The MPEXS series, a CUDA code based on Geant4

13th Geant4 Space Users Workshop
Space Center, Houston, TX
November 30, 2018

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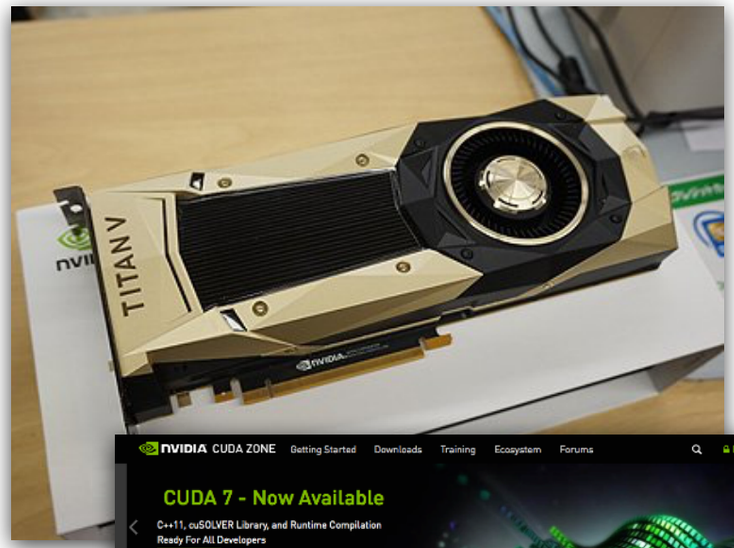
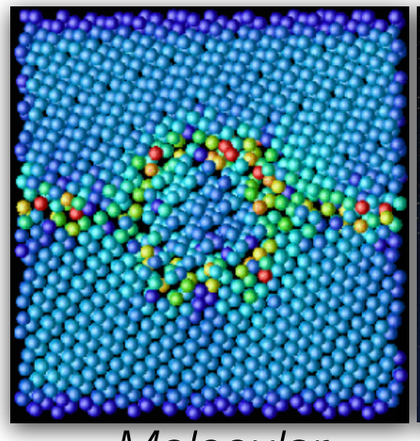
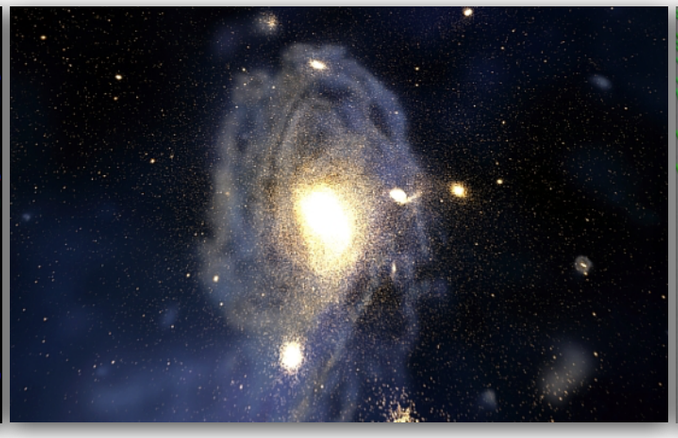
GPGPU: General-Purpose computing on GPU

- **GPU is used as an accelerator for simulations.**
  - NVIDIA TITAN V GPU
    - 5,120 cores (1.46 GHz, FP32)
    - 12 GB Memory (HBM2, GDDR6)
  - CUDA
    - Programing framework for GPU computing
    - Like extension of C/C++
    - Equips APIs, libraries, profiler, debugger, …
- **We have succeeded to boost up Geant4 simulations.**

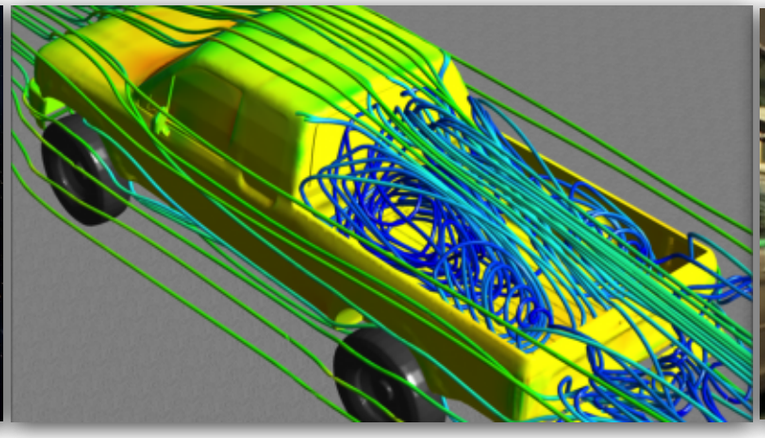




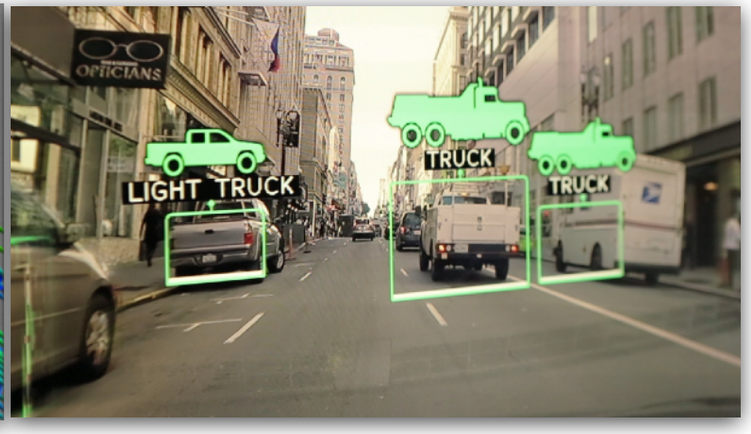
Molecular Dynamics



Multi-body simulation



FEM Simulation



Deep Learning

The MPEXS Project

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

- A state-of-the-art radiation simulator running on GPU devices
  - Developed as a dose calculation engine for radiotherapy to improve the calculation time drastically

- The core algorithms and associated physics data are taken from Geant4.
  - Standard EM physics processes of Geant4 10.2.p3 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:
  - Standard EM physics processes for γ and $e^{\pm}$ below 1 GeV
  - Water equivalent material
  - Voxelized geometry

The joint project among:

SLAC NATIONAL ACCELERATOR LABORATORY

ICME INSTITUTE for COMPUTATIONAL & MATHEMATICAL ENGINEERING at STANFORD UNIVERSITY

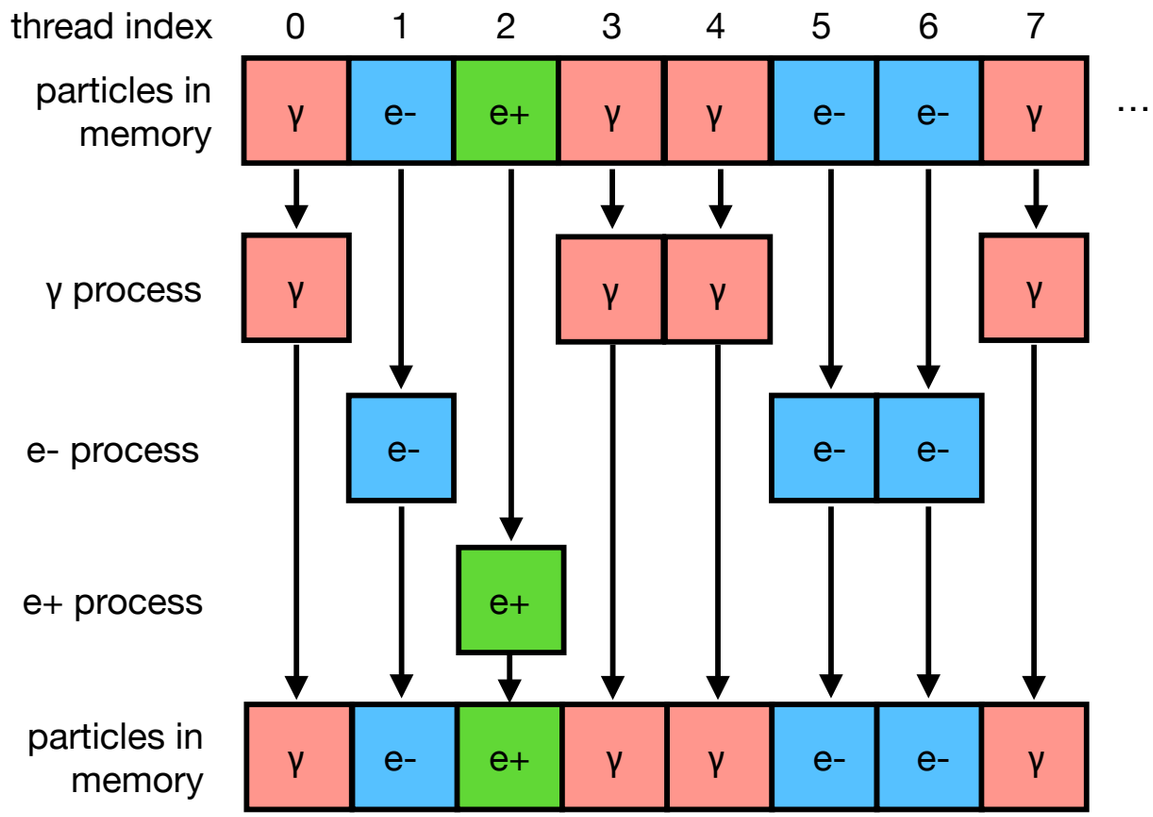
powered by

NVIDIA

Parallel Tracking on GPU

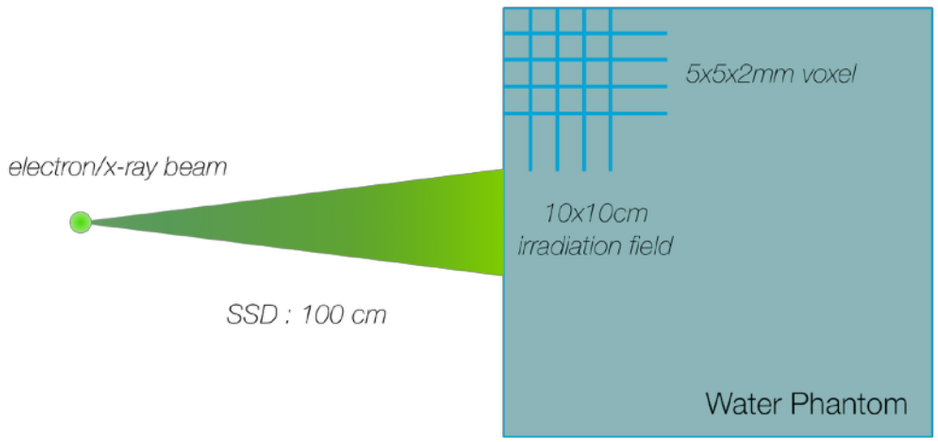
- **Millions of particles are spread over GPU threads and tracked in parallel.**
  - Each track is independent.
  - Each thread has kinematic information of a particle.
    - Track information
      - $(\overrightarrow{x}, \overrightarrow{p}, E, k),\ k \in (\gamma, e^-, e^+)$
    - Secondary stack

- Parallel processing of different particles leads to thread divergence.
  - Thread efficiency: **~ 50%**



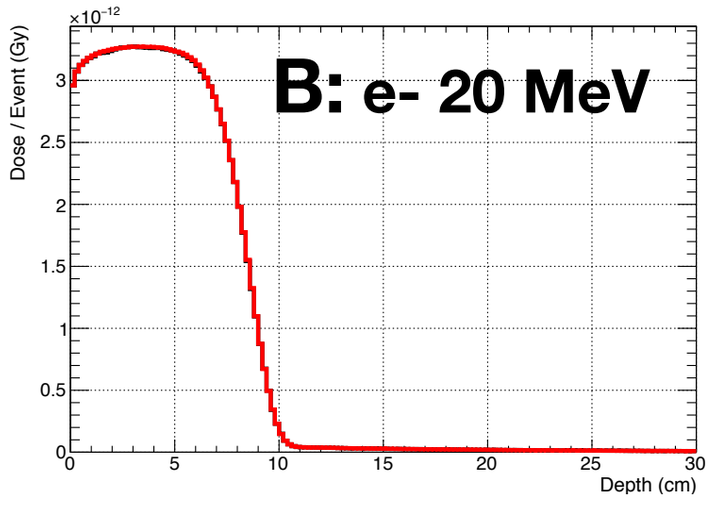
MPEXS Performance

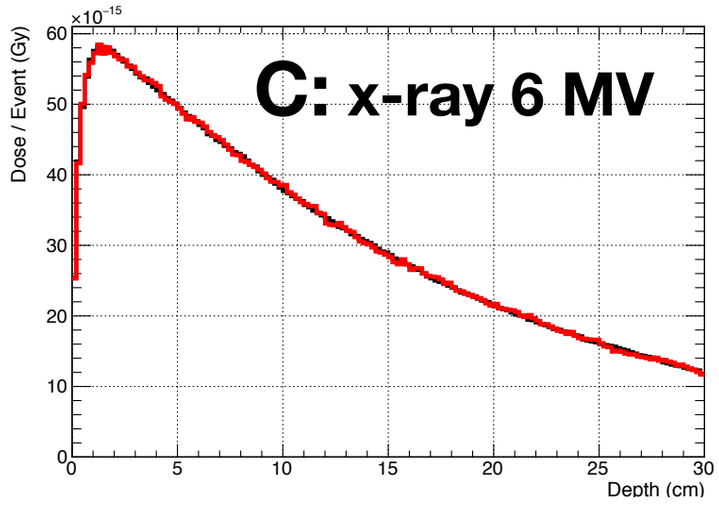
A: Benchmark Model



Depth dose curves (CPU vs GPU)

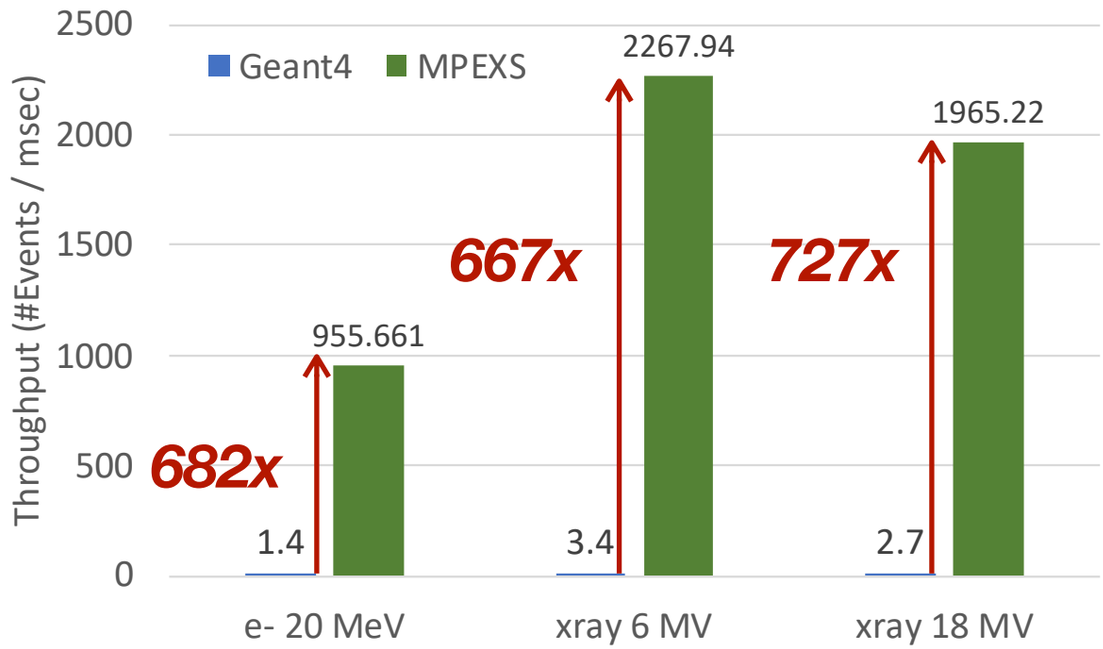
— Geant4 (CPU)
— MPEXS (GPU)





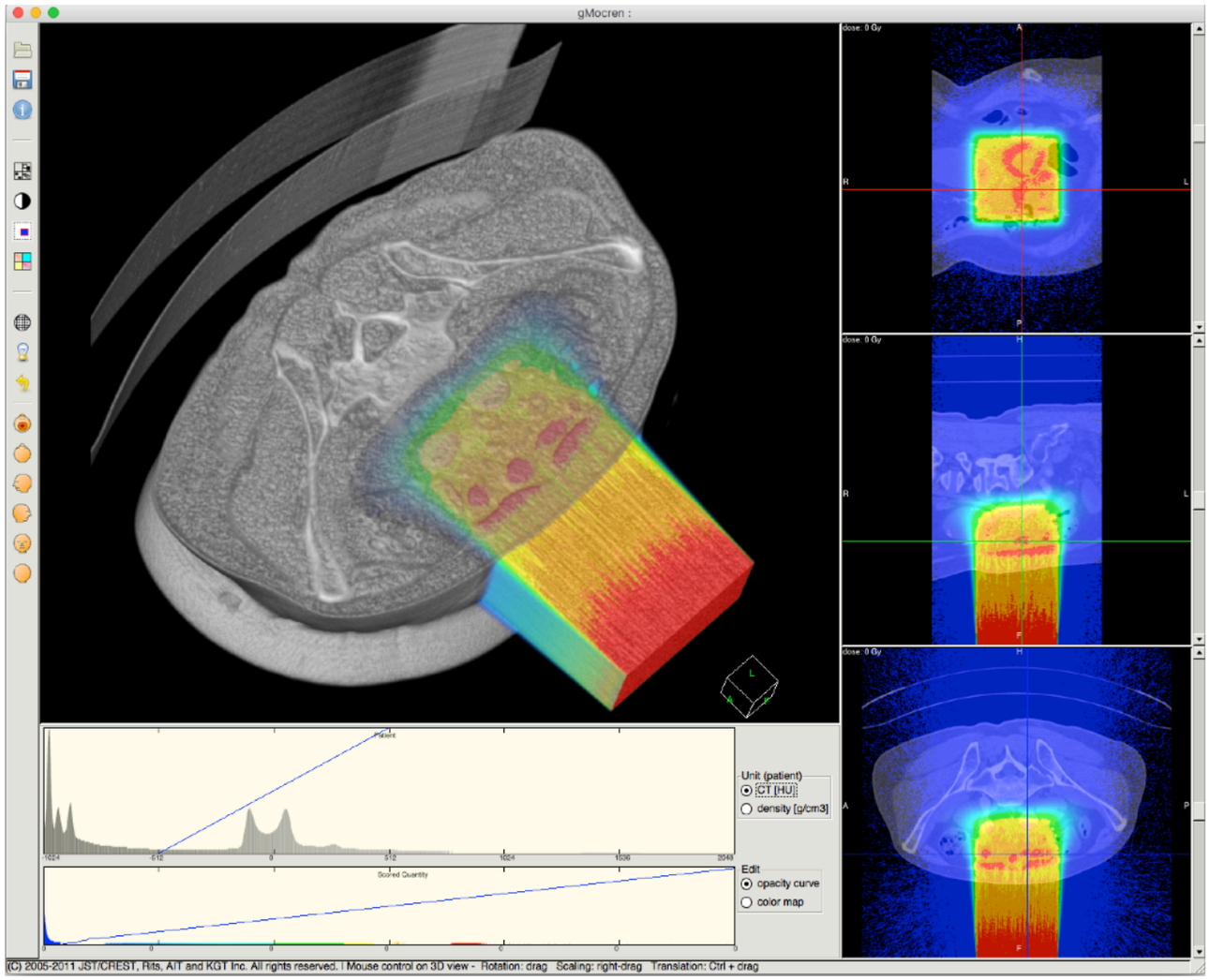
- MPEXS shows agreement with Geant4 simulation within 2%.
- Up to **730 times** speedup against Geant4 with single-core CPU
  - NVIDIA TITAN V GPU for MPEXS
  - Intel Xeon E5-2643 v2 (3.5 GHz) for Geant4

D: Comparisons of events processed per 1 ms



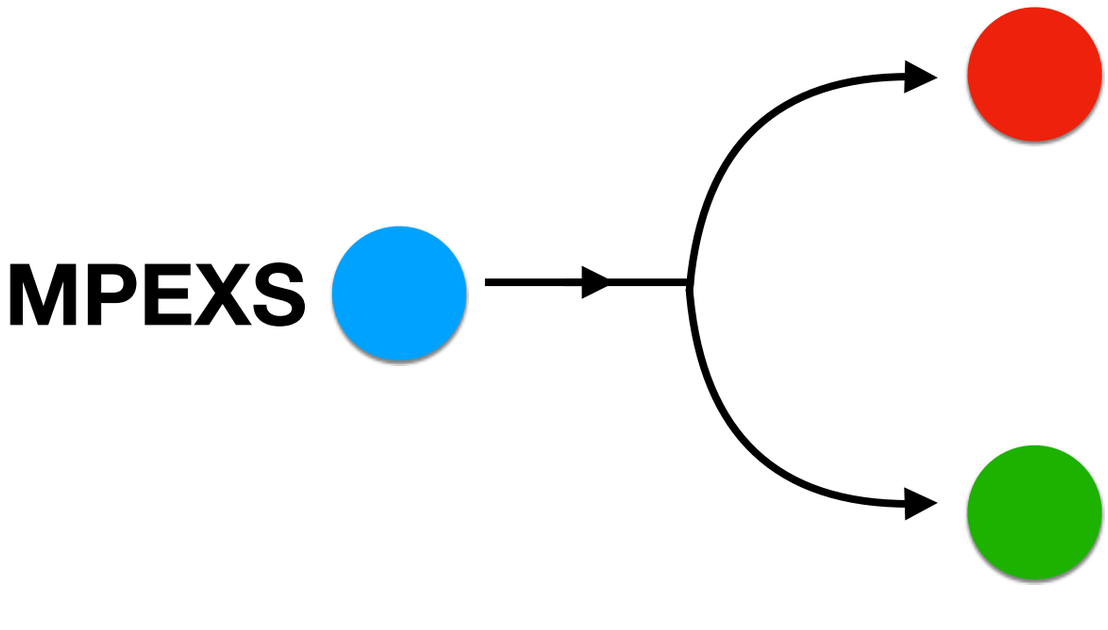
Radiotherapy Simulation on MPEXS

- MPEXS can handle phase-space data for primary beam and DICOM CT data as geometry.
  - LINAC Phase-space data
    - Electrons with E_{kin} = 21 MeV
    - Provided from
      Prof. Bruce Faddegon (@UCSF)
  - DICOM CT data
    - Demo data from Real INTAGE (CYBERNET, JP)



- Speedup factor: **~600 times**

MPEXS Extensions to Hadron and DNA Physics



MPEXS-h

- **A fast dose calculation engine for proton and carbon therapy**
- Development is ongoing.

MPEXS-DNA

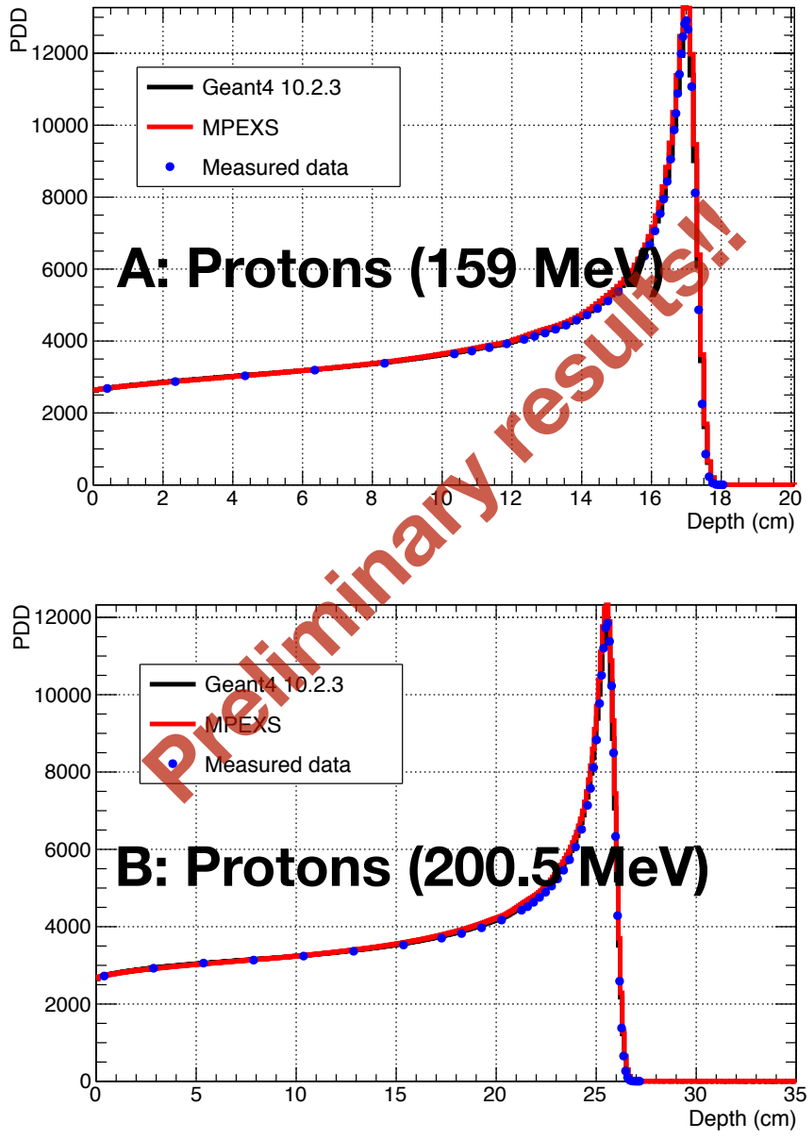
- **Acceleration of Geant4-DNA using GPU power**
- Improve long calculation time of Geant4-DNA simulation
  - Several days on a CPU cluster (80-cores) -> **a few min. (GPU)**

- The kernel mechanisms (e.g. particle transportation, sampling PIL, etc.) are common to MPEXS.
- Additional physics processes are ported for each extension.

MPEXS-h: MPEXS Hadron Extension

- Accelerate dose calculations for proton and carbon therapy
- Rewrite Geant4 hadronic processes (10.2.p3) in CUDA
  - Binary Cascade, Precompound, Fermi Breakup, Evaporation, and Photon Evaporation
- Application for Nagoya Proton Therapy Center (Japan)
- For now, **30 times** speedup against Geant4-based treatment planning
  - Thread divergence is much larger than EM case.
  - Working on optimization of the CUDA code

Percent Depth Dose curves (CPU vs GPU vs measurement)



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

MPEXS-DNA: Microdosimetry Simulation on GPU

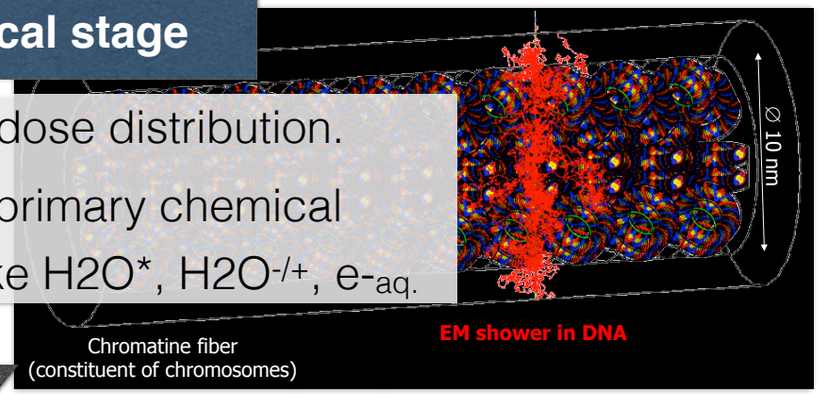
- Extension to DNA physics

- Rewrite Geant4-DNA (10.2.p3) in CUDA.
  - EM Physics with lower energy range (down to meV)
    - Calculate local energy loss and generate primary molecules like H_2O^* and $H_2O^{+/-}$
  - Radiolysis of water
    - Diffusion and reactions for molecular species such as •OH radicals
  - The biological stage not yet implemented

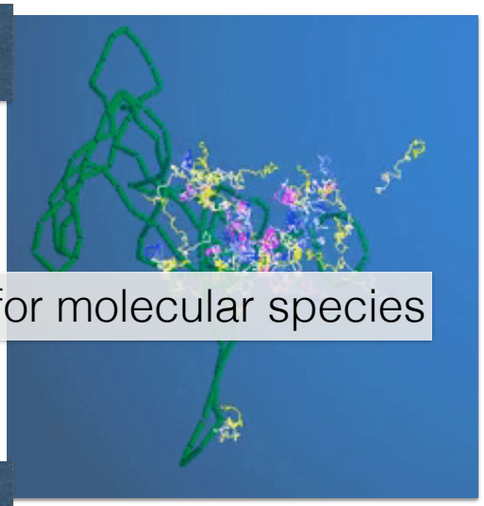
- Collaboration between  and 

1. Physical stage

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

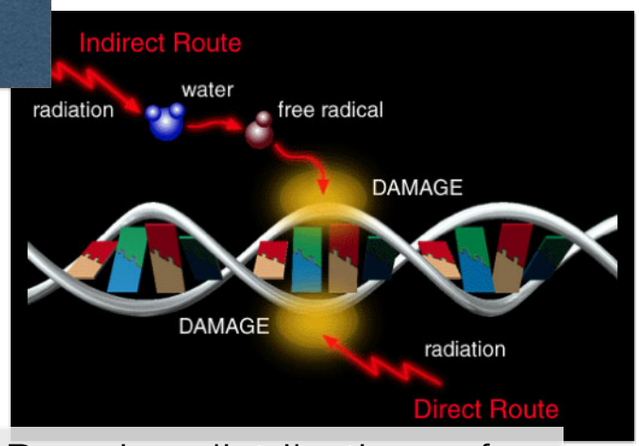


2. Chemical stage



Diffusion and reactions for molecular species

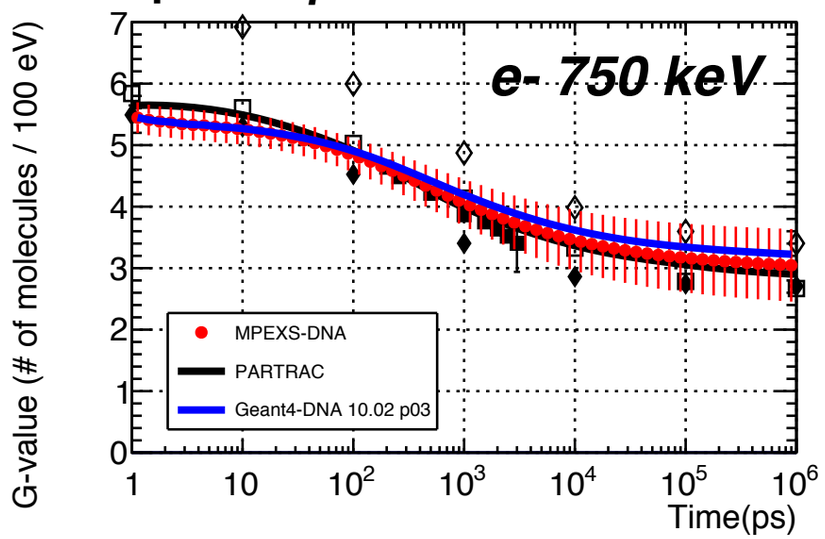
3. Biological stage (Future work)



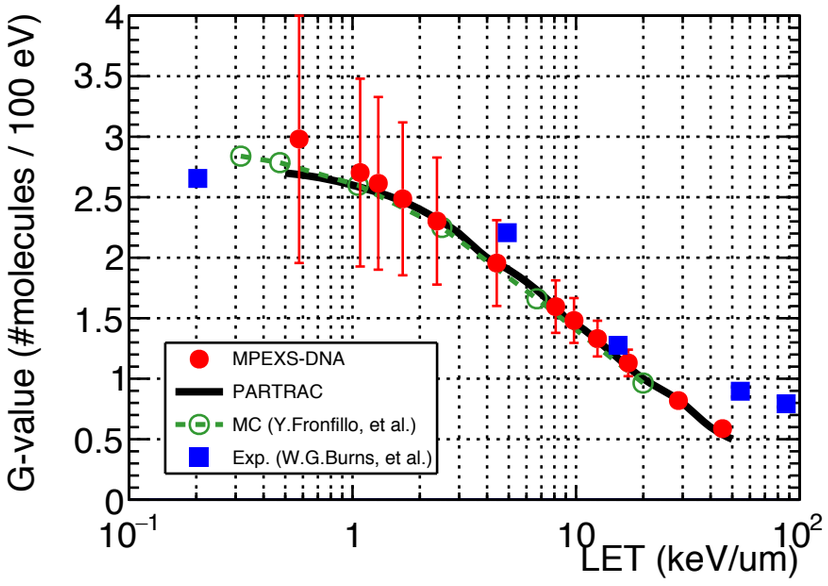
Estimate SSBs and DSBs using distributions of energy loss and molecular species inside the cell nucleus.

MPEXS-DNA Performance

A: G-value time profile for ·OH radicals from 1 ps to 1 μs after irradiation of e-

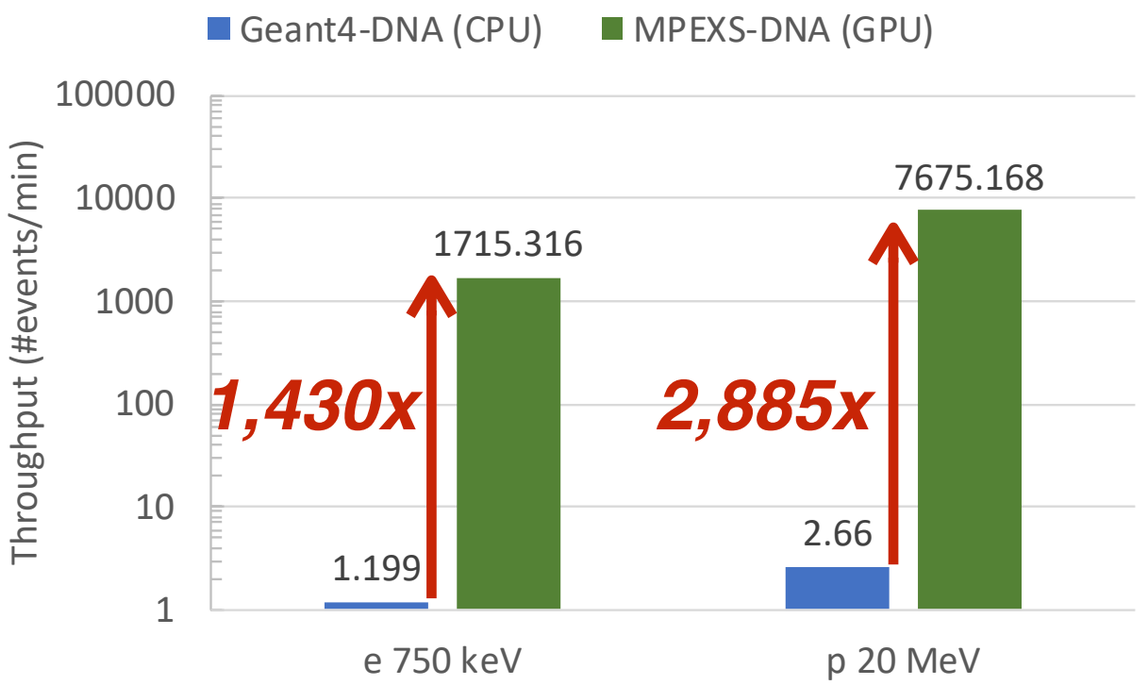


B: LET dependency of G-value for ·OH radicals at 1 μs after proton irradiation



- MPEXS-DNA is consistent with other MC simulations and experiment data.
- Up to **2,900 times** faster than Geant4-DNA with single-core of CPU
  - ~ 4 days (CPU) -> **~ 2 min. (GPU)**

C: Comparisons of event number processed per 1 min.



- GPU: NVIDIA, TITAN V
- CPU: Intel, Xeon E5-2643 v2, 3.5 GHz

MPEXS License Model

- Two models
  - Collaboration license
    - Only for groups who expect to submit a paper jointly within 1 year.
    - Free of charge
    - The newly earned intellectual properties in the collaboration are requested to be donated to KEK or to be put in the public domain.
      - Also shall not exercise the moral rights of the author or any other similar rights

  - General license
    - Contracts with KEK are necessary.
    - A license fee will be requested.

Summary

- MPEXS is a state-of-the-art radiation simulator running on GPU.
  - Developed as a dose calculation engine for radiotherapy
  - Reimplemented the Geant4 Standard EM physics processes in CUDA
  - Up to **730 times** speedup against Geant4 simulation

- MPEXS-h
  - Hadron physics extension for proton and carbon therapy
  - Development is ongoing.

- MPEXS-DNA
  - Improve simulation speed of Geant4-DNA simulation
    - **2,900 times**, at maximum, faster than Geant4-DNA
  - Could facilitate microdosimetry simulation and contribute scientific achievement in radiobiology

- **MPEXS and its extensions are NOT open source.**
  - Collaboration based on license contract
  - Contact: Prof. Takashi Sasaki (KEK, Takashi.Sasaki@kek.jp)

Future Plans

- Publications
  - Papers will be publish soon.

- Performance improvements
  - Calculation speed, especially MPEXS-h
  - Reproducibility of physics

- More functionality
  - Neutron Physics
    - An implementation already exists for a private sponsor.
  - Handling more complex geometry imported from CAD with ray tracing algorithm
  - Handling various materials

- Applications
  - Possibility of collaboration with Geant4-DNA users
    - Dr. Sébastien Incerti (CENBG, incerti@cenbg.in2p3.fr) is our representative in Europe.
  - We are seeking a killer application.

Backup

Lessons learned from Geant4

- The MPEXS series is developed by Geant4 developers.

- People love something in free of charge.
  - Geant4 became very popular rapidly.
    - Lots of citations for the Geant4 general papers in different fields
  - The Geant4 license is very flexible also.
    - Even commercial applications can be made and sold without paying anything.

- Who pays the costs necessary for the development and maintenance of Geant4?
  - Major HEP institutes such as CERN, SLAC, KEK and others
  - Also lots of volunteers
    - Very limited number of people are hired for Geant4.

- Volunteers face the difficulty with funding.
  - Funding agencies do not want to pay for one project in a very long term.
    - They prefer new projects than sustainable development, maintenance and support (at least in Japan).
  - Users never pay anything because Geant4 is open-source software.
  - Developers need your help to provide sustainable development, maintenance, and support, especially, for applications outside of HEP.