KEK
High Energy Accelerator Research Organization

Monte Carlo Applications for Radiological Science

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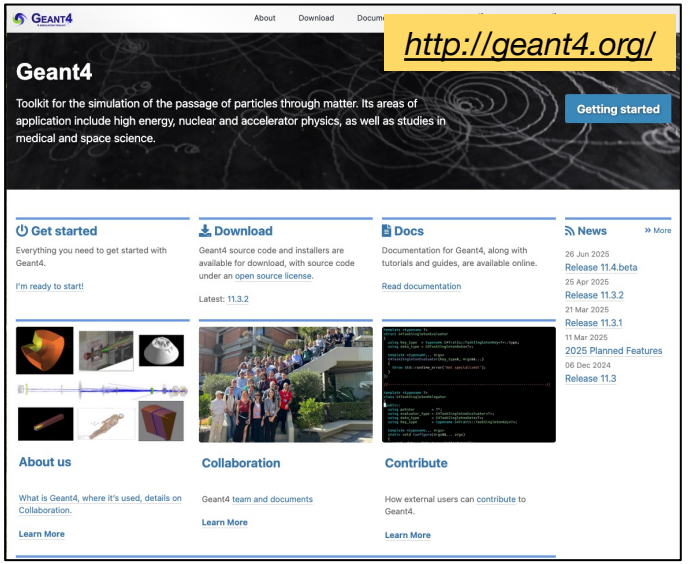
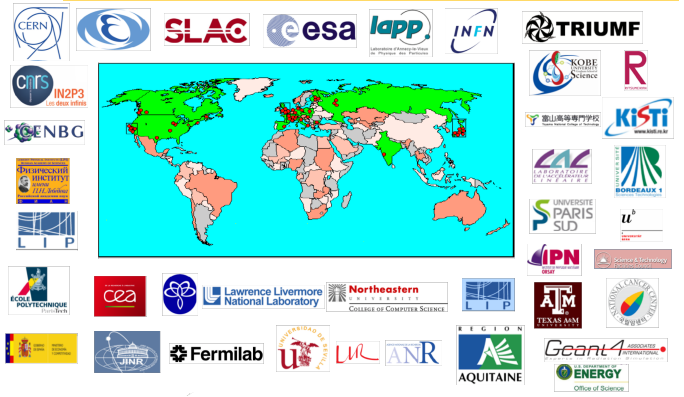
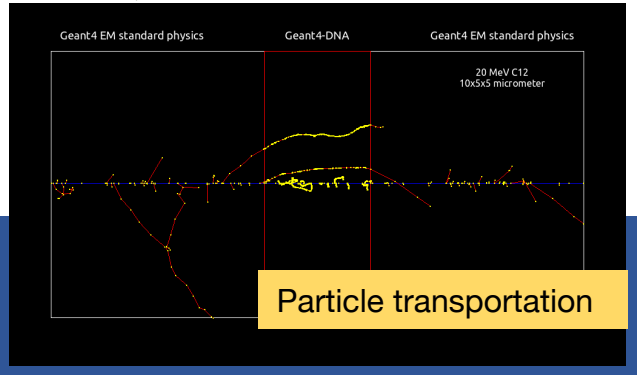
Geant4

- A radiation simulation toolkit for high energy physics (HEP) using the Monte Carlo method
  - International collaboration among KEK, CERN, SLAC, …
  - Geant4 libraries:
    - Simulating EM and hadronic physics processes with wide energy range (meV ~ PeV)
    - Building complex geometries for HEP experiments
    - **Users need to write a main program using Geant4 libraries**
  - Detector simulations, backgroud estimations, etc.
- Major simulation code for radiation physics in the world
  - Spreading out to various research domains
  - The first paper has been cited **+20k**
    - S. Agistinelli et at., “Geant4: a simulation toolkit”, NIM A, vol. 506, no. 3, pp. 250-303, 2003



Geant4 Collaboration
24 countries, 38 institues, 129 members



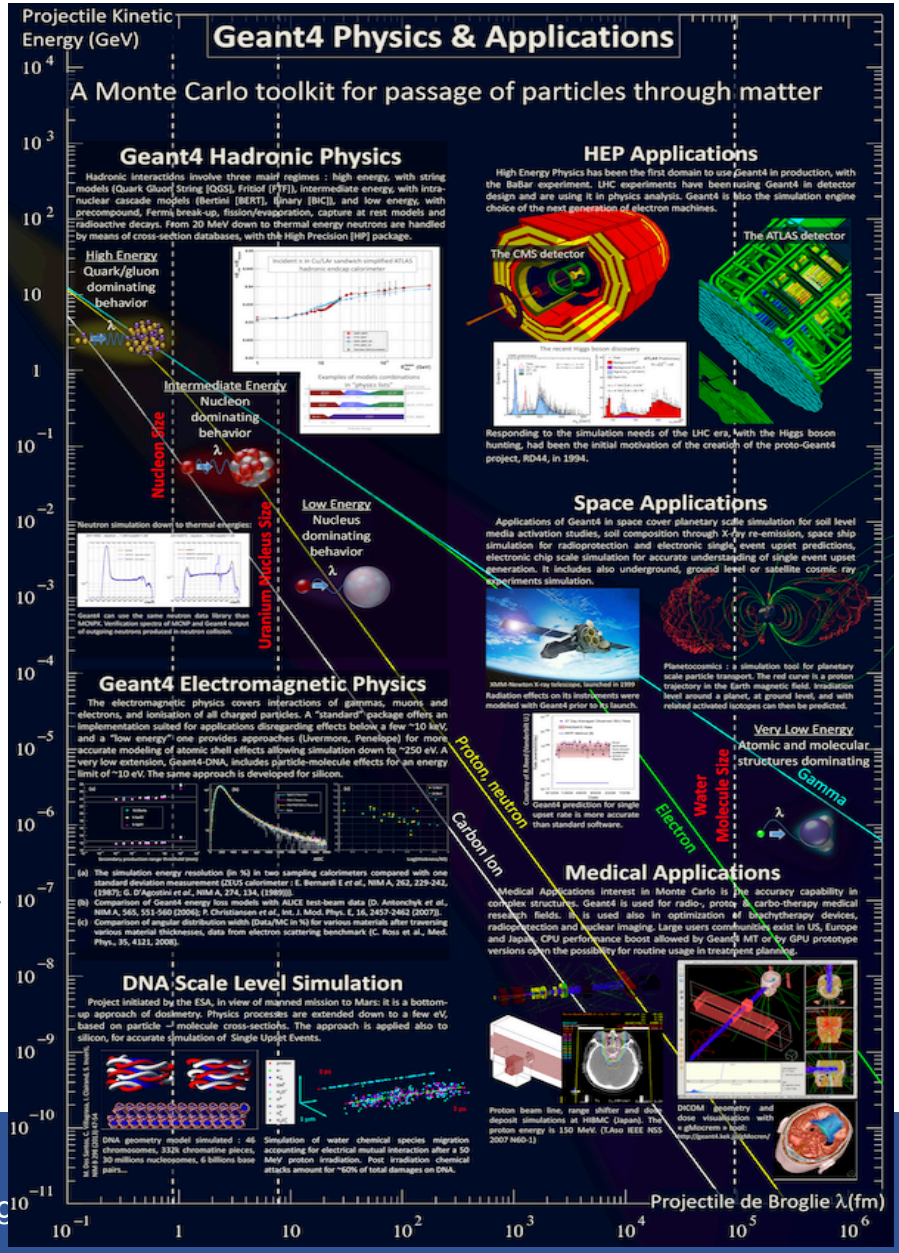


Particle transportation

Geant4 Applications

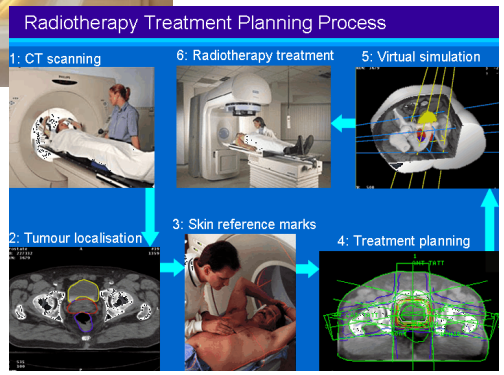
- Transferring simulation technology accumulated through HEP experiments to the other fileds:
  - Nuclear physics
    - Radiation shielding
  - Astrophysics / Spece science
  - Accelerator science
  - Medicine / biology

- The Geant4-Japan group focusing on application study in medicine and biology
  - Extending functionalities of Geant4 for particle therapy and user supports
  - R&D of advanced treatment planning using MC simulations
    - Collaboration research with particle therapy facilities
  - Taking part in the Geant4-DNA project
    - Microdosimetry simulations

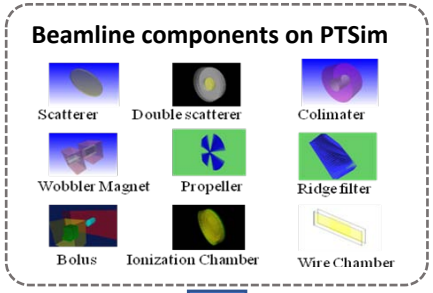


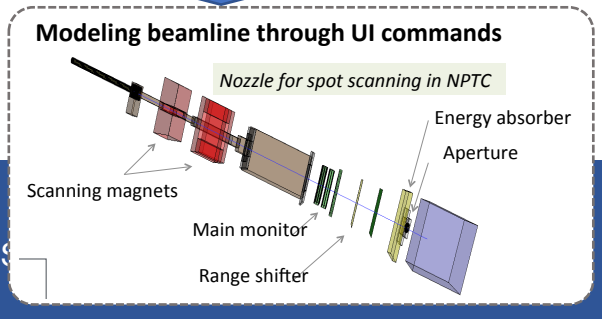
Geant4 in Medicine and PTSim

- **Particle therapy**
  - Uses energetic protons/carbons to irradiate tumors
    - 26 facilities (19 protons, 6 carbons) in Japan
  - Optimizing beam energy, direction, and dose during treatment planning
    - Geant4 is used in QA of treatment planning
      - Higher accuracy than treatment planning system
      - One day simulation per patient on CPU cluster



- **PTSim: A Geant4-based MC platform for medicine**
  - Developed by the Geant4-Japan group
    - JST-CREST project (2003-2010)
      / Representative: Prof. T. Sasaki (KEK-CRC)
  - Runs dose calculation with simple UI commands
    - Models beam-delivery system and treatment head
    - Reconstructs patient geometry from CT images
  - Widely used for QA in Japanese hospitals
    - Our project has inspired other projects in the world
      - TOPAS / GAMOS





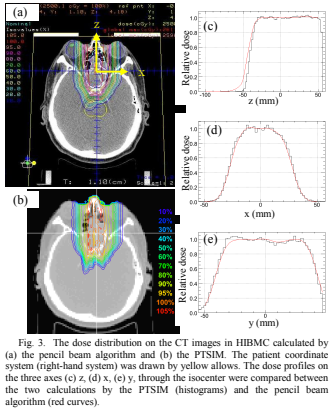
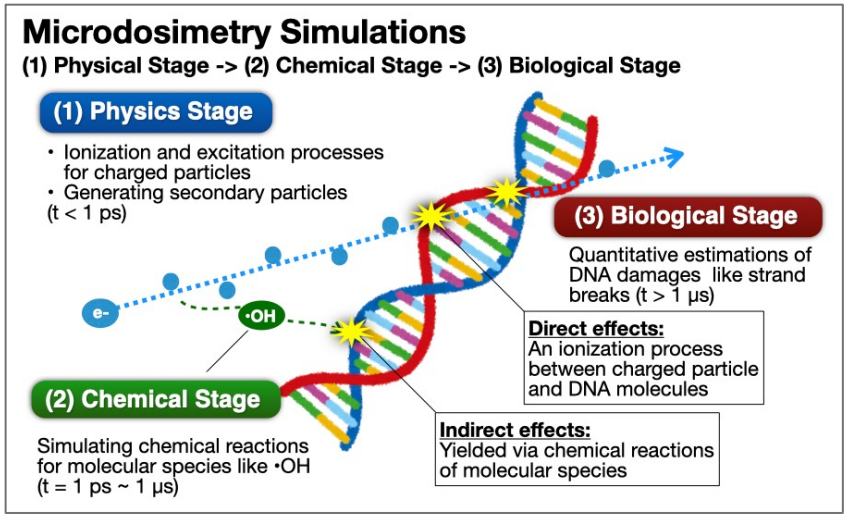


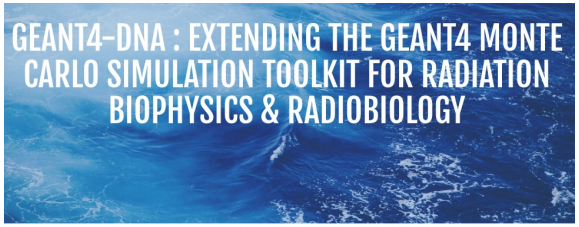
Fig. 3. The dose distribution on the CT images in HIBMC calculated by (a) the pencil beam algorithm and (b) the PTSIM. The patient coordinate system (right-hand system) was drawn by yellow allows. The dose profiles on the three axes (c) z, (d) x, (e) y, through the isocenter were compared between the two calculations by the PTSIM (histograms) and the pencil beam algorithm (red curves).

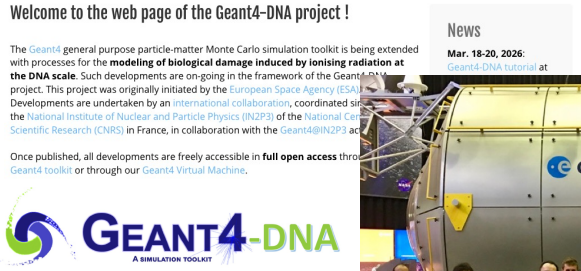
Microdosimetry Simulations

- Understanding radiation phenomenology at a subcellular scale
  - Simulating physical / chemical interactions
  - Evaluating radiation damages quantitatively
    - e.g., strand breaks, base damages, and repairs

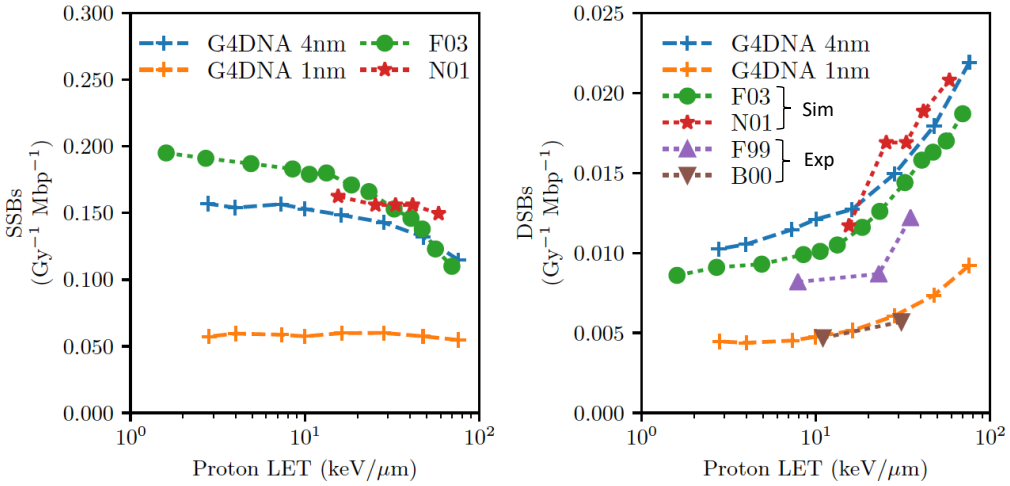
- **The Geant4-DNA Project**
  - An extension of Geant4 to DNA physics
    - Led by Bordeaux Univ. LP2i
    - KEK-Geant4 team taking part in the project
  - Main objective
    - Estimating effects on human health under chronic radation exposure for astronauts in space missions
    - …
  - Functinalities
    - EM physics processes for ultra-low energy range (down to meV) and chemical reactions
    - Estimating early radiation damages to DNA after irradiation
    - Handling the cell nucleus geometries which contains DNA double helix structures



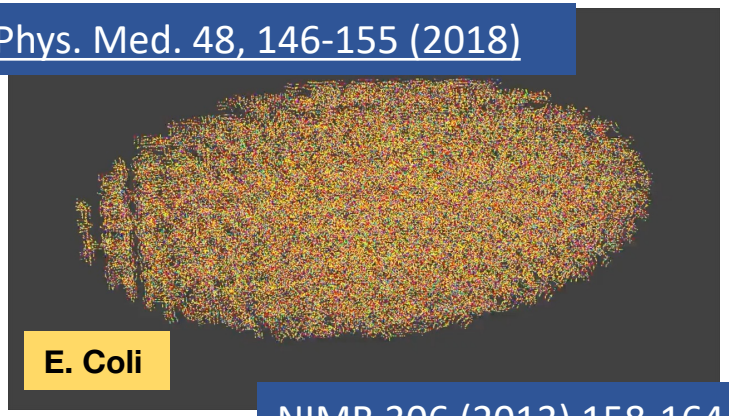




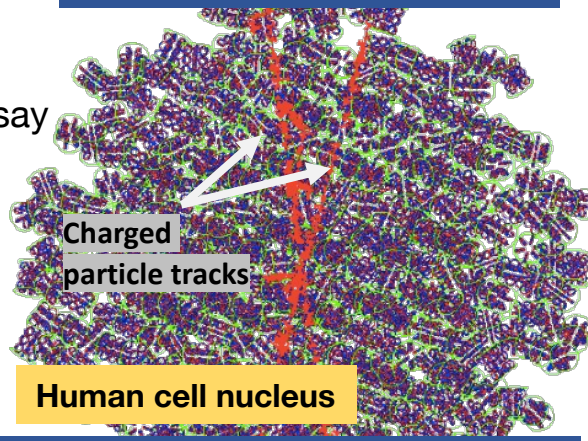
DNA Damage Estimstions through Geant4-DNA Simulations



Phys. Med. 48, 146-155 (2018)

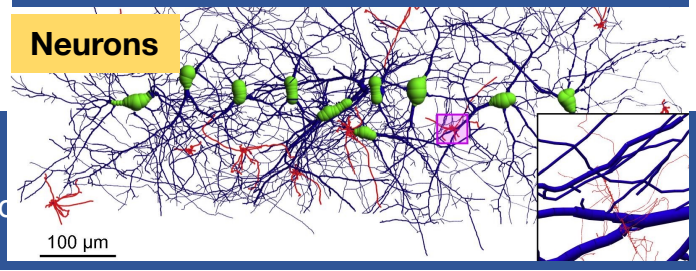


NIMB 306 (2013) 158-164



- Geant4-DNA can reproduce experimental data of radiation damage assay
- Microdosimetry simulations spend significantly longer time
  - Tracking vast number of particles and molecules
    - Yielded +10,000 per one initial particle
  - Taking several days to weeks even on CPU cluster
  - **Accelerating computing performance is required**
- Works in progress:
  - Implementation of repair process
  - Study for gold nano particle, FLASH RT, etc.

Phys. Med. 32(12) 1510-1520 (2016)



Accelerating Medical & Biological Applications by GPGPU

- Requires much more computing power in medicine and biology
  - Particle therapy
    - Higher accuracy for dose calculations by Geant4 (PTSim)

    → One day simulation per patient
  - Microdosimetry
    - Tracking much more particles and molecular species to increase spatial resolution for radiation damage estimations

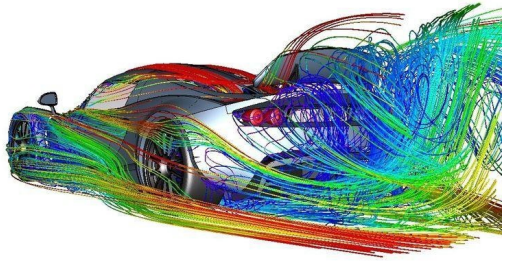
    → Several days to weeks simulation

- Reduces computation time by ultra-parallel processing on GPU
  - Developing MPEXS to make medical and biological simulations more practical

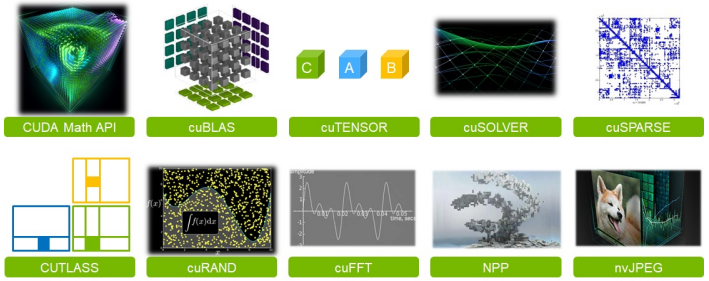
GPGPU

- **GPU: Graphical Processing Unit**
  - Ultra parallel processing devices for graphics
    - GPU: +20,000 cores
    - CPU: Up to 100 cores

- **GPGPU: General-Purpose computing on GPU**
  - Accelerating scientific calculations in various fields:
    - AI
    - FEM simulations
    - Molecular Dynamics
    - Multi-body simulations
    - …



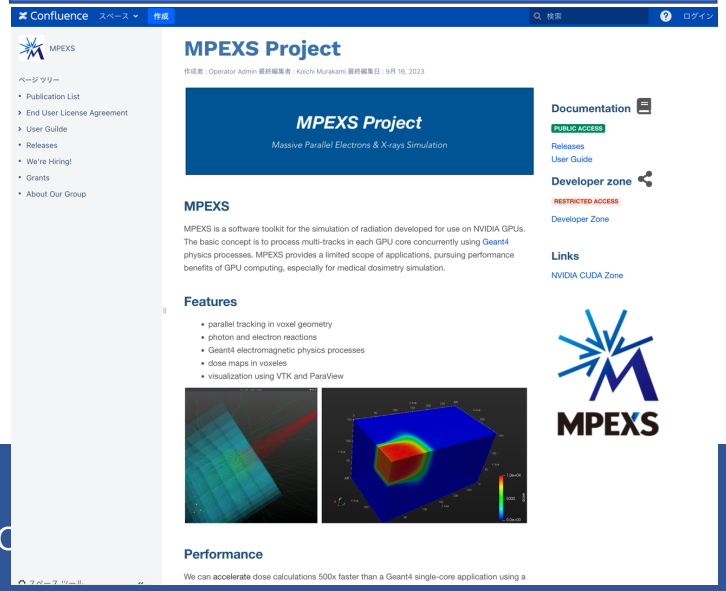
- **CUDA**
  - Programing framework for GPU computing
  - Like a C/C++ language extension
  - Providing APIs, debuggers, and profilers to support developing GPU applications



MPEXS Project

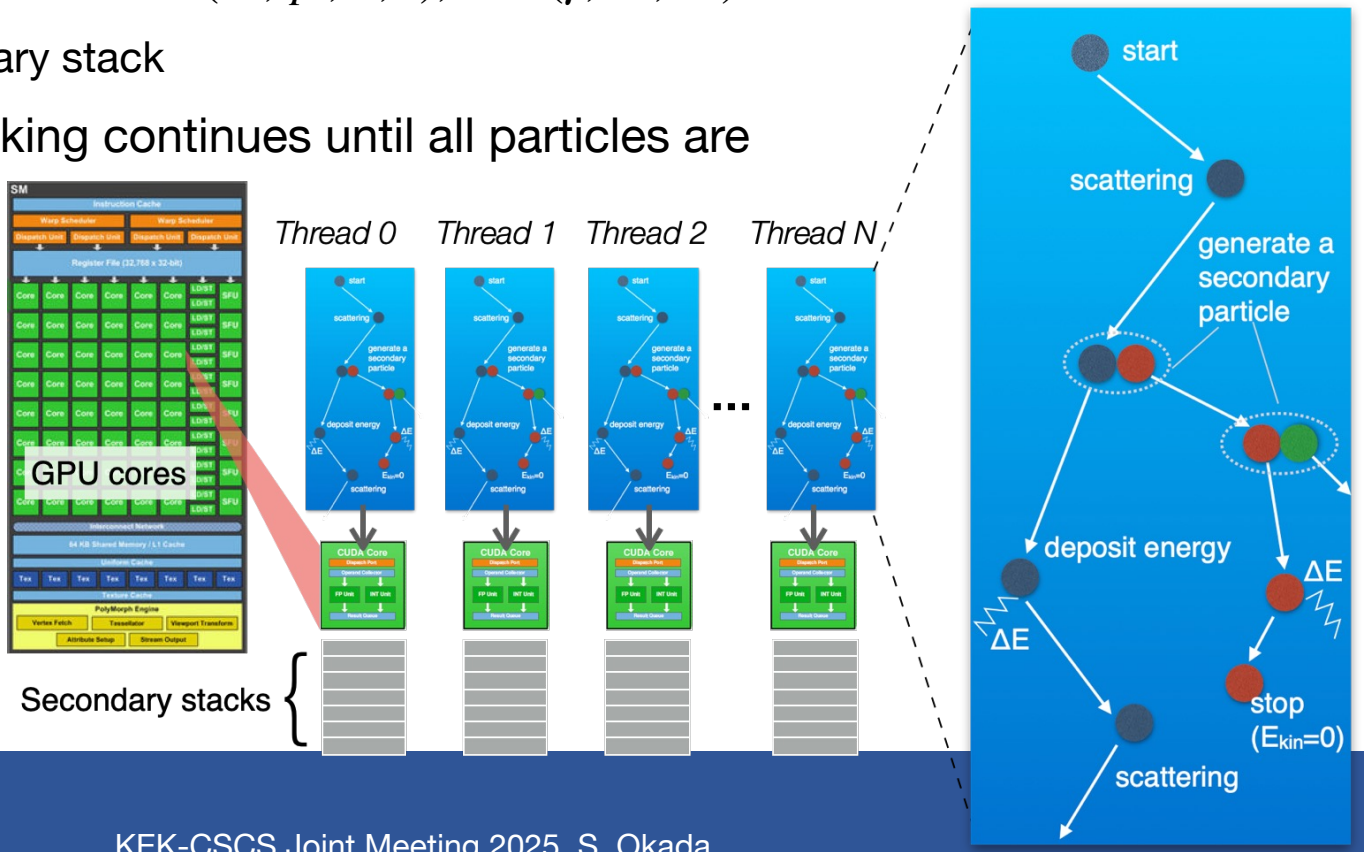
- **A state-of-the-art radiation simulator running on GPU devices**
  - Developed as a dose calculation engine for radiotherapy
- **Core algorithm and associated physics data taken from Geant4**
  - Physics process of Geant4 are reengineered and reimplemented in CUDA
  - Data structure is redesigned from scratch to suite for GPU processing
  - Not machine translation (e.g., OpenACC)
- **Current functionality:**
  - EM / hadron / neutron physics processes with energy range below 1 GeV
  - Water-equivalent material
  - Voxelized geometry

https://wiki.kek.jp/display/mpexs/MPEXS+Project



Parallel Tracking on GPU

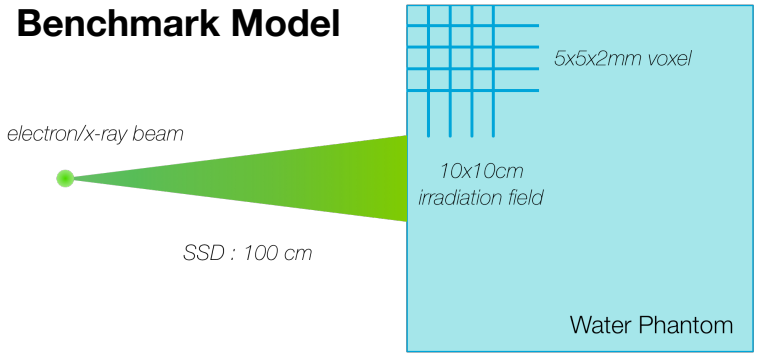
- Millions of particles are tracked in parallel across GPU threads
  - Each track is independent
  - GPU threads hold kinematic information of particles:
    - Track information: $(\vec{x}, \vec{p}, E, k),\ k \in (\gamma, e^-, e^+)$
    - Secondary stack
  - Parallel tracking continues until all particles are processed



MPEXS Performance

- MPEXS shows agreement with Geant4 simulations within 2%
- Up to **1000 times** speedup against Geant4 with a single-core CPU

Benchmark Model



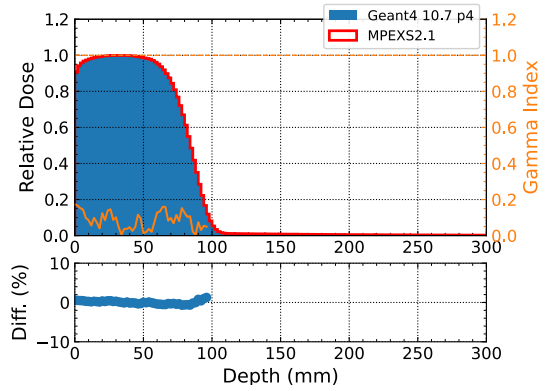
Throughput: number of events processed per milisecond

Primary Particles	Geant4 ver. 10.7 p4	MPEXS	Speedup (MPEXS/G4)
Electron 20 MeV	2.9	2423.7	**x832**
X-ray 6 MV	6.2	5817.5	**x931**
X-ray 18 MV	5.6	4600.8	**x822**

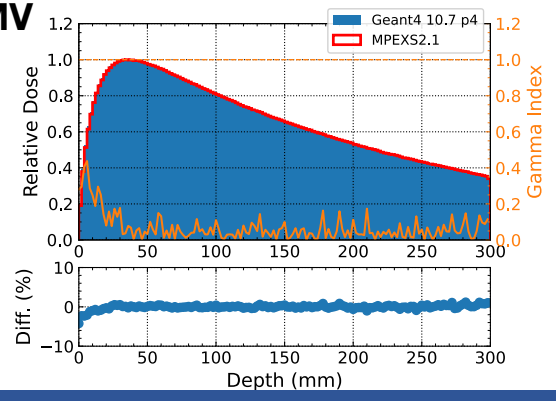
Benchmark hardware:
- CPU: Intel Xeon Gold 6326 (Ice Lake)
- GPU: NVIDIA RTX 6000 Ada Generation

Depth dose curves (Geant4 vs MPEXS)

e^- 20 MeV



X-ray 18 MV



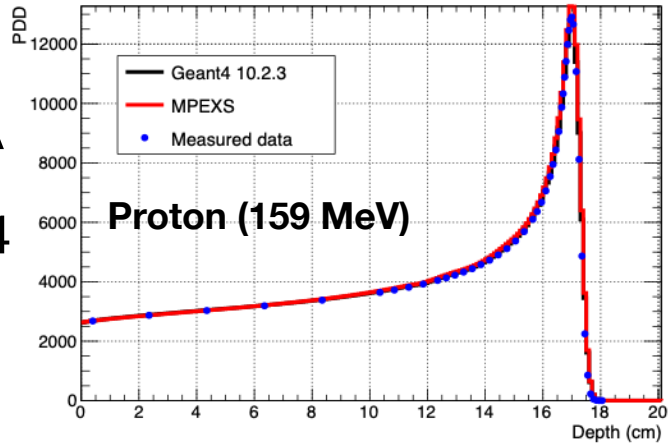
MPEXS Hadron Physics Extension

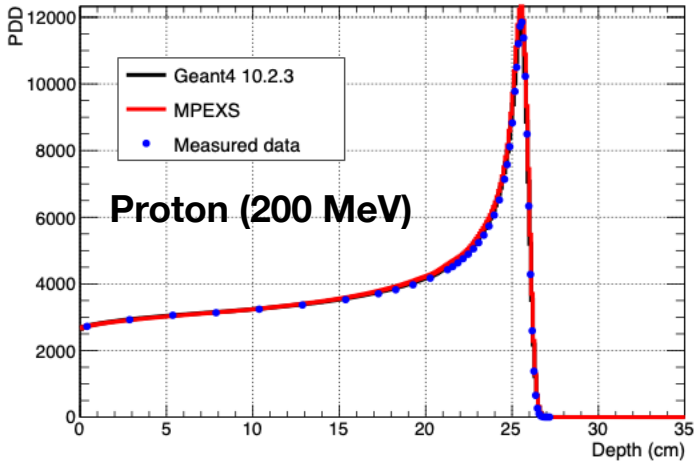
- Accelerate dose calculations for proton/carbon therapy
- Port Geant4 hadronic processes to CUDA
- Up to **230 times*** speedup against Geant4 simulations with a single-core CPU
  - Thread divergency is much larger than EM processes

*Benchmark hardware:
- CPU: Intel Xeon Gold 6132
- GPU: NVIDIA RTX 3090

Ref.) C. Omachi, et al., "Clinical uses of Geant4 and a new GPU Monte Carlo simulation system in proton therapy", PTCOG 57th Annual Conference, Cincinnati, US, 2018 May

Depth dose comparison (Geant4 vs MPEXS-h vs measurement)





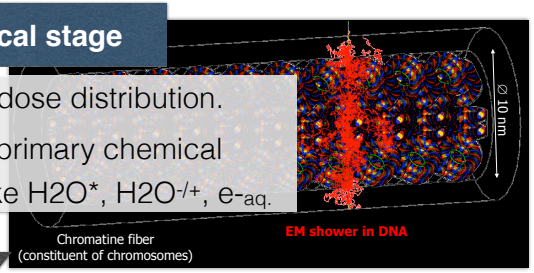
MPEXS-DNA: Microdosimetry Simulation on GPU

- MPEXS Extension to DNA Physics
  - Collaborative study with the Geant4-DNA project

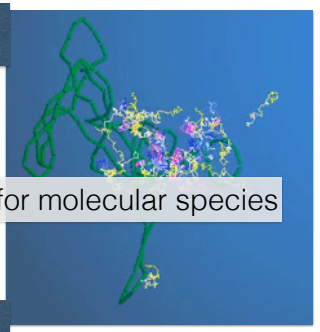
- Based on Geant4-DNA 10.7 Patch-4
  - EM Physics with lower energy range
    - Down to meV
    - Calculate local energy loss and generate primary molecules (H_2O^*, $H_2O^{+/-}$)
  - Radiolysis of water molecules
    - Diffusion and chemical reactions for molecular species like •OH radicals
  - The biological stage not yet implemented

1. Physical stage

- Calculate dose distribution.
- Generate primary chemical species like H2O*, $H2O^{-/+}$, $e^-_{aq.}$

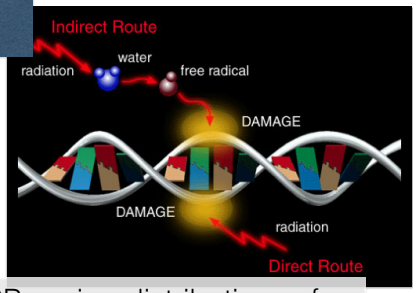


2. Chemical stage



Diffusion and reactions for molecular species

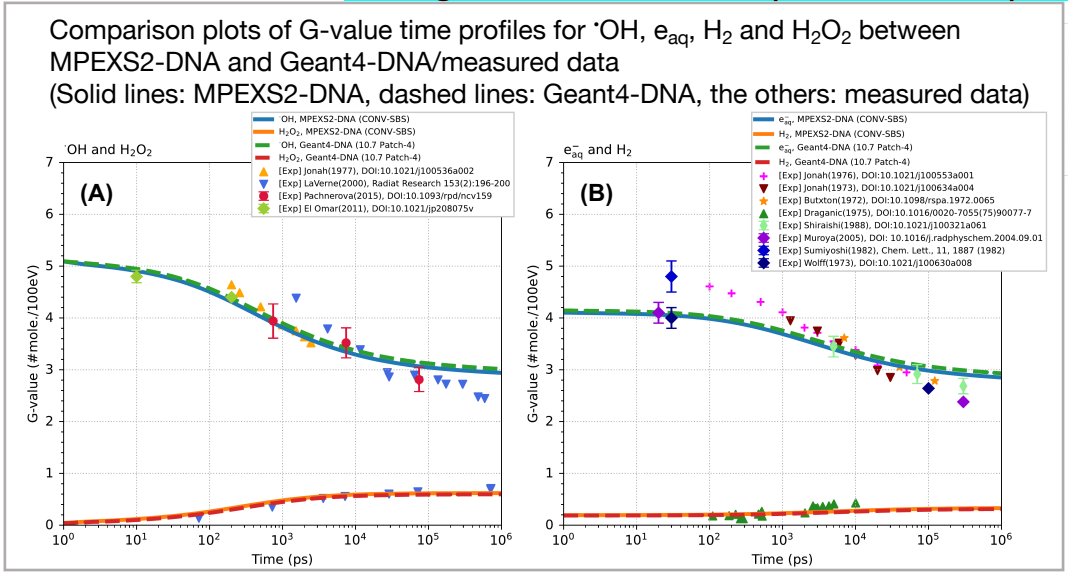
3. Biological stage (Future work)

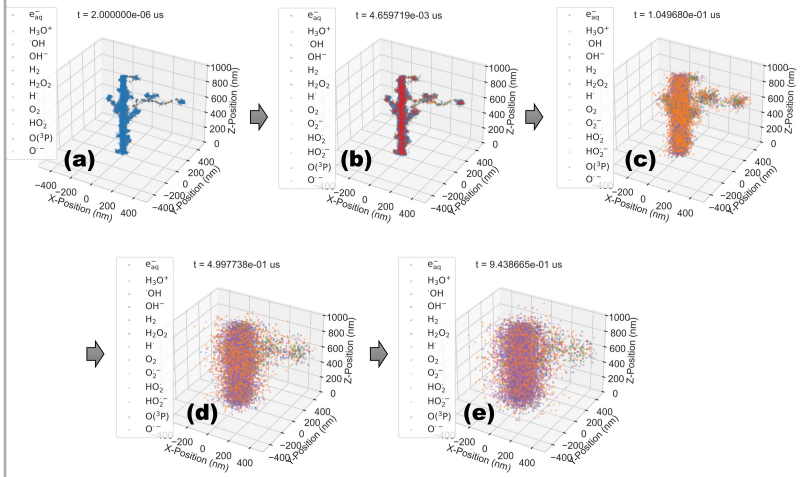


Estimate SSBs and DSBs using distributions of energy loss and molecular species inside the cell nucleus.

MPEXS-DNA Performance

- Water radiolysis under 750 keV electron irradiations
  - Reproducing measured data reasonably well
  - MPEXS2-DNA is much faster than Geant4-DNA
    - A single GPU has the equivalent computing performance of 7,600 CPU cores





Benchmark hardware:

- CPU: Intel Xeon Gold 6326 (Ice Lake)
- GPU: NVIDIA RTX 6000 Ada Generation

	Geant4-DNA 10.7.4	MPEXS-DNA
Throughput (#histories / min.)	5.69	43564.97
Speedup Factor (MPEXS / Geant4)	-	**x7,656**

References:

[1] S.Okada et al., *Medical Physics*, 2019, doi: 10.1002/mp.13370

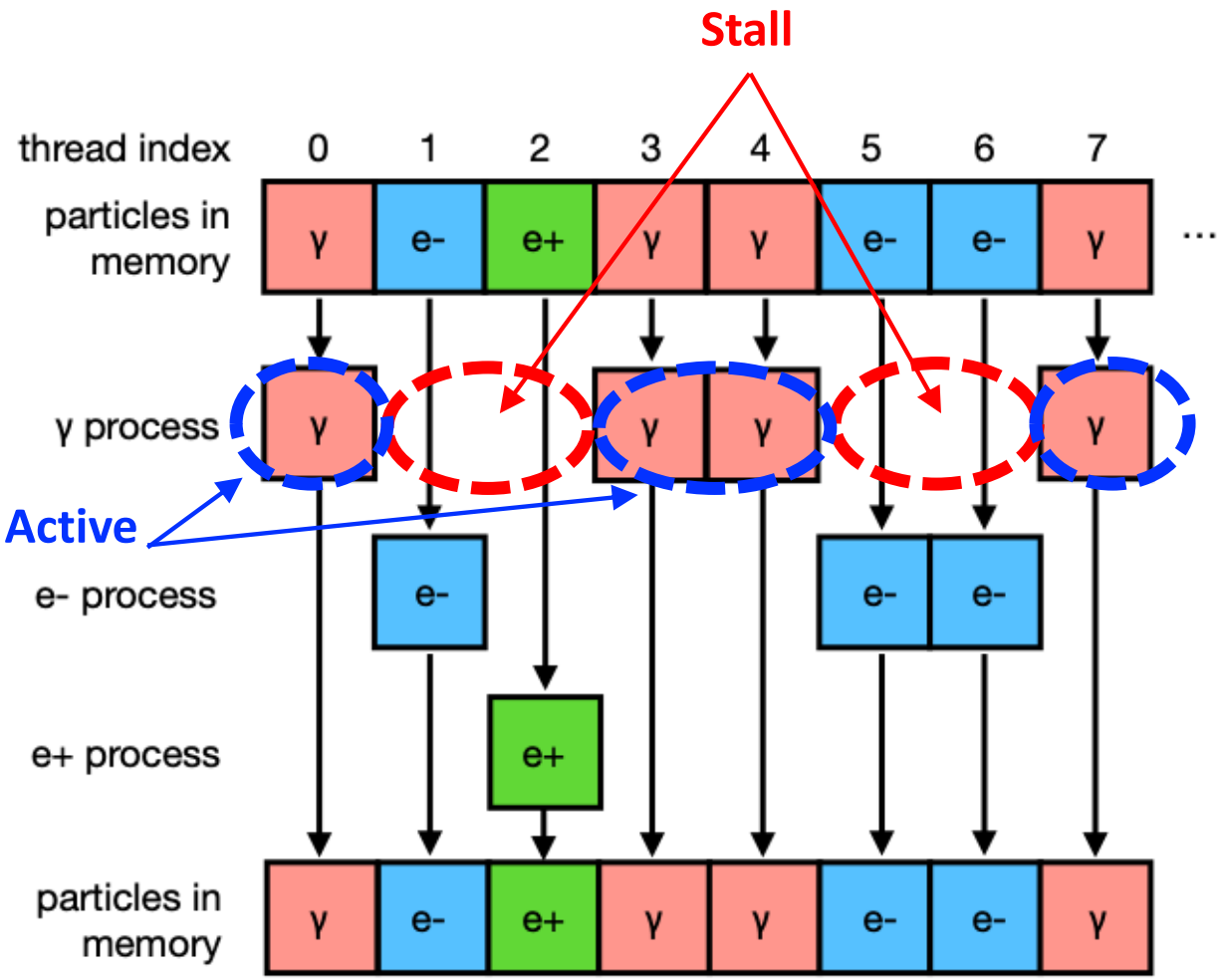
[2] S.Okada et al., *Scientific Reports*, 2025, doi: 10.1038/s41598-025-00875-w

[3] S.Okada et al., *Medical Physics*, 2025, doi: 10.1002/mp.70071

Summary

- Geant4 has been applied to medicine and biology, transferring simulation technologies from HEP experiments
  - Collaboration with particle therapy facilities for developing a Monte Carlo–based platform (PTSim) for QA of treatment planning
  - Participation in the Geant4-DNA project to reveal radiation-induced phenomenology

- Developed a GPU-based Monte Carlo simulator, MPEXS
  - Achieving thousands-fold speedup while maintaining good accuracy
  - Ongoing improvements for faster and more functional radiation simulations in medicine and biology



- Parallel processing of different particls leads to thread divergence
  - Thread efficiency: ~50%