Physics Implementation and Computing Costs for Gold Nano Particle (GNP) Simulations

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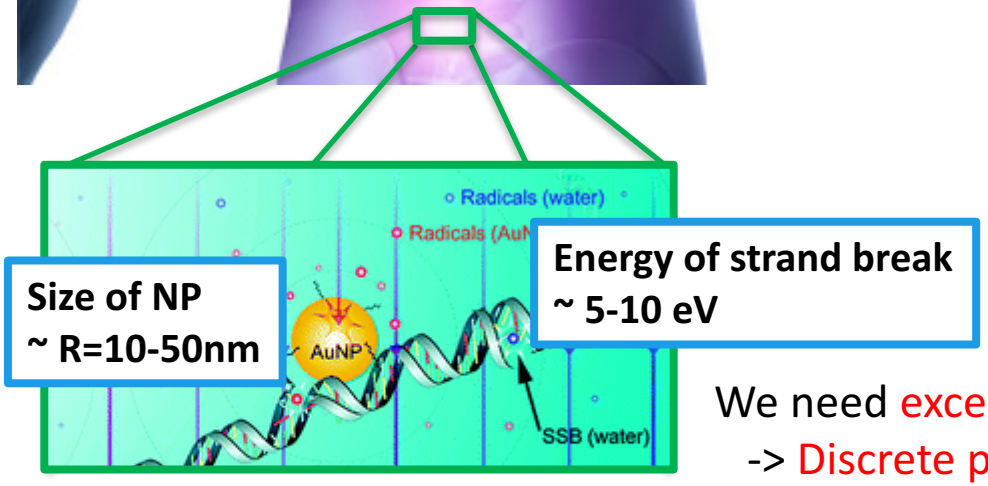
Outline

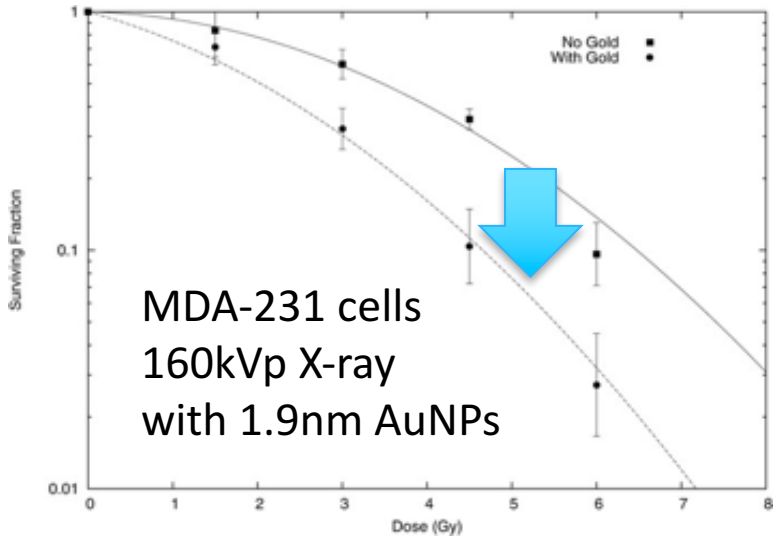
- Introduction
- Modeling Description
  - Physics models for electrons in Gold
  - Verification and Validation
- Simulation Description
  - NP simulation configuration
  - Computing resource and calculation costs

GNP Boosted Radiation Therapy



J.D. Carter et al, J. Phys. Chem. B, 2007, 111 (40), 11622

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



- Interest Energy Range
  - 1 eV to 10 MeV
- Interest Space Range
  - 1 nm to 10 cm

We need excellent resolution and large dynamic range.
-> Discrete physics models with huge calculation resource

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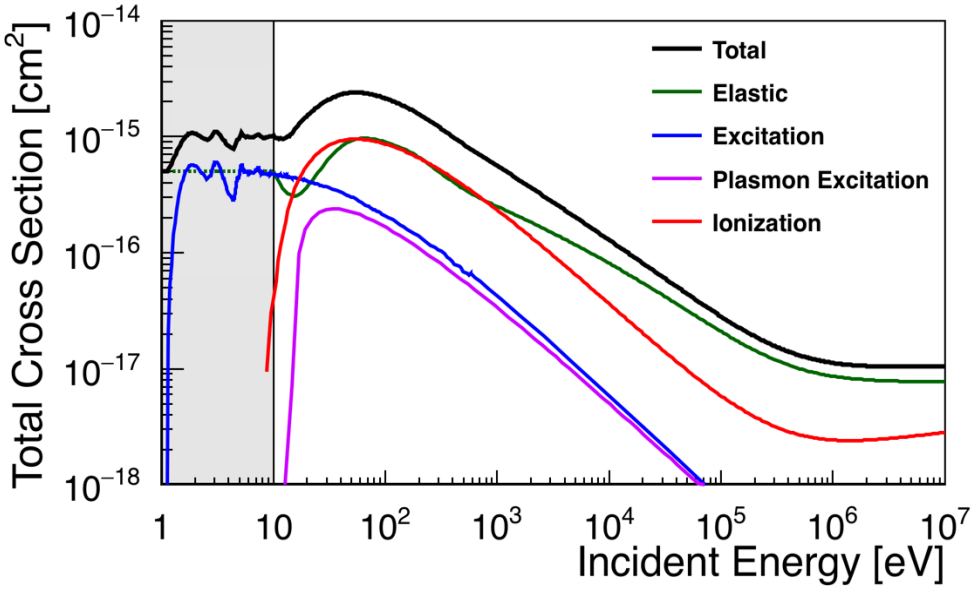
Physics Models for electrons



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.

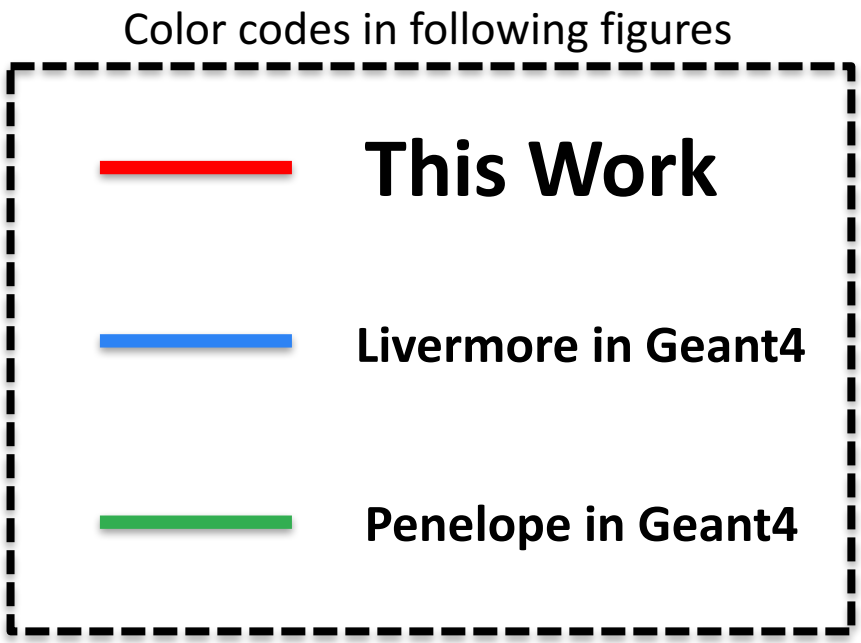
Physics	Model
Elastic	Partial Wave Analysis (ELSEPA)
Ionization	Relativistic Binary-Encounter Bethe Vriens
Excitation	Experiment + Dirac B-Spline R-Matrix
Plasmon Excitation	Quinn Model
Bremsstrahlung	Seltzer and Berger Model

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

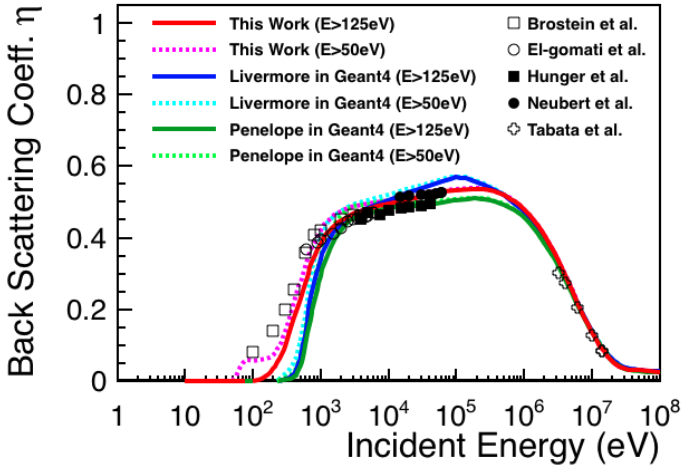
D. Sakata et al, J. Appl. Phys. 120 (2016) 244901

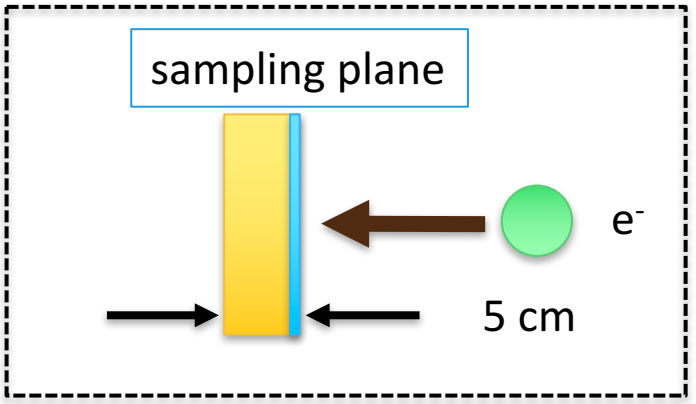
Verification and Validation

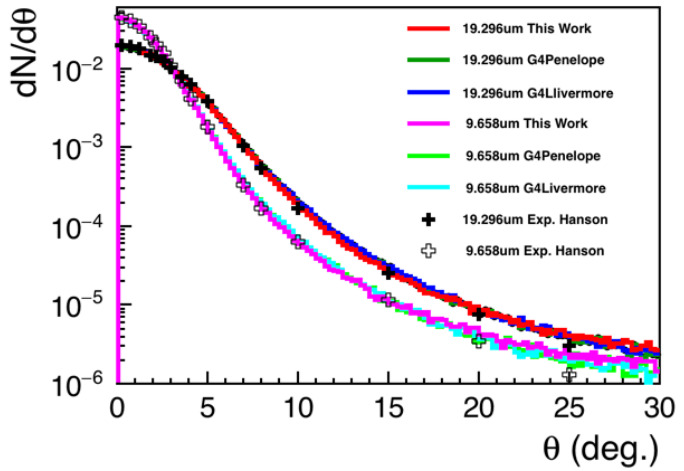
- Back scattering
- Transmission

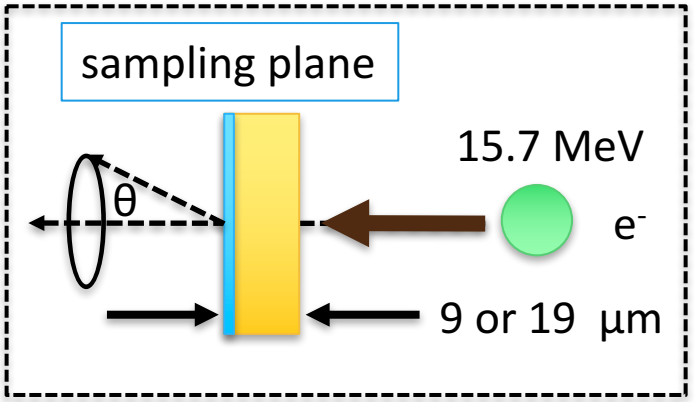


Back Scattering & Transmission









Computing resource and costs

- **10 nodes in CENBG cluster for Geant4-DNA projects**
  - **CPU : Intel(R) Xeon(R) X5550 [Bi-Quard core] 2.67GHz**
  - **RAM : 48GB/node**

		Number of events	Calculation time
GNP	1 keV	500 M events	3 days
	10 keV	300 M events	2 days
	100 keV	100 M events	2 hours
	1,000 keV	100 M events	3 hours
WNP	1 keV	5 G events	8 days
	10 keV	3 G events	3days
	100 keV	1 G events	1 day
	1,000 keV	1 G events	1 day

Summary

- We implemented electro-magnetic interaction models for electron transportation in gold.
- **The physics models presented excellent agreement with experimental data.**
- For NP simulations, we need more calculation resource.