What's new in 11.2: Electromagnetic physics

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for the Geant4 EM physics group

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Agenda

- Update of infrastructure for EM physics
  - *EM data structure*
  - *Ion ionisation*
  - *Selected results*
- New EM model development
- Geant4-DNA developments

Disclaimer:

not all developments are discussed and not all authors are not shown in these slides

Update of infrastructure for EM physics

- **New dataset G4EMLOW8.5**
  - *Updated directory structure and cleanup of all README*
  - *Recommended access to G4LEDATA data without get of environment variable*
    - *const G4String& G4EmParameters::GetDirLEDATA();*
- **Initialization of static data**
  - *The problem report #2546 shown the problem of creation/destruction of static data of EM models*
    - *It was understood that the check G4VEmModel::IsMaster() in the case of more that 1 model object in the master thread may provide problems*
  - *The solution of the problem was found and released in Geant4 11.2*
    - *The class G4ElementData was extended to keep and destroy the data*
    - *Initialisation of the data is performed once, which is controlled by static std::once_flag applyOnce*
    - *Data are stored and destroyed by the G4ElementData class*
  - *This approach is implemented for the part of EM models and will be done for all in newer release*

G4ElementData class

- **G4ElementData is used for many years**
  - *It keeps G4PhysicsVectors and G4Physics2DVector data and fast run time access via Z and A*
- **Some concerns:**
  - *It was using C-arrays with fixed length Zmax=99*
  - *Data deleted by the consume class (it is the main problem!)*
- **Updated version for 11.2 of the class uses std::vector and std::pair instead of C-arrays**
  - *Zmax is defined by the consume class*
  - *Registered in G4ElementDataRegistry*
  - *Allowed extra structures for vector and 2D-vector per isotope*
- **G4ElementDataRegistry – new store**
  - *Has access method by the G4ElementData name*
  - *Is responsible for deletion end of job*
  - *Now G4ElementData may be shared between threads and be non-static*

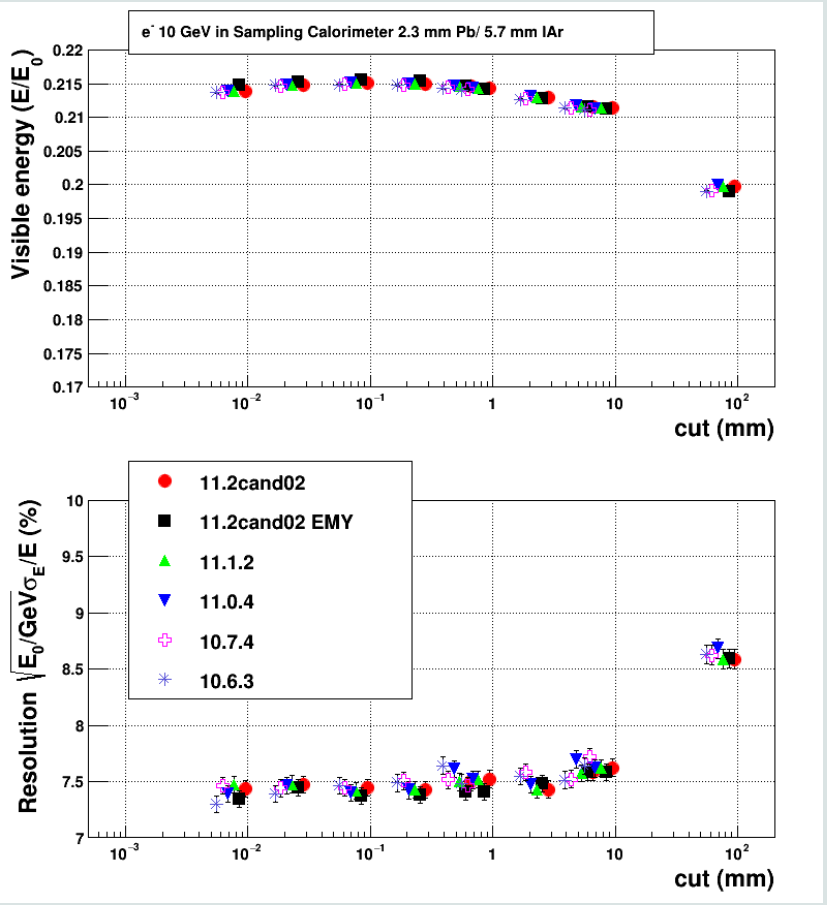
Ion ionisation

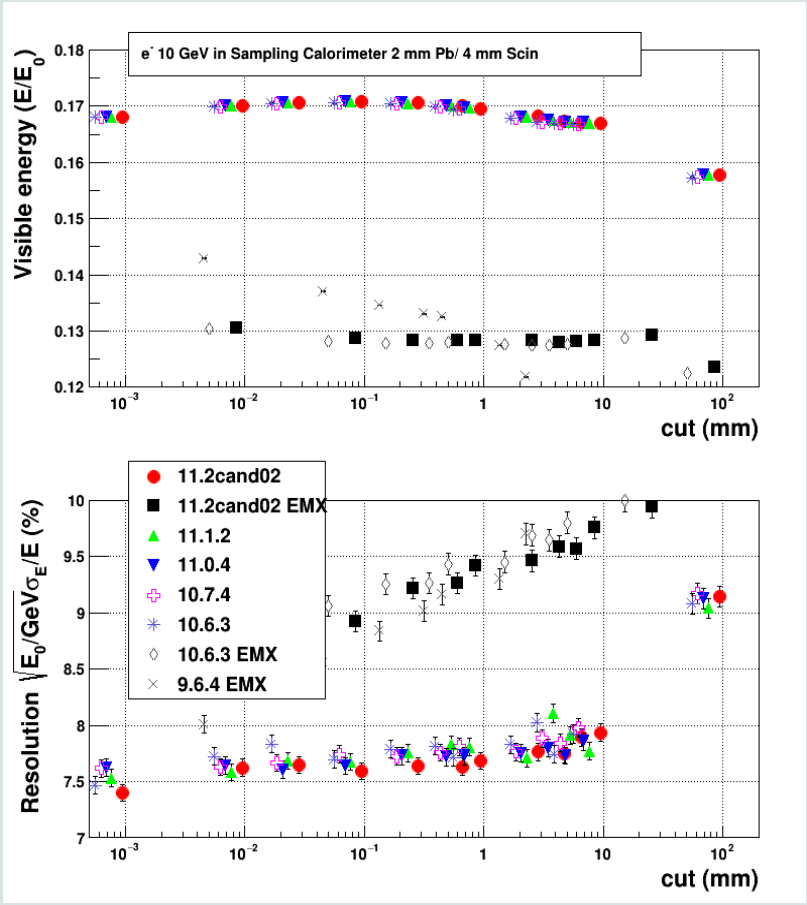
- **In recent Geant4 release ICRU90 data with proton, alpha, and ion data on stopping power were added**
  - *This improving accuracy so some applications but makes technical problems and provokes bug reports*
- **Some reorganization of ion ionization model was introduced in 11.2**
  - *G4BraggModel – is used for low energy protons and backup for any ion/target pair*
  - *G4BraggIonModel – for alpha particles at any target*
  - *G4LindhardSorensenModel – for all other ions*
- **Low-energy stopping power data are used for $E_{kin}*M_{proton}/M_{ion} < 2$ MeV/u**
  - *For protons - ICRU90 (if available for a material), PSTAR for the rest*
  - *For alpha - ICRU90 (if available for a material), ASTAR for the rest*
  - *For other ions ICRU90 (if available for a material), alternatively ICRU73 (if available for a material), for the rest PSTAR and effective charge model*
  - *New stopping power data may be added (even custom data)*

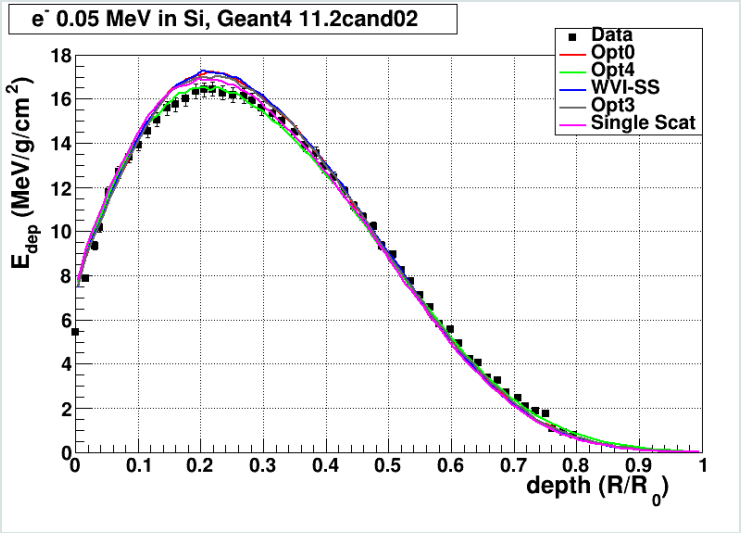
Other developments

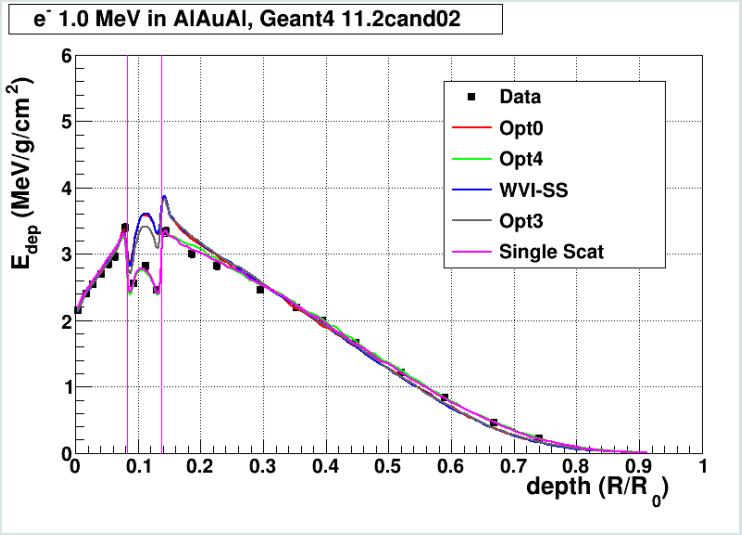
- **Number of bug reports are fixed**
  - *Bugzilla #2511, #2530, #2531, #2532, #2542, #2543, #2546, #2555, #2568, #2569, #2572*
  - *Git issues: #168, #182*
- **Added extra flag**
  - *MscPositronCorrection – may be used to enable/disable L. Urban positron correction introduced in early Geant4 releases (ATLAS problem)*
    - UI command and C++ interface
- **Update for quantum entanglement**
  - *Allowing definition in G4State_Idle*
  - *Postpone one of correlated track into waiting stack, this allows to keep track on correlations after 1st Compton scattering*

Few validation results









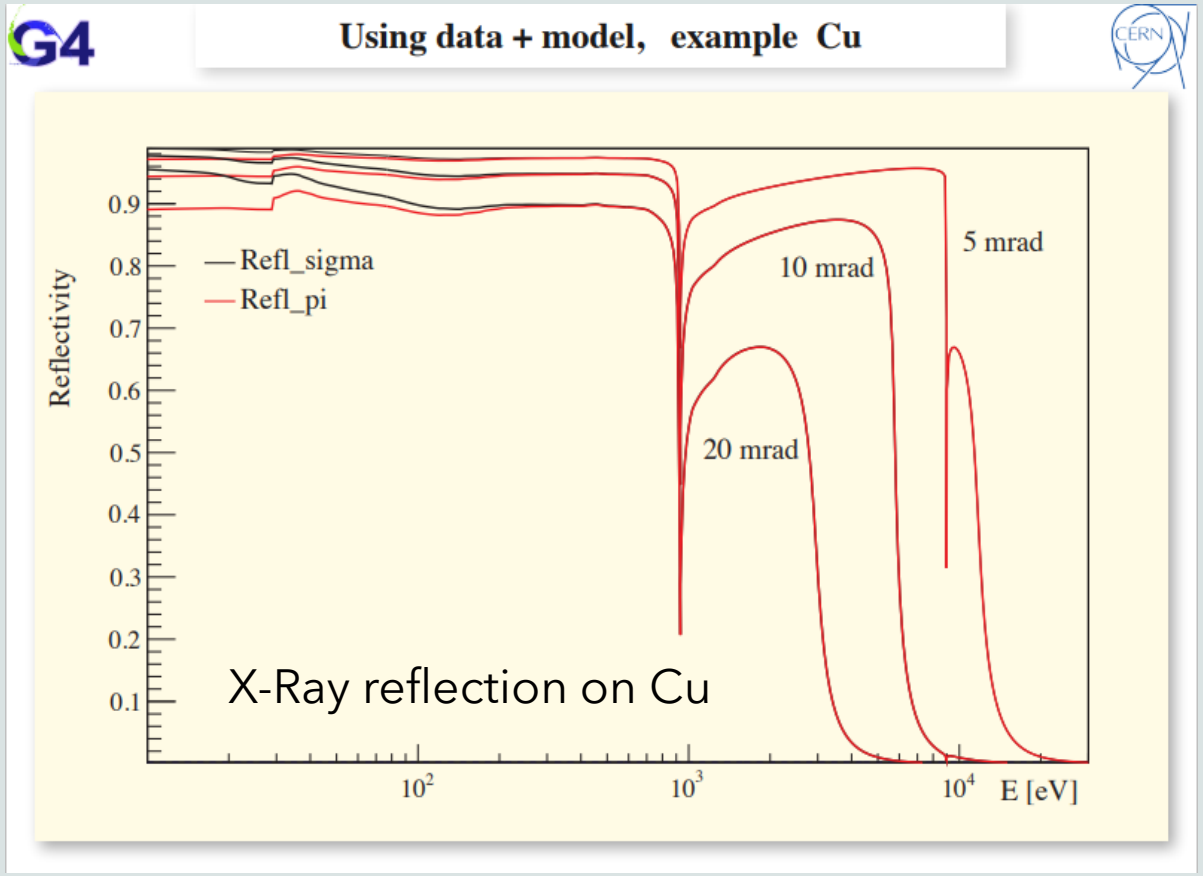
- Results for 11.1/11.2 are stable in general, now major problems reported so far

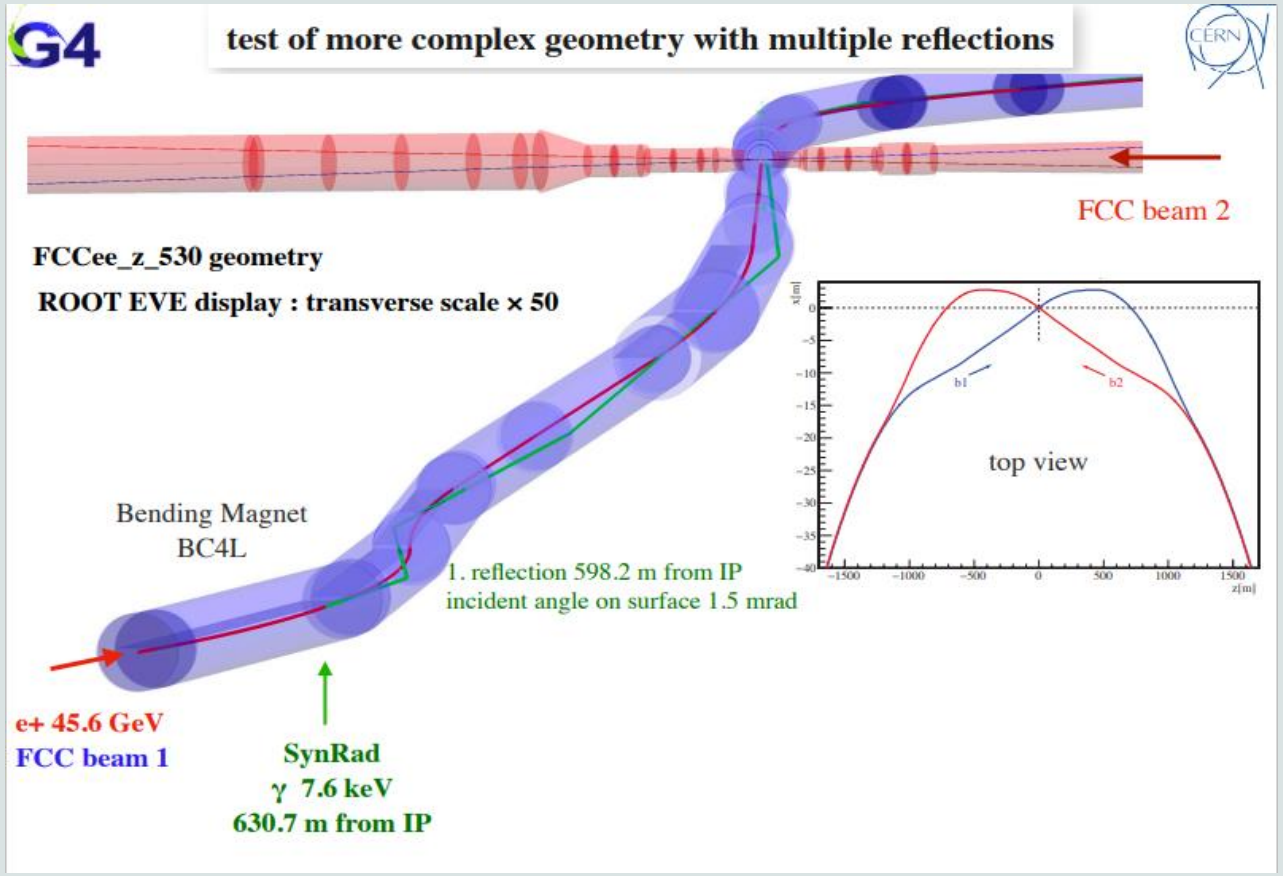
New model developments

- **Components of EM physics in crystals are implemented via fast simulation interface**
  - *Processes are released within $G4INSTALL/parameterisations/channeling*
- **X-Ray surface reflection process**
  - *Needed for many applications in accelerator physics, space science, …*
  - *B.L. Henke, E.M. Gullikson, and J.C. Davis. X-ray interactions: photoabsorption, scattering, transmission, and reflection at E=50-30000 eV, Z=1-92, Atomic Data and Nuclear Data Tables Vol. 54 (no.2), 181-342 (July 1993)*
- **New MicroElec models and data**
  - *New photon model applicable to projectile electrons and ions*
  - *Elastic and inelastic scattering for extra materials*
    - Previously the models were applicable to Silicon only
    - Now Aluminium oxide, Boron nitride, and Silicon dioxide are added

X-Ray Reflection (H. Burkhardt, Geant4 annual workshop, 2023)

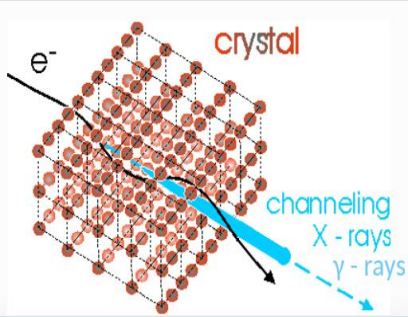
https://indico.cern.ch/event/1307331/contributions/5575553/attachments/2719822/4726354/G4coll_XrayReflection_2023_09_25.pdf

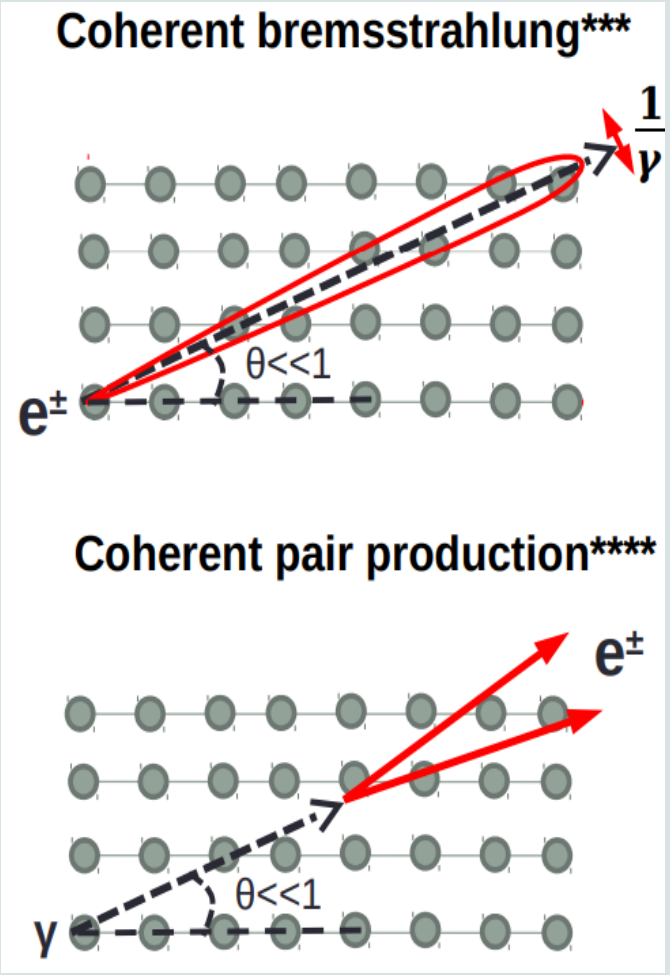


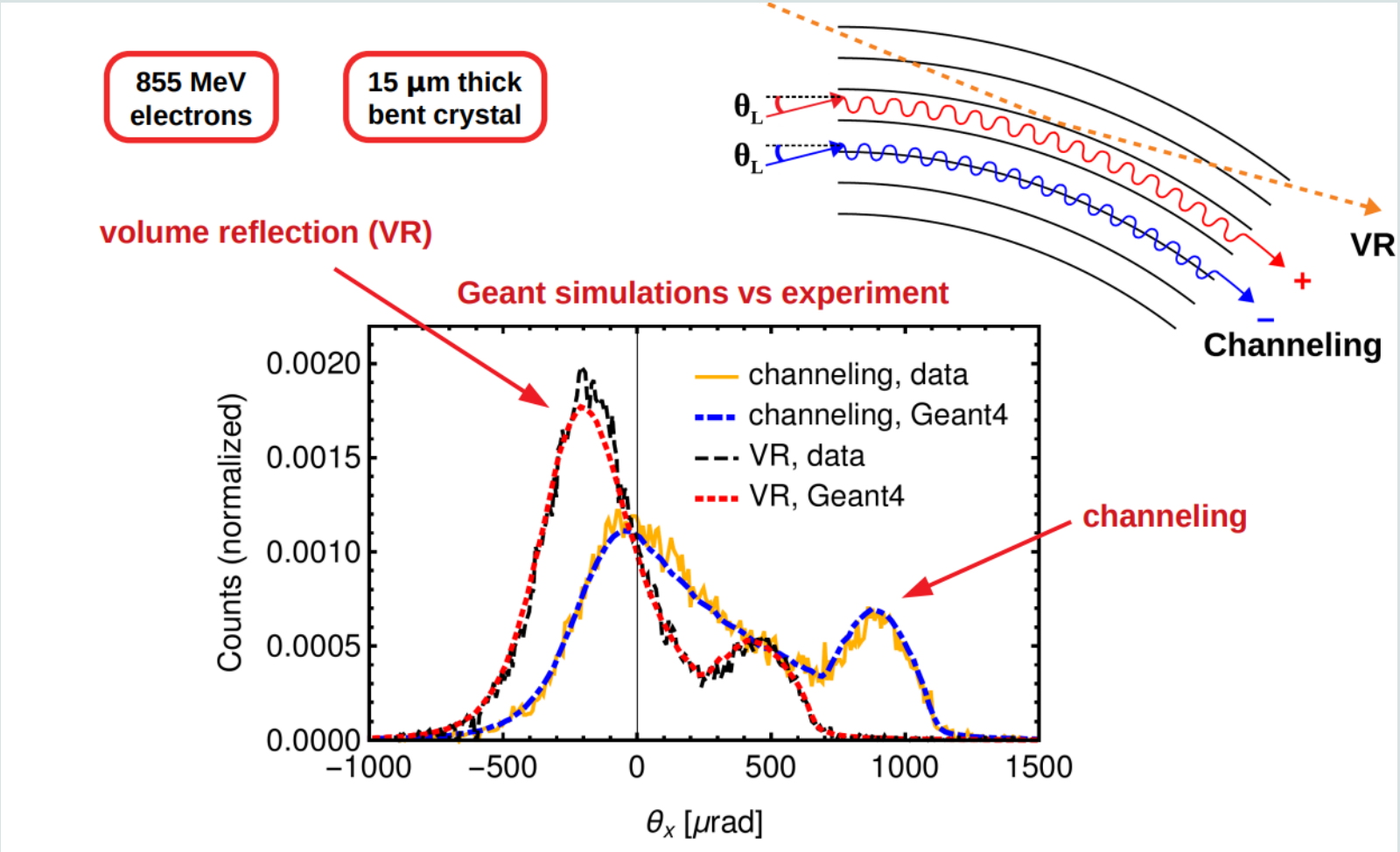


Simulation of beam channeling (A. Sytov, Geant4 annual workshop, 2023)

https://indico.cern.ch/event/1307331/contributions/5575555/attachments/2720674/4726621/Sytov_Channeling2023-to-publish.pdf





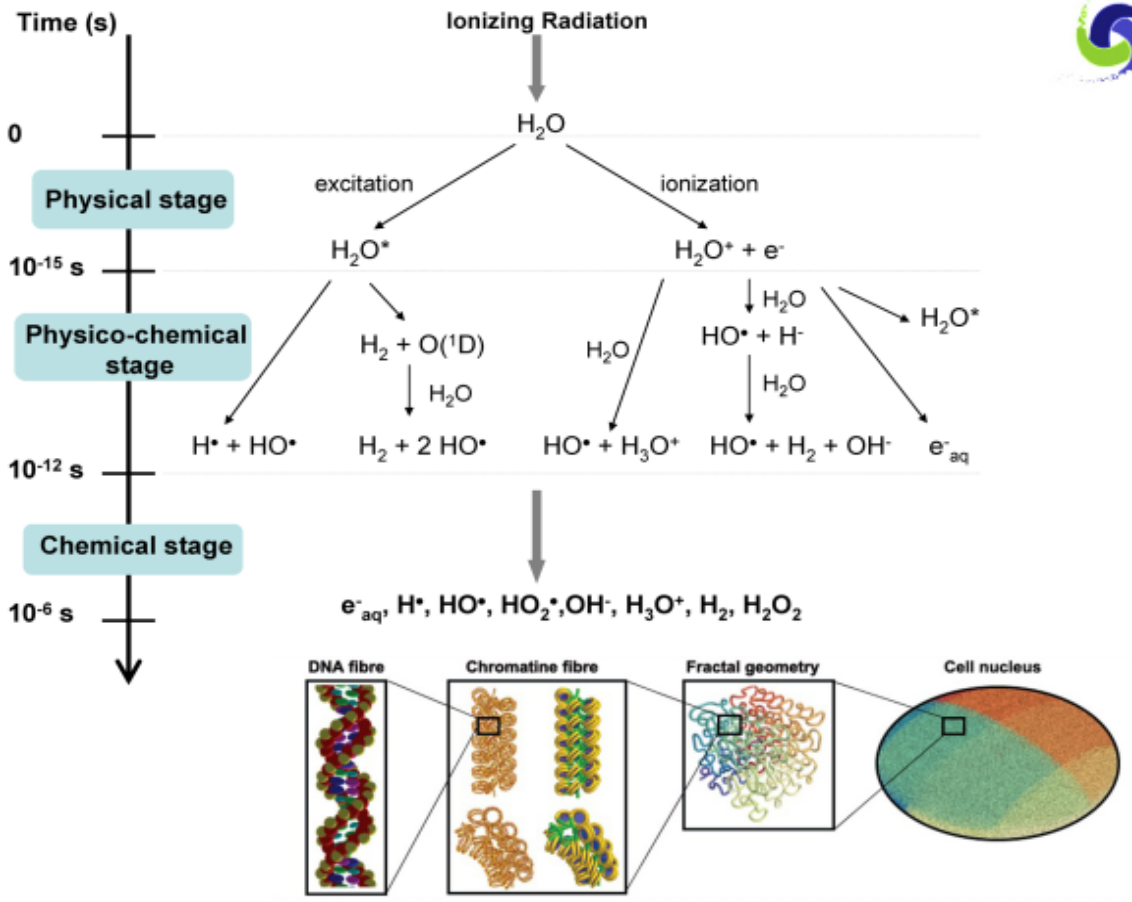


Geant4-DNA developments

S. Incerti & Ngoc Hoang Tran

On behalf of Geant4-DNA collaboration

Geant4-DNA for radiobiology



GEANT4-DNA
A SIMULATION TOOLKIT

Extension of the Geant4 Monte Carlo simulation toolkit for radiobiology

- **Track structure code**: simulates each particle-matter interaction
  - **physical stage**
- Simulate the production and tracking of radiolytic species, together with their mutual interactions
- DNA-scale geometries

GEANT4-DNA

List of recent updates for DNA physics models

- **New DNA_Option4 model developed at the Univ. of Ioannina**
  - *A robust and updated model that permits electron transport in liquid water from 10 eV to 10 MeV*
  - *Validation versus ICRU90 data agreement better than 5%*
- **The new model for proton ionisation developed at the Univ. of Sevilla**
  - *energy from 100 MeV up to 300 MeV*
  - *A. D. Domínguez-Muñoz et al., Radiat. Phys. Chem 199: 110363 (2022)*
- **New models for additional DNA materials**
  - *Elastic, Inelastic, Excitation model*
  - *DNA bases and backbone from 11 eV to 1 MeV*
    - Adenine, Guanine, Thymine, Cytosine, Deoxyribose, Phosphoric acid
    - S. Zein et al. NIMB (2021) and (2023)
  - *Atmosphere: N2 and O2 cross section models up to 10 MeV*
    - Agreement with ESTAR data better than 6%
    - F. Nicolanti, et al, . Phys Med. (2023)

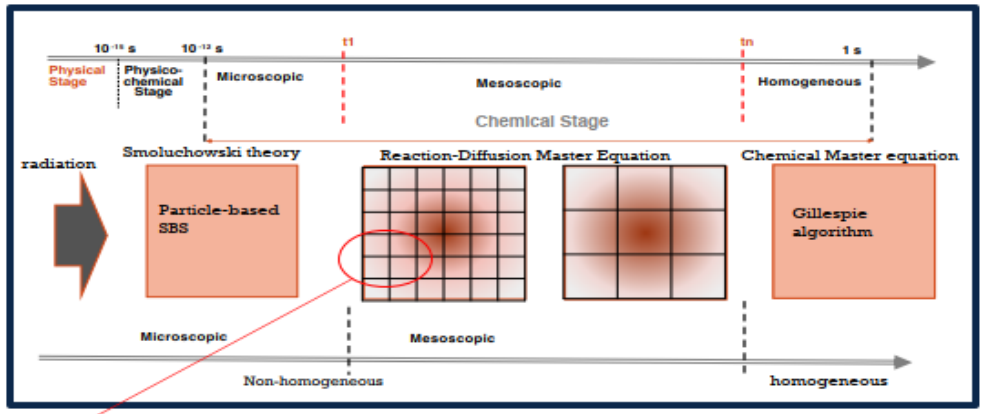
List of recent updates for chemistry and DNA examples

- **New « mesoscopic » approach**
  - *Advance method to simulate chemistry processes in liquid water*
  - *Tran et al., Int. J. Mol. Sci. (2021) 22*
- **Modelling of ultra-high dose rate (UHDR) electron beams**
  - *UHDR extended example*
- **New biological geometries and applications**
  - *moleculardna : simulate early DNA damage in a full DNA geometries of cell nucleus.*
  - *dnadamage2 : this examples provides scoring of plasmid DNA strand breaks.*
  - *dsbandrepair : a new biological geometry application from IRSN*

New « mesoscopic » approach

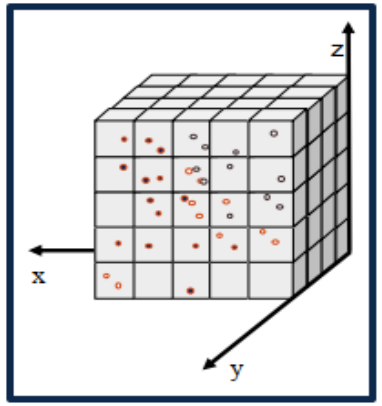
- Use new « mesoscopic » approach to study the production and evolution of reactive oxygen species generated under irradiation with
  different dose rate conditions, such as in FLASH RT
- Coarse-grained model: "compartment based"
- Simulation from heterogeneous (SBS, microsecond) to homogeneous states (beyond)
- Developed in Geant4-DNA by the MAGIC Collaboration
  - CHUV, Switzerland & CNRS/LP2i, France

Tran et al., Int. J. Mol. Sci. (2021) 22 (link)



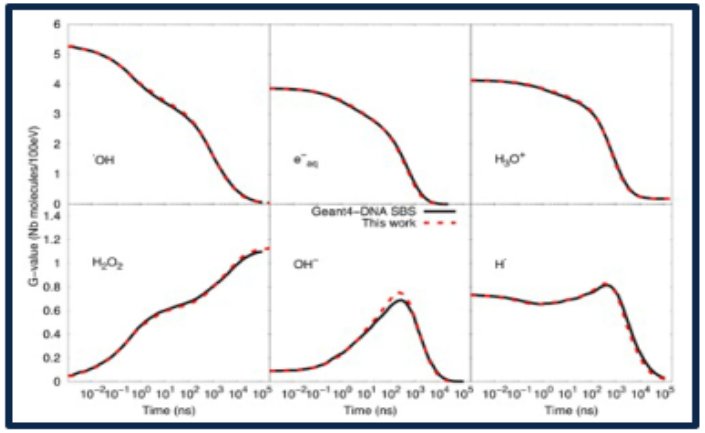
Principle of the combination of the particle-based SBS model with the compartment-based model

1. *Well mixed species in voxels*
2. *Species can react with each other in the voxels*
3. *Diffusion is modelled by jumps between adjacent voxels*

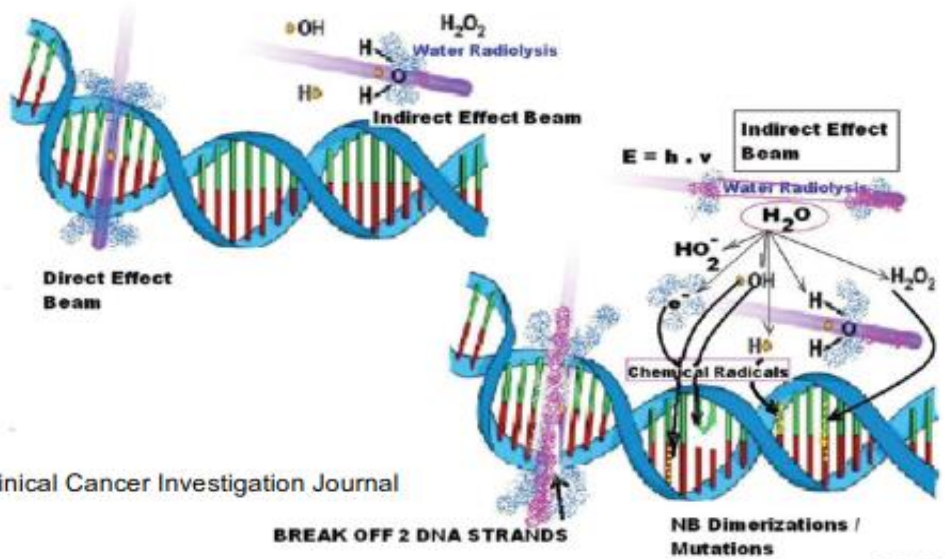


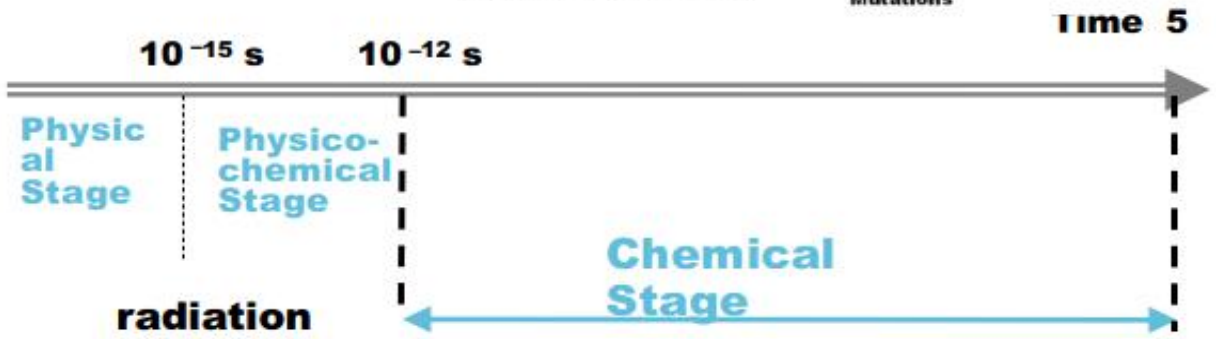
Voxelization of the simulation volume into smaller sub-volumes. Species are represented by different types of circles

Comparison of time-dependent G-values as computed with the particle-based SBS model and the SBS-RDME model (this work) from 1 ns until 100 us, for 1 MeV e-.



Moleculardna: simulate early DNA damage using only Geant4 macro commands - No C++ skills needed





Simulation of physics, physico-chemistry and chemistry processes in DNA geometries.

GEANT4-DNA

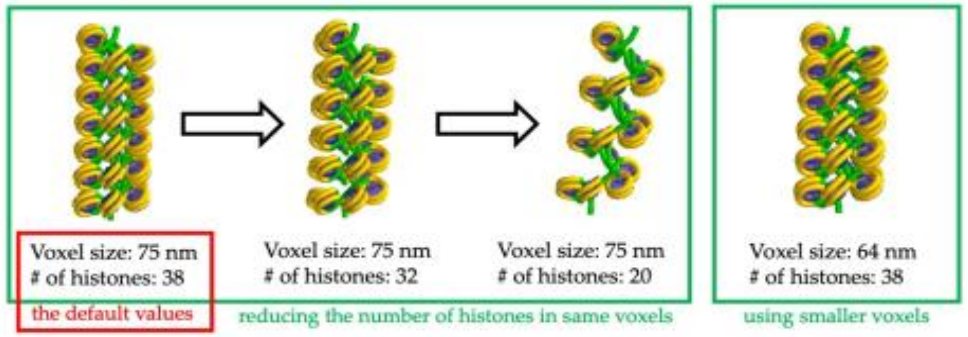
```
/world/worldSize 10200 nm
/cell/radiusSize 3 3 3 um

/dnageom/setSmartVoxels 1
/dnageom/checkOverlaps false

/dnageom/radicalKillDistance 9 nm
/dnageom/interactionDirectRange 7 angstrom

/dnageom/placementSize 30 30 100 nm
/dnageom/fractalScaling 1 1 1 nm
/dnageom/definitionFile geometries/prisms200k_r3000.txt
/dnageom/placementVolume prism geometries/straight-216-0.txt

# Damage Model
/dnadamage/directDamageLower 17.5 eV
/dnadamage/directDamageUpper 17.5 eV

/dnadamage/indirectOHBaseChance 1.0
/dnadamage/indirectOHStrandChance 0.65
/dnadamage/inductionOHChance 0.0

/dnadamage/indirectHBaseChance 1.0
/dnadamage/indirectHStrandChance 0.65
/dnadamage/inductionHChance 0.00

/gps/particle e-
/gps/ang/type iso
/gps/energy 4.5 keV
/gps/pos/type Volume
/gps/pos/shape Sphere
/gps/pos/radius 500 nm
/gps/pos/centre 0 0 0 nm
/run/beamOn 1000
```

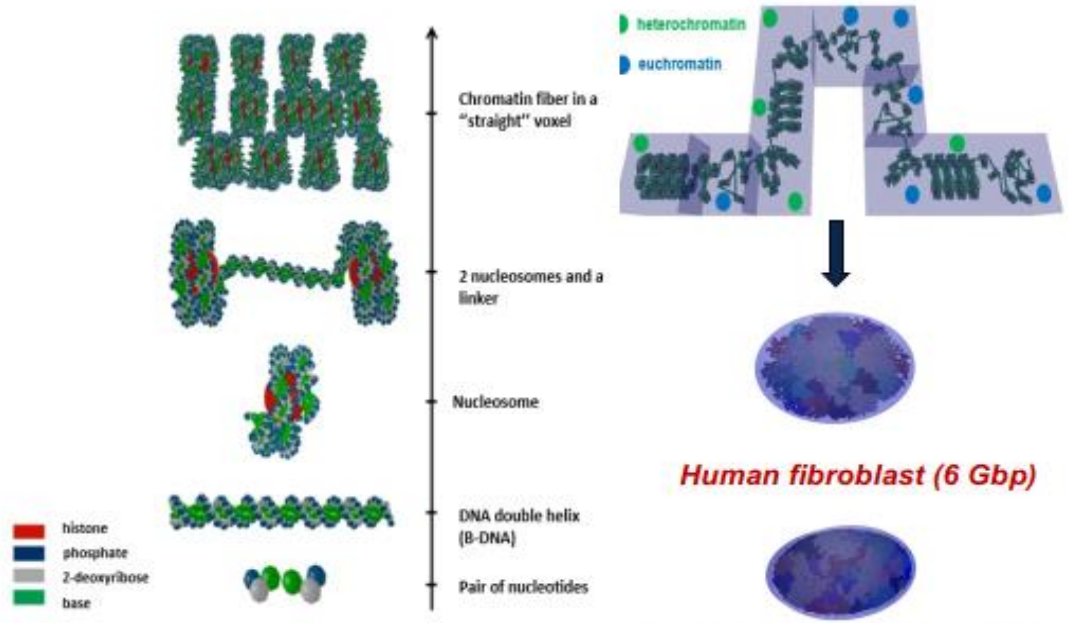
Geometry info

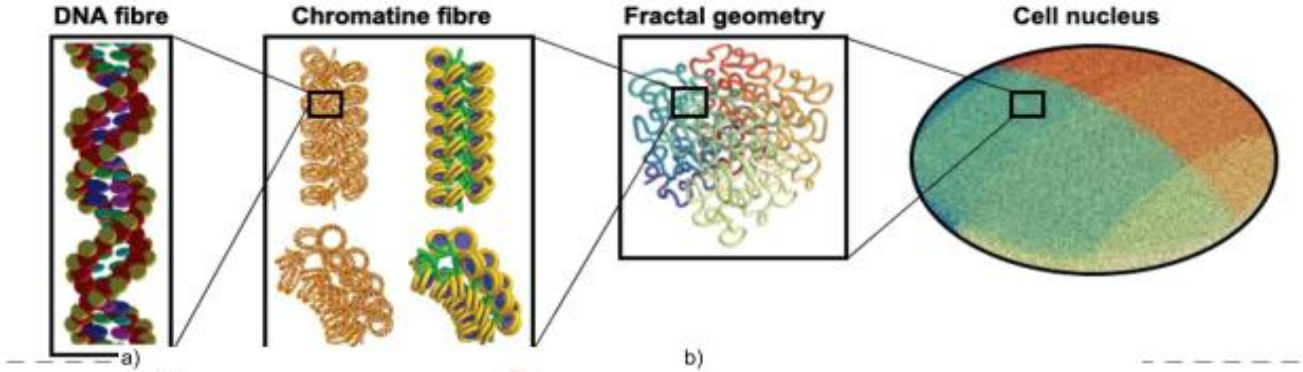
Damage model

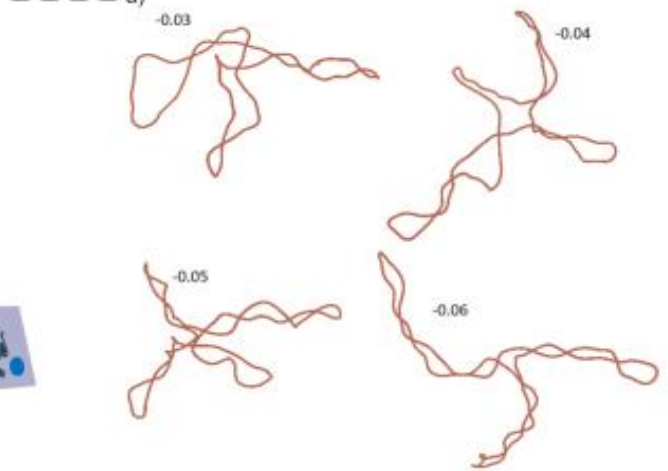
Particle source

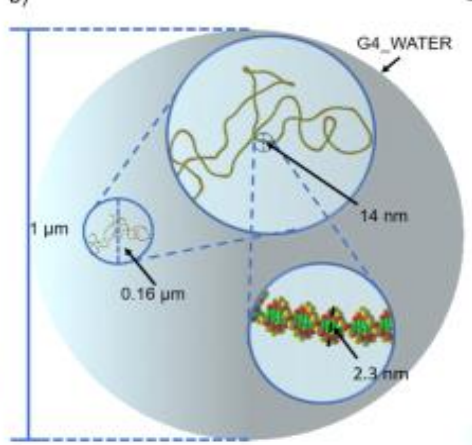
Geometry library

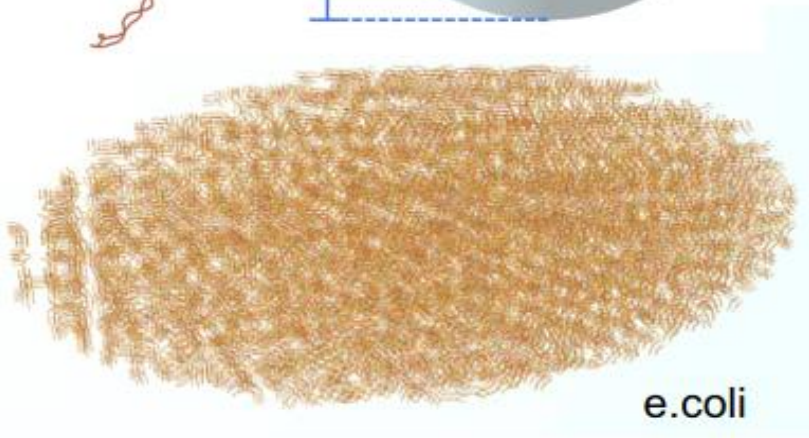












GEANT4-DNA

Thank you