Electromagnetic Physics Updates

Dennis Wright (SLAC)
(from presentations by
Sebastien Incerti (IN2P3-CENBG) and
Vladimir Ivantchenko (CERN, Tomsk State U.)

Geant4 Space Users Workshop
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Outline

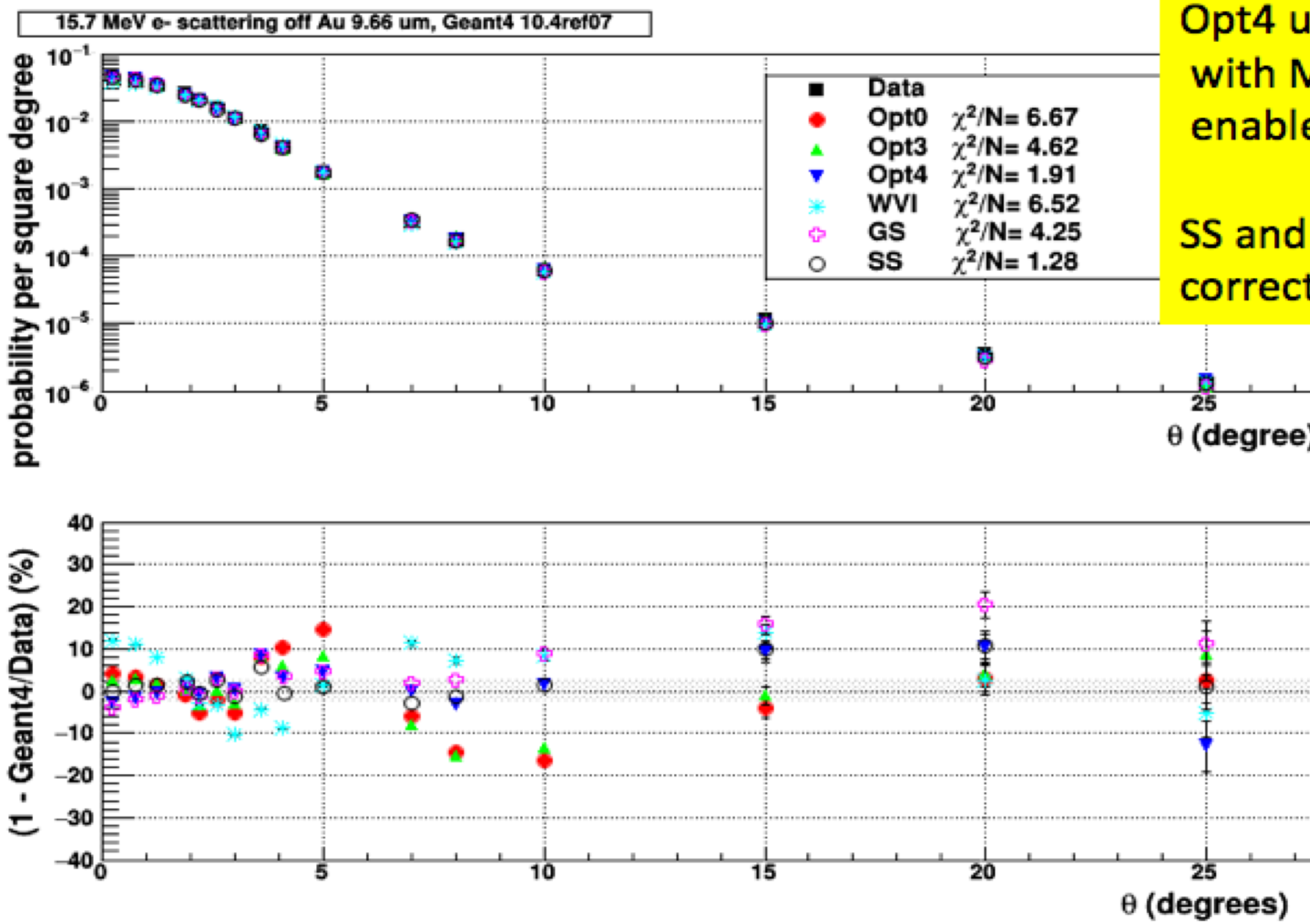
- Standard and high energy
- Low energy
- DNA (really low energy)

EM Model Development (1/5)

- Multiple scattering
  - GoudsmitSaunderson e^+/e^- multiple scattering code cleaned up and optimized
  - Urban model: new parameterization for lateral displacement sampling

- Mott corrections included in WentzelVI and Goudsmit-Saunderson MS
  - Mott differential cross section (dcs) is more precise
  - for speed we sample from screened Rutherford dcs
  - then apply ratio of (unscreened Rutherford dcs)/(Mott dcs) as a rejection function

Mott corrections in WentzelVI



Opt4 uses GS model with Mott corrections enabled

SS and WVI use Mott corrections

This is essential for sampling of high energy $e^{\pm}$ scattering

EM Model Development (2/5)

- Bremsstrahlung
  - reviewed and optimized sampling algorithm (now faster)

- Gamma conversion
  - reviewed and optimized sampling algorithm (now faster)
  - angular generators -> improved e^+/e^- final state angles
  - new 5D model: Bethe-Heitler pair production cross section sampled in 5 variables (θ_+ , θ_- , ϕ_+ , ϕ_- , x_+)

- Optical photons
  - substantial speedup of optical photon transport
  - G4RealSurface-2.1: expanded database for optical surfaces

EM Model Development (3/5)

- Triplet production (gamma conversion near atomic electron) now possible for low energy models:
  - G4LivermoreNuclearGammaConversionModel
  - G4BoldyshevTripletModel

- Updated EM low energy database
  - G4EMLOW-7.3 required as of Geant4 10.4

- Extended coverage of shell ionization models
  - K, L and M shell form factors improved
  - covers $5 < Z < 93$
  - also for PIXE (incident p, α)

EM Model Development (4/5) (new models, work in progress)

- Gamma processes
  - 3-gamma annihilation ($e^+ e^- \rightarrow \gamma\gamma\gamma$)
    - rare but useful in PET (non-colinear gammas)
    - more likely at very high energies

- Implementation of ICRU90 stopping power data
  - up to now Geant4 used mostly ICRU73 standard at lower energies
  - ICRU90 has accurate data for a limited number of materials

EM Model Development (5/5) (new models, work in progress)

- G4LinhardSorensenIonModel
  - nuclear size correction to stopping power
  - important at high energies

- G4AtimaEnergyLossModel and G4AtimaFluctuations
  - precise energy loss of heavy ions in materials
  - uses approach of ATIMA program for stopping power

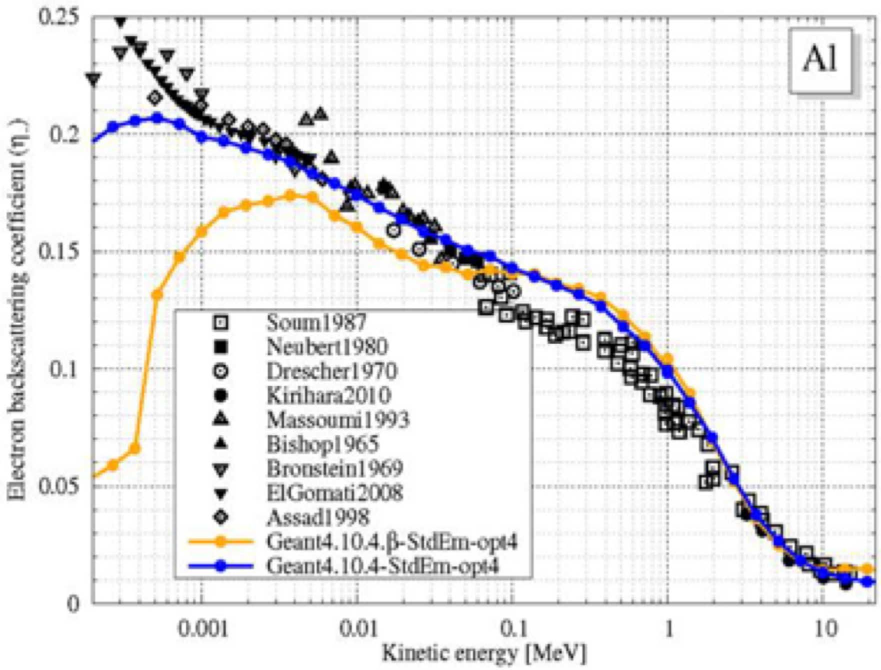
- Above 4 models released for first time in Geant4 10.5
  - maybe not completely ready for production

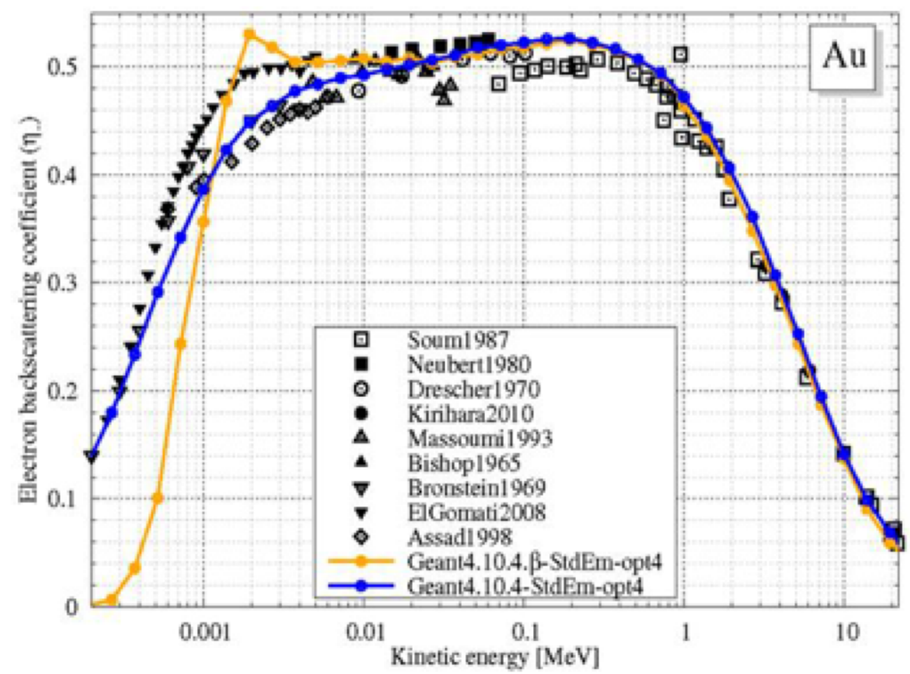
Configuration of EM physics

- 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 and Opt2 with simplified multiple scattering and other options
  - The alternative Opt4 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
  - Opt3 is kind of intermediate between Opt0 and Opt4
- 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
  - EM physics configuration and PAI ionization model may be defined for or more G4Region(s)
    - This feature is used by ALICE and CMS experiments at LHC

Backscattering validation for 10.4

(CHEF-2017 Conference JINST 13 (2018) C02054)





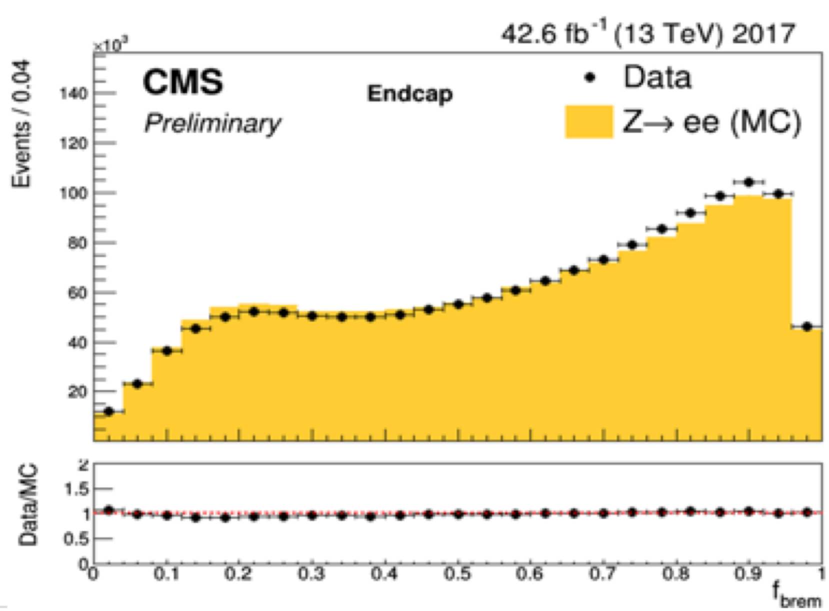
- *Simulation of electron backscattering from Al (left) and Au (right) targets versus data from different experiments.*
- *Opt4 EM configuration is with the Urban model (yellow) and the GS model with “error-free” stepping (blue)*

EM Physics List approach

- We are trying keep stable
  - Opt0 – for ATLAS (default or _EM0)
  - Opt1 – for CMS (_EMV)
- Improved models are included in
  - Livermore (_LIV)
  - Penelope (_PEN)
  - Opt3 – standard models (_EMY)
  - Opt4 – our recommendation for the most accurate physics (_EMZ)
- New models/features are tested in
  - Opt0 with GS msc for $e^{\pm}$ (__GS)
  - WentzelVI model (_WVI)
  - Single scattering (__SS)
  - lowenergy - 5D-pair production, LS ion ionization (__LE)

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 .

Going Forward in HEP

- High energy/high luminosity at LHC (Run3)
  - need more statistics
  - current EM physics modeling uncertainties may contribute to systematic uncertainty of physics observables
  - rare EM processes (order % and below) may create non-standard event patterns

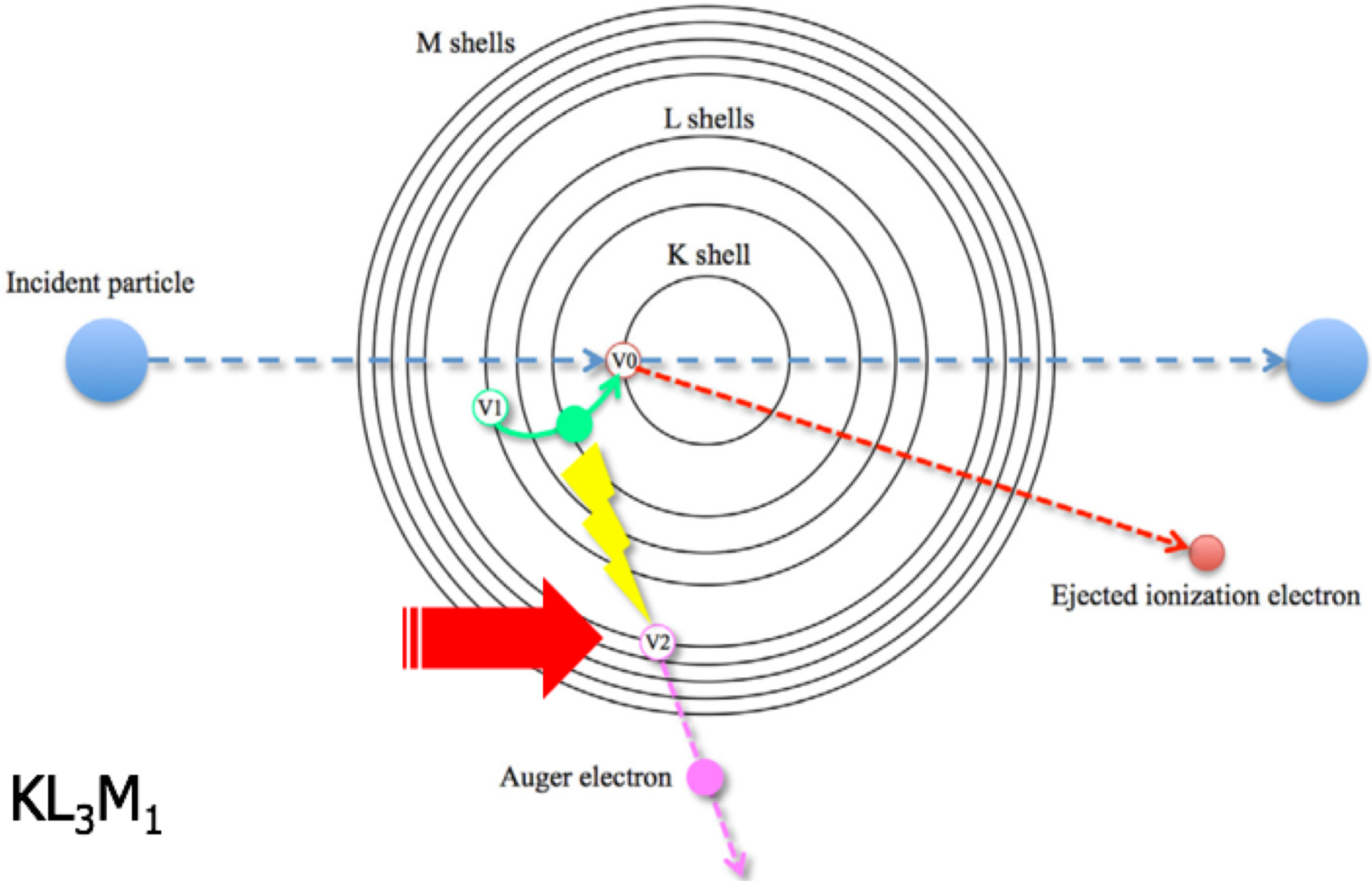
- FCC (Future Circular Collider)
  - EM simulation up to 100 TeV required
  - LPM suppression for gamma conversion and bremsstrahlung
  - EM processes for interaction region
  - nuclear recoil effects

Current Priorities in HEP

- Review/update all models to state of the art
- Extensions of existing models to deal with next-to-leading order for cross sections
- Add sampling of second-order final states
  - additional recoiling atomic electrons
  - extra gammas or e+/e- pairs
  - more recoil nuclei

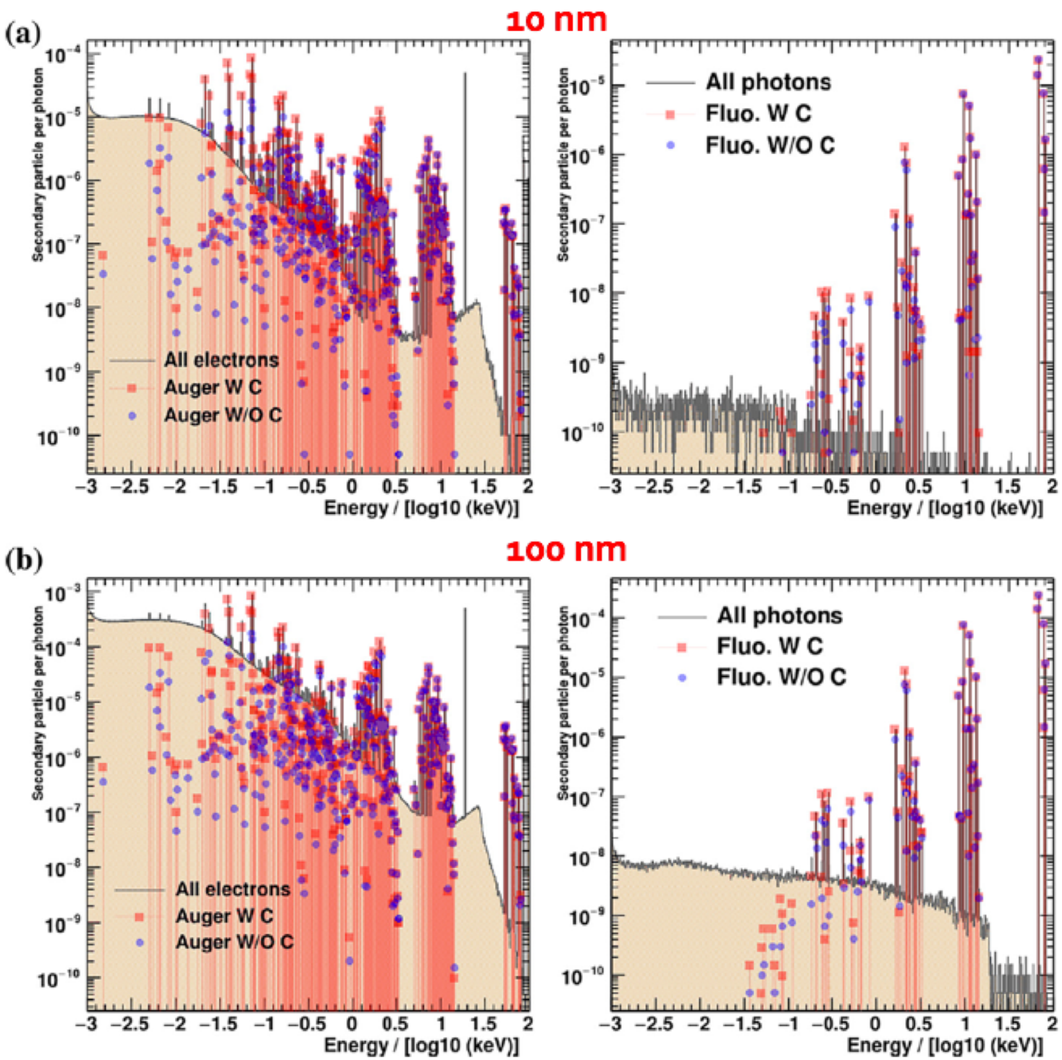
- Speeding up the code (for hadronics, too)
  - more physical detail → slower code
  - higher luminosity → many more statistics required

Full Auger Cascade Added



KL_3M_1

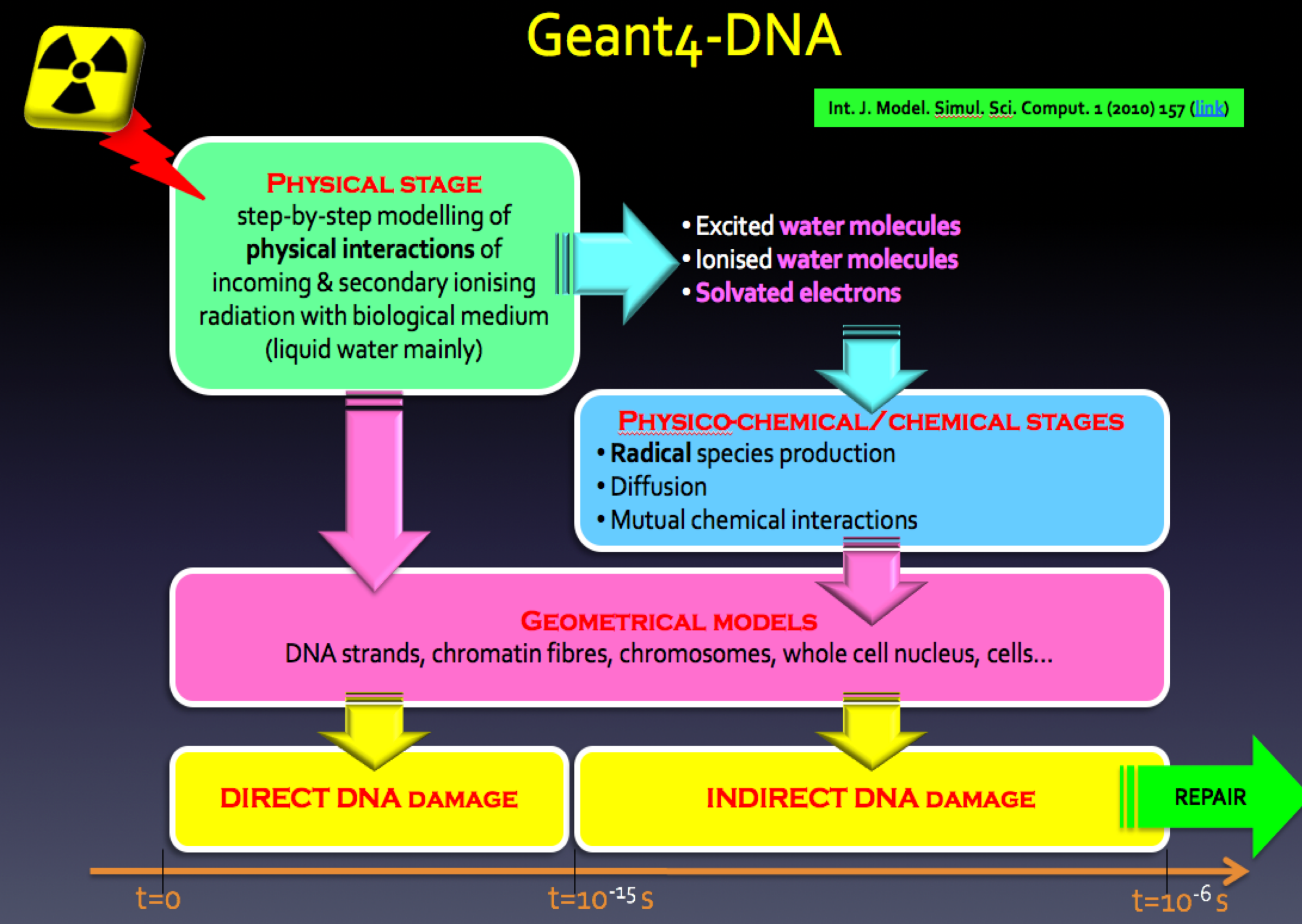
Atomic De-excitation Cascade in GNPs



- γ and e^- energy spectra from 100 keV γs on GNP (gold nano-particles)
- NIM B 372, 91 (2016).

Atomic Deexcitation

- New experiment-derived electron binding energies
  - whenever possible, BEs taken from LBL (XDB) X-Ray Data Booklet
  - all others from theory
  - up to Z = 120
  - this version is still optional – old (all theory) version still the default
- Auger emission and fluorescence are switched off by default
  - too time-consuming


Geant4-DNA
Int. J. Model. Simul. Sci. Comput. 1 (2010) 157 (link)
PHYSICAL STAGE
step-by-step modelling of physical interactions of incoming & secondary ionising radiation with biological medium (liquid water mainly)
• Excited water molecules
• Ionised water molecules
• Solvated electrons
PHYSICO-CHEMICAL / CHEMICAL STAGES
• Radical species production
• Diffusion
• Mutual chemical interactions
GEOMETRICAL MODELS
DNA strands, chromatin fibres, chromosomes, whole cell nucleus, cells…
DIRECT DNA DAMAGE
INDIRECT DNA DAMAGE
REPAIR
t=0
t=10^-15 s
t=10^-6 s

Overview of physics models for TS simulations in liquid water

Geant4 10.4
December 2017

Electrons

- Elastic scattering
  - Screened Rutherford and Brenner-Zaider below 200 eV
  - Updated alternative version by Uehara with vapor screening param.
  - Independent Atom Method (IAM) by Mott et al. & VLE data in ice from CPA100
  - Partial wave framework model by Champion et al., 3 contributions to the interaction potential
- Ionisation (5 shells)
  - Dielectric formalism & FBA using Heller optical data up to 1 MeV, and low energy corrections (exchange, interference and Coulomb-field) by Emfietzoglou et al.
  - Improved alternative version by Emfietzoglou and Kyriakou including low energy corrections (« Ioannina U. »)
  - Relativistic Binary Encounter Bethe (RBEB) by Terrissol from CPA100 TS code
- Electronic excitation (5 levels) (*)
  - Dielectric formalism & FBA using Heller optical data and semi-empirical low energy corrections, , derived from the work of Emfietzoglou et al.
  - Improved alternative version by Emfietzoglou and Kyriakou
  - Dielectric formalism by Dingfelder from CPA100 TS code
- Vibrational excitation (*)
  - Michaud *et al.* xs measurements in amorphous ice with factor 2 to account for phase effect
- Dissociative attachment (*)
  - Melton xs measurements

Med. Phys. 37 (2010) 4692 (link)
Appl. Radiat. Isot. 69 (2011) 220 (link)
Med. Phys. 42 (2015) 3870 (link)
Phys. Med. 31 (2015) 861 (link)
Nucl. Instrum. and Meth. B 343 (2015) 132 (link)
Phys. Med. 32 (2016) 1833 (link)
Med. Phys. 45 (2018) e722-e739 (link)

(*) only available in Geant4-DNA

- **Protons & H**
  - Excitation (*)
    - Miller & Green speed scaling of e^- excitation at low energies and Born and Bethe theories above 500 keV, from Dingfelder *et al.*
  - Ionisation
    - Rudd semi-empirical approach by Dingfelder *et al.* and Born and Bethe theories & dielectric formalism above 500 keV (relativistic + Fermi density)
  - Charge change (*)
    - Analytical parametrizations by Dingfelder *et al.*
  - Nuclear scattering
    - Classical approach by Everhart *et al.*
- **He^0, He^+, He^{2+}**
  - Excitation (*) and ionisation
    - Speed and effective charge scaling from protons by Dingfelder *et al.*
  - Charge change (*)
    - Semi-empirical models from Dingfelder *et al.*
  - Nuclear scattering
    - Classical approach by Everhart *et al.*
- **Li, Be, B, C, N, O, Si, Fe**
  - Ionisation
    - Speed scaling and global effective charge by Booth and Grant
- **Photons**
  - from EM « standard » and « low energy »
    - Default: « Livermore » (EPDL97)

PhD theses of
H. N. Tran (2012)
Q. T. Pham (2014)
J. Bordes (2017)

Recommended Geant4-DNA Constructors and Examples for Liquid Water

Process	Geant4-DNA physics constructors electron models		
	G4EmDNAPhysics_option2	G4EmDNAPhysics_option4	G4EmDNAPhysics_option6
Ionization (inelastic)	Emfietzoglou dielectric model (11 eV–1 MeV)[5]	Emfietzoglou–Kyriakou dielectric model (10 eV–10 keV)[47]	Relativistic binary encounter Bethe model from CPA100 code (11 eV–256 keV)[48]
Electronic excitation (inelastic)	Emfietzoglou dielectric model (9 eV–1 MeV)[5]	Emfietzoglou–Kyriakou dielectric model (8 eV–10 keV)[47]	Dielectric model from CPA100 code (11 eV–256 keV)[48]
Elastic scattering (elastic)	Partial wave model (7.4 eV–1 MeV)[5]	Uehara screened Rutherford model (9 eV–10 keV)[47]	Independent Atom Method model from CPA100 code (11 eV–256 keV)[48]
Vibrational excitation (inelastic subexcitation)	Sanche data (2 eV–100 eV)[49]	n/a	n/a
Attachment (inelastic subexcitation)	Melton data (4 eV–13 eV)[50]	n/a	n/a
Auger electron emission	From the EADL database[51] and the Geant4 atomic relaxation interface[52,53]		
Default tracking cut[(*)]	7.4 eV	10 eV	11 eV

Extended example name	Purpose	Macro file	Other related reference(s)
dnaphysics	Detail of tracking, automatic combination with Geant4 standard EM physics models, modification of medium density	dnaphysics.in	[6]
microdosimetry	Combination "by hand" of Geant4 standard EM and Geant4-DNA processes and models in different regions	microdosimetry.in	[6]
range	Range, projected range, penetration	range.in	[59]
spower	Stopping power	spower.in	[72]
mfp	Mean free path	mfp.in	–
wvalue	Mean energy required for the creation of an ion pair in liquid water (the so-called "W-value")	wvalue.in	[47]
svalue	Dose to a liquid water target per unit of cumulated activity in a source region (the so-called "S-value")	svalue.in	[6,73,74]
slowing	Slowing-down electron spectra	slowing.in	[72]
microyz	Microdosimetric distributions (lineal energy y, specific energy z) and related quantities	microyz.in	[60]
TestEm12[(+)]	Dose point kernel	dna.mac	[6,59,75]
TestEm5[(+)]	Identification of atomic de-excitation products for Geant4-DNA processes	dna.mac	–

(link)

Geometries: realistic molecules using an interface to PDB

Developed @ LPC Clermont (L. Maigne et al.)

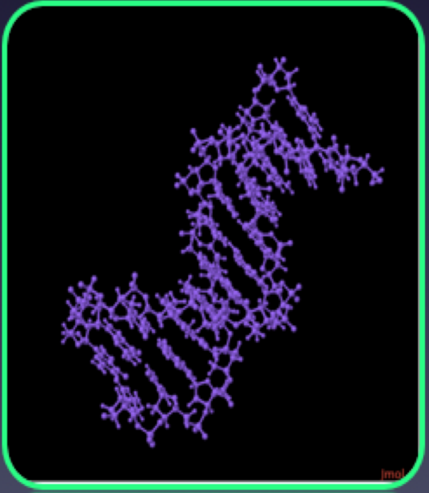
- PDB : Protein Data Bank

  http://www.rcsb.org/pdb/

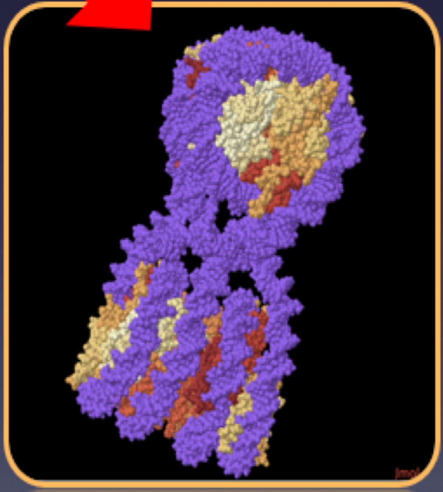
  - 3D structure of molecules
  - Proteins
  - Nucleic acids
- Description of DNA molecules
  - 1FZX.pdb
    - Dodecamer
    - 12 DNA base pairs
    - (2,8 x 2,3 x 4,01 nm³)
  - 1ZBB.pdb
    - Tetranucleosome
    - (9,5 x 15,0 x 25,1 nm³)

```
HEADER   STRUCTURAL PROTEIN/DNA              08-APR-05   1ZBB
TITLE    STRUCTURE OF THE 4_601_167 TETRANUCLEOSOME
...
ATOM      1  O5'  DA I   1      70.094  16.969 123.433  0.50238.00    O
ATOM      2  C5'  DA I   1      70.682  18.216 123.054  0.50238.00    C
ATOM      3  C4'  DA I   1      69.655  19.289 122.776  0.50238.00    C
...
TER   14223      DT J 347
...
HELIX    1   1 GLY A   44  SER A   57  1                            14
HELIX    2   2 ARG A   63  ASP A   77  1                            15
...
SHEET    1   A 2 ARG A  83  PHE A  84  0
SHEET    2   A 2 THR B  80  VAL B  81  1  O  VAL B  81   N  ARG A  83
```

1ZBB.pdb

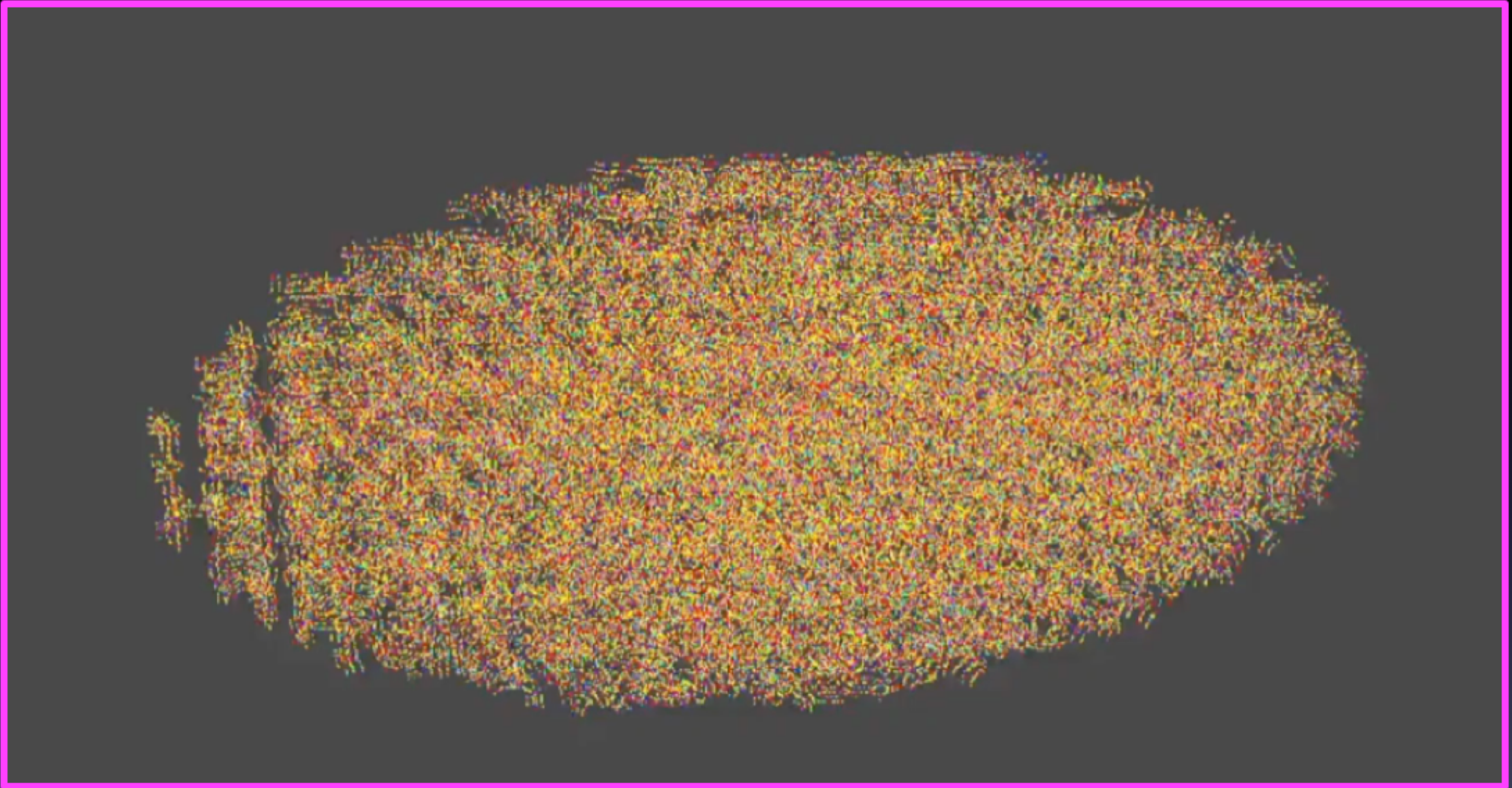


1FZX.pdb



1ZBB.pdb 15

Bacterium: modeling E. coli… in 2017



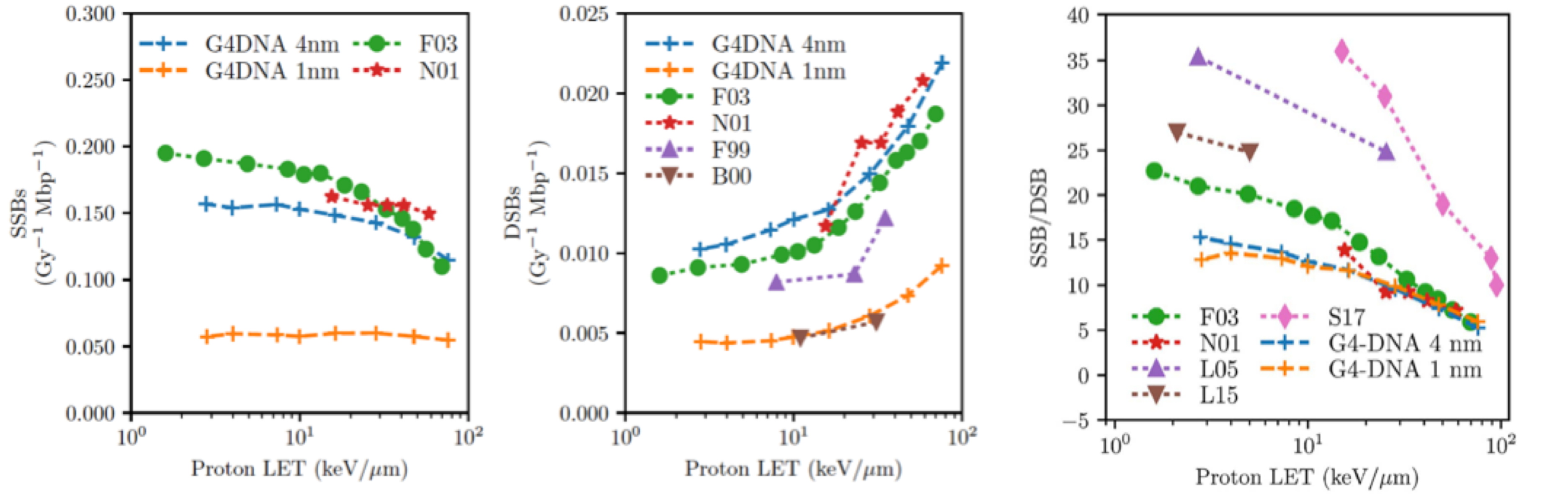
PhD thesis of N. Lampe @ LPCC and CENBG (2017)

Hilbert, 1.9 mm x 0.8 mm, 4.63 Mbp

Phys. Med. 48 (2018) 146 (link)

Phys. Med. 48 (2018) 146 (link)

E. coli : DNA damage from proton irradiation



More chemical plasmid damage from distant radicals ?

- Based on the faster « Independent Reaction Time » approach for the modeling of water radiolysis, developed by M. Karamitros (2017)
- Plausibility: SSB and DSB yields from proton damage simulated using Geant4-DNA, compared to results from the PARTRAC (F03) and the KURBUC (N01) simulation codes.
- Experimental DSB yields are indicated by F99 for human fibroblast cells, and B00 for V79 Chinese hamster cells.
- Experimental ratios are for plasmids.

Porting Geant4-DNA Physics to GPU

Developed @ KEK
MPEXS & MPEXS-DNA

Absorbed dose in voxellized water phantom irradiated with 100 keV electrons

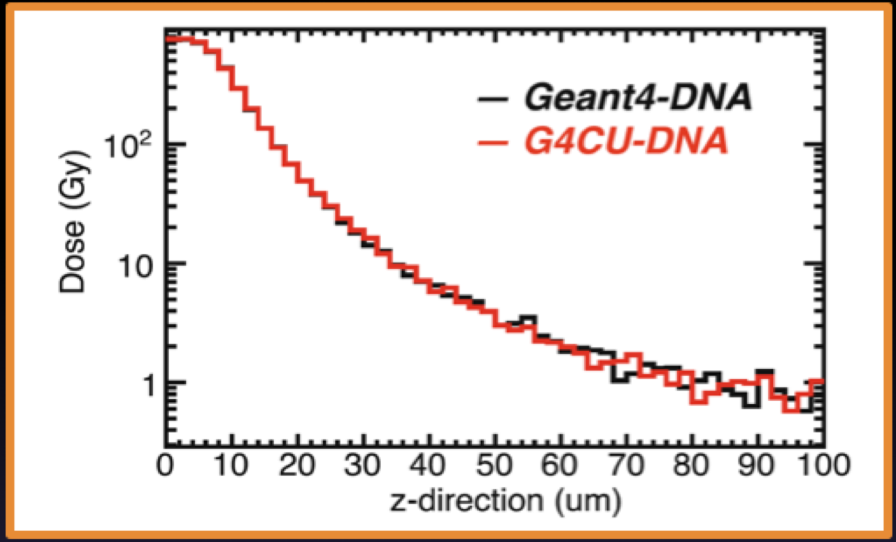


Table 4 Comparisons of computation time between GPU and CPU simulations

Incident particle	Initial energy	Geant4-DNA (CPU) (sec/particle)	G4CU-DNA (GPU) (sec/particle)	Speedup factor (=G4/G4CU)
e^-	100 keV	7.64×10^{-1}	1.05×10^{-2}	**72.9**
p	1 MeV	11.8	6.10×10^{-1}	**19.4**
He^{++}	1 MeV	12.3	6.63×10^{-1}	**18.6**

Achieved up to 70 speedup compared to single CPU (Intel Xeon E5-2643V2) for electron and gamma simulation using NVIDIA Tesla K20 GPU

Smart Innovation, Systems and Technologies 45 (2016) 323 (link)

Summary

- Standard EM code has been updated and optimized
  - expect significant CPU improvement (up to 20%)

- Precision of low energy EM has been improved
  - new models added as well

- Geant4-DNA continues to be expanded and used in many different application areas
  - GPU version being worked on