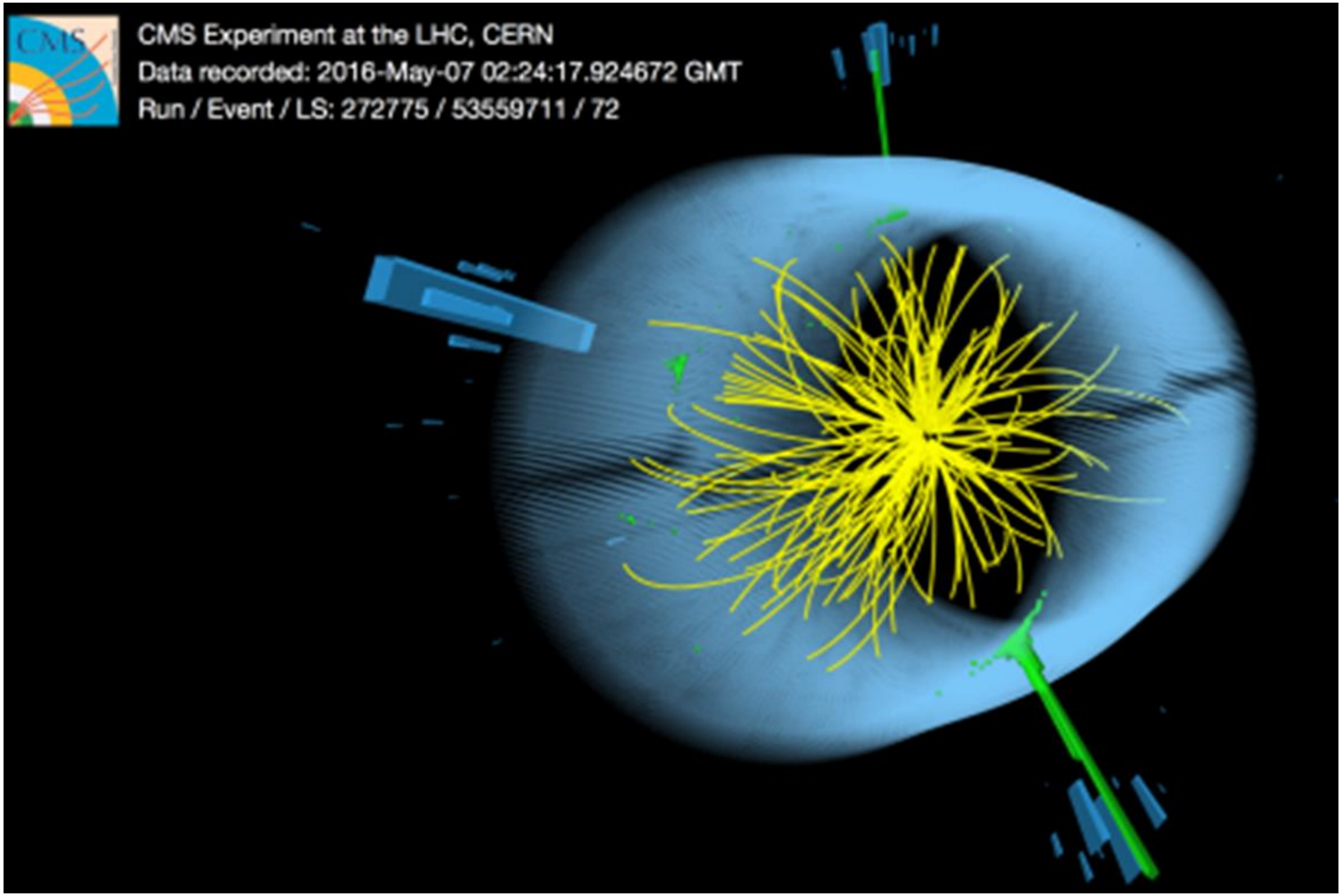
EM Data Sharing for Geant4 MT

- The scalability of Geant4 application in the MT mode depends on how effectivly data management is performed
- Shared EM physics data:
  - tables for cross sections, stopping powers and ranges are kept by processes
  - Differential cross section data are kept by models
  - Material propertes are in material data classes
  - EM parameters established for Physics Lists in the G4EmParameters class



Tables are filled by Master and have read-only access in run time

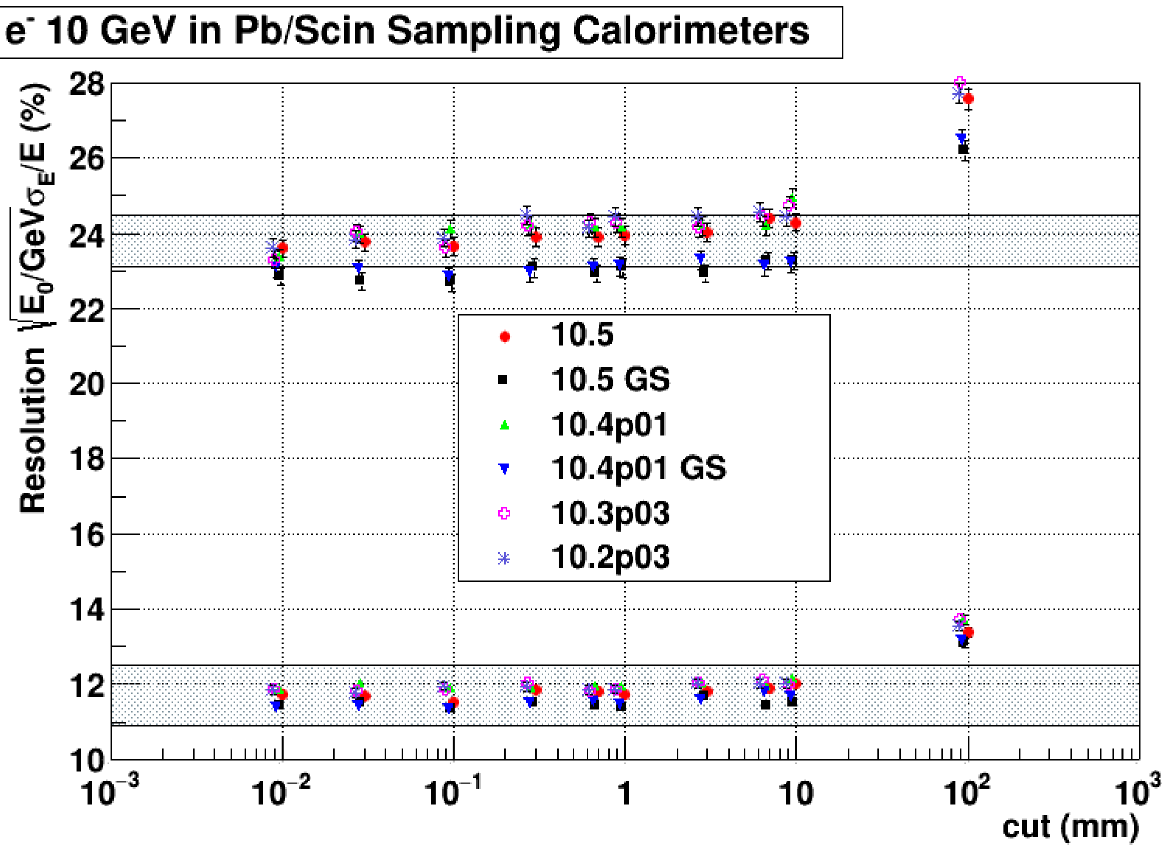
In this scheme number of threads is not limited



Geant4 EM for HEP

Resolution of Pb/Sc calorimeters

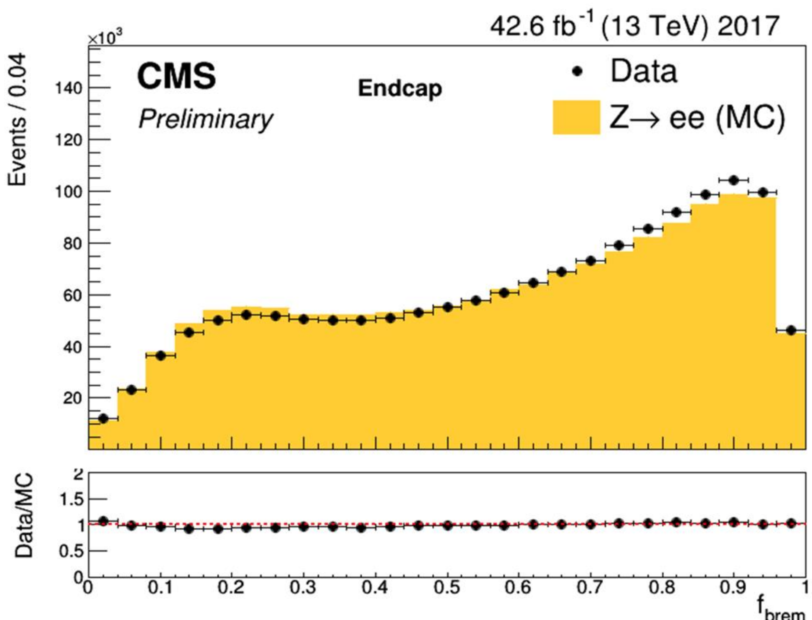
Bernardi E. et al. 1987 Nucl. Instrum. Meth. A **262**, 229



- A classical benchmark (ZEUS test-beam) for two sampling calorimeters with different sampling fractions
  - The same simulation conditions for two setups
- Geant4 results are stable between different releases
  - Goudsmit-Saunderson (GS) model of multiple scattering predicts less width within experimental uncertainty

Current accuracy of Geant4 EM

- Since Geant4 9.6
  - Accuracy of EM cross sections, shower response and resolution O(%)
  - EM shower shapes are monitored in regression on level $O(10^{-3})$
- Some discrepancies observed with LHC data do not clearly indicate the level of inaccuracy of the current EM physics but may be attributed to
  - Inaccuracy of geometry descriptions of detectors
  - Inaccuracy of simulation of digitization including pileup effects
- For more details see materials of the LPCC workshop



Recent example of Run-2 simulation:

CMS-DP-2018/017: Electron and Photon performance in CMS with the full 2017 data sample

Less agreement with data for the endcap than for the barrel

The fraction of the momentum lost to bremsstrahlung measured in the tracker, defined as f_{brem} for ECAL endcap .

Main challenges for EM physics in future experiments

- LHC Run-3 and HL-LHC physics analysis
  - Will require higher statistics of simulation
  - Current EM physics modelling uncertainties may contribute to systematic uncertainty of physics observables
  - Rare EM processes with O(%) cross section and below may potentially create non-standard event patterns
- In dark matter search experiments rare EM processes are background
- For FCC design we need reliable EM simulation up to 100 TeV
  - LPM suppression for gamma conversion and bremsstrahlung
  - Nuclear recoil effects
  - Nuclear and atomic form-factors
  - Specific EM processes for study of interaction region design
- Current priorities in Geant4 EM physics developments:
  - Review and update of all models according to the best state of art
  - Focus on model extensions to implement next to leading order corrections for cross sections
  - Add sampling of second order final states
    - extra recoil atomic electron , extra gamma or e+e- pair, recoil nucleus

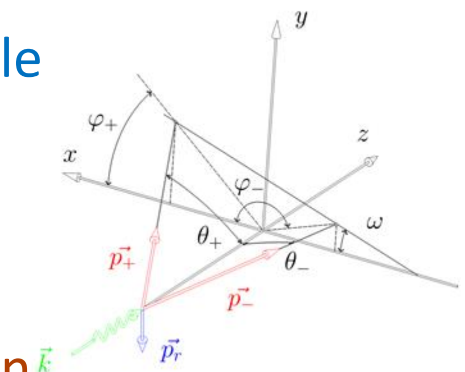
Recent developments

Most important updates for Geant4 10.4 (December 2017)

- Extended Geant4 Goudsmit-Saunderson (GS) model of multiple scattering of electrons and positrons
  - Mott corrections are fully implemented
  - Error free stepping option is available with Opt4 EM physics (EMZ)
- Tuned Urban model of energy loss fluctuations
- Improved photo-electric model and Rayleigh scattering
- Improved computations of LPM suppression corrections
  - Gamma conversion and bremsstrahlung
- Improved model for gamma conversion into $\mu^+\mu^-$ pair
- Provided 1st Geant4 example for light dark matter particle transport
- Improved interfaces for management of EM parameters
  - Models may be activated per detector region in easy way
- Improved handling of material properties for optical processes

Most important updates for Geant4 10.5 (December 2018)

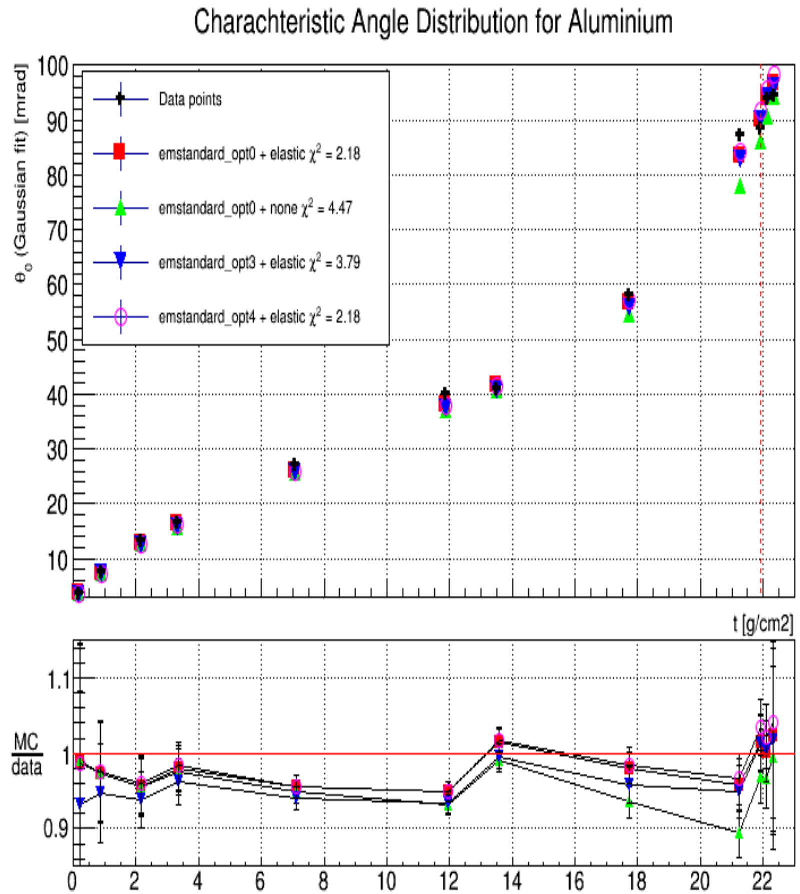
- Inclusion of Mott corrections in WentzelVI and single scattering models used for high energy e+e-
- Improved displacement sampling in Urban multiple scattering model
- Improved final state sampling for default gamma conversion models
- A new alternative 5D model for gamma conversion
  - Accurate simulation of angular correlations for final state
  - Triplet production (recoil e-)
  - Linear polarization of gamma may be taken into account
- A new relativistic models for ion ionization
- 1st variant of positron 3γ annihilation



Selected results

Geant4 Multiple and Single Scattering

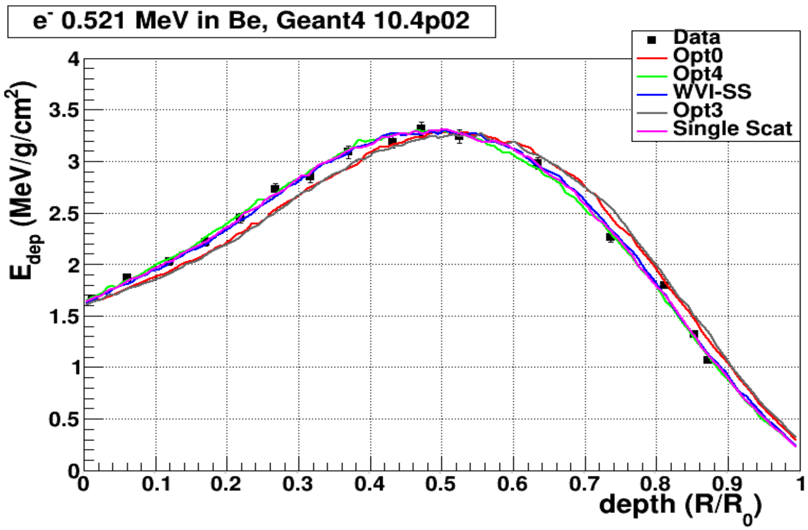
- Combined multiple and single scattering Wentzel-VI models
  - Single scattering for large angles
  - Multiple scattering for small angles
  - For muons and hadrons
  - For e+- above 100 MeV
- Urban multiple scattering
  - By default for e+- below 100 MeV by default
  - For ions
- New GS model
  - Used for e+- below 100 MeV
  - Used single scattering regime in vicinity of geometry boundary
  - Mott corrections since 10.4

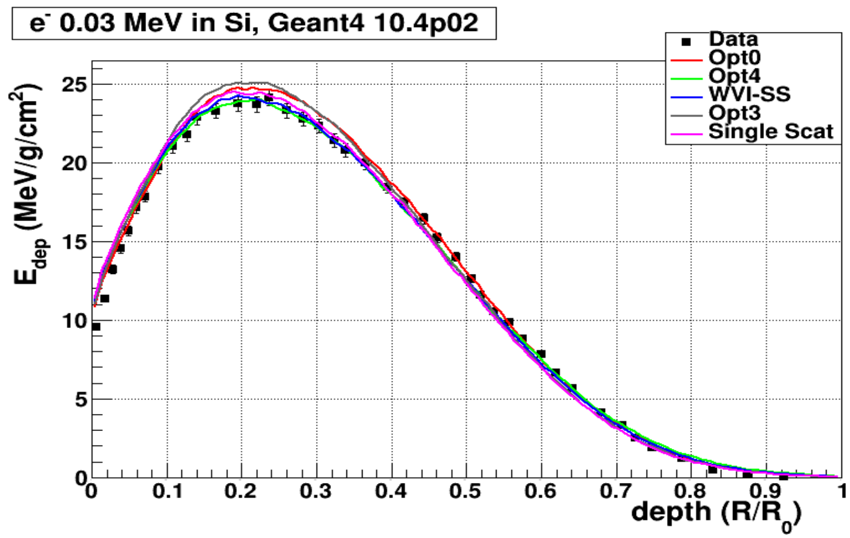


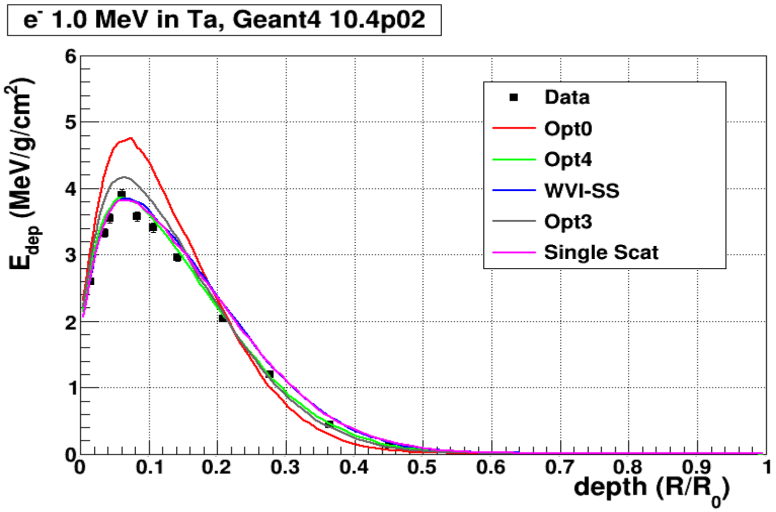
Proton multiple scattering benchmark
Nucl. Instr. Meth. B 74, 467 (1992)

Energy deposition in semi-infinite media

SANDIA REPORT SAND79-0414.UC-34a



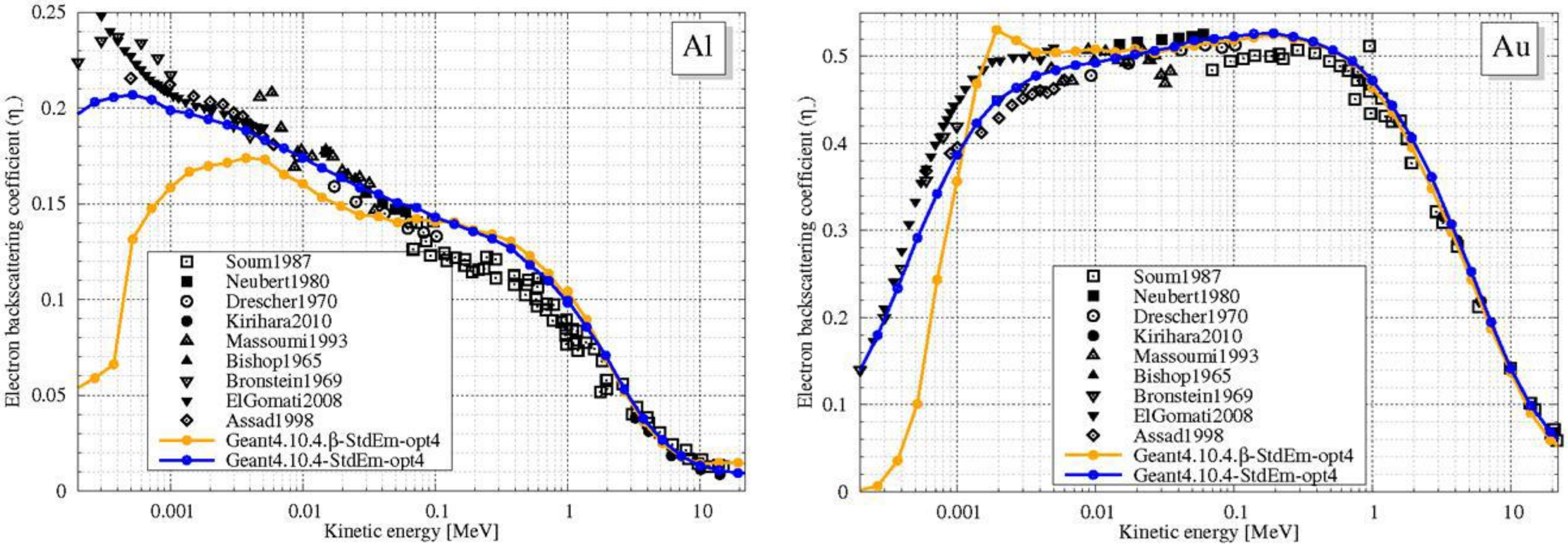




- Recent GS model now describes data for both low and high density media
- Opt0 (default) is not so accurate but is fast
- Opt4 (EMZ) is recommended as an alternative if increased precision is needed but is slower

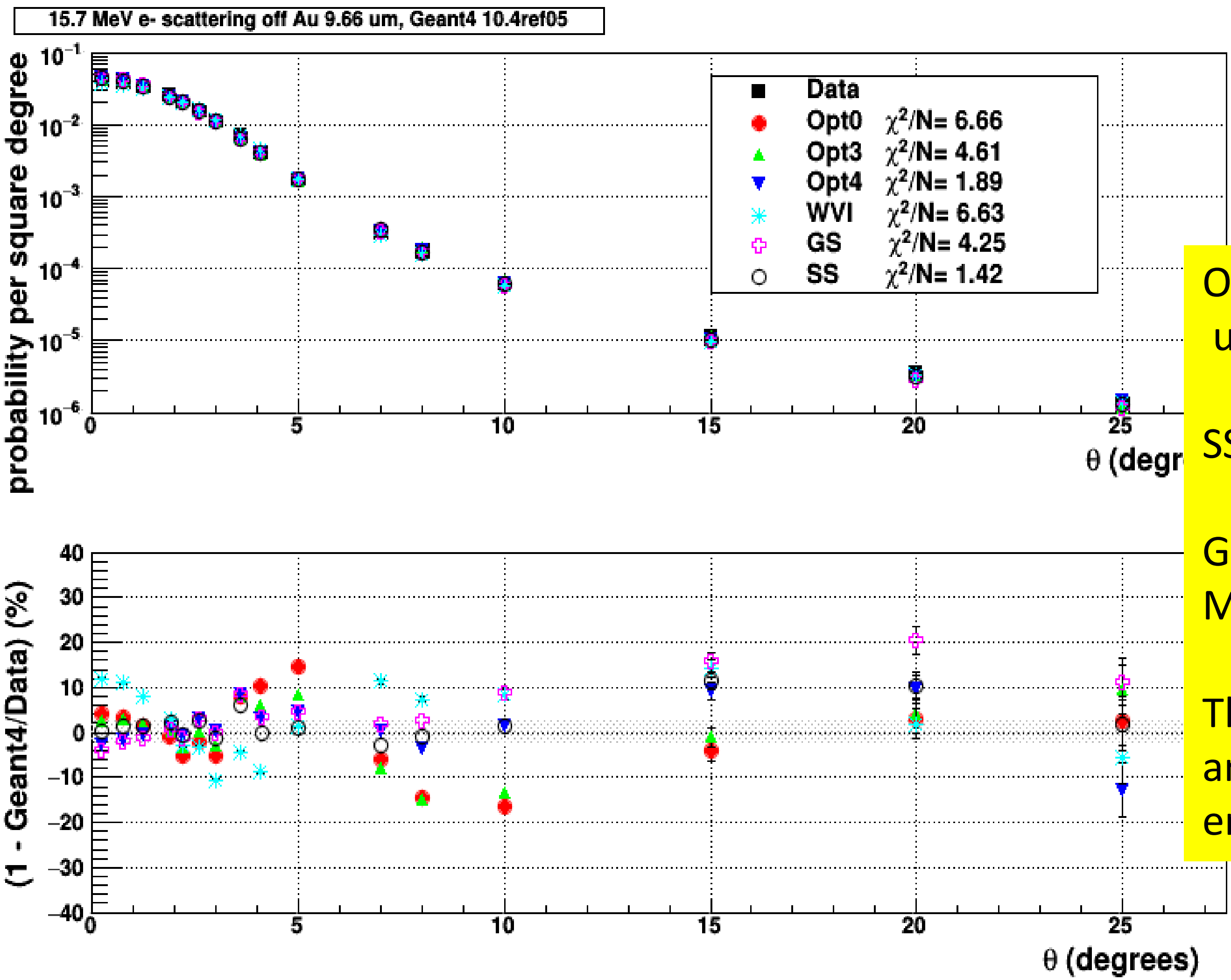
Backscattering validation results

CHEF-2017 Conference (JINST 13 C02054, 2018)



- Validation of electron backscattering from light (Al) and heavy (Au) targets versus data from different experiments.
- Old Opt4 (EMZ) EM configuration uses the Urban model (yellow), the final variant of Opt4 uses GS with “error-free” stepping (blue)
- Simulation with GS is substantially more accurate below 10 keV

Hanson data for electron scattering off Gold target (*Phys. Rev.* **84**, 634-637, 1951)



Opt4 Physics List uses the GS model

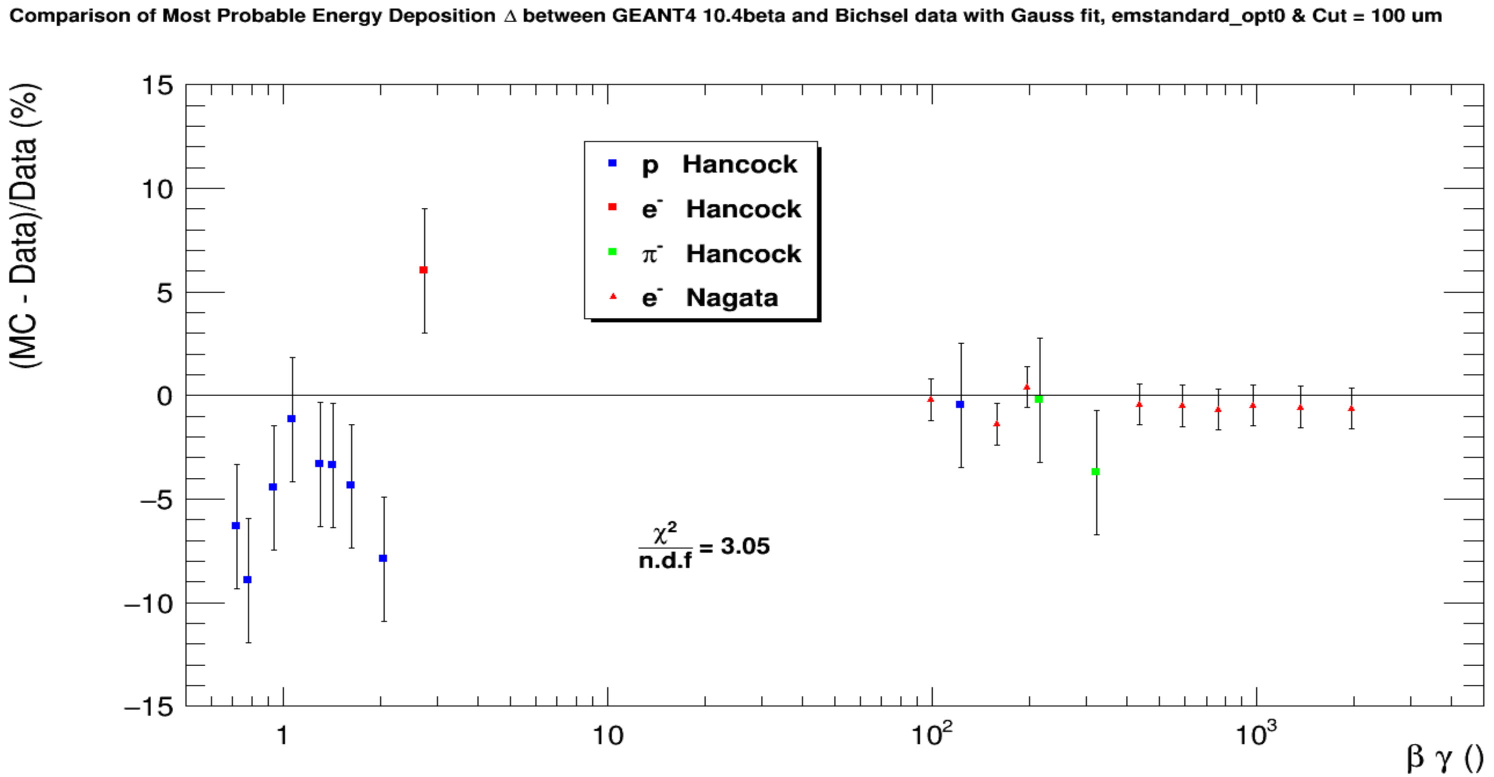
SS is single scattering

GS and SS are using Mott corrections

These improvements are also valid for all energies

Energy depositions in Silicon detectors

H. Bichsel data collection: Rev. Mod. Phys. **60**, 663, 1988

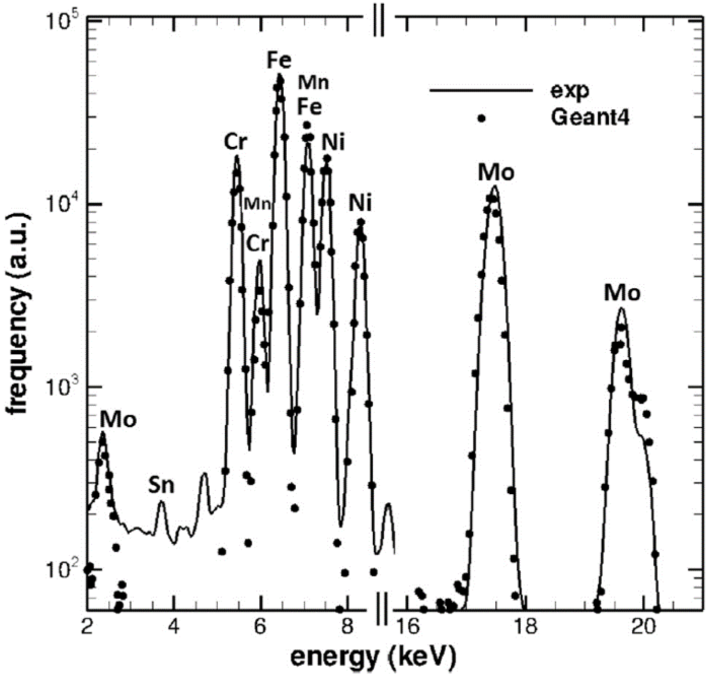


- Geant4 results for 0.3 and 1.4 mm thick Silicon detectors
  - Both Urban and PAI models reproduce well data for relativistic beams
  - Less accurate for e- and proton data for $\beta\gamma \sim 1$
    - There are questions to experiments

Atomic de-excitation module

NIM B 316 (2013) 1-5

- Is used by
  - Photoelectric effect
  - Compton scattering
  - Ionisation
  - Radioactive decay
- For discrete processes full gamma and Auger electron cascade are simulated
- For ionization and internal conversion of gamma in nuclear de-excitation
  - K-, L-, M- cross sections are implemented



Stainless steel sample simulation compared to data, taking into account Al' 'funny filter'' of 250 um and 0.26% hole-detector surface proportion.

Ion ionisation

Geant4 models of ionisation

- By default, classical models are used for simulation of ionisation
  - Moller-Bhabha for electrons and positrons
  - Bethe-Bloch for muons, hadrons, and ions above 2 MeV/u
  - NIST parameterization of dEdx below 2 MeV/u (PSTAR, ASTAR)
  - Parameterized model of fluctuation of energy loss (L.Urban)
    - Recommended do not reduce step size below 5 μm
- Alternative models:
  - Livermore and Penelope $e^{\pm}$ ionisation below 1 MeV
  - PAI model applicable for relativistic particles
    - More accurate absolute energy deposition in thin layers
  - MicroElec models for Silicon for electrons, protons, and ions below 100 MeV
    - Sampling of each elastic or inelastic collision below
- Since Geant4 10.4 it is possible on top of any EM physics to enable models for G4Region:
  - PAI model per particle type or for all particles
  - MicroElec model for electron, proton, ions
  - Atomic de-excitation for ionization (PIXE) and for photo-effect and Compton with emission of gammas and electrons

Geant4 treatment of ions

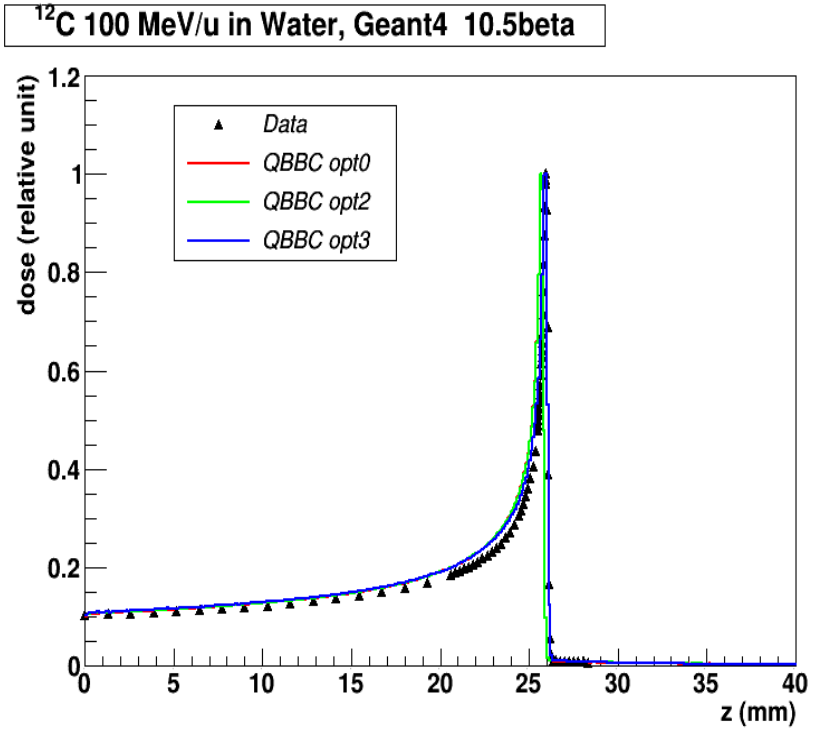
- Number of "stable" charged particles in Geant4 is 44
  - For $\mu^{\pm}$ $\pi^{\pm}$ p, pbar are «base» particles
    - dEdx, Range and Inverse range, and δ-electron cross section tables are created per material-cuts-couple
  - For any charged particle (Z_1, M_1) scaling relation for stopping power: $S_1(E) = S_b\left(E \cdot M_b / M_1\right) \cdot Z_1^2$,
  - Majority of "stable" particles have charge ±1
- Number of known isotopes ~5000
  - G4GenericIon is used as a «base» particle for all ions with Z>2
  - G4GenericIon has parameters of proton
  - For low energies we need substitute $Z_1 \rightarrow Z_{1eff}$
    - This is used in the default model and Opt0
    - Scaling is not accurate, so more accurate approach is needed

ICRU73 Ion Ionisation Model

- A. Lechner, V. N. Ivanchenko, J. Knobloch, Nucl. Instrum. and Meth. B 268 (2010) 2343-2354
- G4IonParameterisedLossModel implements ion ionisation using ICRU73 stopping power tables
  - Initially we used only tables from the report
  - Later we get full set of projectile/target tables computed specially for Geant4
    - We have all targets for pure elements up to Uranium
    - Additionally for G4_WATER
  - A table for stopping power is uploaded by request for each new projectile/target combination
    - A user can add a custom table
  - Energy interval E/A from 0.025 keV to 1 GeV

Specifics of Ion Transport

- Ion have much higher energy deposit than protons
- In order to sample narrow Bragg peak for ions we use more strong step limitation
- Stepping function:
  - Opt0 (0.1, 0.1mm)
  - Opt4 (0.1, 0.01mm)
- In order to have an accurate transport additionally to dEdx table for each projectile/target couple range and inverse range tables are created



Issues and New Models

- ICRU73 stopping has good but not infinite accuracy and limited energy range for stopping powers
- It requires a substantial memory to keep all tables
  - In LHC experiments simulation all possible isotopes are produced and hundreds of different materials describing geometry – this model cannot be used effectively
- Various activities are caring out in 2018
  - GATE group is working with ICRU90 data
    - We are trying include a variant for p, α as an option
  - Jose-Luis Rodriguez-Sanchez (CEA) has implemented for 10.5 the new class
    - Will be available with WVI experimental Physics List
  - We implemented G4LinhardSoremsenIonModel
    - Will be discussed below

Stopping Power of Relativistic Ions

Lindhard J., Sorensen A.H., Relativistic theory of stopping for heavy ions.
Phys. Rev. A 53 (1996) 2443

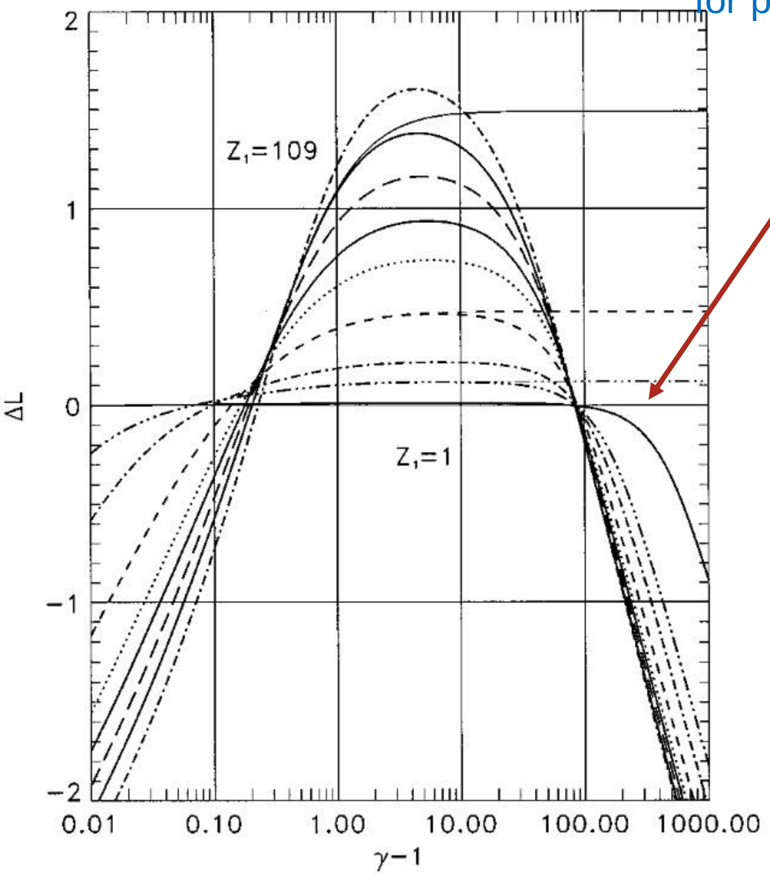
$$-\frac{dE}{dx} = \frac{4\pi Z_1^2 e^4}{mv^2} N Z_2 L$$

$$L_{stand} = ln\left(\frac{2mv^2}{I}\right) - \frac{v^2}{c^2} - \frac{1}{2}\delta$$

$$L - L_{stand} =$$
$$\Delta L + \delta L_{shell} + L_{Barkas} + L_{scr}$$

ΔL is the function of energy and projectile ion size
It has been parameterized
in the form f(γ, Z)

for point nuclei



Stopping for finite nuclear size. The curves display the values of ΔL for atomic numbers Z1 = 1, 10, 18, 36, 54, 66, 79, 92, and 109

Configuration of EM physics

Recommendations for Geant4 10.5

- A set of EM physics constructors are provided together with each recent Geant4 version
  - The default (Opt0) EM physics is optimized for use in HEP
  - There are variants Opt1 (EMV) and Opt2 (EMY) with simplified multiple scattering and other options
  - The alternative Opt4 (EMZ) physics is combination of the most accurate EM models
    - It is substantially slower than the default
    - Is recommended for R&D and detector performance studies
    - May be recommended for simulation of nuclear physics setups
- On top of any EM physics configuration it is possible to customize EM parameters via UI commands and C++ interface
  - G4EmParameters class may be called via UI commands
  - EM physics configuration and PAI ionization model may be defined for or more G4Region(s)

EM physics constructors for HEP

- Urban multipe scattering for e^{+-} below 100 MeV only
  - WentzelVI + Single scattering above 100 MeV
- WentzelVI + single scattering for muons and hadrons
- Urban multiple scattering model for ions

Constructor	Components	Comments
G4EmStandardPhysics	Default (QGSP_BERT, FTFP_BERT…)	ATLAS, and other HEP productions, other applications
G4EmStandardPhysics_option1	Fast due to simple step limitation, cuts used by photon processes (FTFP_BERT_EMV)	Similar to one used by CMS, good for crystals, not good for sampling calorimeters
G4EmStandardPhysics_option2	Fast due to simple step limitation, updated photon models and bremsstrahlung angular generator	Similar to one used by LHCb

EM physics for accurate simulations

- Focus on accuracy instead of maximum simulation speed
- Ion stopping model based on the ICRU'73 data
  - Step limitation for multiple scattering using UseDistanceToBoundary option
- Strong step limitation by the ionisation process defined per particle type
- Recommended for hadron/ion therapy, space applications

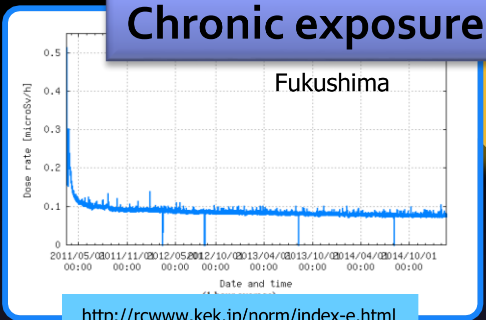
Constructor	Components	Comments
G4EmStandardPhysics_option3	Urban MSC model for all particles	Proton/ion therapy
G4EmStandardPhysics_option4	The best combination of models per particle type and energy range, GS multiple scattering model for e+- below 100 MeV with error free stepping approach and Mott corrections	Goal to have the most accurate EM physics
G4EmLivermorePhysics	Livermore models for γ, e^- below 1 GeV, Standard models above 1 GeV 5D pair production model	Livermore low-energy electron and gamma transport
G4EmPenelopePhysics	Penelope models for γ, $e^\pm$ below 1 GeV, Standard models above 1 GeV	Penelope low-energy $e^\pm$ and gamma transport

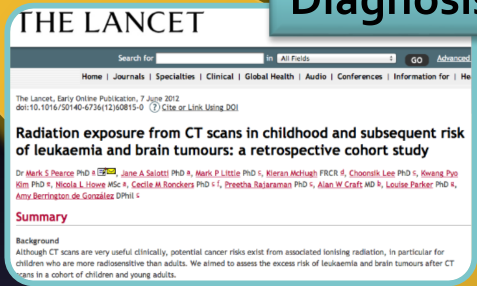
Special EM Physics List constructors

Constructor	Components	Comments
G4EmStandardPhysicsGS	GS multiple scattering model for e+- below 100 MeV with loose step limitation	May be considered as an alternative to standard Opt0
G4EmStandardPhysicsWVI	WVI + SS combination ATIMA ion ionisation	Is good for high energy interactions
G4EmStandardPhysicsSS	Single elastic scattering for all charged particles	Mainly for validation and verification
G4EmLowEPPhysics	Monarsh University Compton scattering model, WVI-LE model, GS model, 5D pair production	Used new low-energy models
G4EmLivermorePolarized	Polarized gamma models	An extention of Livermore physics

Geant4-DNA

Modelling biological effects of ionising radiation remains a major scientific challenge





THE LANCET

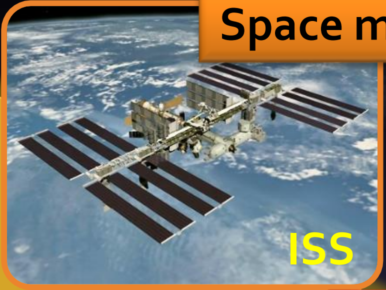
The Lancet, Early Online Publication, 7 June 2012
doi:10.1016/S0140-6736(12)60815-0

Radiation exposure from CT scans in childhood and subsequent risk of leukaemia and brain tumours: a retrospective cohort study

Summary

Background

Although CT scans are very useful clinically, potential cancer risks exist from associated ionising radiation, in particular for children who are more radiosensitive than adults. We aimed to assess the excess risk of leukaemia and brain tumours after CT scans in a cohort of children and young adults.



« A MAJOR CHALLENGE LIES IN PROVIDING A SOUND MECHANISTIC UNDERSTANDING OF LOW-DOSE RADIATION CARCINOGENESIS »

L. MULLENDERS *ET AL.*

ASSESSING CANCER RISKS OF LOW-DOSE RADIATION

NATURE REVIEWS CANCER (2009)

Geant4-DNA time-line

Main objective

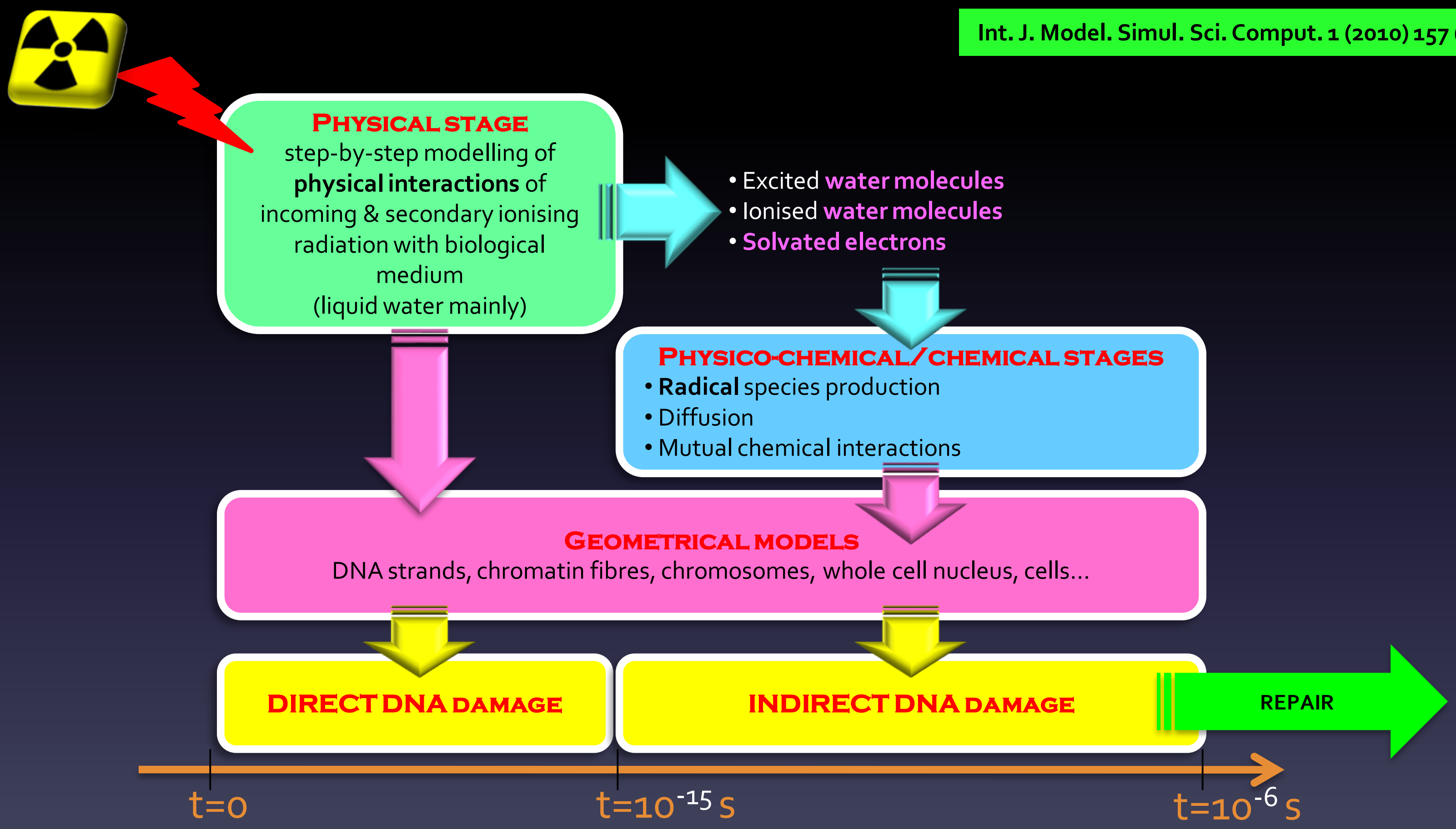
Extend the general purpose Geant4 Monte Carlo toolkit for the simulation of interactions of radiation with biological systems at the cellular and DNA level in order to predict early and late DNA damage in the context of manned space exploration missions (« bottom-up » approach).

C++ extension included in Geant4 designed to be developed and delivered in a FREE software spirit under the Geant4 license, easy to upgrade and improve.

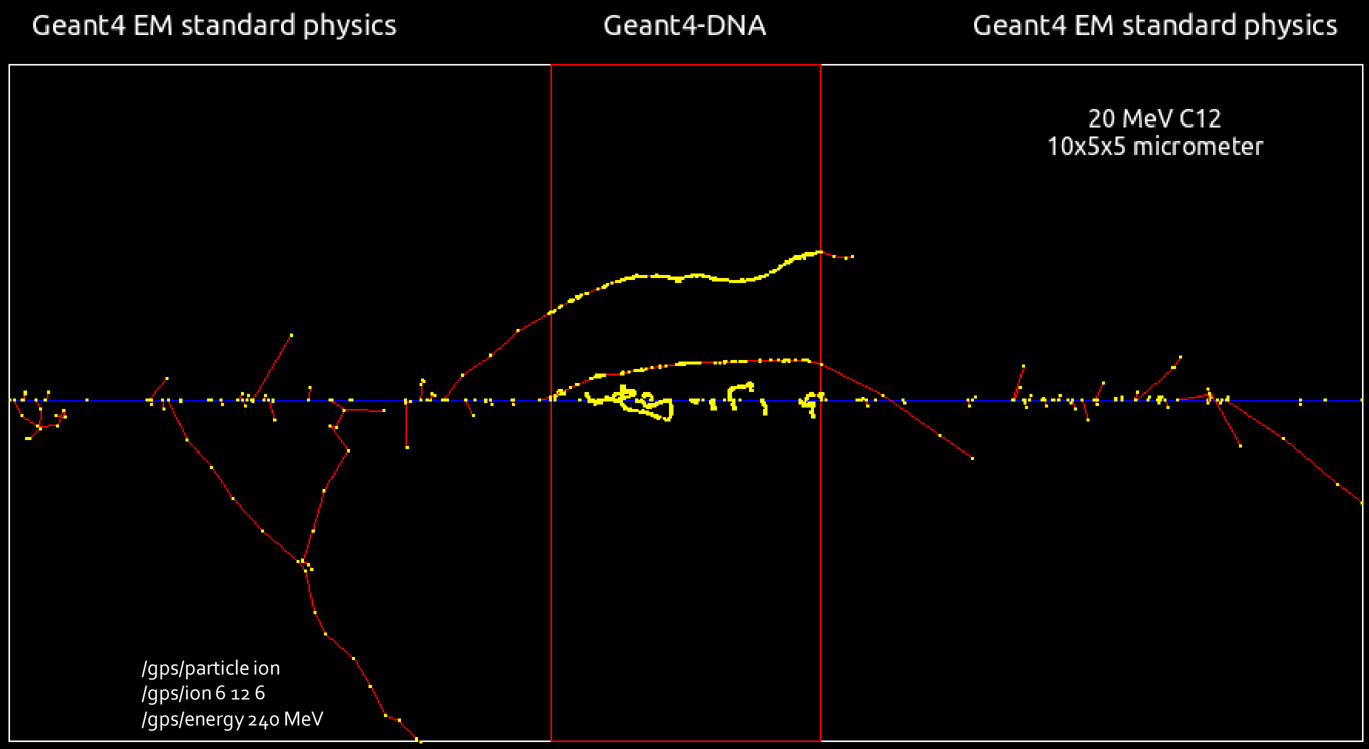
- **2001** – Initiated at the **European Space Agency/ESTEC** by **Petteri Nieminen**
- **2007** – First prototypes of **physics models** for liquid water added to Geant4 **9.1**
  - W. Friedland, D. Emfietzoglou, M. Dingfelder
- **2008** – Development coordinated by **CNRS/IN2P3** (physics, chemistry, geometries)
- **2014** – **Chemistry stage** extension ready for end users in Geant4 **10.1**
- **2015-18** – **New alternative models** for electron tracking & geometries **10.2 – 10.5**

How can Geant4-DNA model early DNA damage ?

Int. J. Model. Simul. Sci. Comput. 1 (2010) 157 (link)



Simulation of track structures



Courtesy of V. Stepan (CENBG)

See extended/medical/dna/dnaphysics example

Nucl. Instrum. and Meth. B 273 (2012) 95 (link)
Prog. Nucl. Sci. Tec. 2 (2011) 898 (link)

Summary

- Geant4 EM physics is well established
  - High energy physics
  - Radiation medicine
  - Radiation effect for space science
  - Opened for new developments
- Main challenges and activity areas
  - CPU/memory performance
  - Review and update of all models according to the best state of art
  - Focus on model extensions to implement next to leading order corrections for cross sections and final states
  - Developments of rare EM processes
  - Introduce gamma polarisation as an option on top of any EM physics
- Geant4 DNA is a radiobiology extension of Geant4
  - Is a part of EM physics libraries
  - Is under intensive development