EM low energy / Geant4-DNA extended examples

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List of 6 new examples

- icsd
- mfp
- microyz (update)
- slowing
- spower
- splitting

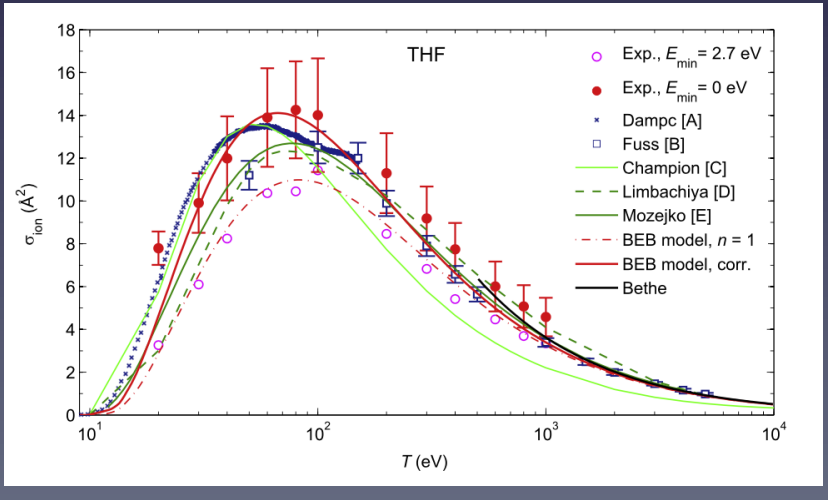
All located in extended/medical/dna

1) icsd

New bio-materials discrete XS

- New cross sections available for biomaterials in Geant4-DNA: part of the effort to extend Geant4-DNA models to other materials than liquid water
- Cross sections for biological materials are proposed since Geant4 10.4 Beta, they are applicable to DNA constituents
  - tetrahydrofuran (THF), trimethylphosphate (TMP), pyrimidine (PY) and purine (PU)
  - serving as models for the deoxyribose and phosphate groups in the DNA backbone as well as for DNA bases
- For the following incident particles
  - electrons (12 eV-1keV, elastic + excitation + ionisation) : from measurements @ PTB, Germany
  - protons (70 keV-10 MeV, ionisation) from the HKS approach

Eg. total electron ionisation cross sections in THF



More details in
Rad. Phys. Chem. 130 (2017) 459–479

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June 2017

IonizationClusterSizeDistribution

- developed by IRSN team (C. Villagrasa, S. Meylan)
- explains to user how to use these new "bio" cross sections
  - PhysicsList by 'hand' (including elastic, ionisation and excitation processes for electrons)
  - Material is TetraHydroFuran (THF) precursor of DNA deoxyribose (density is 1.346 g/cm3)
- output: two ROOT ntuples
  - information for calculating the ionisation cluster size distribution per event
  - interaction information at the step level

2) mfp

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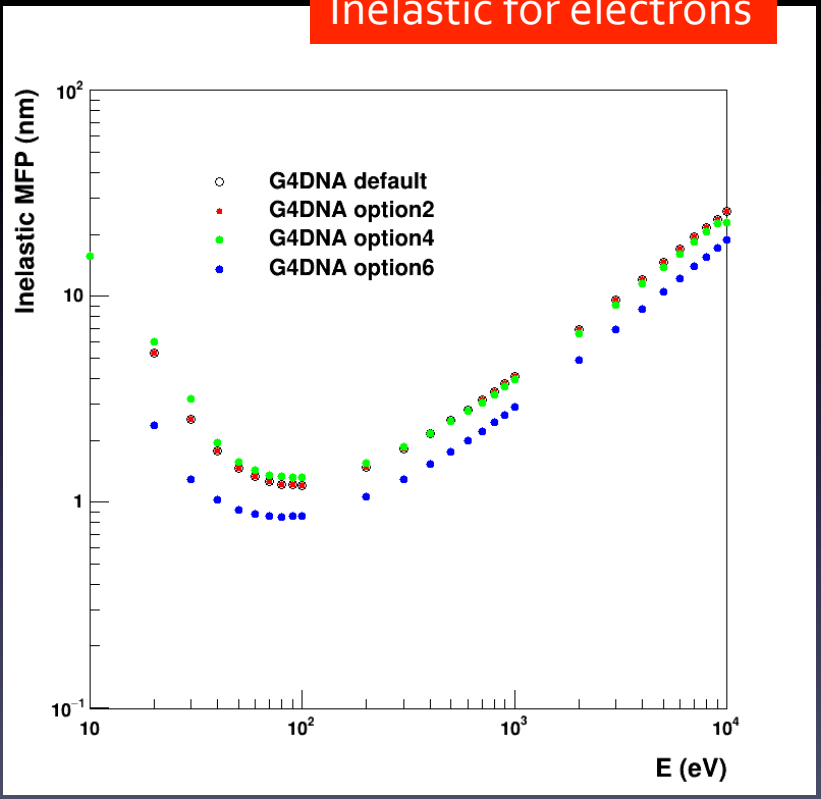
MeanFreePath

- a test to evaluate the accuracy of the code compared to other track structure (discrete) codes of the literature:
  - calculation of Mean Free Path in liq. water (using Gean4-DNA)
  - regular request by users

- the user can simulate MFP activating discrete processes of his/her choice
  - inelastic
  - full
  - with or without Geant4-DNA sub-excitation processes

Inelastic for electrons



See extended/medical/dna/mfp example

3) microyz

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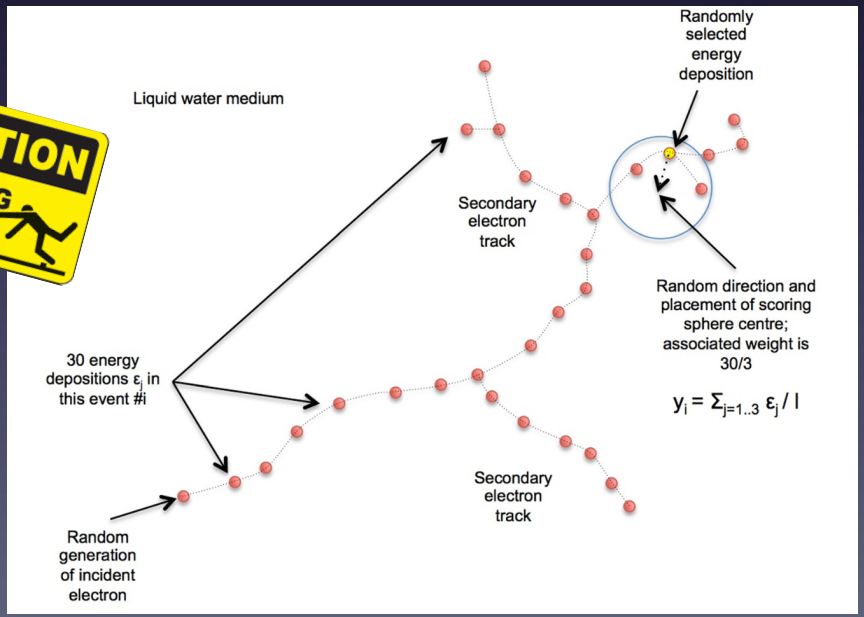
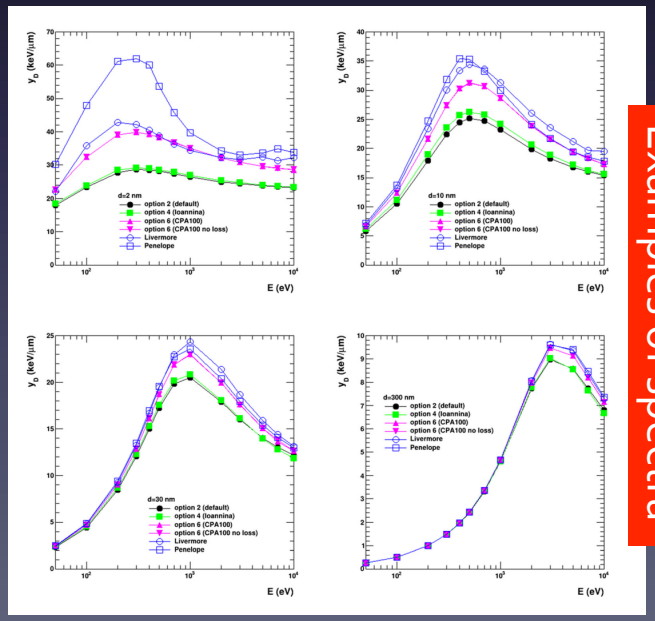
J. Appl. Phys. 122 (2017) 024303 (link)

microyz

- For the first time, we provide an extended example capable of simulating microdosimetry spectra: lineal energy (y), specific energy (z), frequency-mean lineal energy, dose-mean lineal energy, frequency-mean specific energy, dose-mean specific energy
- energy scored in spheres of selected radius
- particular care for weighting of energy scoring… (many users ignore weighting)

$\overline{y}_F$ $\overline{y}_D$ $\overline{z}_F$ $\overline{z}_D$





Examples of spectra

See extended/medical/dna/microyz example

4) slowing

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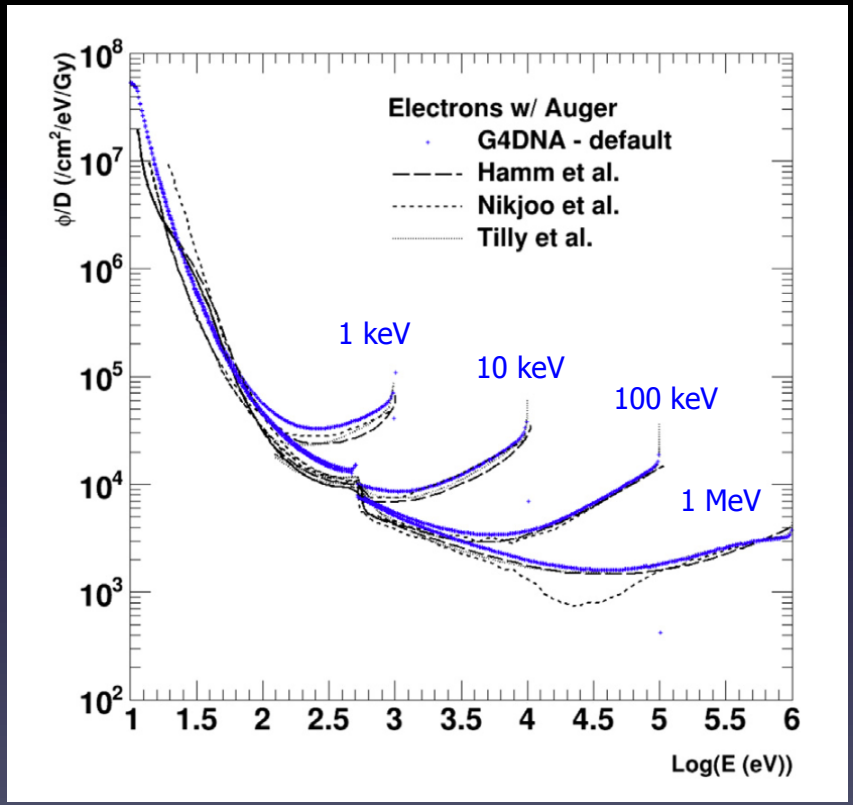
slowing down spectra

- a reliable test to evaluate the performance of track structure codes
- represent the fluence distribution (differential in energy) of both the primary and all subsequent generations of secondary electrons generated through the full slowing-down process in liquid water
- ∅(E)dE is the total distance travelled by electrons while their energy is in the interval E, E+dE (Vassiliev, 2012)
- method: we record for each simulation step the kinetic energy of each electron undergoing a Geant4-DNA inelastic process in a log-binned histogram, setting for each record a statistical weight equal to the size of the step.
- small influence of sub-excitation processes at low energy; Auger electron production from Oxygen should be considered.
- includes UI tracking cut selection



Nucl. Instrum. Meth. B 397 (2017) 45 (link)

See extended/medical/dna/slowing example

5) spower

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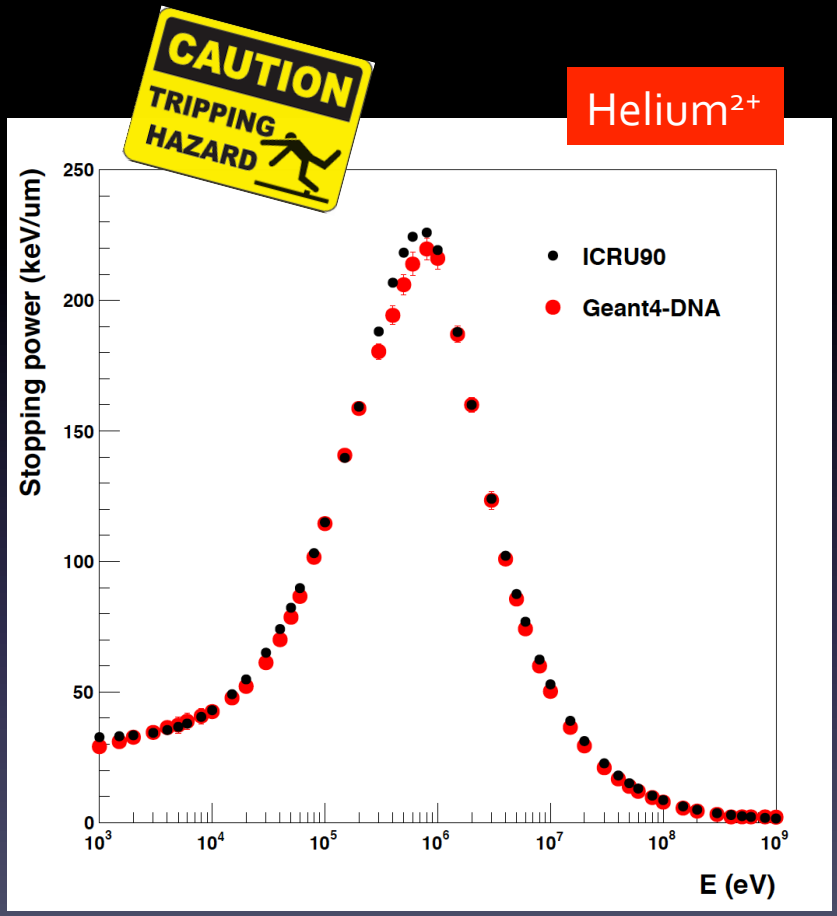
stopping power

- a reliable test to evaluate the accuracy of the code
- Geant4-DNA does not use SP tables: then how can we calculate SP ?
- users usually try to simulate SP by dividing energy loss over step length but forget to select stationnary regime
  - (alternative analytical calculation is always possible from differential ionisation cross sections and excitation cross sections)
- we provide specific stationary Geant4-DNA physics constructors for liquid water which activate stationary regime in all inelastic models



Nucl. Instrum. Meth. B 397 (2017) 45 (link)

See extended/medical/dna/spower example

6) splitting: acceleration of Geant4-DNA Physics

See next slides by José Ramos Mendez

Thanks

Backup

Phys. Med. Biol. 62 (2017) 5908-5925 (link)

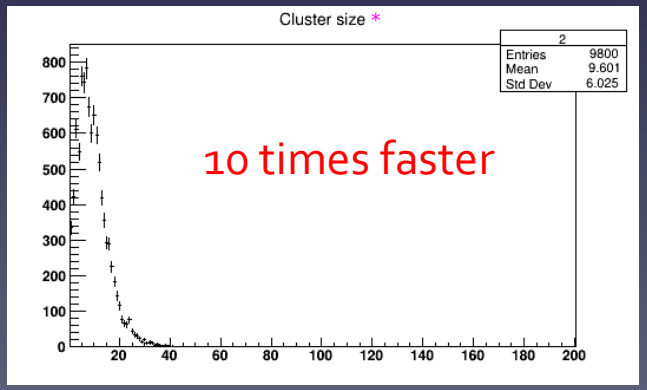
Accelerating simulations: variance reduction

- An new extended example, "splitting", provided by J. Ramos-Mendez (UCSF) is provided to illustrate variance reduction technique in the Geant4-DNA ionisation process
- Method:
  - ionisation events are scored in a nanoscaled cylinder (6 nm x 10 nm).
  - ionised electrons generated by the first generation of secondary electrons are split (via G4WrappedProcess), i.e. new "clone electrons" are generated, labeled and propagated. The label is used to classify those new particles as if they were produced by independent histories to avoid overlapping of tracks at final analysis.
  - the splitting is performed only if the ionization event occurred in the cylinder.
- The user can define the split number using a UI command:

  `/vrt/numberOfSplit 10` (default is 1, no split)

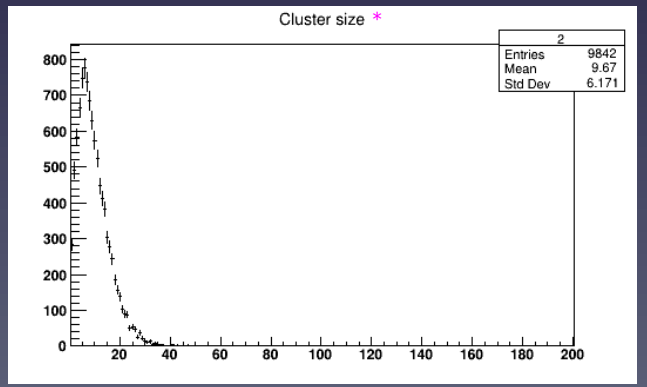
Example of He^{2+} of 4 MeV

100 primaries & numberOfSplit = 10



*number of ionisations produced within the scoring volume produced by a single history

1000 primaries & numberOfSplit = 1



See extended/medical/dna/splitting example