Implementation of EM physics for nano-scale gold electron simulations

16/June/2017

International Multidisciplinary Workshop on Geant4

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University of Bordeaux, CNRS/CENBG

Outline

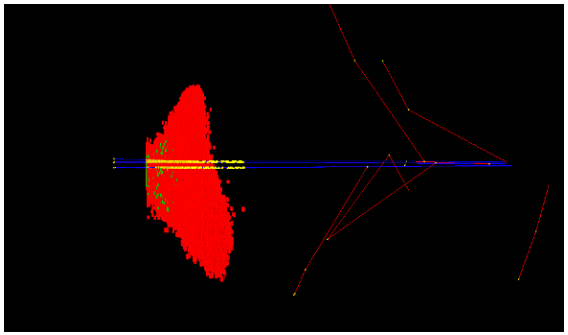
- Introduction
- Physics modeling for electron transportation in Gold
- Verification and validation of new models
- Impact of new physics models for GNP simulations

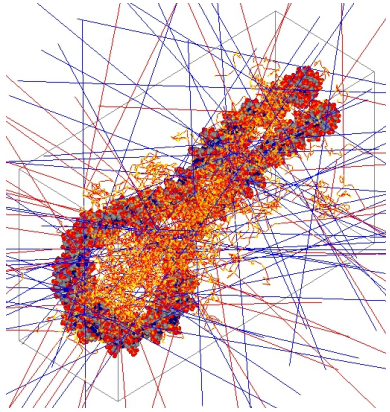
What is Geant4-DNA?

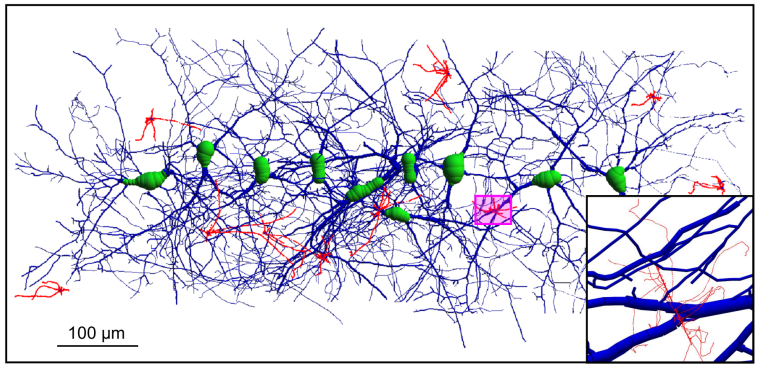
Geant4-DNA

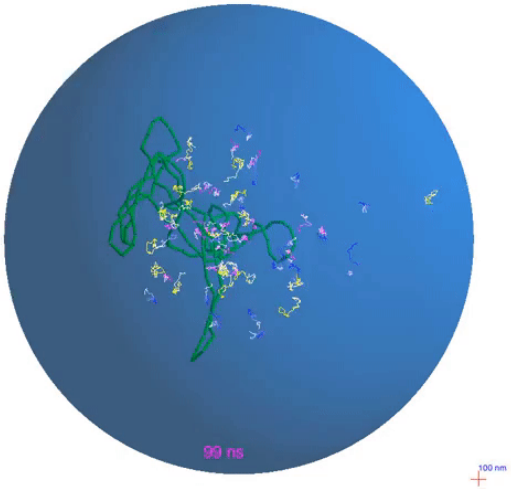
An extension of Geant4 for low energy particle transport simulations and radiochemistry, allowing in particular biological simulations.

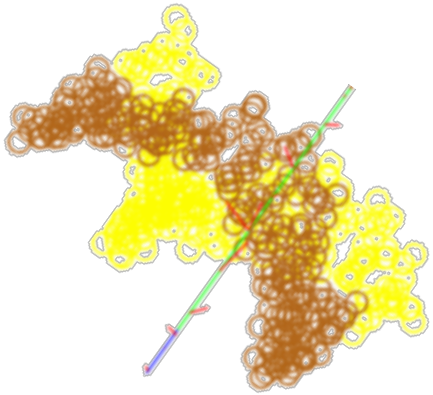
http://geant4-dna.org/

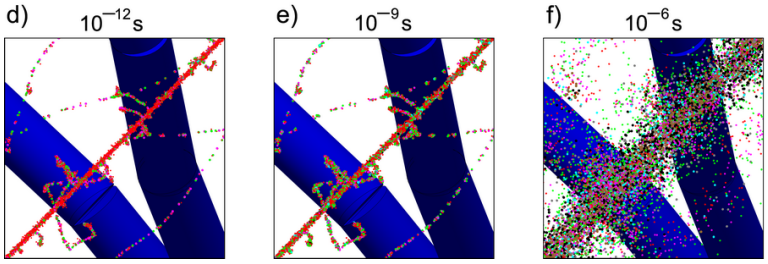




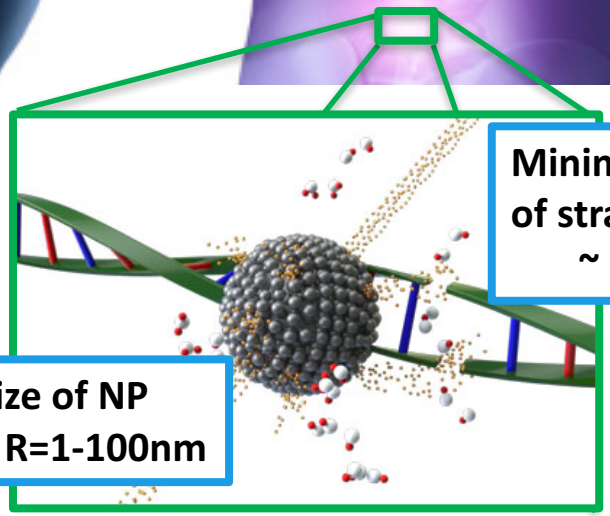








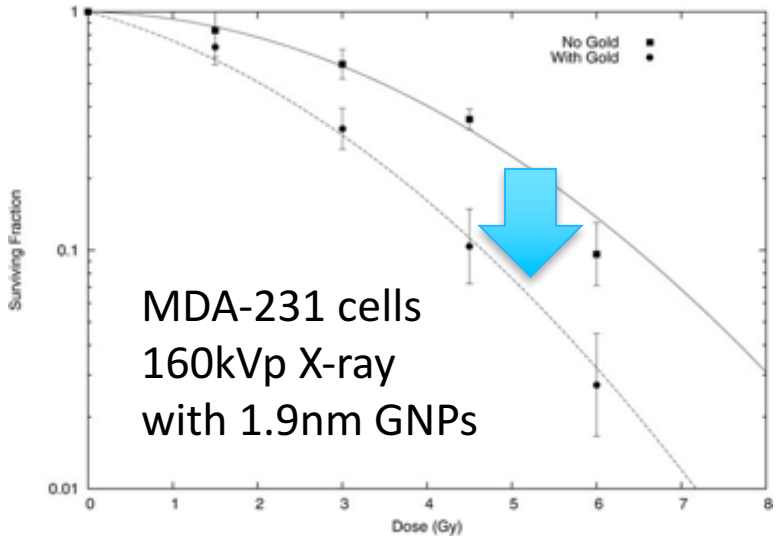
Gold nanoparticle boosted radiation treatment



Minimum energy of strand break ~ 5-10 eV

Size of NP ~ R=1-100nm

S.J McMahon et al, Scientific Reports 1, Article number: 18 (2011)



MDA-231 cells
160kVp X-ray
with 1.9nm GNPs

It is necessary to implement accurate physics models which are applicable for low energy particles in very small volumes.

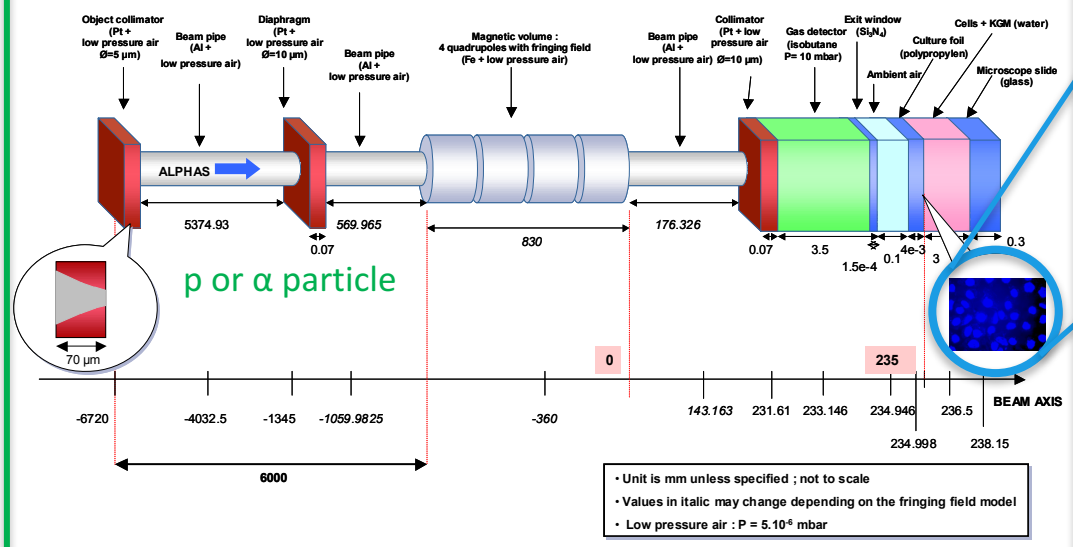
Goal and Agenda of This Study

Problems

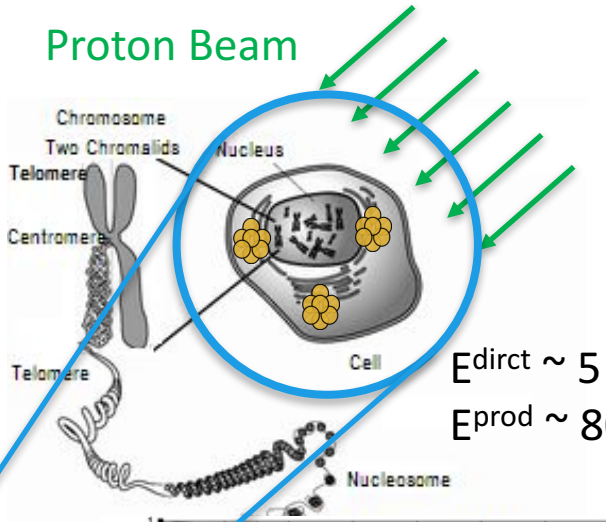
① Large uncertainties on low energy particle transportation in very small volume.

② Too high secondary production energy cut in inelastic interactions by proton impact.

Micro Beam Line for Cellular Irradiation at CENBG

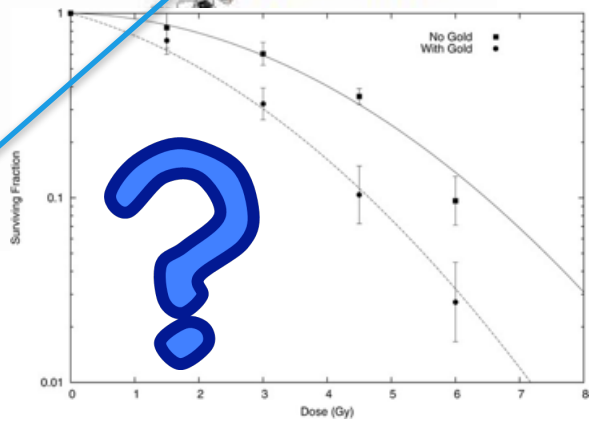


Proton Beam



E^{dirct} ~ 5 - 10 eV

E^{prod} ~ 800 eV



Current Trials of Geant4-DNA

Physics (for Au)

Photon
- Rayleigh scattering
- Photo-electric ionization
- Compton scattering
- Pair production

Electron
- Bremsstrahlung
- Elastic scattering
- Electronic excitation
- Plasmon excitation
- Ionization

This Work

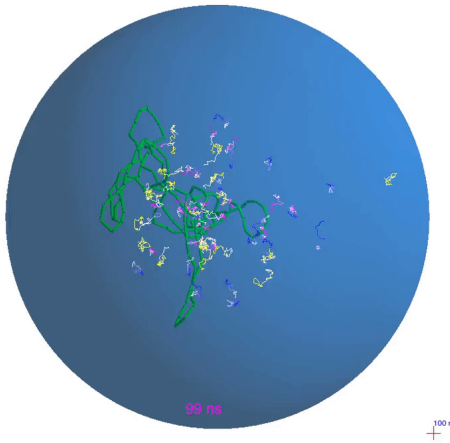
Proton
- Elastic scattering
- Excitation
- Ionization
- Charge exchange

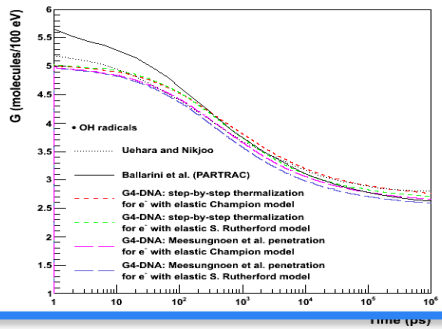
On Going

- Bremsstrahlung

Chemistry(for water)

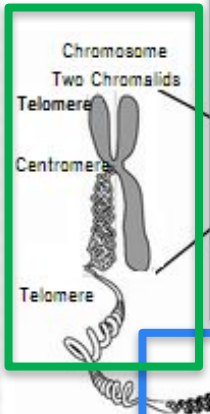
Done!





Geometry

On Going



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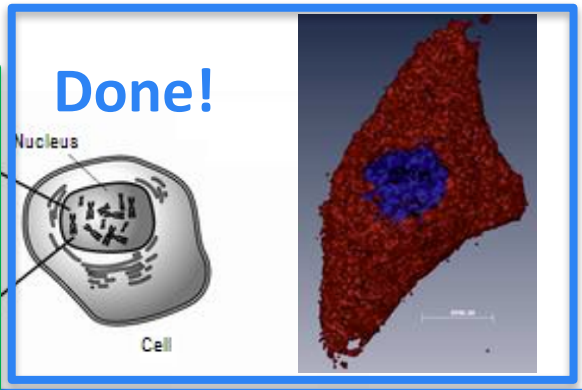

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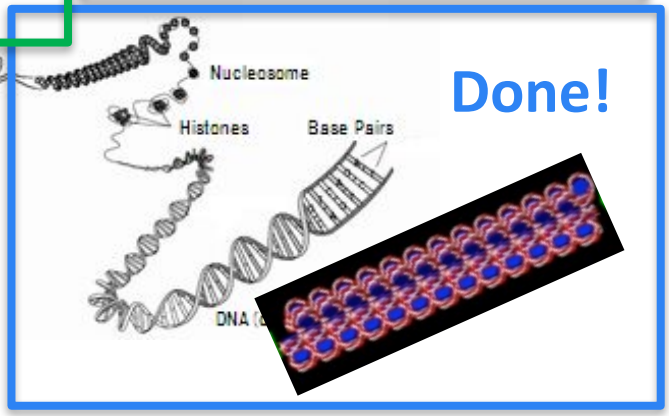

Physics modeling for electron transportation in Gold

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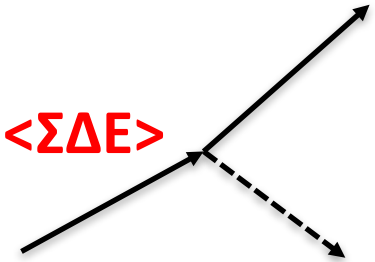
Physics improvement for electron transportation

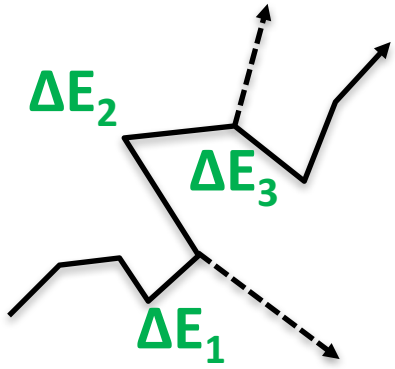
Condensed history models

- One multiple-scattering deflection
- One average total energy loss + fluctuation
  are sampled for each step
- Usage of production cut



Discrete models

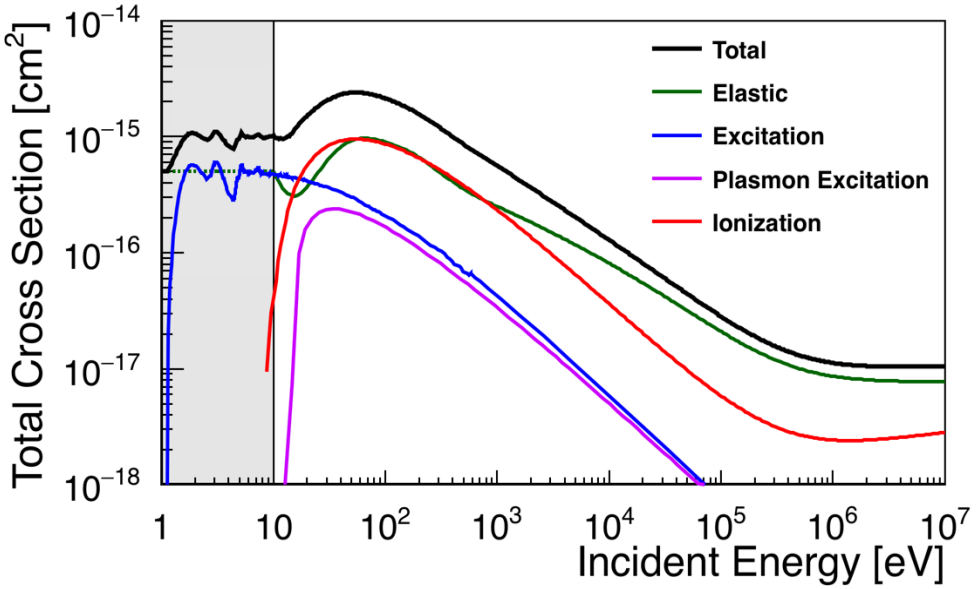
- One single deflection
- One single energy loss
  are calculated for each physics process.
- No production cut



To improve accuracy for low energy and small scale simulations, implementation of discrete physics models is needed !

New discrete physics models for Gold

D. Sakata et al, J. Appl. Phys. 120 (2016) 244901



Integrated electron cross sections in gold. Bremsstrahlung is not shown. All particles with energy below 10 eV (shown in gray) are killed and their energy is dumped locally.

Physics	Model
Elastic	Partial Wave Analysis (ELSEPA)
Ionization	M. Relativistic Binary-Encounter Bethe Vriens
Excitation	Experiment + Dirac B-Spline R Matrix
Plasmon Excitation	Quinn Model
Bremsstrahlung	Seltzer and Berger Model

Energy Range of the models
10 eV < E < 1 GeV

Verification and Validation

- This Work
- Livermore
- Penelope

Stopping Power

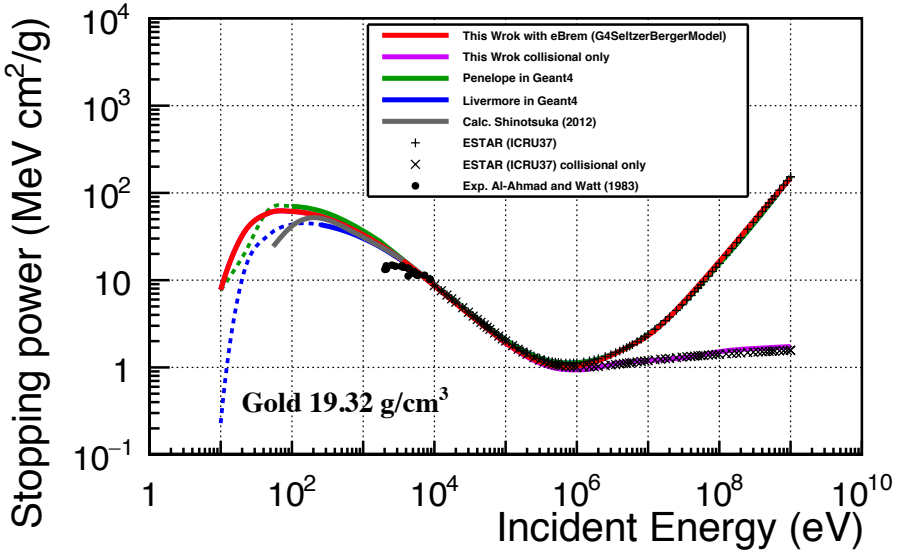
Range

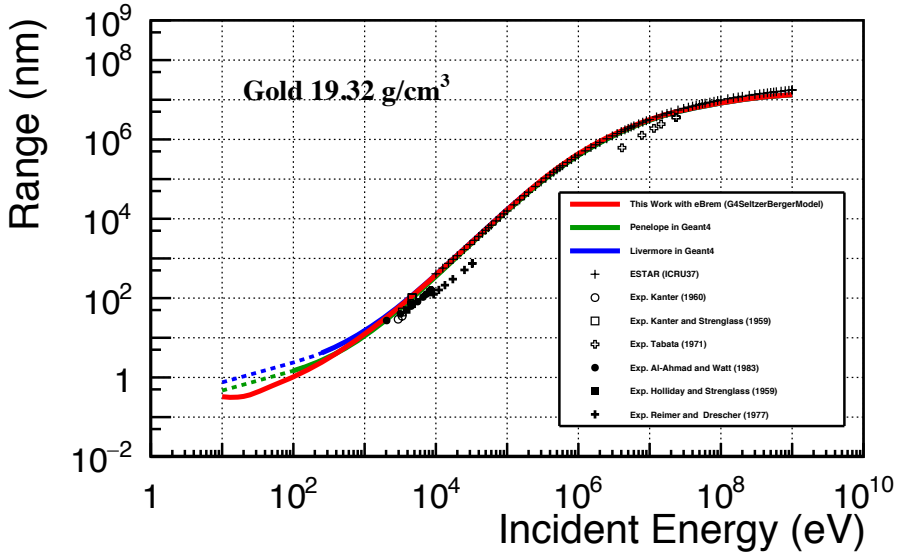
Back scattering Coefficient

Transmission Coefficient

Stopping Power and Range

D. Sakata et al, J. Appl. Phys. 120 (2016) 244901





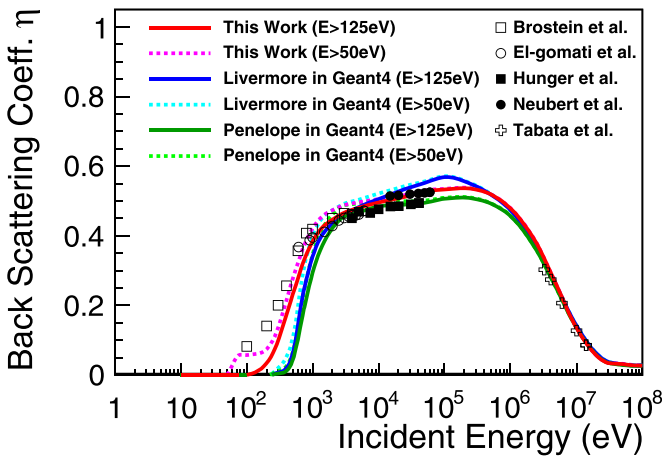
This Work

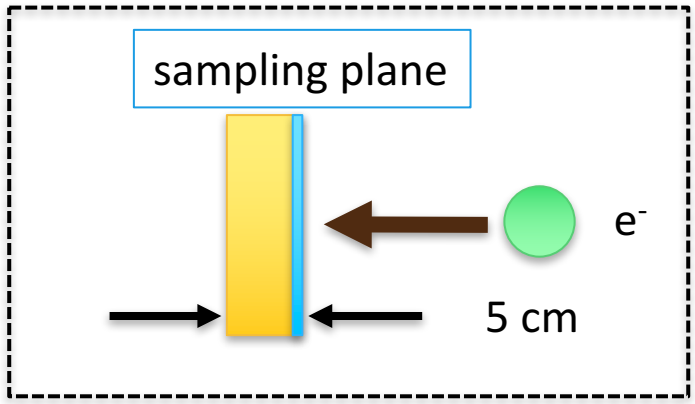
Livermore

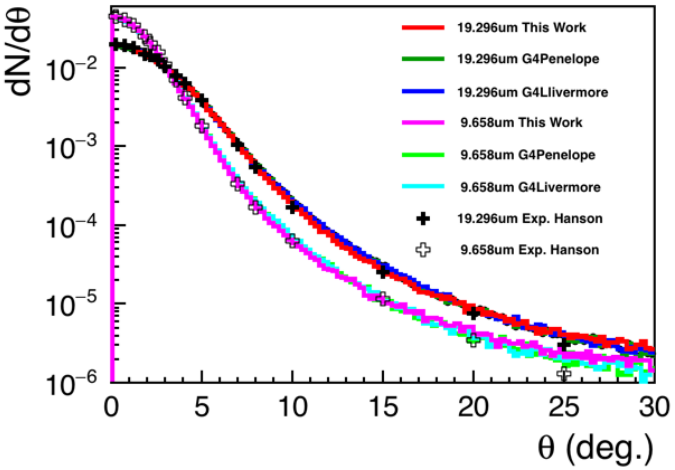
Penelope

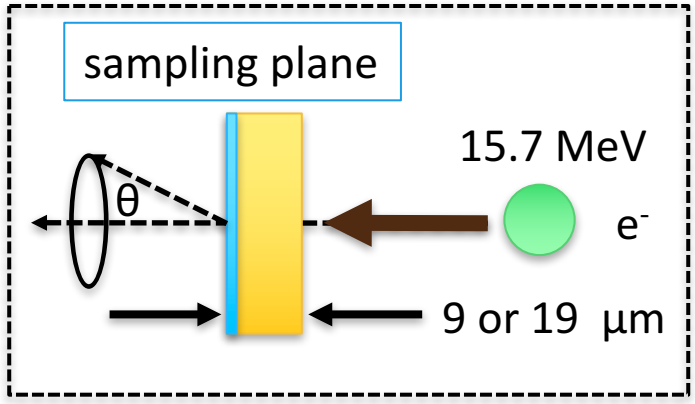
- We have good agreements with existing physics models in high energy on Geant4 and ICRU37 recommendation.

Back Scattering & Transmission









D. Sakata et al, J. Appl. Phys. 120 (2016) 244901

Impact of new physics models for GNP simulations

- This Work
- Livermore
- Penelope

Simulation Configuration
Secondary Spectra
Model Dependence
NP Size Dependence
Energy Dependence

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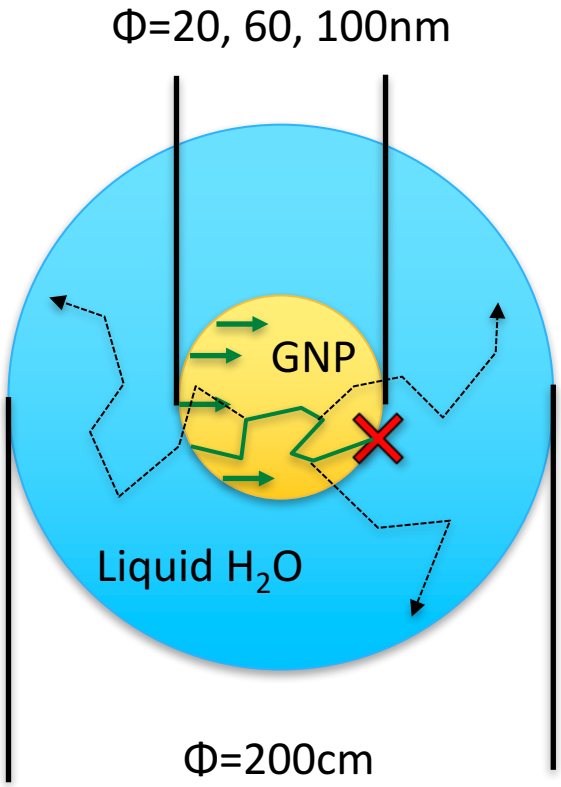
Simulation Configuration



- Incident configuration
  - Particle : electron
  - Energy : 1,10,100,1000 keV
  - Beam shape : uniform beam from hemi-sphere
- NP: Gold (R=10,30,50nm)
- Absorber : Water (R=100cm)
- Particle transportation limits
  - Maximum step length in NP : R/2
  - Incident particle : killed at end NP
  - Secondary particle : killed below 10 eV

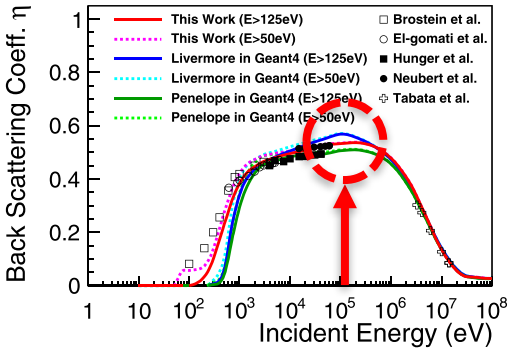
Secondary particle spectra

1D absorbed dose

- **Large difference could be found in close region of GNP. Condensed history model less estimate self absorption of secondary particles.**

2D absorbed dose

Back scatt. coef. for 5cm gold plate



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All physics models show high back scattering coefficient in large gold bulk.

Only new physics models describe high absorbed dose in backward direction.

R = 50 nm **E_{inc}=100 keV**

This Work (GNP) Livermore (GNP) Penelope (GNP) WNP

Size dependence in 2D dose

R = 10 nm (Liv) **R = 10 nm** **R = 30 nm** **R = 50 nm**

E_{inc}=100 keV

The new physics models seems to be applicable for very small GNP down to diameter is 10 nm.

Energy dependence in 2D dose

1keV 10keV 100keV 1000keV

Back scattered

Punch through

Emit large number of secondary particles

Mean free path is comparable with NP size

R=50nm

Summary and Outlook

- New alternative Geant4-DNA physics models for electron in gold have been implemented.
- The models well validated, and working well for nano-mater scale simulations.
- Estimate GNP effect in X-ray radiation field.
- Improve inelastic interaction models.
- Extend the models to be applicable for protons.
- Extend the models for more low Z elements.