APP_01: The Geant4-DNA and MPEXS-DNA projects at the Physics-Biology frontier

11/May/2017 FJPPL-FKPPL Joint Meeting

Dousatsu Sakata, University of Bordeaux,
CNRS/CENBG

Current Project Members

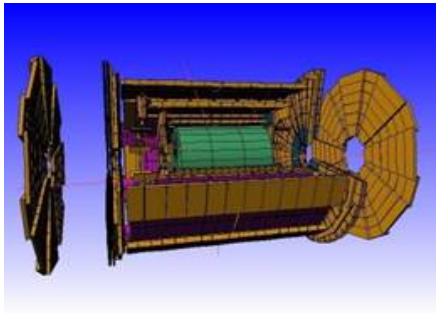
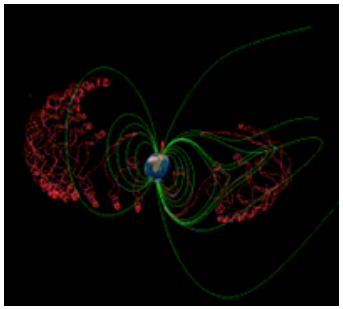
Sebastien Incerti	Dr.	CENBG	Takashi Sasaki	Prof.	KEK
Dousatsu Sakata	Dr.	University of Bordeaux	Katsuya Amako	Prof.	KEK
Hoang Tran	Dr.	CEA/SPhN	Koichi Murakami	Dr.	KEK
Stephanie Mora	Mrs.	CHU Bordeaux	Chihiro Omachi	Dr.	Nagoya City
			Akinori Kimura	Prof.	Ashikaga Inst. Tech.
			Yoshiyuki Hirano	Dr.	Gunma University
			Shogo Okada	Dr.	Kobe University
			Toshiyuki Toshito	Dr.	Nagoya City
			Tsukasa Aso	Dr.	Toyama National Collage

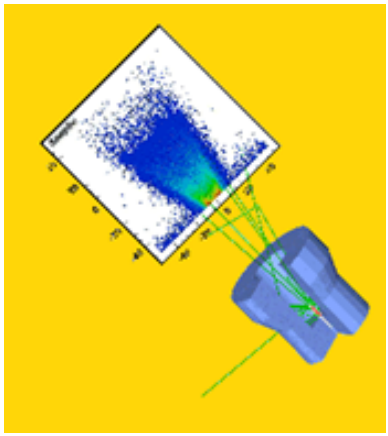
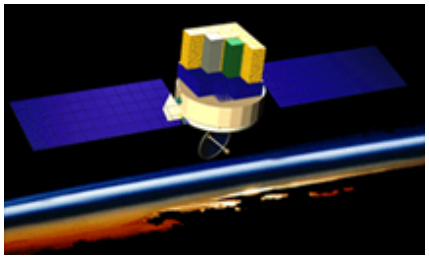
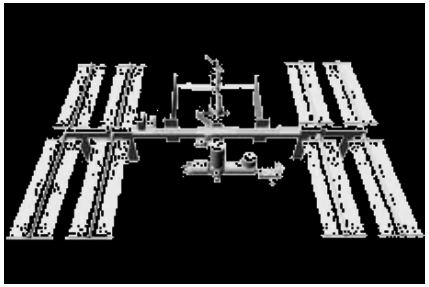
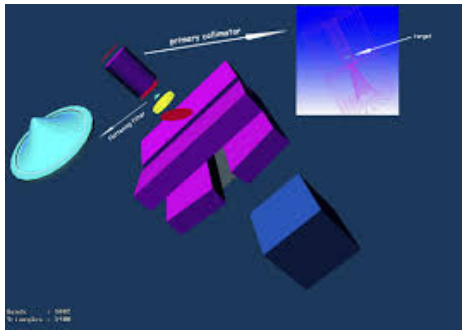
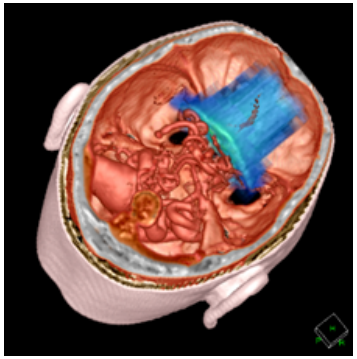
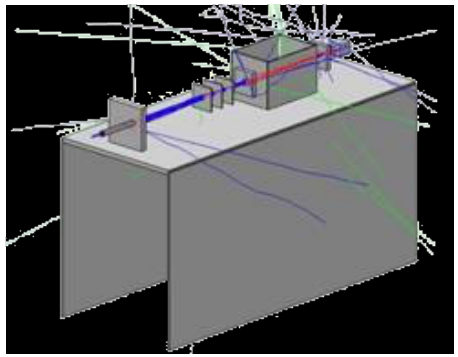
Overview of 2013-2016 activity

Bio2

“The Geant4-DNA project at the Physics-Medicine-Biology frontier”

What is Geant4?

Geant 4

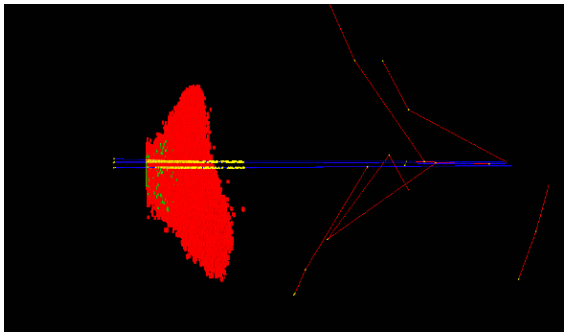
http://geant4.org

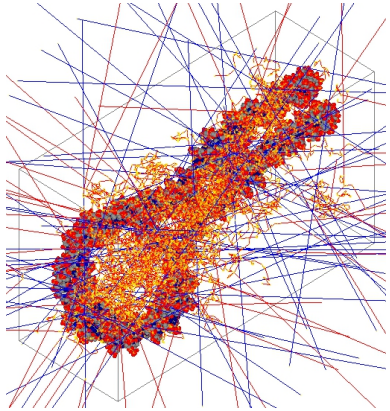
What is Geant4-DNA?

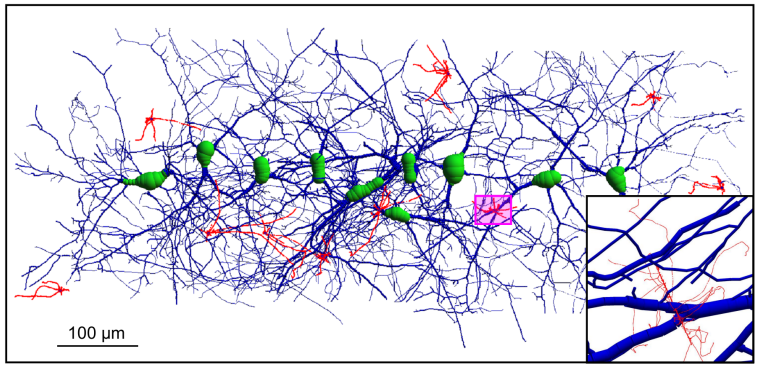
Geant4-DNA

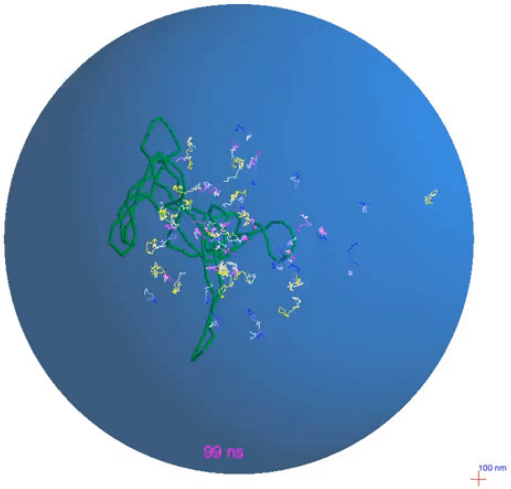
An extension of Geant4 for low energy particle transport simulations and radiochemistry, allowing in particular biological simulations.

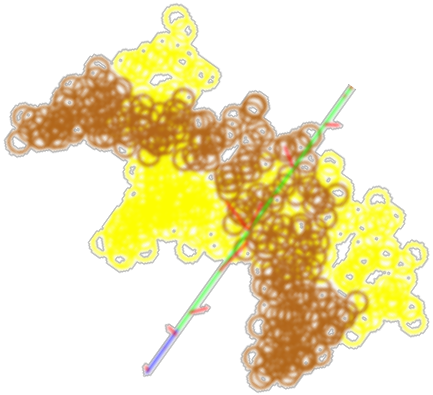
http://geant4-dna.org/

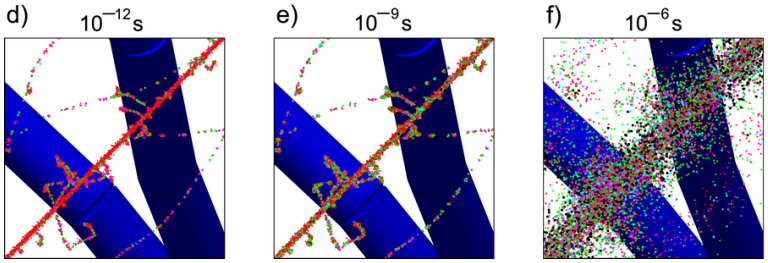






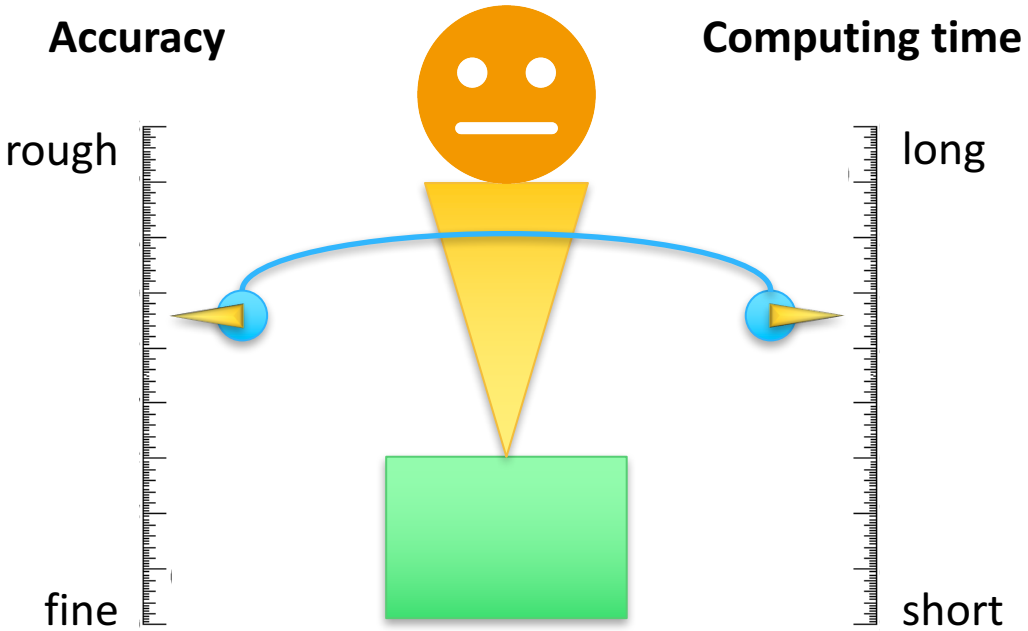






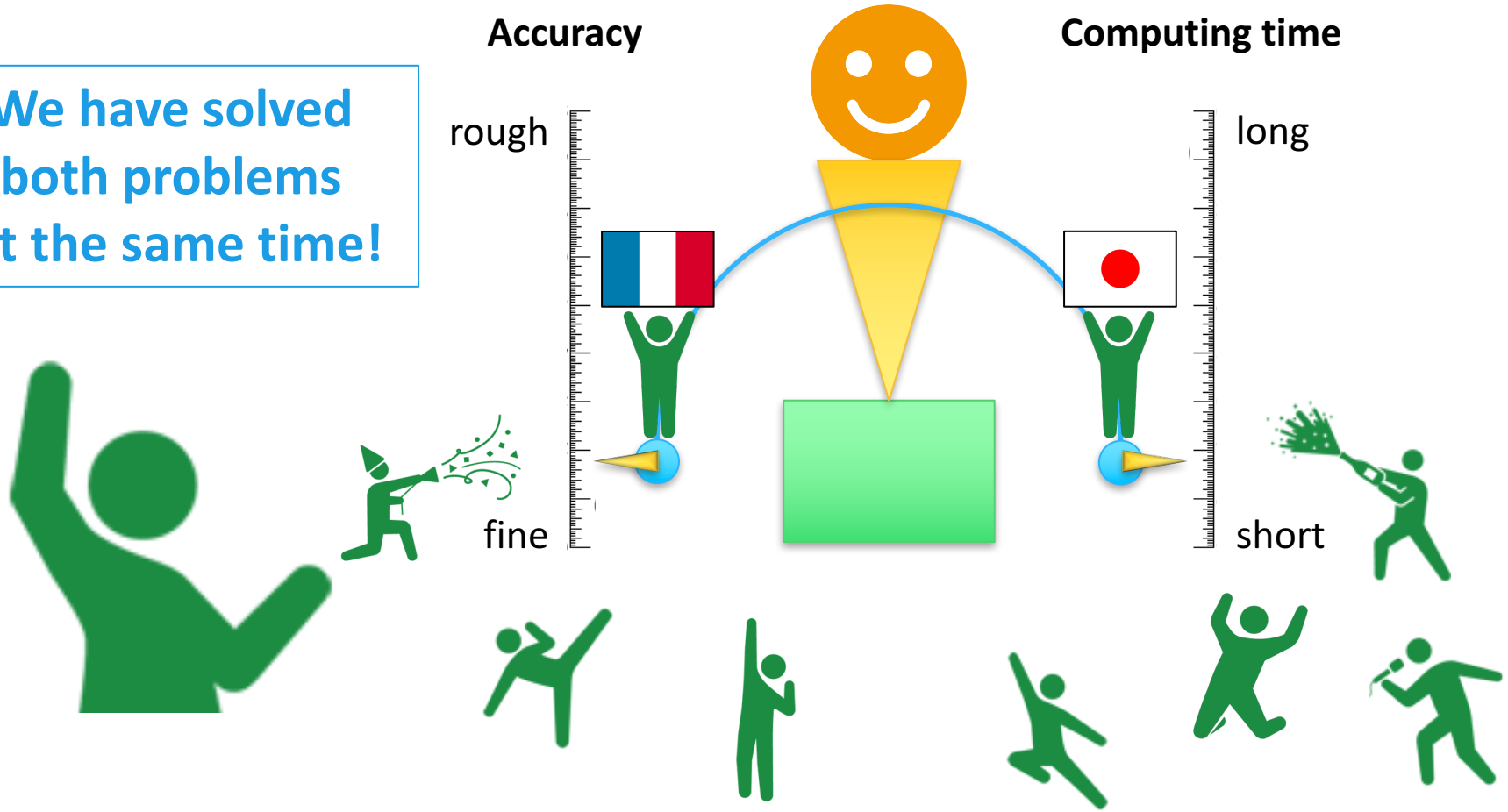
Improving Monte Carlo simulations

Accuracy and computing time is tradeoff…



Improving Monte Carlo simulations

We have solved both problems at the same time!



Highlights in 2013-2015

- Development of Geant4-DNA
  - Geant4-DNA physics models have been improved in order to simulate electron transportation in liquid water.
  - A Geant4-DNA interface able to simulate chemical reactions in liquid water was also developed.

- MPEXS-DNA: Porting of Geant4-DNA to GPGPU
  - Up to **280 times** faster on GPU(K40c) than CPU for Geant4-DNA physics (2015)

- Organization of the 11th Geant4 Space User's Workshop
  - 11th Geant4 Space User's Workshop in Hiroshima, Japan, on August 26-28th, 2015 (http://nsl.iis.it-hiroshima.ac.jp/geant4/).
  - Geant4-DNA tutorial on August 23-24, 2015 at the same location, and attracted 26 participants, mainly from Japan (https://indico.esa.int/indico/event/82/).

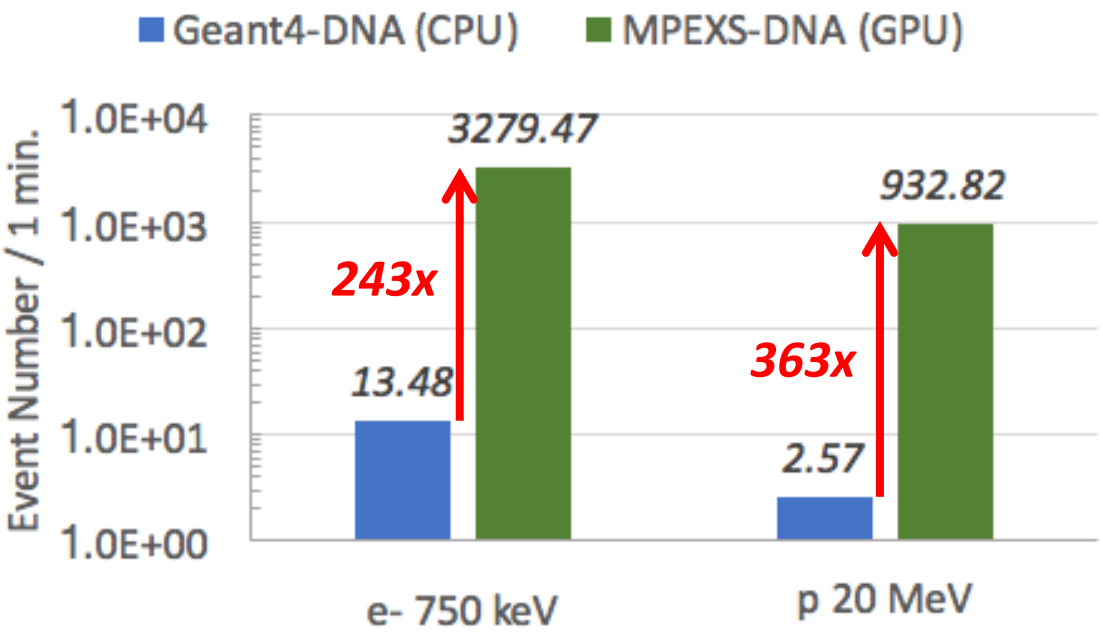
Highlights in 2016

- **MPEX-DNA: porting physics and chemistry interface to GPGPU**
  - The chemistry interface in Geant4-DNA has been ported to GPGPU.
  - The calculation speed on MPEX-DNA including chemistry interface is up to **1,178 times** faster on GPU(P100) than single-CPU.
- **Development of Geant4-DNA physics**
  - **New discrete physics models** for electron transportation **in Gold**.
  - The physics models are validated by experimental data for large gold bulk.
  - The physics models are working well compared with existing Geant4 models in very small gold bulk.

1) Computing performance improvement

- MPEXS: *Massive Parallel Electro X-ray Simulator*
  - GPU-powered Geant4 standard EM physics
  - Up to 250 times speedup against single core CPU (2015)
  - Collaborators: SLAC NATIONAL ACCELERATOR LABORATORY, ICME Stanford Institute for Computational & Mathematical Engineering, 
- MPEXS-DNA
  - An extension of MPEXS to Geant4-DNA Physics
  - Up to 280 times speedup against single core CPU (2015)
  - Collaborators: CENBG, 

- Up to ***1,178 times*** speed up against single-core CPU including physics and chemical interface
  - 4 days (single-core CPU) -> **~ 5 min.** (p 20 MeV, 10k events: P100)



K40c→ P100 (Preliminary)

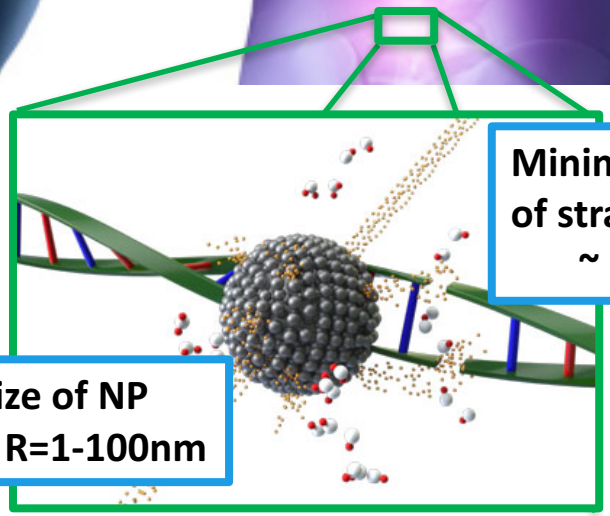
e^- 750 keV : **3.06x**

p 20 MeV : **3.24x**

S. Okada et al, GTC2017

- GPU (NVIDIA, Tesla K40c, 2,880 cores, 745 MHz)
- CPU single core (Intel, Xeon E5-2643 v2, 3.50 GHz)

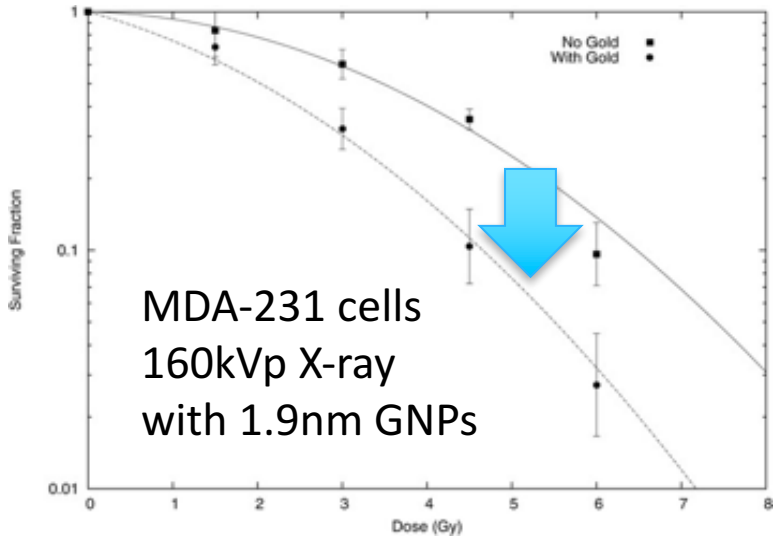
2) Physics models accuracy improvement for Gold NP



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)



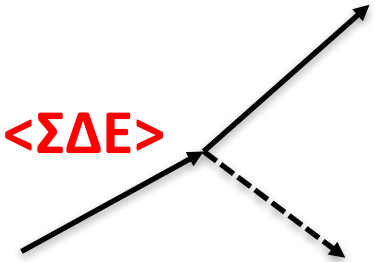
MDA-231 cells
160kVp X-ray
with 1.9nm GNPs

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

Physics models accuracy improvement for Gold NP

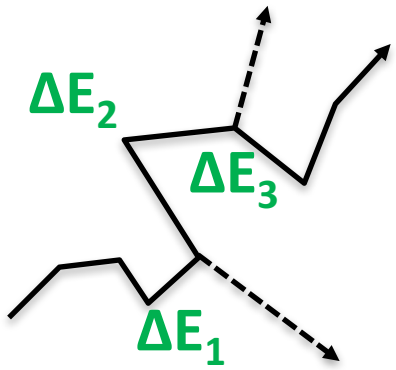
Condensed history models

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



Discrete models

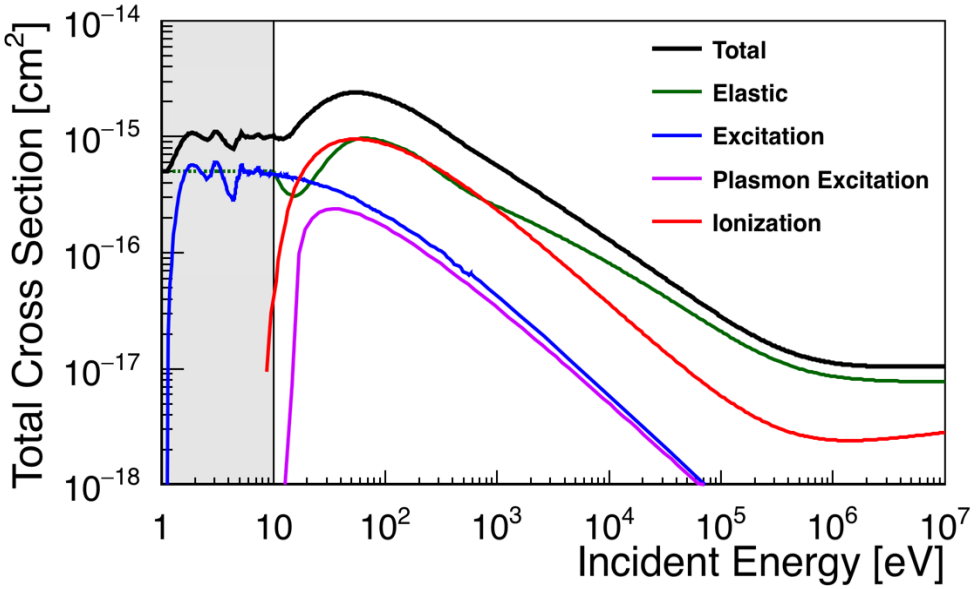
- One single deflection
- One single energy loss
  are calculated for each physics process.
- No production cut



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



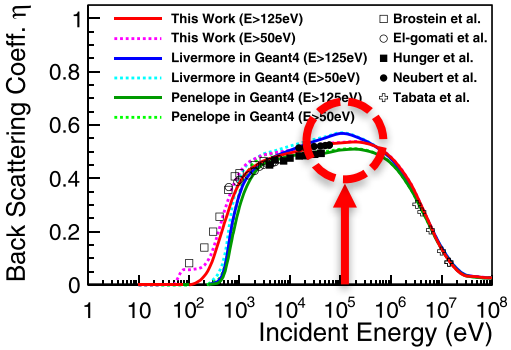
Integrated electron cross sections in gold. Bremsstrahlung is not shown. All particles with energy below 10 eV (shown in gray) are killed and their energy is dumped locally.

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

New physics models in gold nanoparticle (GNP)

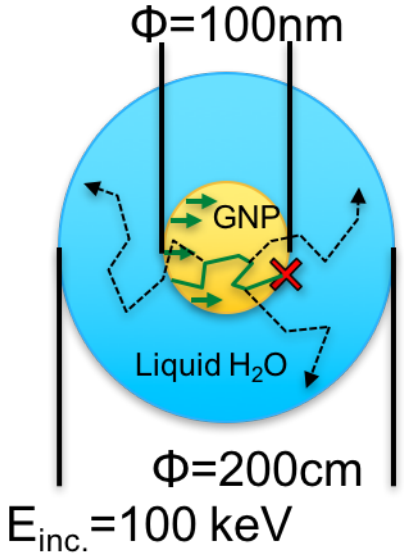
Back scatt. coef. for 5cm gold plate

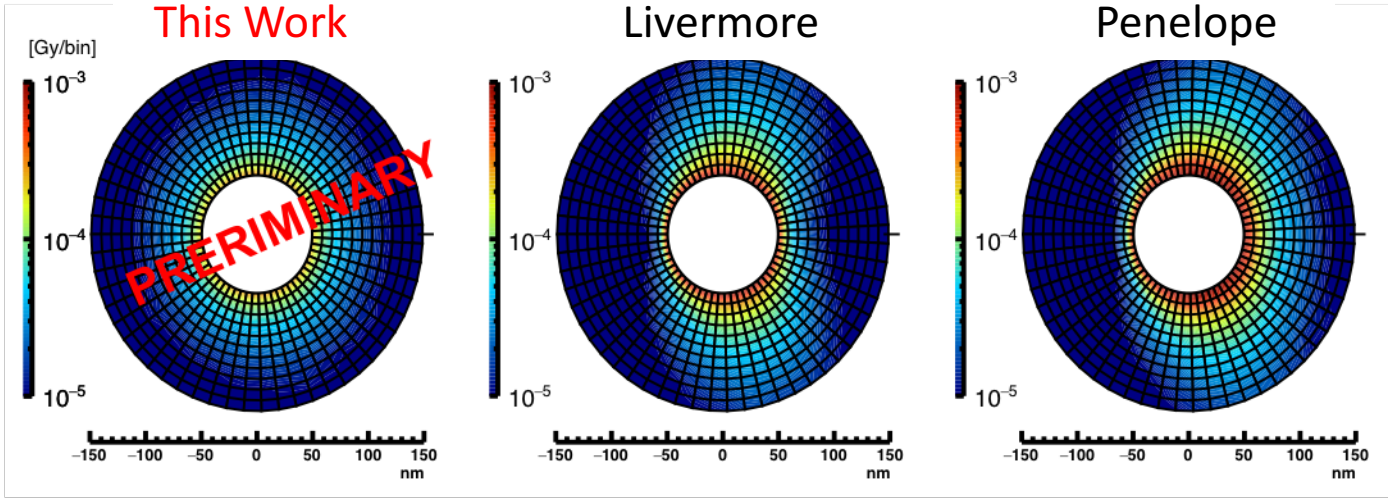


All physics models show high back scattering coefficient in large gold bulk.

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

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





Outcome 2013-2016

- Award
  - NDIVIA award (Best poster award) by **S.Okada** at GPU Technology Conference Japan, 2016

- 5 publications
  - *"An implementation of discrete electron transport models for gold in the Geant4 simulation toolkit"*, **D. Sakata et al**, **J. Appl. Phys. 120 (2016) 244901**
  - *" Recent developments in Geant4 "* , Geant4 Collaboration, **Nucl. Instrum. Meth. A 835 (2016) 186-225**
  - *"Geant4 Monte Carlo simulation of absorbed dose and radiolysis yields enhancement from a gold nanoparticle under MeV proton irradiation"*, **H. Tran et al**, **Nucl. Instrum. Meth. B 373 (2016) 126-139**
  - *" GPU Acceleration of Monte Carlo Simulation at the Cellular and DNA Levels "*, **S. Okada et al**, **Sma. Inn. Sys. Tech. 45 (2016) 323-332**
  - Track structure modeling in liquid water: A review of the Geant4-DNA very low energy extension of the Geant4 Monte Carlo simulation toolkit, M. A. Bernal et al, **Phys. Med. 31 (2015) 861-874**

Access papers from http://geant4.in2p3.fr

- 1 international workshop and tutorial
  - 11th Geant4 Space User's Workshop/Second Geant4-DNA tutorial, August 23-24, 2015 - Hiroshima, Japan

New proposal for 2017-2020

Bio3

"GPU acceleration for Geant4 applications at the Physics-Medicine-Biology frontier "

Proposed workplan from 2017

- Continuation of development of Geant4-DNA for MPEXS-DNA.
  - New physics models from the CPA100 track structure code will be ported to MPEXS-DNA.
- Inclusion of Geant4 hadronic physics into MPEXS.
  - The hadronic physics models of Geant4 (e.g. binary cascades) will be ported to MPEXS.
- Investigation of radiation therapy boost using high-Z nanoparticles
  - The newly developed EM physics models for Gold will be extended for proton transportation.
  - Fundamental study to investigate boost effect in radiation therapy will be done (clinical photons, electrons, protons).
- Development of a medical physics application for interventional radiology.
  - Develop an application to simulate absorbed dose in patient (realistic human phantom) and medical doctor during interventional radiology will be started.

Summary and Outlook

- The Geant4-DNA physics and chemistry have been ported to MPEXS-DNA GPGPU based MC simulation platform.
- The calculation speed on MPEXS-DNA including chemistry interface is up to 1,178 times faster on GPU(P100) than single-CPU(Xeon E5-2643 v2).
- New alternative Geant4-DNA physics models for electron in gold have been implemented.
- Geant4 hadronic interface and Geant4-DNA physics models for Gold will be ported to MPEXS and MPEXS-DNA
- Development of application for medical physics (interventional radiology) will be started.

Current Project Members

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			Toshiyuki Toshito	Dr.	Nagoya City
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Thank you !!!