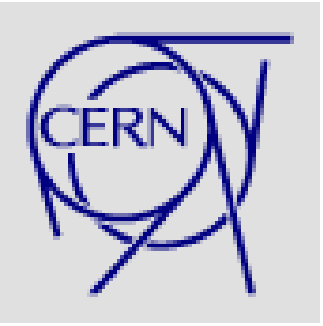

Geant4 Electromagnetic Physics Updates

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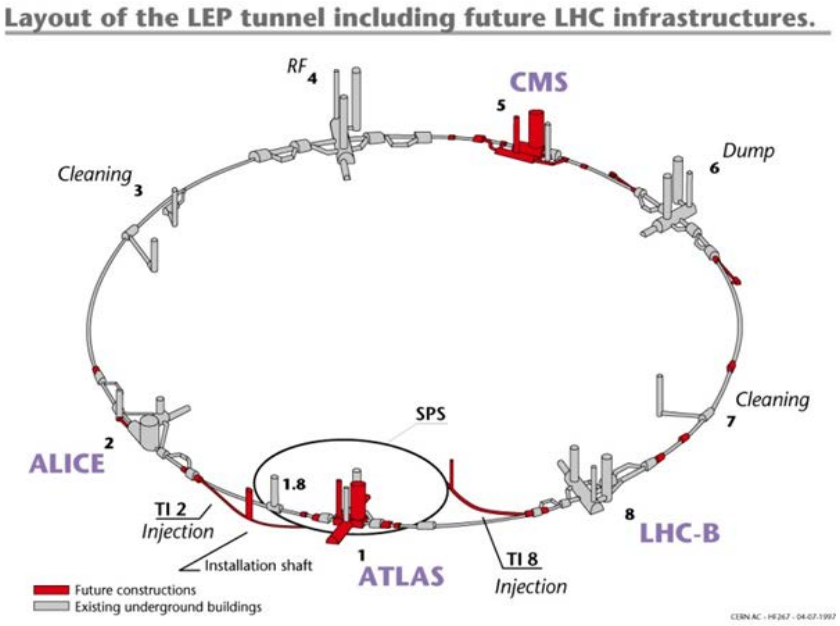
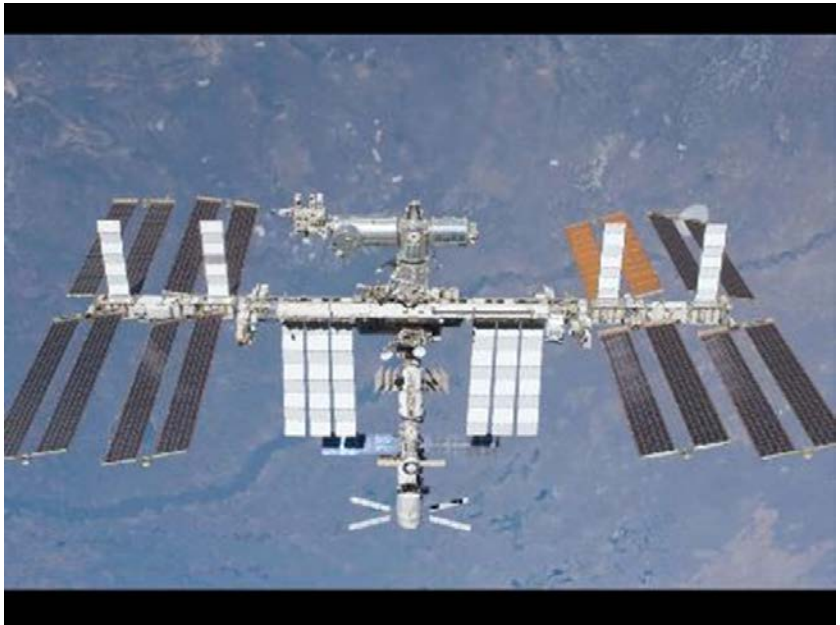
S. Incerti, CNRS, IN2P3, CENBG, France

12th Geant4 Space User Workshop
10-12 April 2017
University of Surrey, Guildford, United Kingdom

Outline

- Recent developemnts
- EM model evolutions
- Geant4 DNA project
- EM physics configuration
- Plans





- There are many similar requirements to Geant4 EM physics coming from between HEP, Space science and medical physics

- EM physics groups of Geant4 trying to address all these requirements

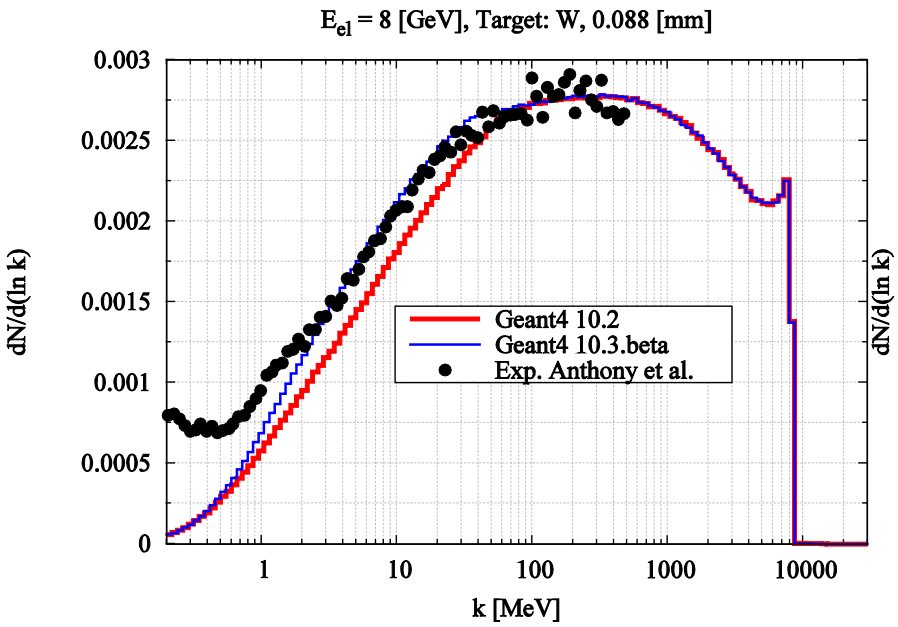
Recent Developments
Technical improvements in Geant4 10.3

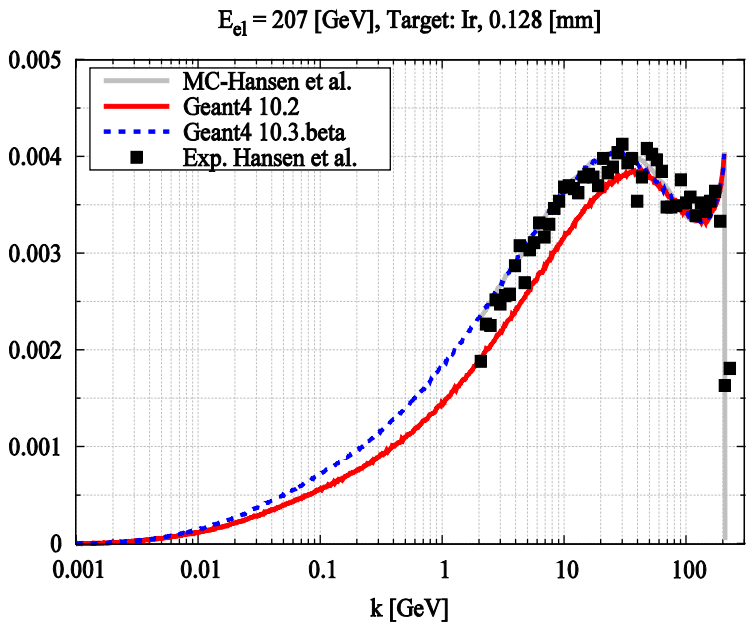
- Fixed several data races in MT mode
  - Material and EM physics
- Elements of C++11 features and keywords are added
- G4EmParameters is fully implemened
  - moved all remaning parameters from G4EmProcessOptions class
    - this class becomes obsolete and not recommended anymore
    - it is kept for backward compatibility but will be removed soon
  - Initialisation is allowed only from master thread
    - Each parameter now has UI command and C++ interface
    - Now UI command order becomes not so important as before
  - EM process or model at initialization reads these parameters
    - There is a “lock” mechanism allowing to provide specific configuration of a model per G4Region
  - Information on set of parameters is available via Dump() method

Recent developments highlights
Standard EM in Geant4 10.3

- The default upper energy of EM physics 100 TeV
  - Needed for FCC design studies
- Ionisation:
  - G4UniversalFluctuations – small fix for Glandz part
  - Fixed density effect parameterisation for compounds
  - Fixed dEdx computations for He3 and He4 in G4EmCalculator
  - G4EmSaturation (Birks effect)
    - make this helper class thread safe and reuse it between threads in run time
    - updated Birks constants using ATLAS and CMS values
- Bremsstrahlung:
  - G4eBremsstrahlungRelModel – improved LPM effect treatments
  - G4SeltzerBergerModel – fixed for Z > 92
- New process is added of e+e- pair creation by e+ and e-
- Multiple scattering – moved final position change from PostStep to AlongStep
  - Before sampling was done AlongStep but position was changed only PostStep
- G4UrbanMscModel – a new algorithm for sampling of lateral displacement is added.
  - Providing similar results as GS and WVI models
  - Added to Opt3, Opt4, Livermore and Penelope Physics Lists
- Three different parameterisations of nuclear formfactors
  - Used by single scattering models: None, Exponential, Gaussian, Flat
- Fixed correlations of linear polarizations of gamma from two gamma annihilation

LPM supression formula is fixed (CHEP'2016)





A classical formula for LPM effect description has been restored by M.Novak
(in the framework of GeantV project)

Shape of distribution is described now with better accuracy

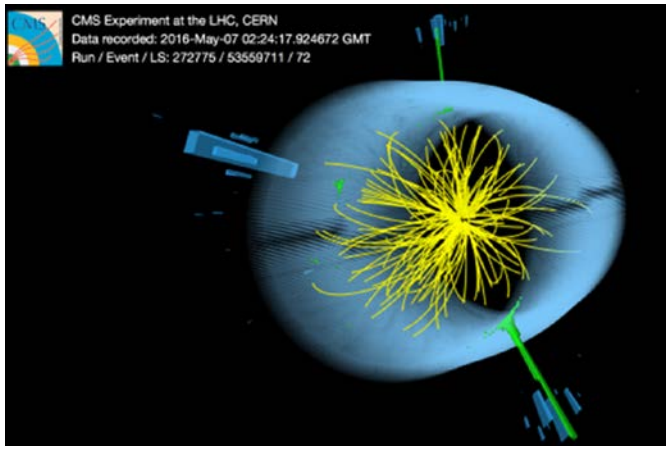
We do not observe a visible effect of this fix on HEP calorimtry response

Recent developments highlights
Low-energy EM in Geant4 10.3

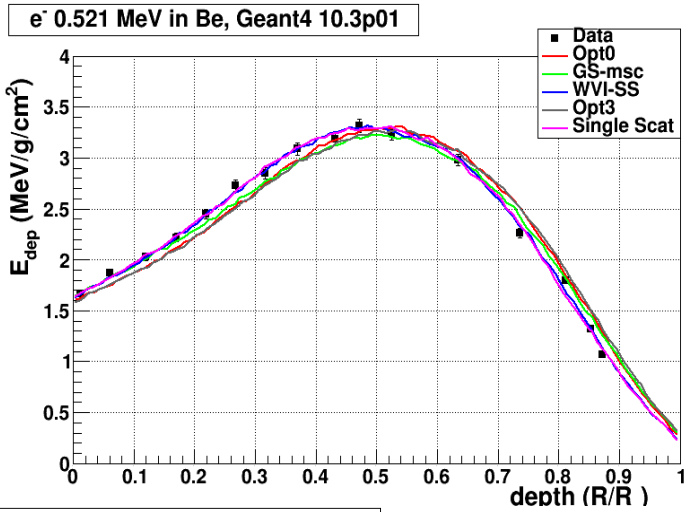
- Atomic de-excitation
  - Fixed initialisation/activation per G4Region
  - fluorescence and Auger cascade are now activated by default in all Geant4-DNA constructors.
- MicroElec models for Silicon
  - acceleration of single elastic scattering for electrons.
- Fixed several DNA classes concern chemistry
  - G4ITNavigator, G4MolecularCounter and G4DNATransformElectronModel
- G4EmDNAPhysicsActivator is a new class for easier Geant4-DNA physics models configuration per particle type.
  - The « dnaphysics » example illustrates its usage.
- Provided a new example application (« chem4 ») for the simulation of radiochemical yields for water radiolysis simulation and benchmarking.
- Data set G4EMLOW-6.50 is required

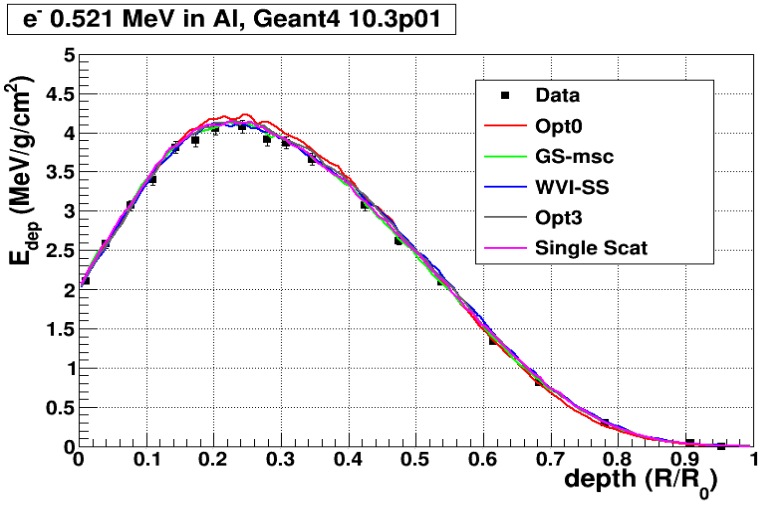
EM physics model evolutions

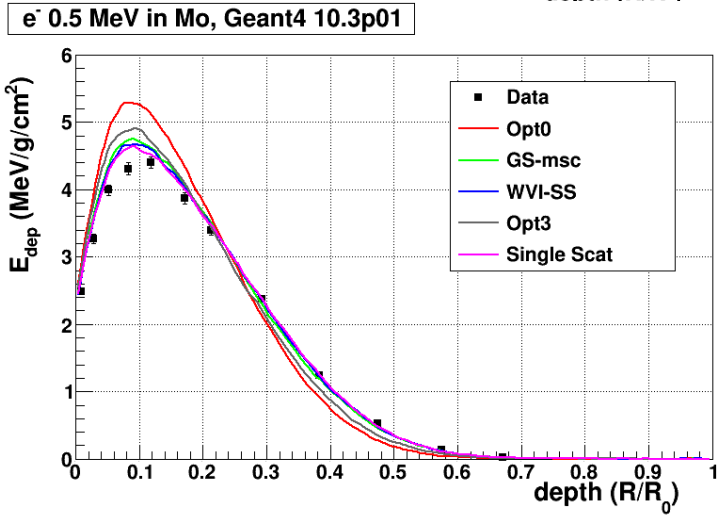
- Since Geant4 9.6 the consolidation of EM physics models are completed
  - Full energy range is covered by each EM physics List
  - High energy and low energy models may work in the same run
  - Components are interchangeable
    - angular generators, de-excitation module..
- With Geant4 10.3 EM sub-library are fully migrated to MT
  - Main data shared between threads
  - Models are thread safe
- Current focus of model developments is on accuracy
  - Replacing old parameterizations by more theory based models
    - GS and WVI models for multiple scattering
    - Bremsstrahlung
    - Gamma conversion
  - Addition next to leading order corrections
  - Addition of nuclear form-factors
  - Improving simulation of effects of polarization
- Extension of testing suite

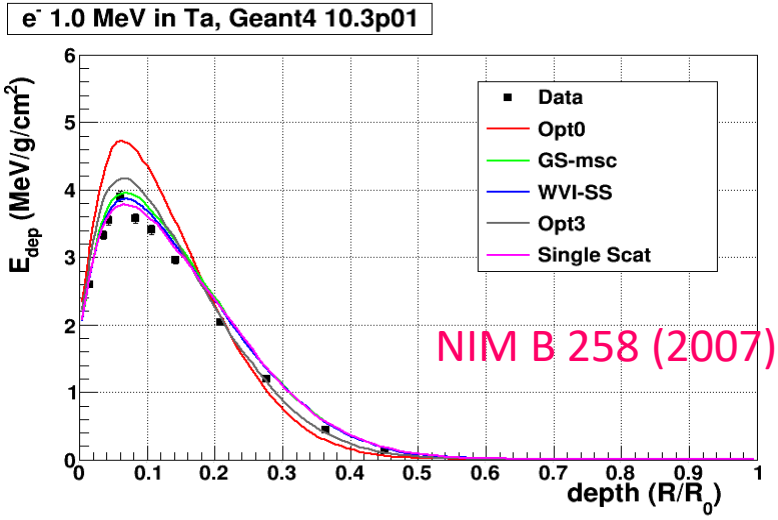


Electron tracking in semi-infinite media SANDIA data







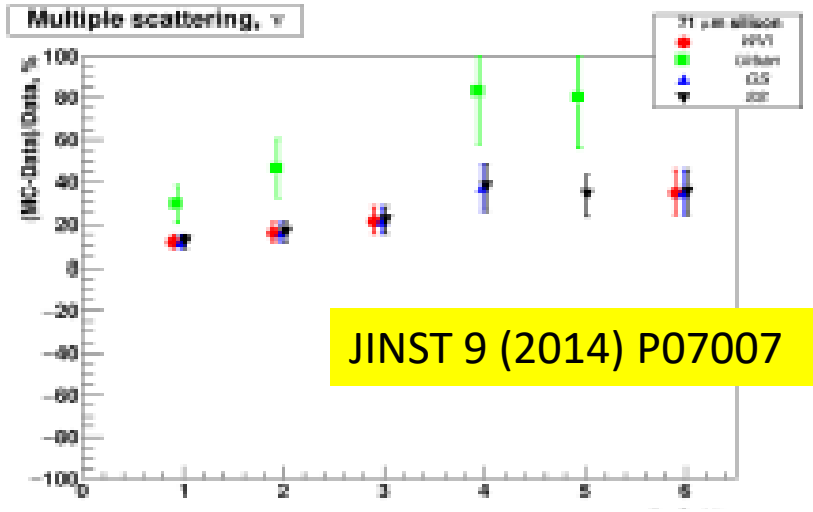


NIM B 258 (2007) 381

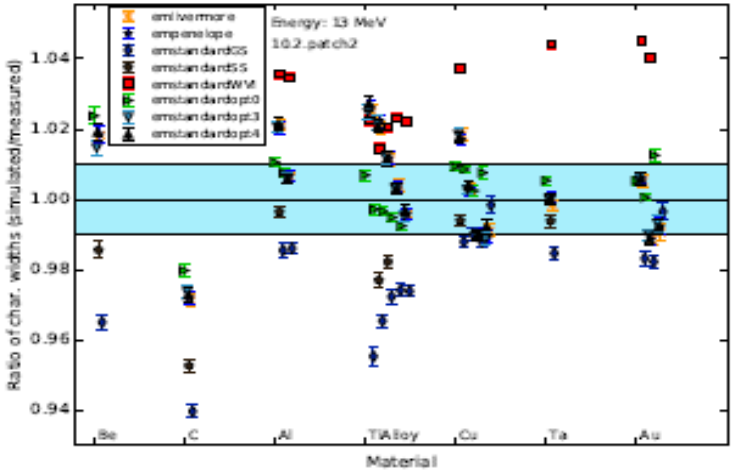
WVI-SS model is most accurate, GS has problems in low Z media
Urban model has problem for high Z media

Recent validation of multiple scattering (CHEP'16)

- Two scattering benchmarks:
  - High energy (1-6 GeV) electron scattering in thin silicon
    - A.Bagulya (Lebedev Institute)
    - WVI, GS and SS are the best
    - There are concerns to publication itself
  - Electron scattered 13 MeV e– beam for different scattering targets and physics lists.
    - D. Sawkey (Varian Medical System)
    - Urban model is the best for this benchmark



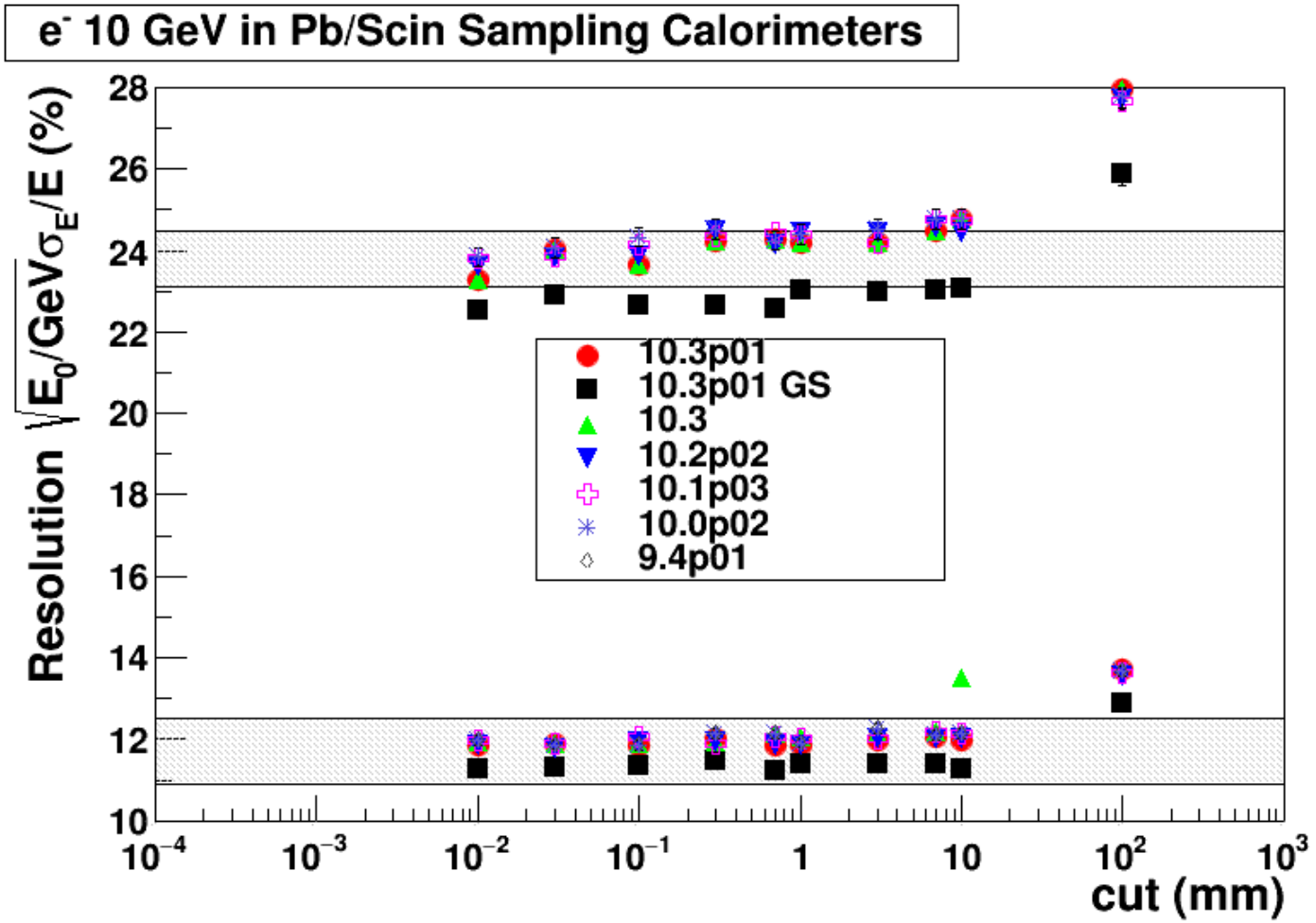
JINST 9 (2014) P07007



Med. Phys. 35 (2008) 4121

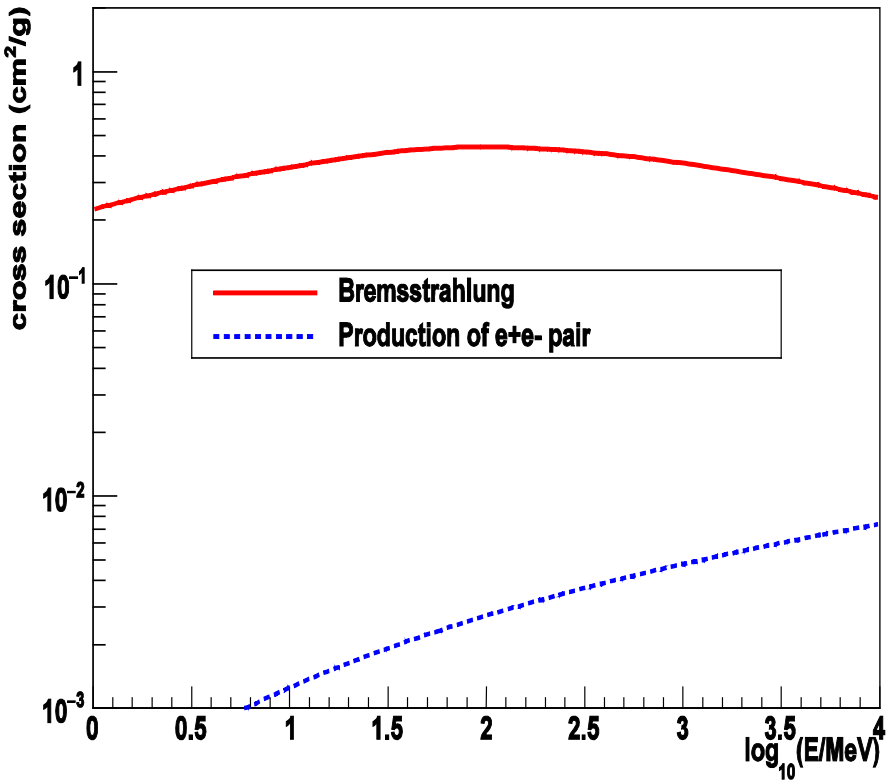
Simplified lead/scintillator calorimeter

NIM A 262 (1987) 229; 274 (1989) 134



Urban model of multiple scattering is still Geant4 default for e+- < 100 MeV
WVI + SS is the default for the rest

Cross section of e+e- pair production by e+ or e-

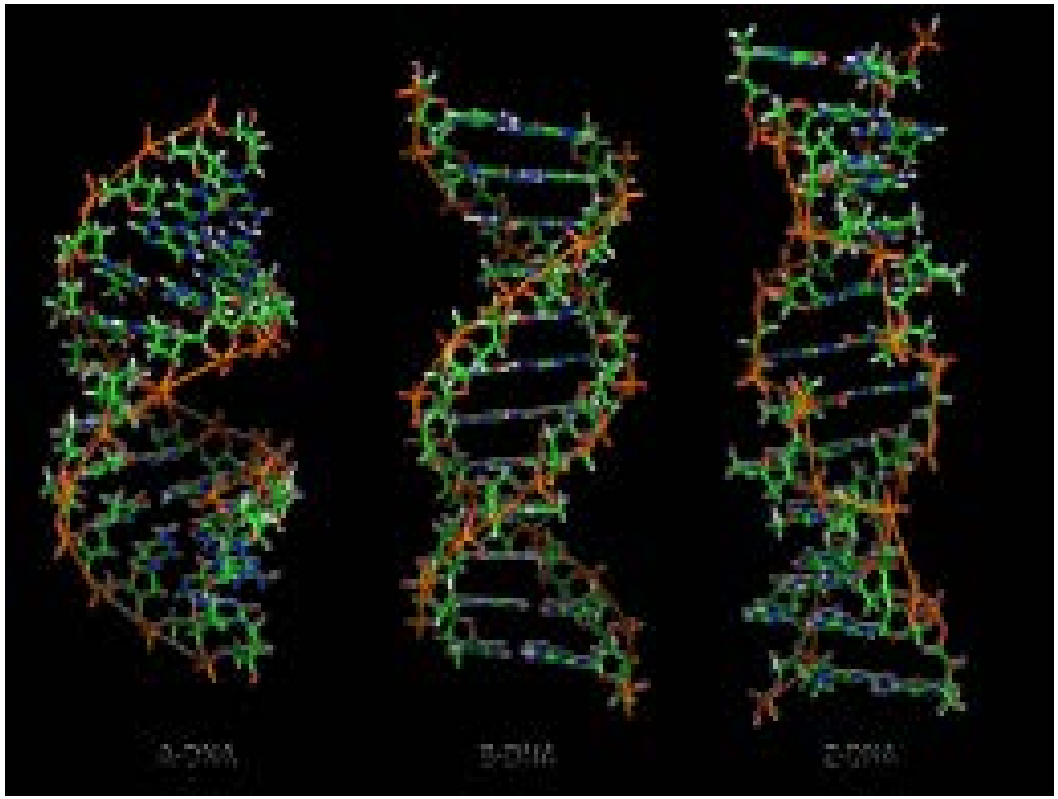


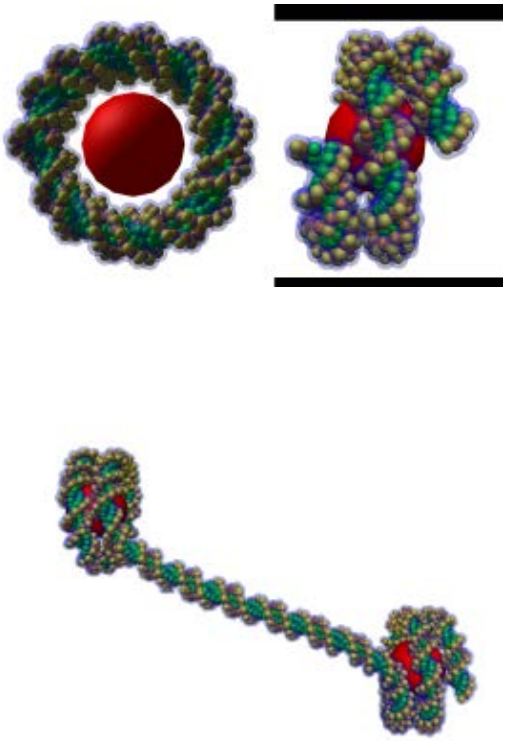
In this plot partial cross sections are shown for energy transfer > 10 MeV

The cross section of e+e- pair production is significantly lower than bremsstrahlung

This new process is not important for simulation of EM shower shape but may be a background in an experiment for a dark matter search

This new process is included in Opt3 and Opt4 Physics Lists



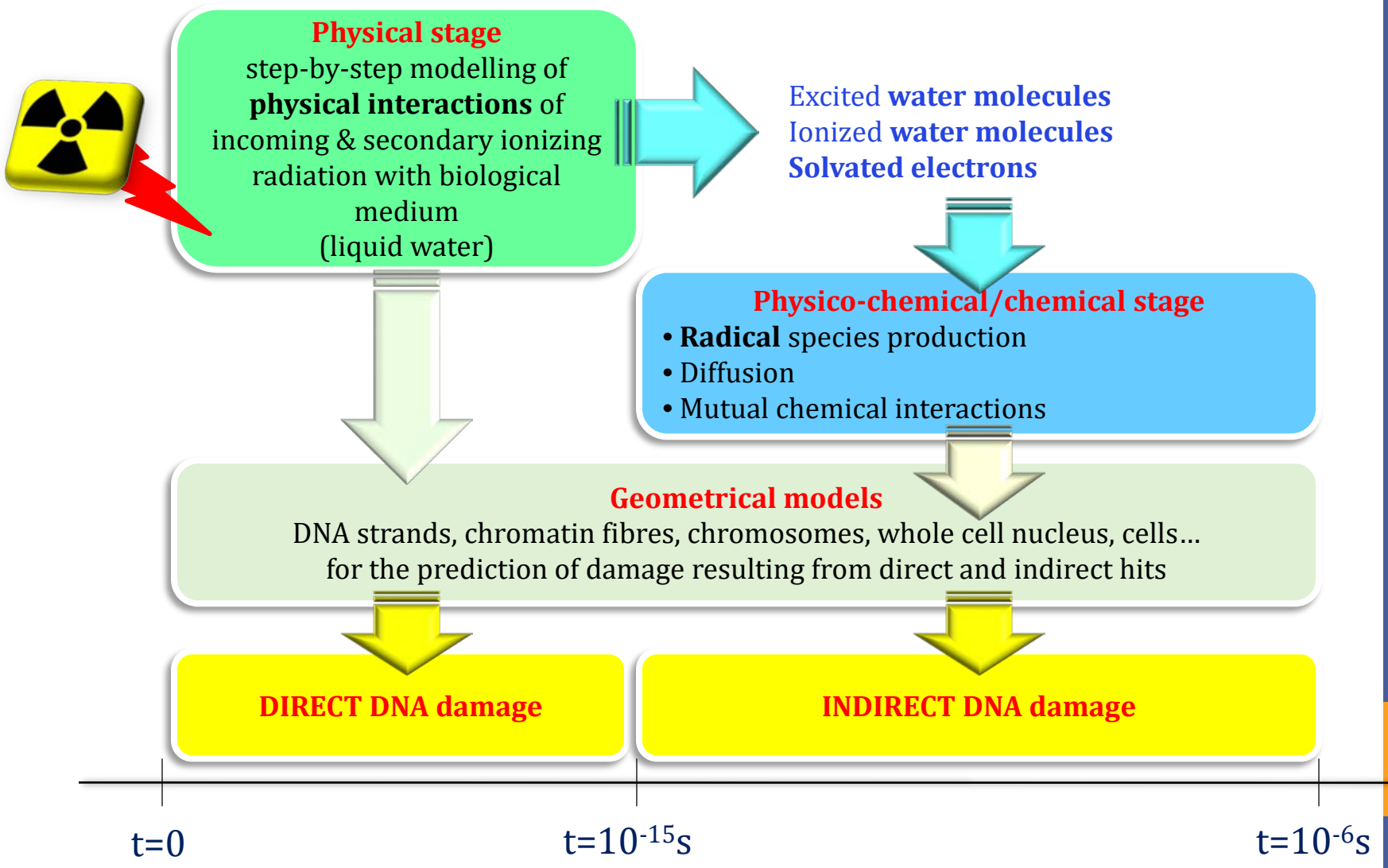


GEANT4 DNA PROJECT

HTTP://GEANT4-DNA.ORG/

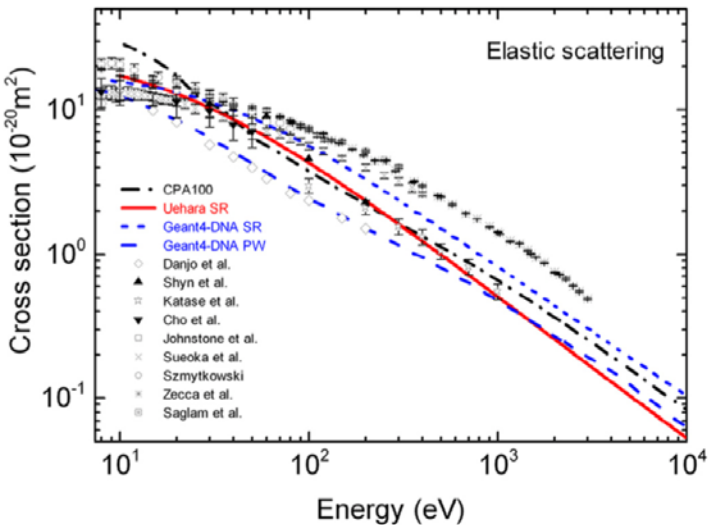
How can Geant4-DNA simulate early DNA damage ?

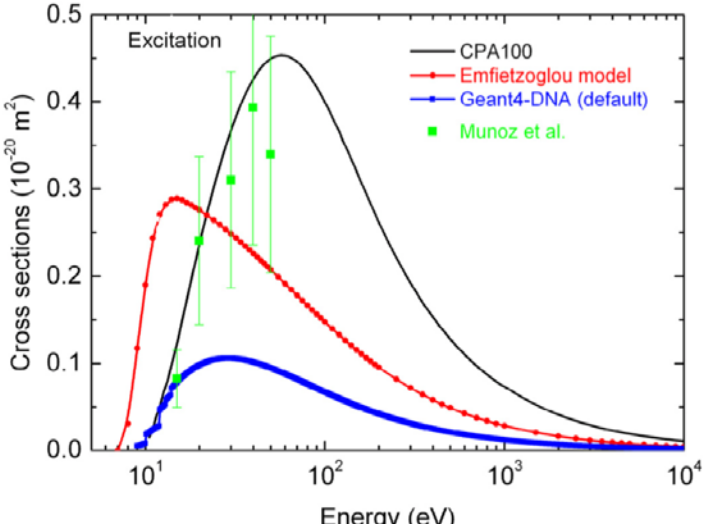
Phys. Med. 31 (2015) 861-87; 32 (2016) 1187-1200

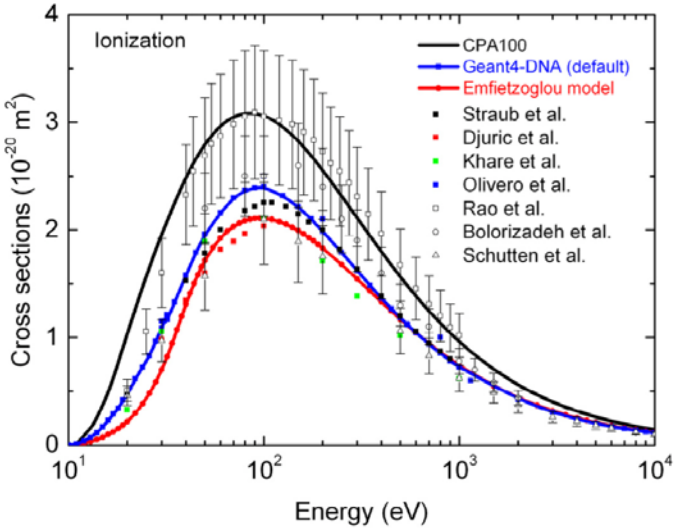


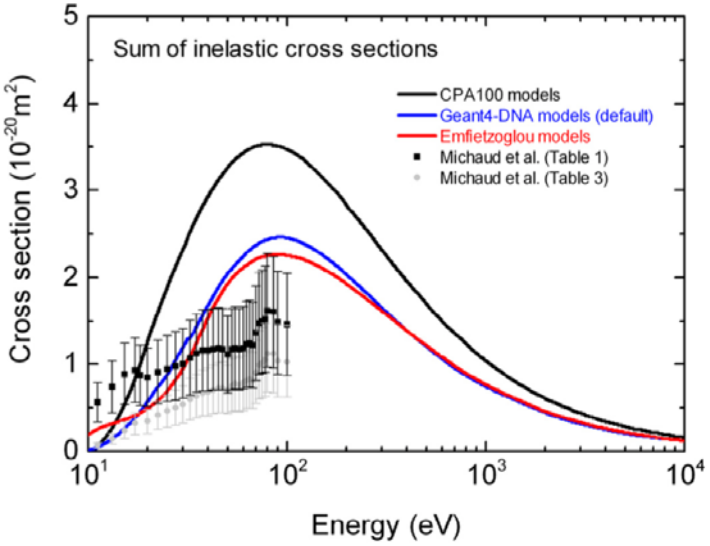
New CPA100 electron cross section models for liquid water in Geant4 10.4 Beta

Phys. Med. 31 (2015) 861









In total, 3 alternative sets of models for electrons in Geant4-DNA

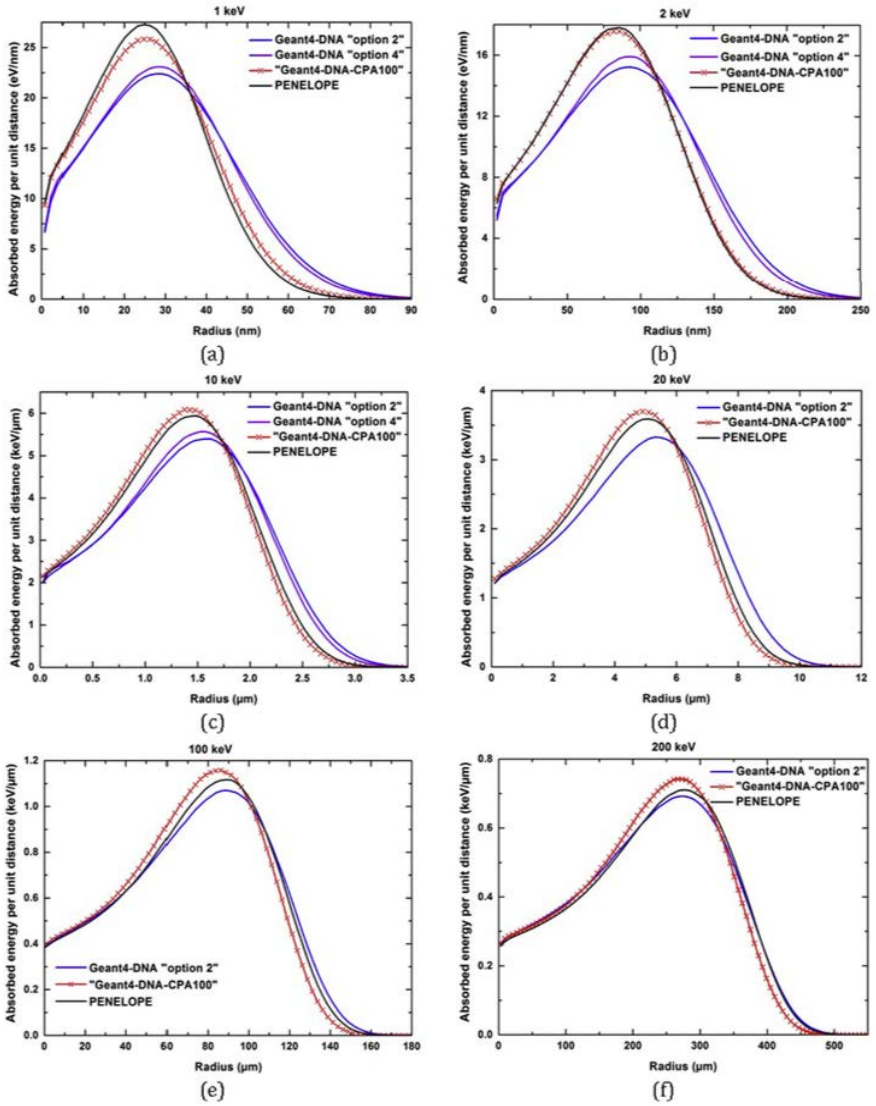
Dose point kernel simulations

Example of DPK comparison in liquid water between

- Geant4-DNA option 2 (default)
- Geant4-DNA option 4 (Ioannina)
- Geant4-DNA CPA100 models
- PENELOPE 2011

The comparison with the reference Monte Carlo code PENELOPE, set to perform step-by-step simulation, showed very good agreement.

For all tested energies, the maximum relative difference between simulated DPK, which occurs for 1 keV electrons, is less than 10%.



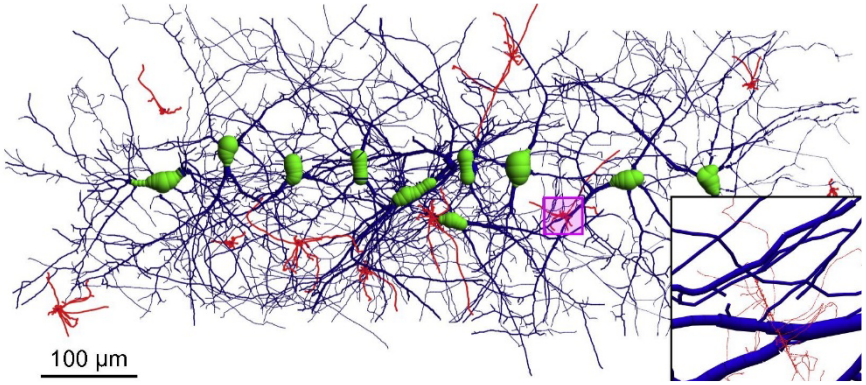
Nucl. Instrum. Meth. B 398 (2017) 13-20

Investigating radiation damage to central nervous system in astronauts thanks to Geant4-DNA

Radiation damage to the central nervous system has been an on-going challenge for the last decades primarily due to the issues of brain radiotherapy and radiation protection for astronauts during space travel.

Now it becomes possible to investigate early biological damage induced by ionizing radiations in a sample neural network by means of modelling physico-chemical processes occurring in the medium after exposure, thanks to Geant4-DNA

« neuron » extended example will be released in Geant4 10.4 Beta

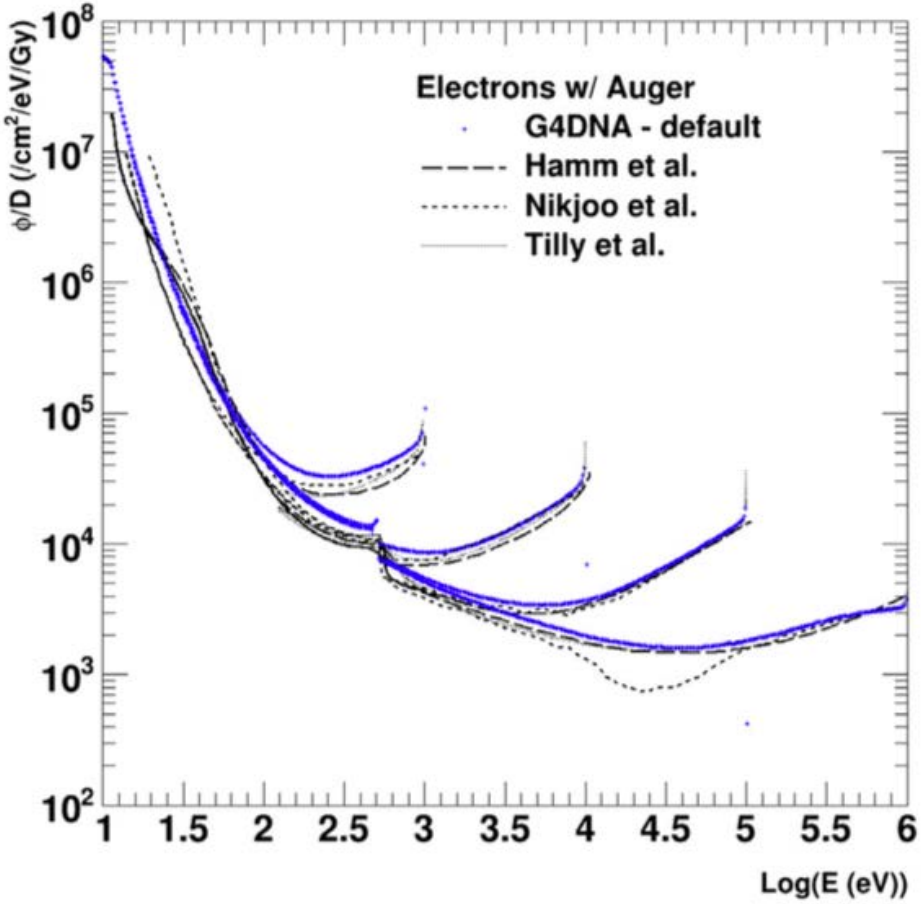


Phys. Med. 32(12) 1510–1520 (2016)

National University of Mongolia, Oulan Baator, June 2016

Geant4-DNA: slowing down spectra

Slowing-down electron spectra for 1 keV, 10 keV, 100 keV and 1 MeV incident electrons simulated with Geant4-DNA ‘‘default” models (blue points), compared to literature data. Auger electron production has been activated as well as electron sub-excitation processes.

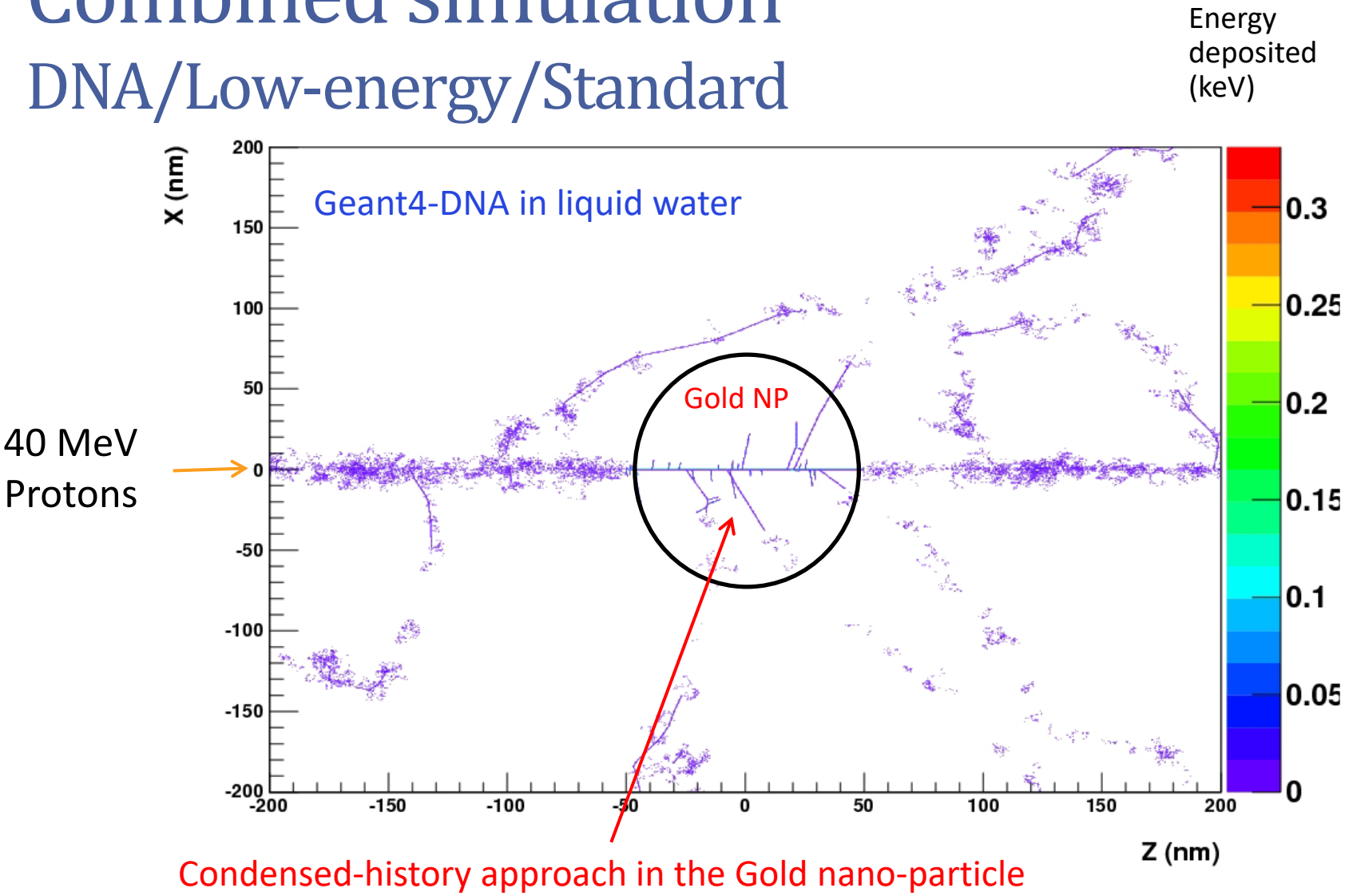


New « slowing » extended example

Geant4-DNA : perspectives

- Physics
  - Inclusion of alternative cross section models for electrons and ions
    - Liquid water + DNA-like materials + gas materials for nanodosimeters + metals
- Physico-chemistry/chemistry
  - Faster alternative approach for the simulation of water radiolysis
  - Combination of geometry & chemistry
  - Addition of scavenger species and reactions
- Biology
  - Multi-scale geometrical models of biological targets, including « deformable » geometries
  - Prediction of direct and non-direct DNA simple & complex damages in realistic cells
  - Time evolution of damage: repair processes, in collaboration with JINR Dubna, Russia
- Computing acceleration
  - GPU for chemistry in collaboration with KEK, Japan
- Continue verification (with other codes) and validation
  - using experimental data
- Budget and manpower remain an important issue

Combined simulation
DNA/Low-energy/Standard



The gold NP can be substituted with Ta_2O_5 and water

J. Appl. Phys. 120 (2016) 244901

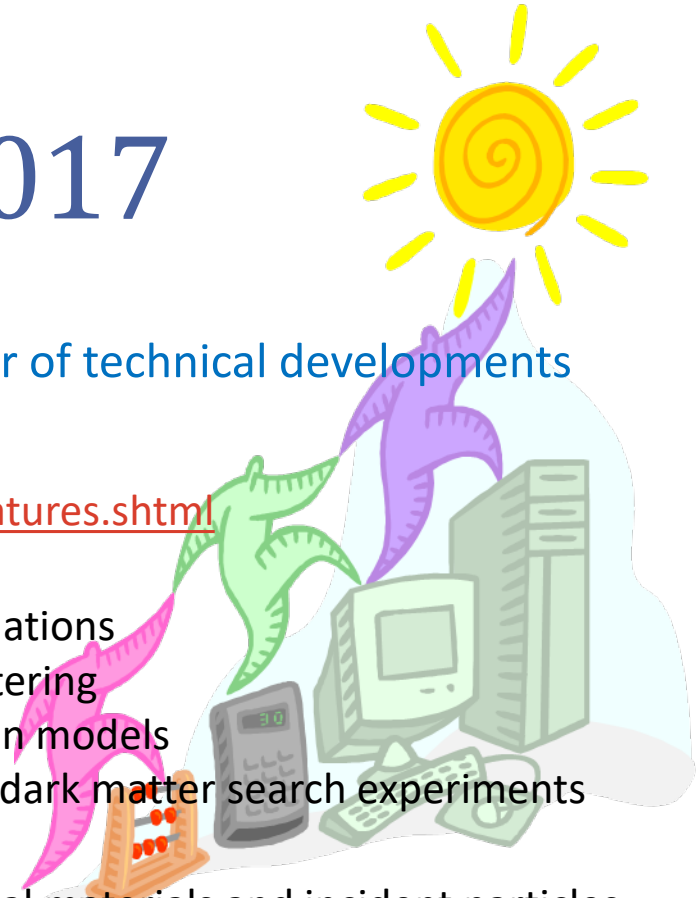
Phys. Med. 32 (2016) 1852-1861, 1216-1224

Nucl. Instrum. Meth. B 373 (2016)

EM physics configuration

- Until Geant4 10.2 we had a limitation Geant4 EM physics should be customized by a user for any special needs:
  - Different models for G4Region
  - Different model options for G4Region
  - Standard/DNA models
- This customisation can be done properly only by an expert user
  - make problems even for top experts
- For 10.2 we provide new UI commands which allow addition of models on top of any Physics List:
  - /process/em/AddPAIRegion all myregion PAI
  - /process/em/AddMicroElecRegion myregion
  - /process/em/AddDNARegion myregion DNA_Opt0
- For 10.3 we provide new UI command:
  - /process/em/AddEmRegion myregion G4EmStandard_Opt3
- This is not full PhysicsList per G4Region but EM physics configuration per G4Region similar to it
  - By this new command we do not fully emulate Opt0, Opt1,..Opt3,..GS, SS
  - Mainly multiple scattering models and atom de-excitation
  - Not all EM options can be configured per G4Region
- This approach is accepted by the CMS collaboration for 2017 large scale simulation production
  - FTFP_BERT_EMM is current default for CMS

Geant4 plans for 2017



- Geant4 plan for 2017 includes less number of technical developments and more physics model refinements
  - Detailed list of work items: http://geant4.cern.ch/support/planned_features.shtml
- EM standard
  - Improve default model of energy loss fluctuations
  - Improve models of single and multiple scattering
  - Improve bremsstrahlung and pair production models
  - Add necessary extensions for simulation of dark matter search experiments
- EM low-energy
  - DNA cross-section models for extra biological materials and incident particles
  - New chemistry models
  - MicroElec models
    - Update to more easily implementation for different materials
  - Addition of Remizovich scattering model for grazing angles
  - RBE modules for biological damage computation
- The new project GeantV is under development:
  - https://geant.web.cern.ch/content/publications