

Advancements in a GPU Monte Carlo simulator for radiotherapy

2016 GPU Technology Conference

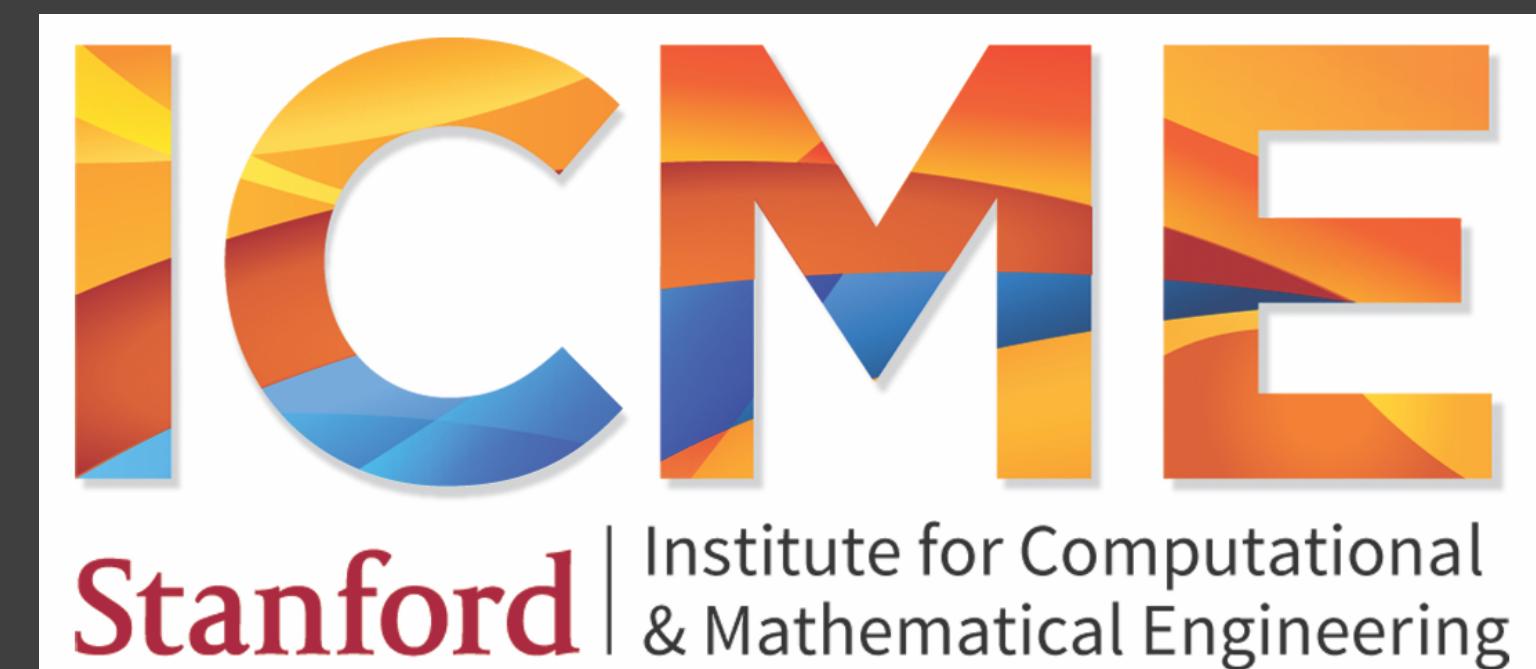
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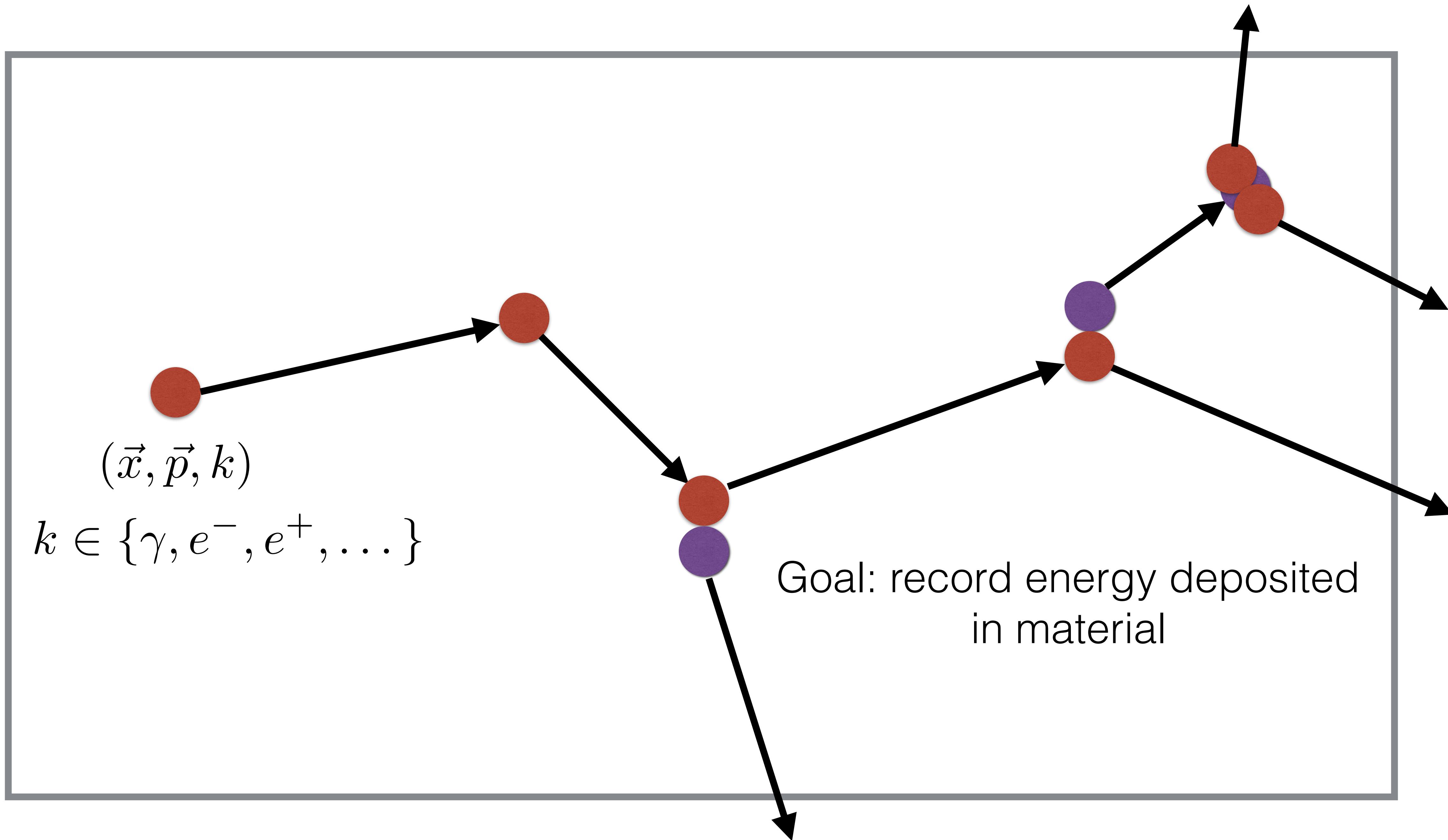
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Collaboration

- Makoto Asai, SLAC
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- Andrea Dotti, SLAC
- Takashi Sasaki, KEK
- Akinori Kimura, Ashikaga Institute of Technology
- Margot Gerritsen, ICME, Stanford



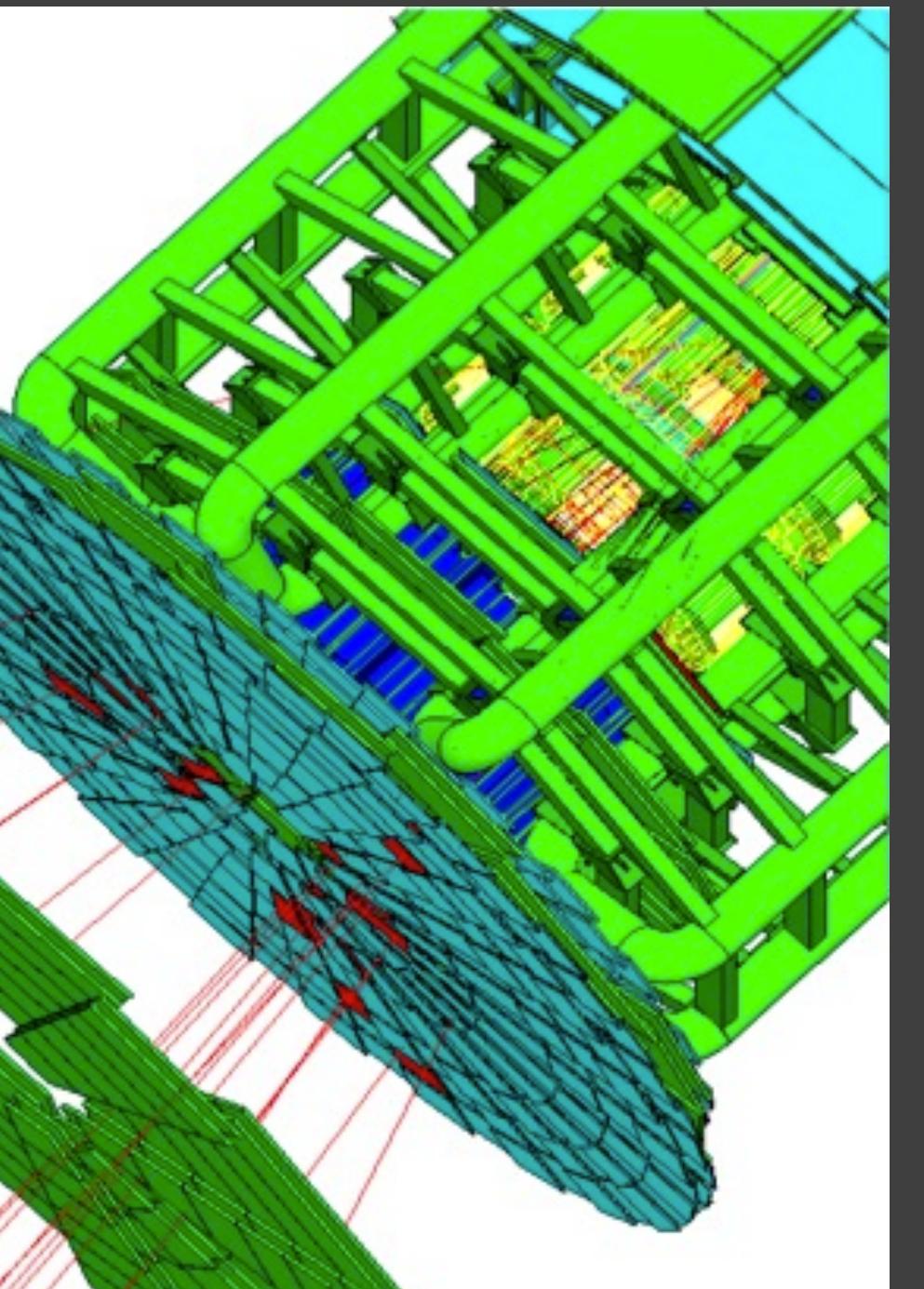
Big Picture



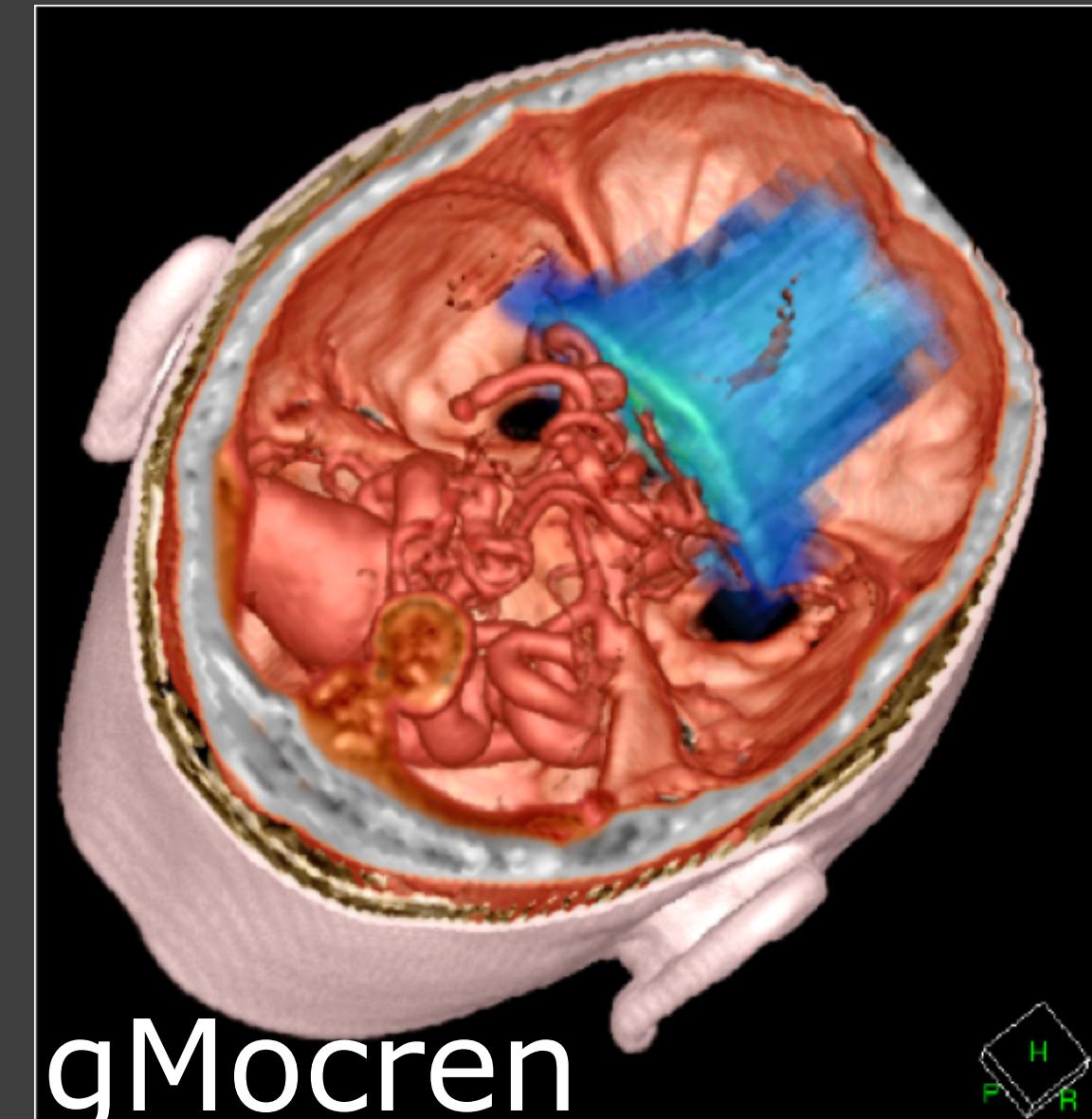
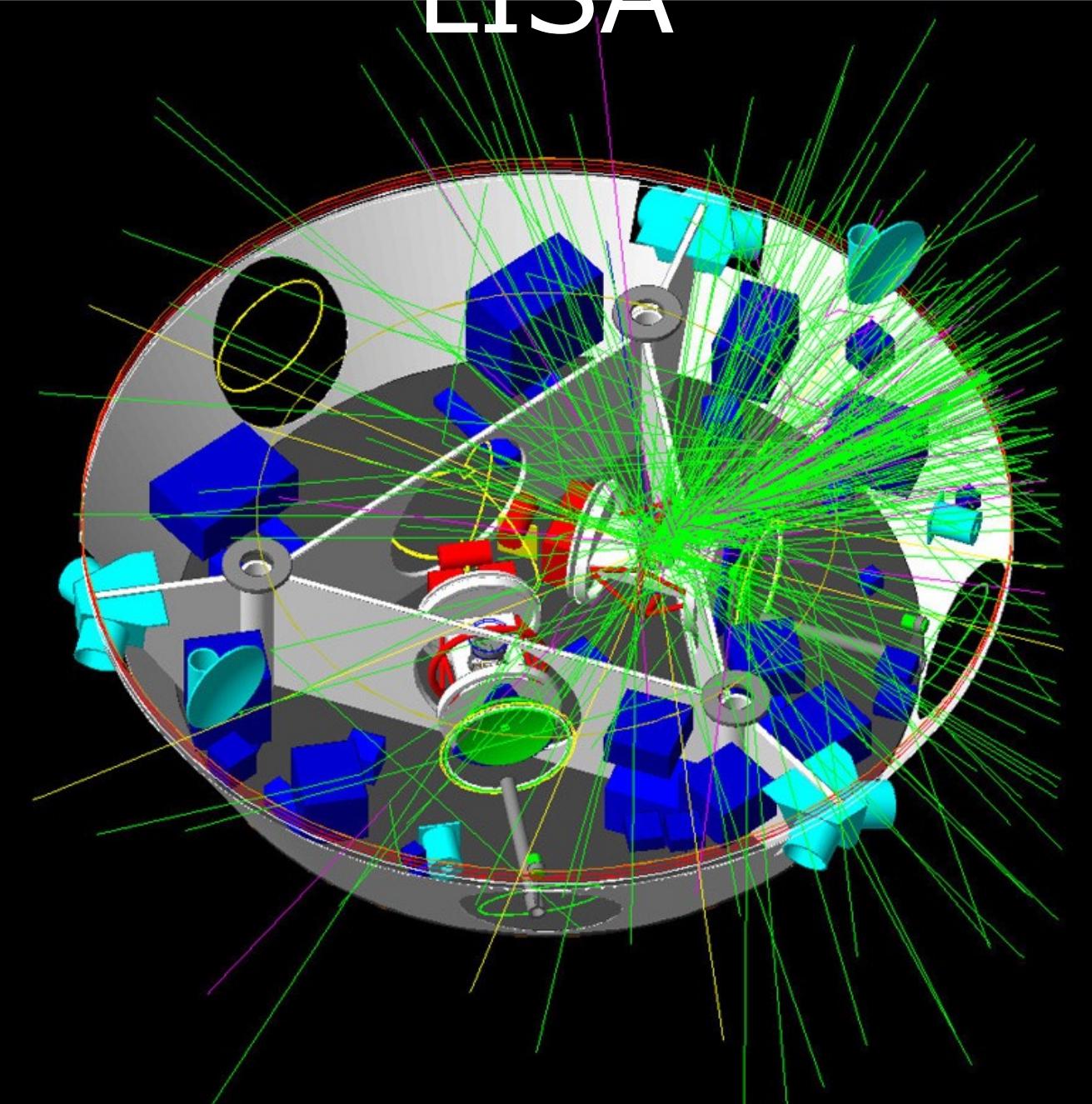
Geant4

- Extensive toolkit for simulation of particles traveling through matter
- Supports wide variety of physics models, geometries, and materials
- Users can add their own
- Used in numerous and diverse application areas
 - high energy physics
 - medical physics
 - spacecraft
 - semiconductor devices
 - biology research

ATLAS



LISA



gMocren



MPEXS

- Adaptation of core Geant4 algorithm to CUDA
- Design inspired by structure of Geant4 in terms of modularization and separation of concerns
- Low energy electromagnetic physics models suitable for simulation of X-ray radiotherapy
- Model material as water with variable density, a common practice in medical physics for X-ray therapy
- Supported particles: photon, electron, positron (easily extended)

MPEXS – algorithm details

- Each CUDA thread tracks an active particle
- Physics processes store secondary particles in thread-local stacks
- Energy is atomically deposited to a global dose array (via `atomicAdd`)

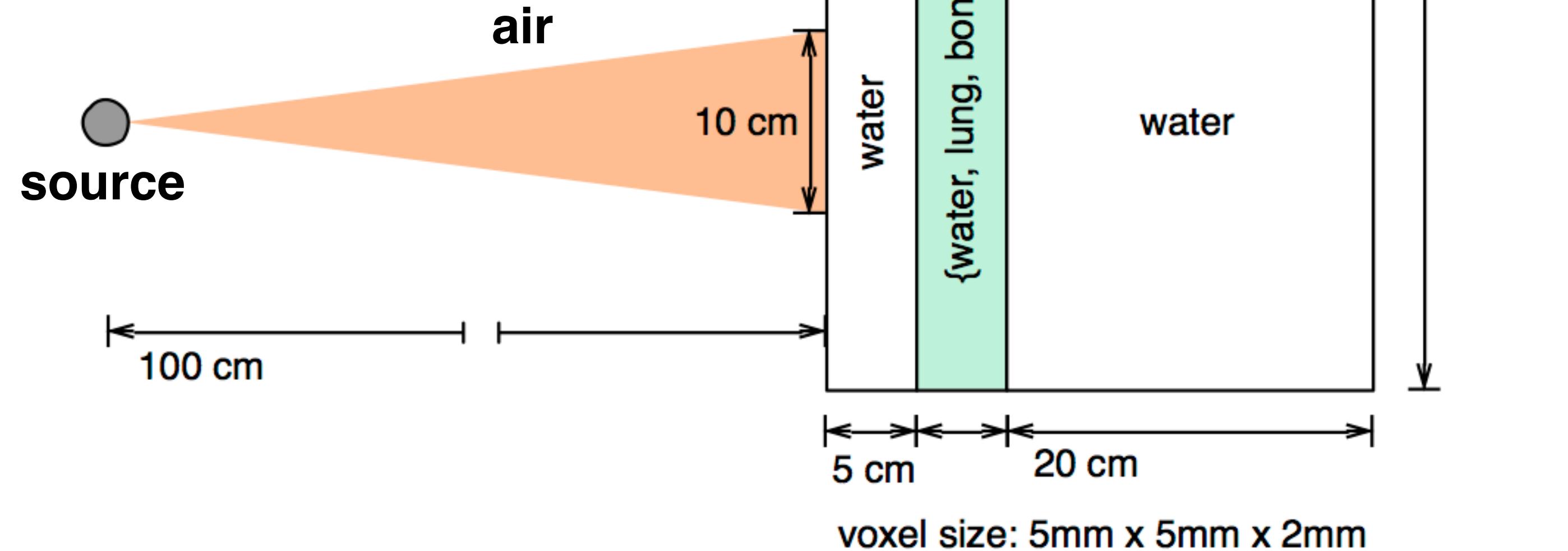
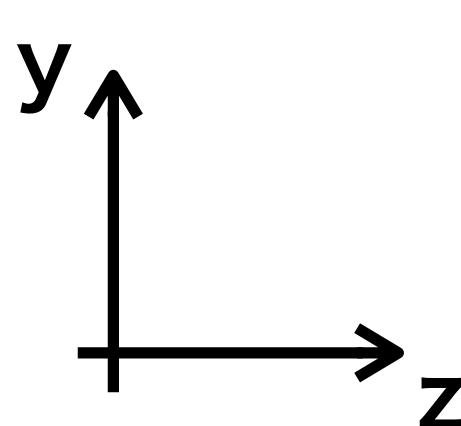
MPEXS – validation & performance

Verification for Dose Distribution

Dose Distribution of slab phantoms

- phantom size : $30.5 \times 30.5 \times 30$ cm
- voxel size : $5 \times 5 \times 2$ mm
- field size : 10 cm^2
- SSD : 100 cm
- slab materials :

- (1) water
- (2) lung
- (3) bone



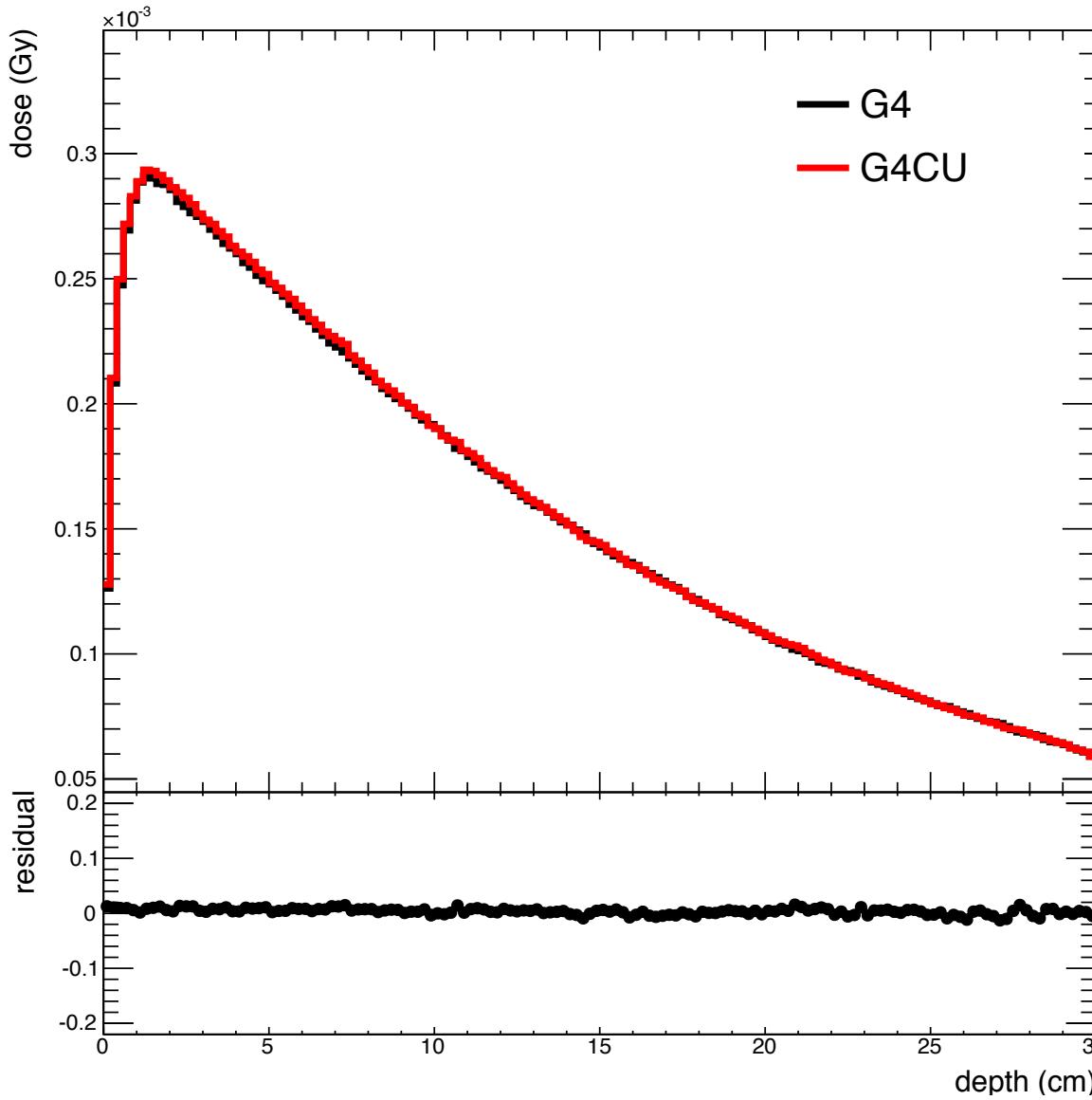
Beam particle and its initial kinetic energy:

- electron with 20MeV
- photon with 6MV Linac
- photon with 18MV Linac

	density
water	1.0 g/cm^3
lung	0.26 g/cm^3
bone	1.85 g/cm^3
air	0.0012 g/cm^3

Comparison of depth dose for γ 6MV

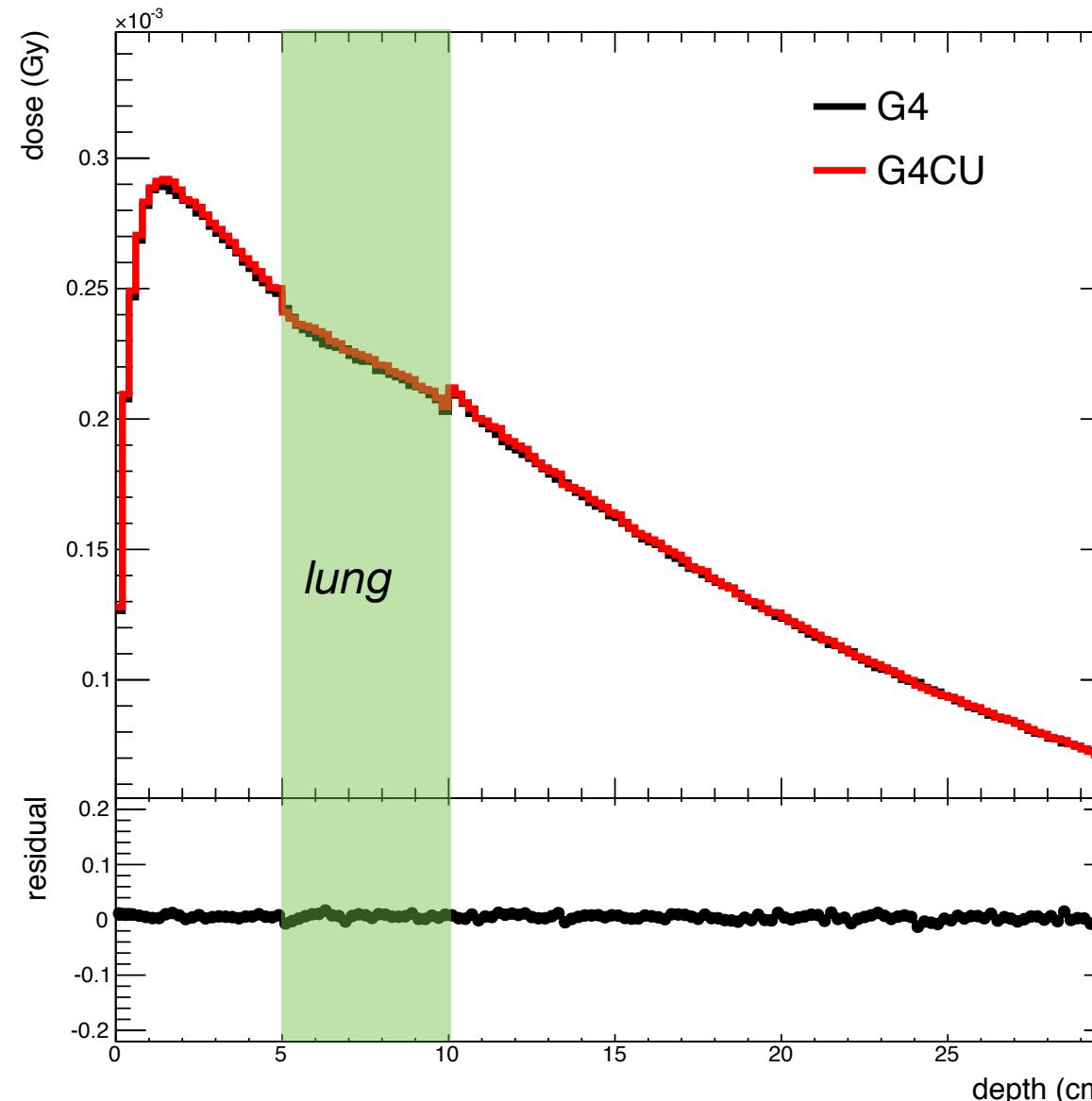
(1) water



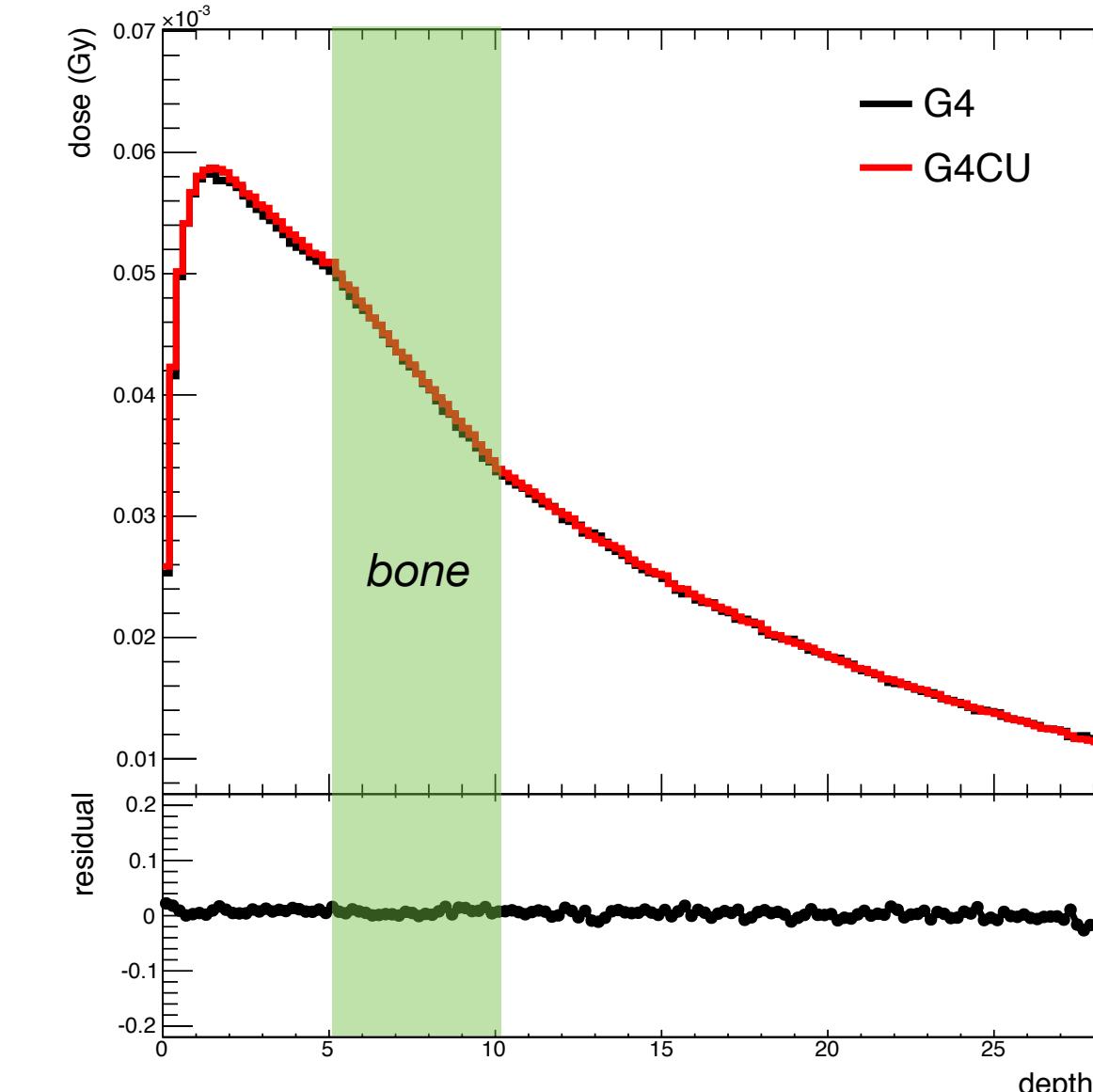
– G4 v9.6.3
– G4CU

- x-axis: z-direction (cm)
- y-axis: dose (Gy)
- residual = (G4CU – G4) / G4

(2) lung

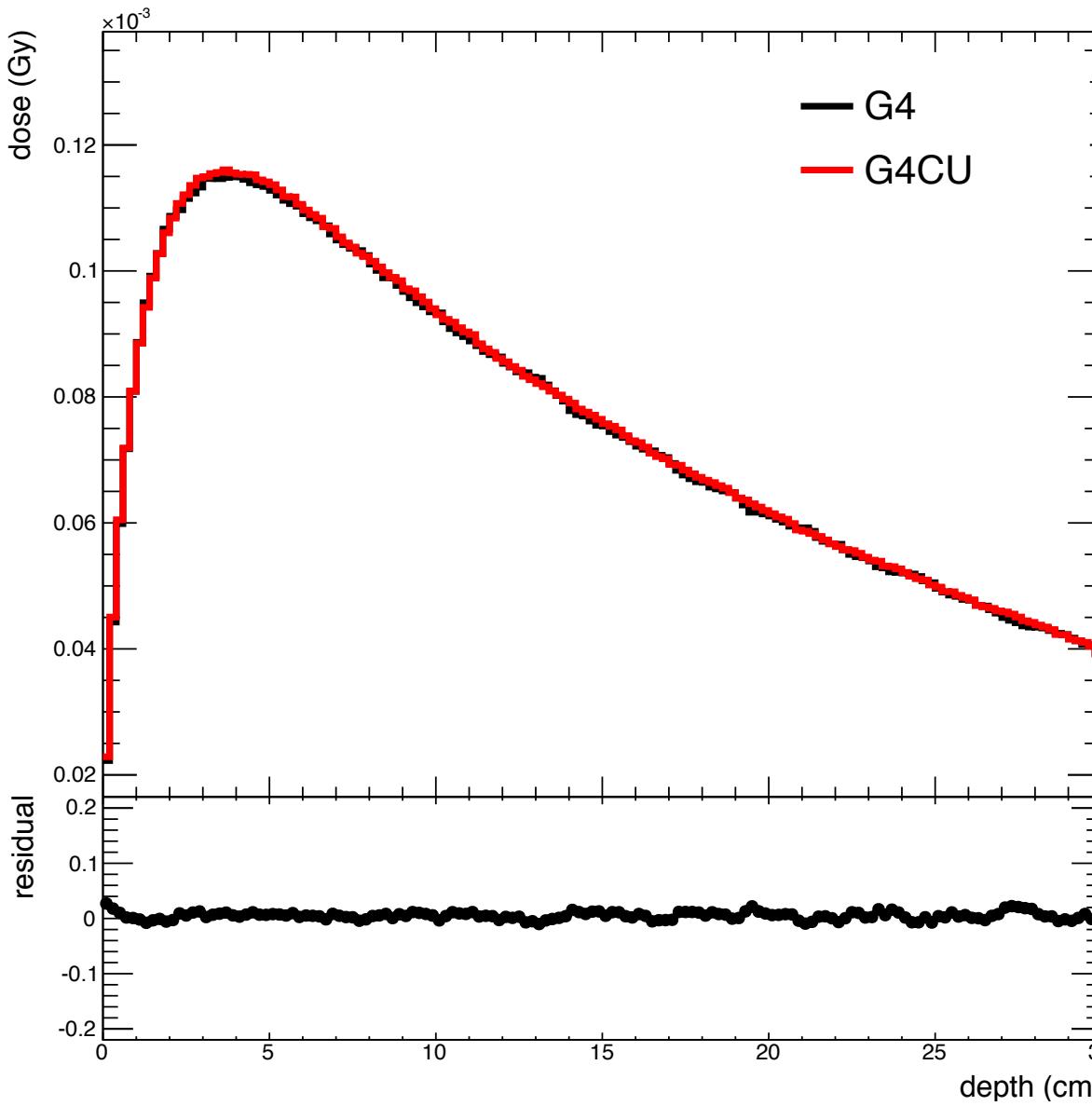


(3) bone



Comparison of depth dose for γ 18MV

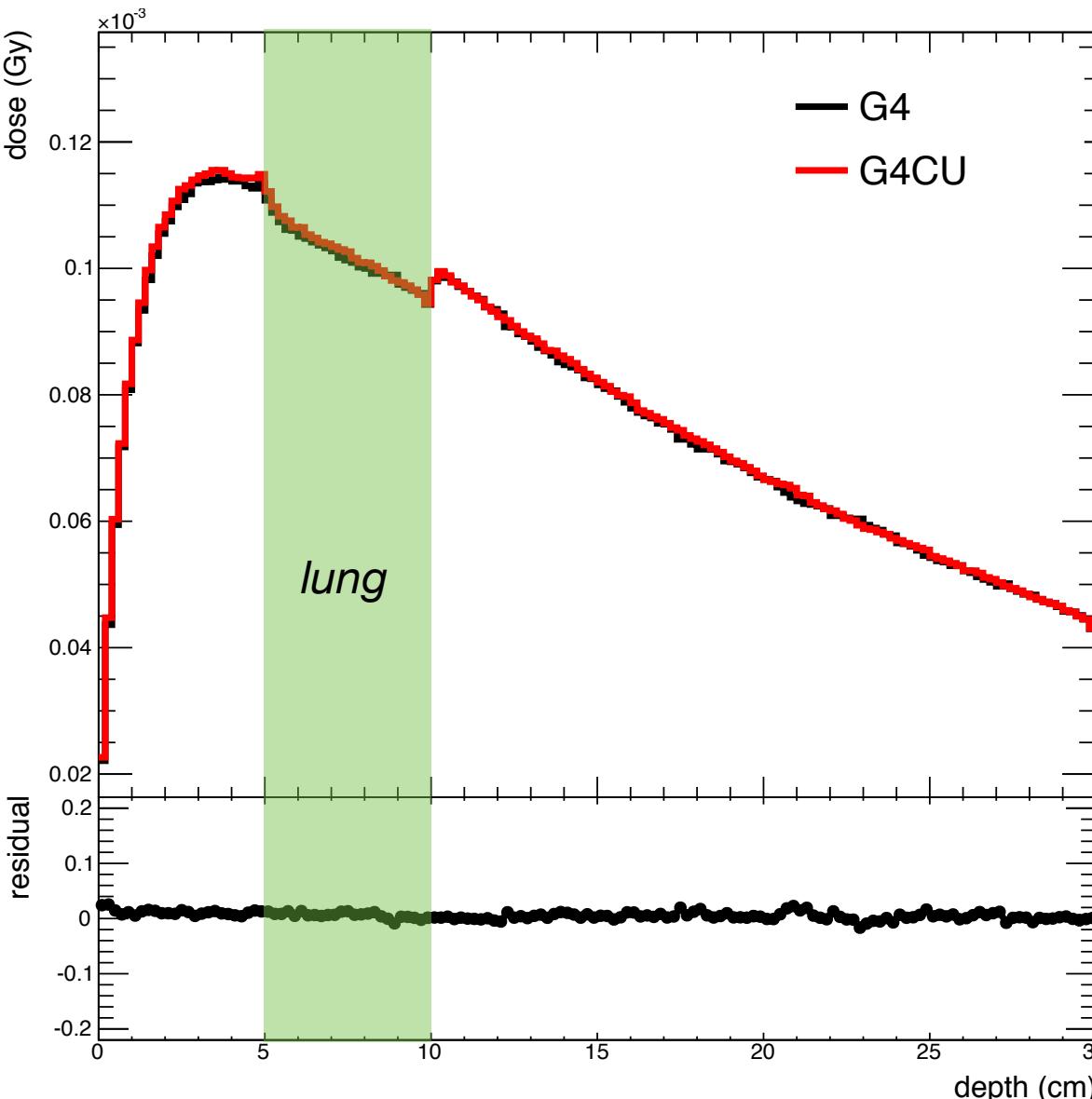
(1) water



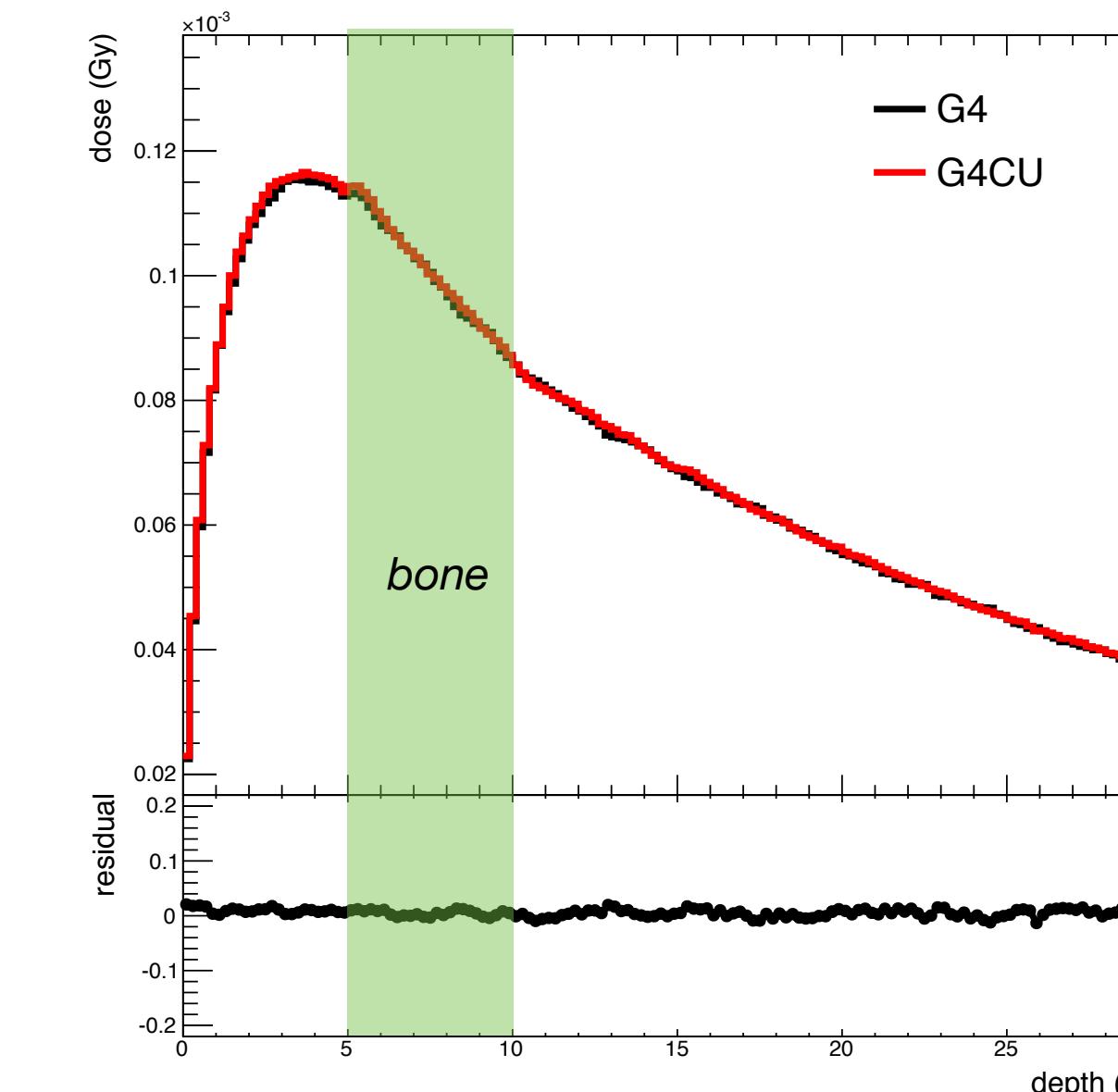
– G4 v9.6.3
– G4CU

- x-axis: z-direction (cm)
- y-axis: dose (Gy)
- residual = (G4CU – G4) / G4

(2) lung

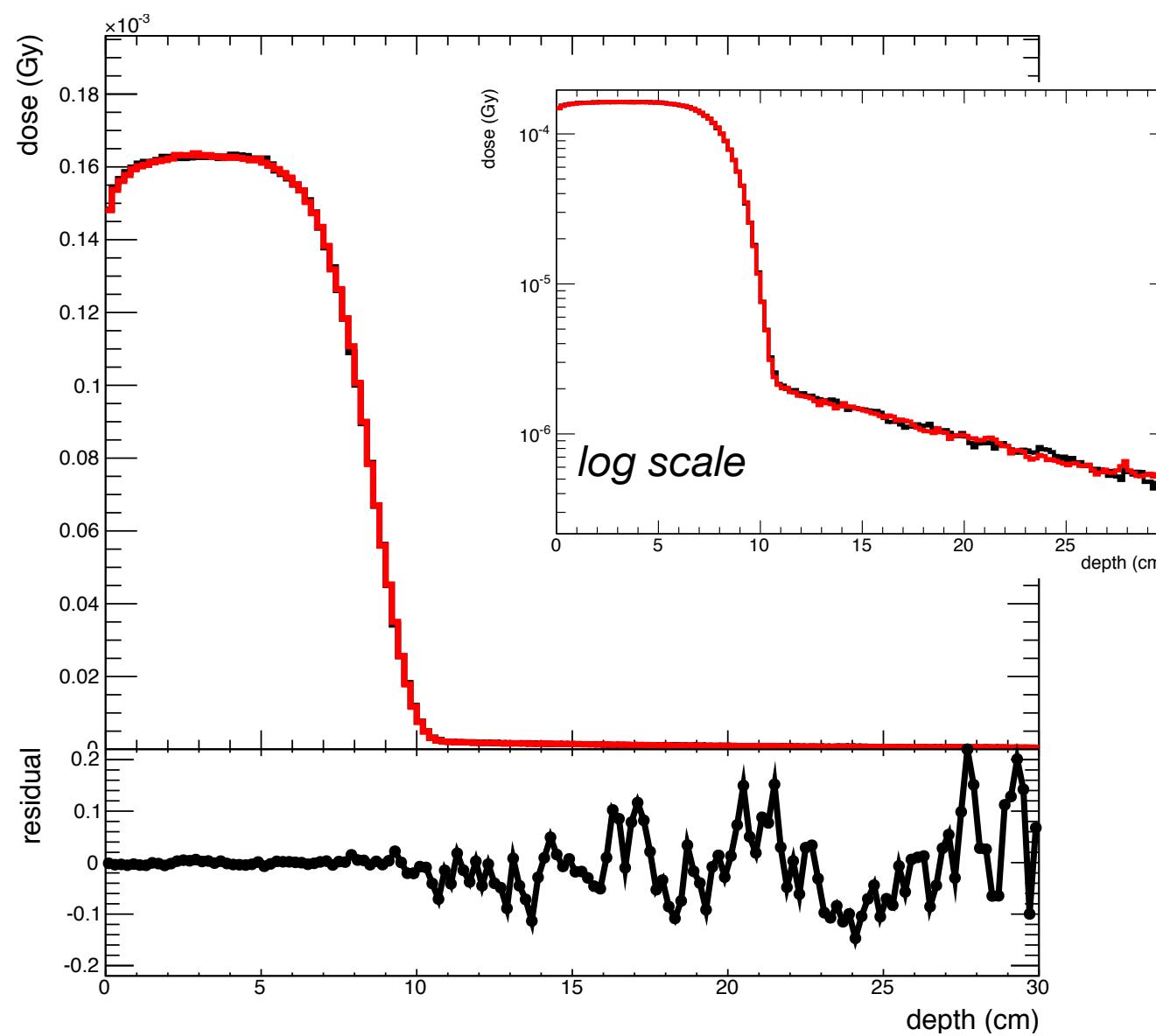


(3) bone



Comparison of depth dose for e- 20MeV

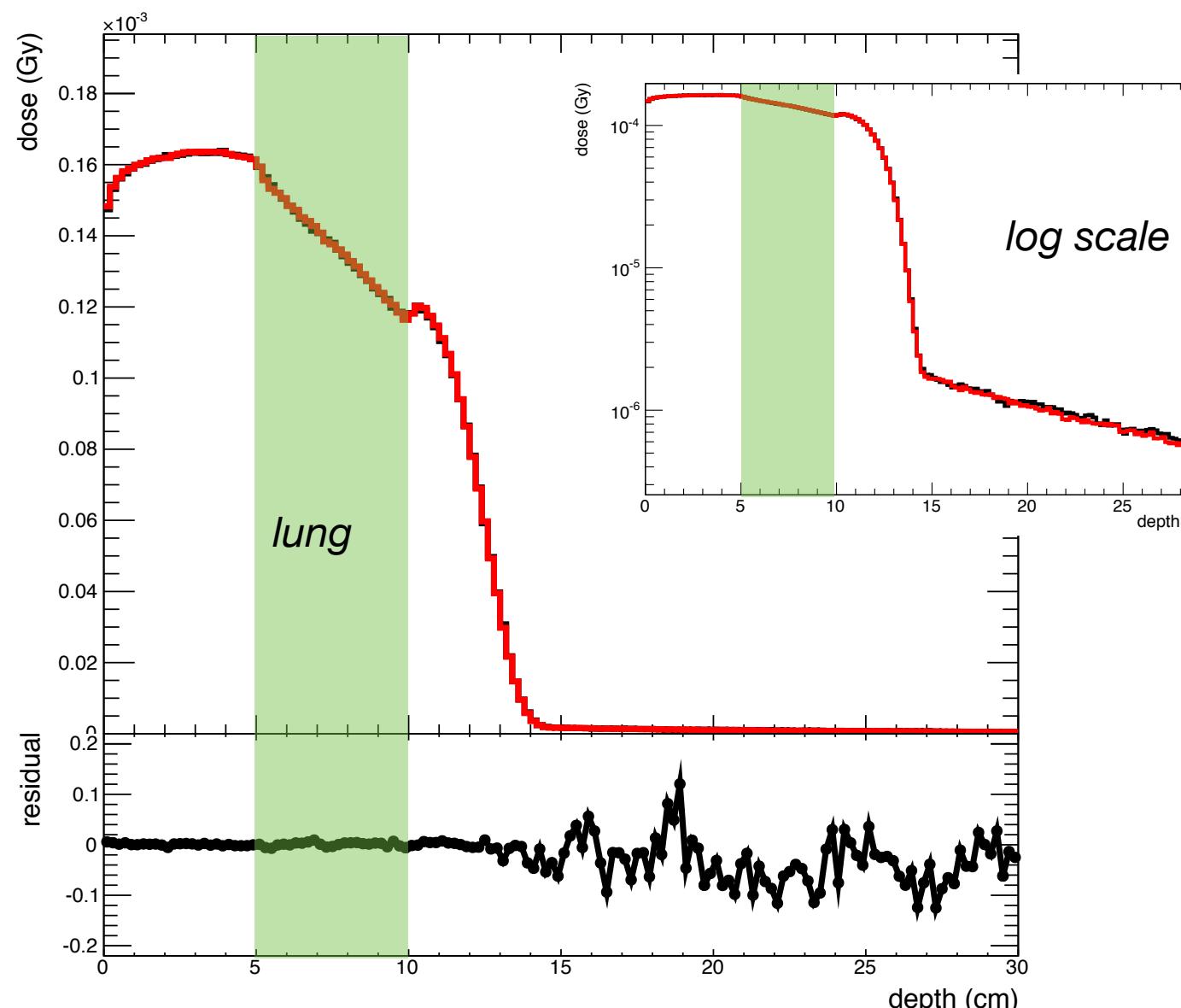
(1) water



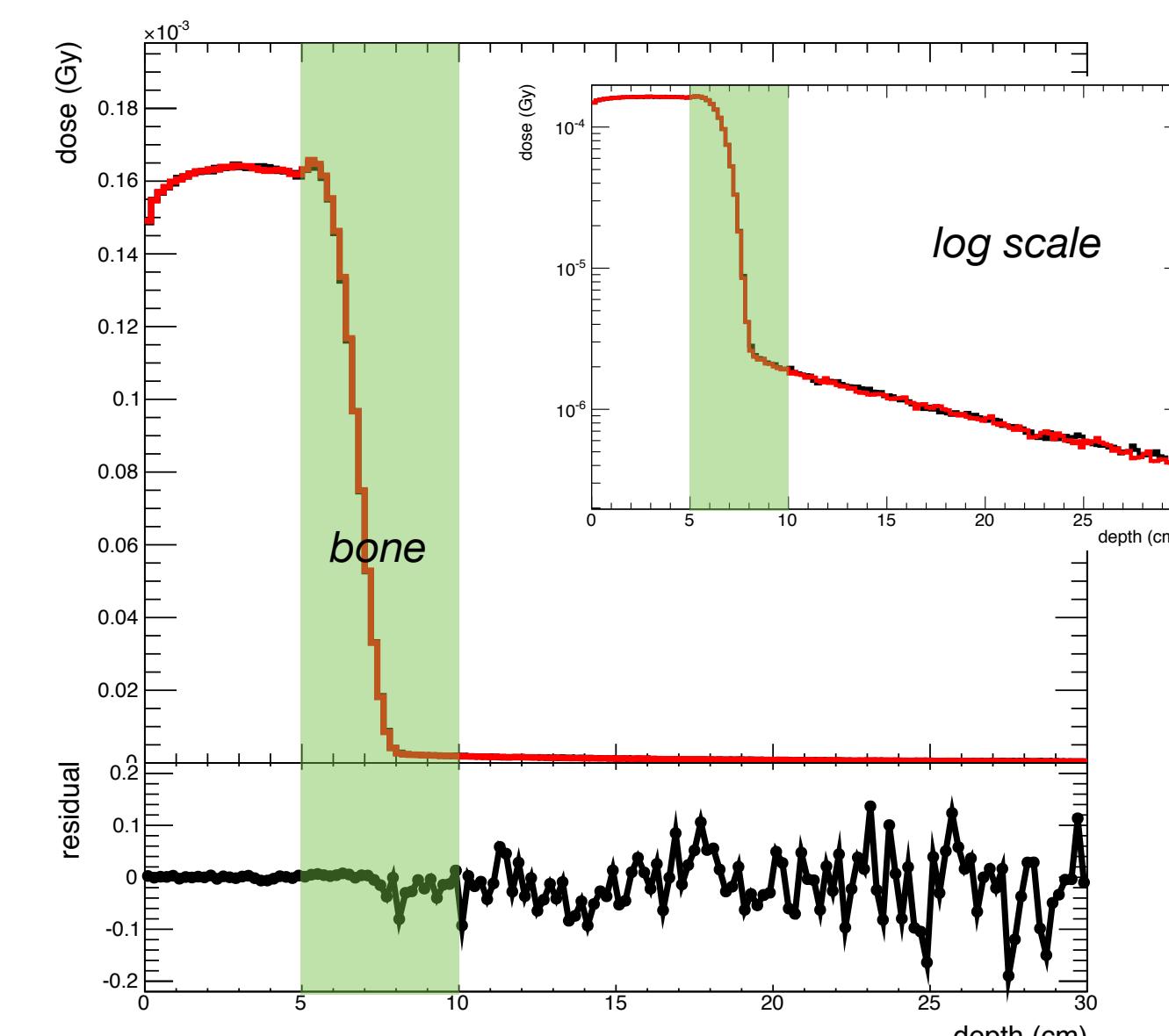
– G4 v9.6.3
– G4CU

- x-axis: z-direction (cm)
- y-axis: dose (Gy)
- residual = $(G4CU - G4) / G4$

(2) lung



(3) bone



Computation Time Performance

185~250 times speedup against single-core G4 simulation!!

	e- beam with 20MeV		
	(1) water	(2) lung	(3) bone
G4 [msec/particle]	1.84	1.87	1.65
G4CU [msec/particle]	0.00881	0.00958	0.00885
x speedup factor (= G4 / G4CU)	208	195	193

GPU:

- Tesla K20c (Kepler architecture)
- 2496 cores, 706 MHz
- **4096 x 128 threads**
- **# of primaries**
 - **50M particles -> e- 20MeV**
 - **500M particles -> γ 6MV, 18MV**

CPU:

- Xeon E5-2643 v2 3.50 GHz

	γ beam with 6MV			γ beam with 18MV		
	(1) water	(2) lung	(3) bone	(1) water	(2) lung	(3) bone
G4 [msec/particle]	0.780	0.822	0.819	0.803	0.857	0.924
G4CU [msec/particle]	0.00336	0.00331	0.00341	0.00433	0.00425	0.00443
x speedup factor (= G4 / G4CU)	232	248	240	185	201	208

MPEXS – key challenges

- main challenge: thread divergence
- other issues:
 - interpolation tables
 - memory bandwidth
 - many kernel launches?

MPEXS-DNA

Geant4-DNA / MPEXS-DNA

- Geant4-DNA: an extension of Geant4 for DNA scale particle simulation (Microdosimetry simulation)
 - Electromagnetic interactions (*down to meV*)
 - Radiolysis of water
 - Estimate DNA damages using energy loss
- MPEXS-DNA — An extension of MPEXS to DNA Physics
 - Up to **280 times** faster than single-CPU core simulation
 - Collaborators: CENBG (France), KEK (Japan)

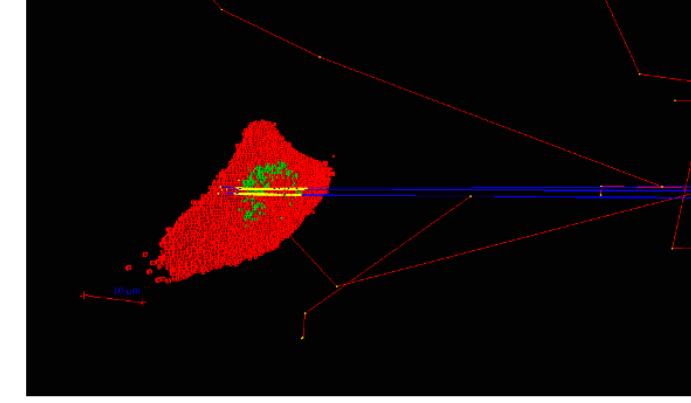
<http://geant4-dna.org>

The Geant4-DNA project
Extending the Geant4 Monte Carlo simulation toolkit for radiobiology

Geant4-DNA Software Physics Chemistry Examples & tutorials Publications Collaboration Funding

Welcome to the Internet page of the Geant4-DNA project.
The Geant4 general purpose particle-matter Monte Carlo simulation toolkit is being extended with processes for the modeling of early biological damage induced by ionising radiation at the DNA scale. Such developments are on-going in the framework of the Geant4-DNA project, originally initiated by the European Space Agency/ESTEC.

Recent posts
Geant4 10.1 has been released.

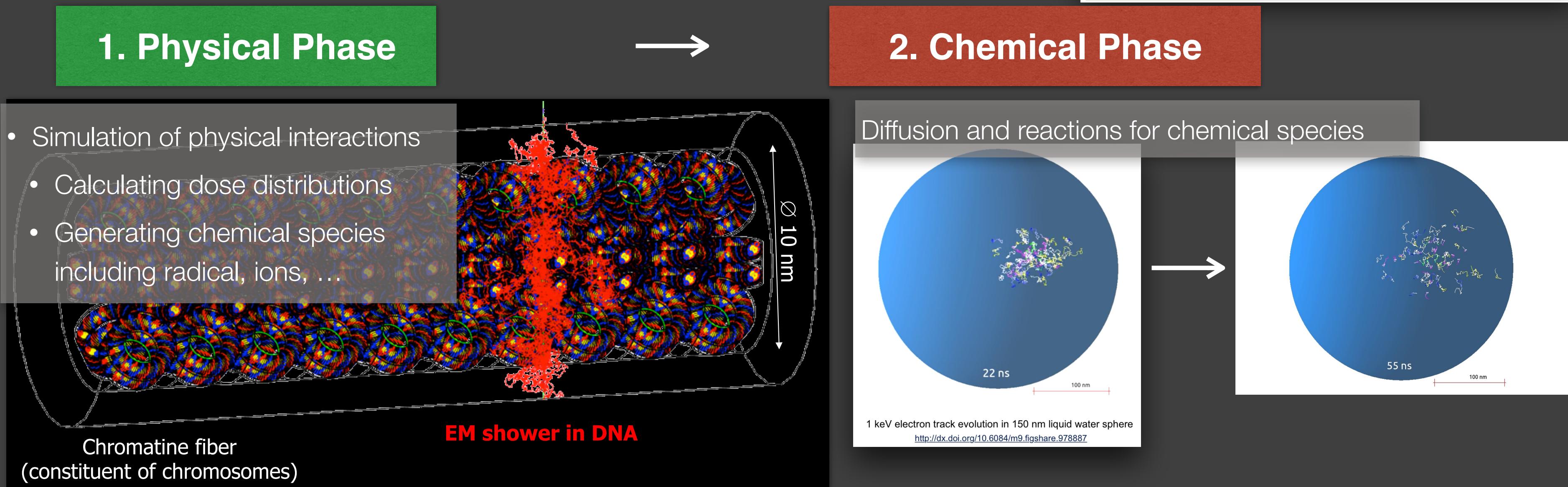


Microbeam irradiation of a keratinocyte with alpha particles
(see the « microbeam » Geant4 advanced example)
- courtesy of L. Garnier (CNRS/IN2P3) -

On-going developments include

- Physics processes in liquid water and other biological materials
- Physico-chemistry and chemistry processes for water radiolysis
- Molecular geometries
- Quantification of damage (such as single-strand, double-strand breaks, base oxidation...)

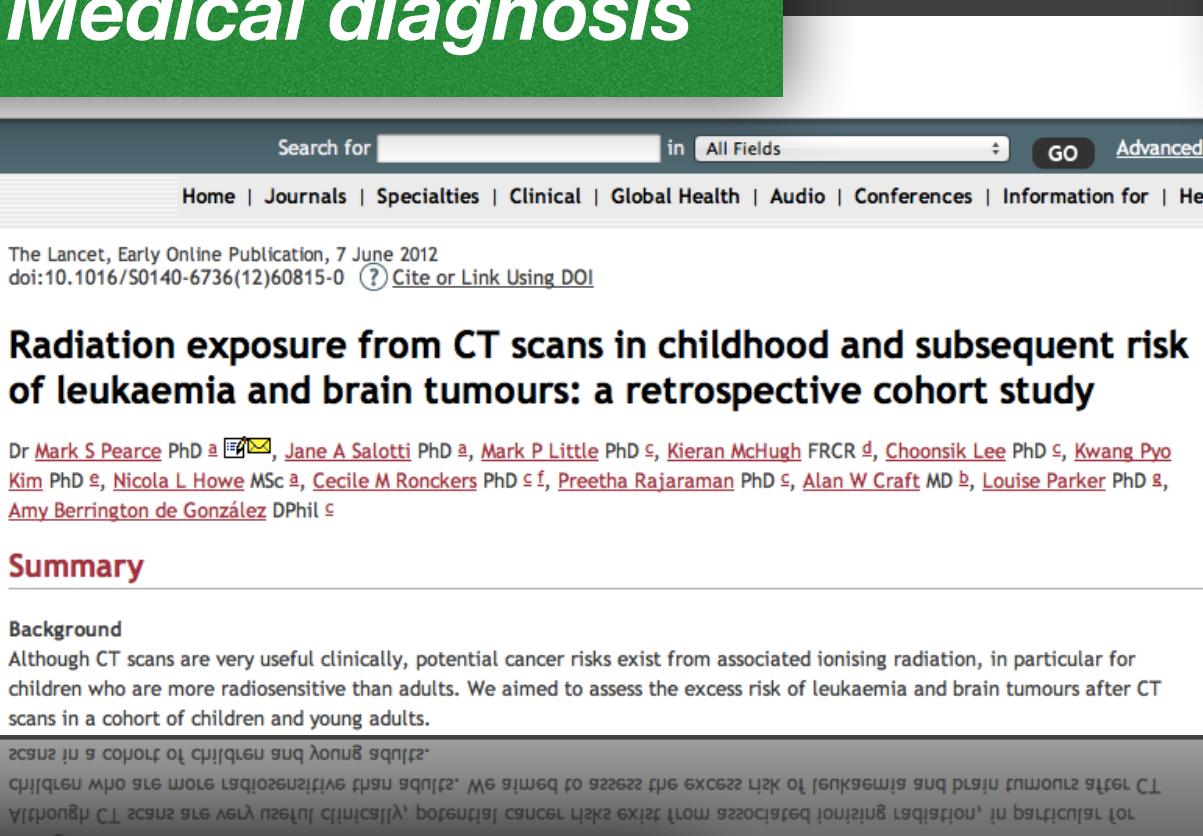
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Use cases of microdosimetry simulation

- Estimation of effects on human health by chronic radiation exposure
- Medical diagnosis, Arline crew, Astronauts in space mission, ...
- Understanding mechanisms of radiation therapy

Medical diagnosis



Airline crew



Space missions

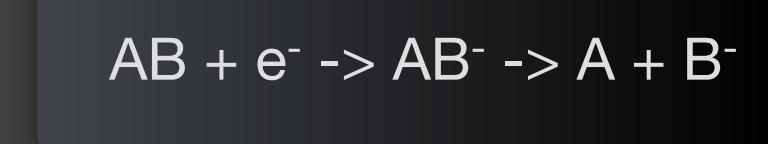
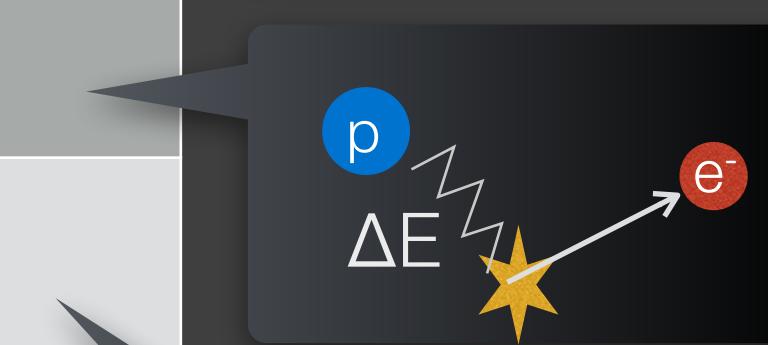
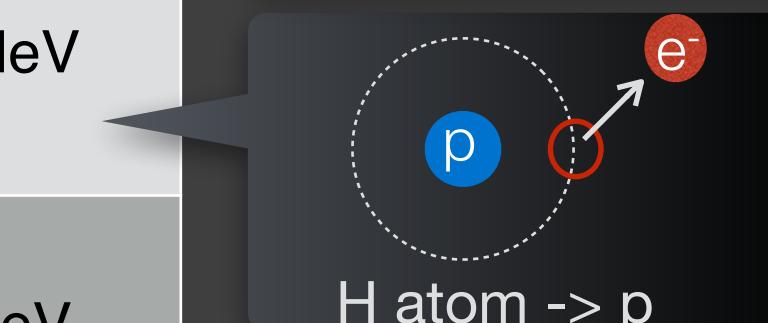
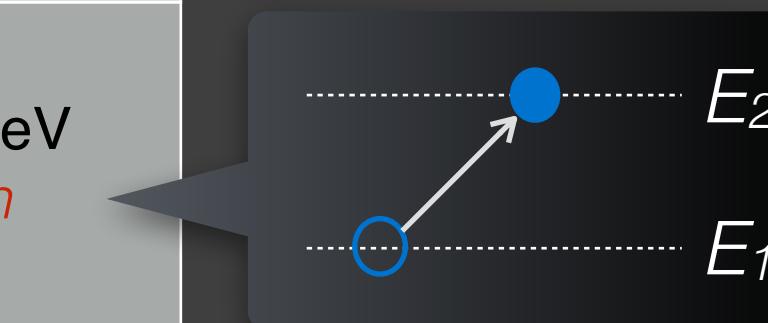
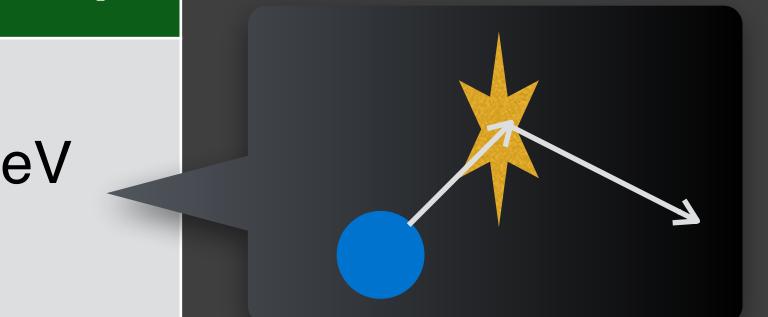


Radiation therapy



DNA Physics Processes

Particles		Electrons	Protons	Hydrogen atoms	Helium atoms (He ⁺⁺ , He ⁺ , He ⁰)
Physics Processes	Elastic scattering	9 eV - 10 keV <i>Uehara</i> 10 keV - 1 MeV <i>Champion</i>	100 eV - 1 MeV <i>Hoang</i>		100 eV - 10 MeV <i>Hoang</i>
	Excitation	10 eV - 10 keV <i>Emfietzoglou</i> 10 keV - 1 MeV <i>Born</i>	10 eV - 500 keV <i>Miller Green</i> 500 keV - 100 MeV <i>Born</i>	10 eV - 500 keV <i>Miller Green</i>	1 keV - 400 MeV <i>Miller Green</i>
	Charge change	—	100 eV - 10 MeV <i>Dingfelder</i>	100 eV - 10 MeV <i>Dingfelder</i>	1 keV - 400 MeV <i>Dingfelder</i>
	Ionization	10 eV - 10 keV <i>Emfietzoglou</i> 10 keV - 1 MeV <i>Born</i>	100 eV - 500 keV <i>Rudd</i> 500 keV - 100 MeV <i>Born</i>	100 eV - 100 MeV <i>Rudd</i>	1 keV - 400 MeV <i>Rudd</i>
	Vibrational excitation	2 - 100 eV <i>Michaud et al.</i>	—	—	—
	Disociative attachment	4 - 13 eV <i>Melton</i>	—	—	—



An issue of DNA Physics Process

The difference in energy loss process (EM vs DNA)

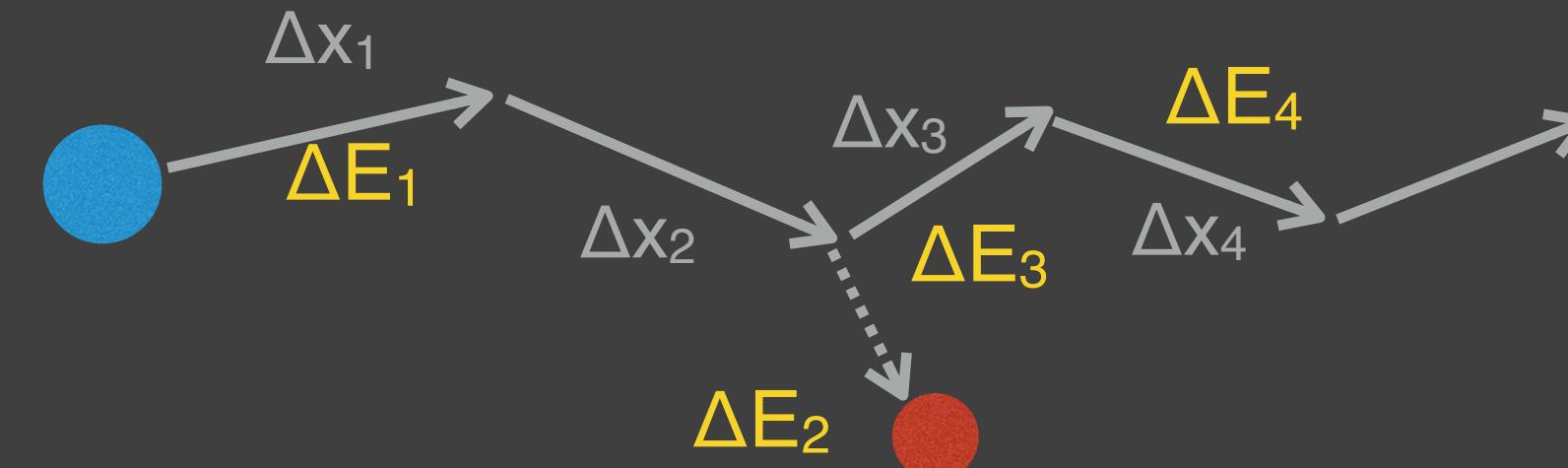
Standard EM Physics

- Continues process
 - Calculating average energy loss at each step with the Bethe-Bloch formula
 - No secondaries are generated
- Discrete process
 - Generating a secondary if energy loss is above threshold

Standard EM Physics

Bethe-Bloch formula

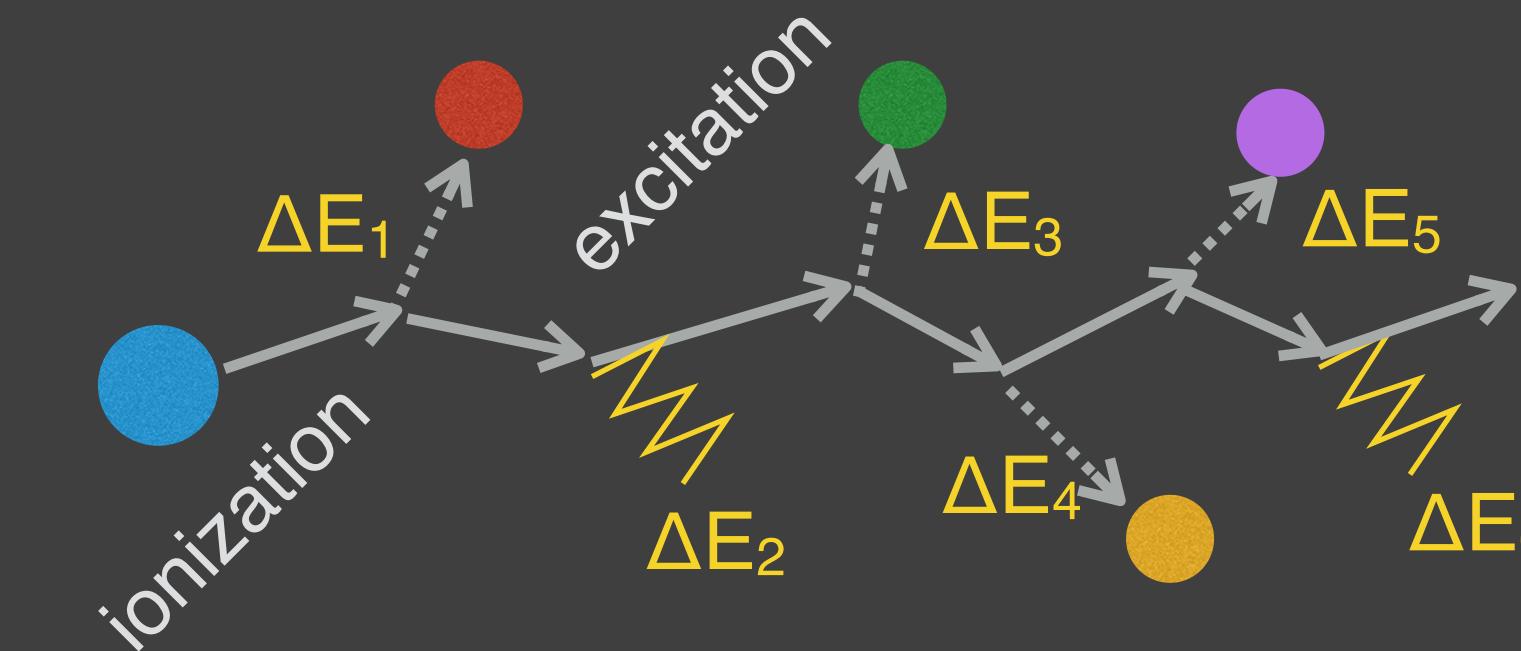
$$-\frac{dE}{dx} = K z^2 \frac{Z}{A} \frac{1}{\beta^2} \left[\frac{1}{2} \ln \frac{2m_e c^2 \beta^2 \gamma^2 T_{\max}}{I^2} - \beta^2 - \frac{\delta}{2} \right]$$



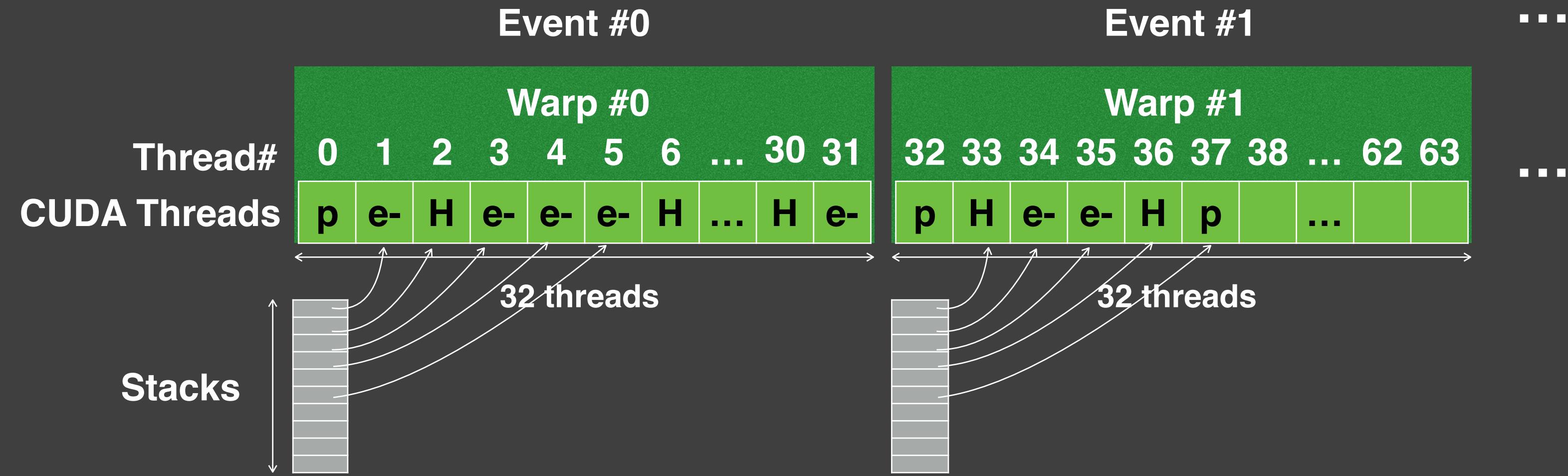
DNA physics

- Handling as a discrete process
 - Particles lose their kinetic energy in ionization and excitation processes
- Ionization process has no energy threshold
 - > **Generating large amount of secondary particles**
 - > **Need longer time for tracking all particles**

DNA Physics



CUDA Thread Assignment For MPEXS-DNA Physics Simulation



- Assign a group of 32 CUDA threads per event
 - Every groups have common stack storing secondaries
 - Allows for tracking up to 32 particles in parallel
 - A CUDA thread in every groups start to track a primary particle
 - As secondaries are generated, vacant threads start to track them
 - If there are no vacant threads, stores secondary particles in the stacks temporally and wait until threads are available

Chemical Phase

- Chemical phase simulates radiolysis of water.
 - Physics processes generate primary chemical species: $(\text{H}_2\text{O}^+, \text{H}_2\text{O}^*, \text{e}^-_{\text{aq}})$.
 - Then, H_2O^+ dissociates. H_2O^* dissociates or releases energy into water.
 - These processes occurs within 1 ps after irradiation.

Electronic state	Process	Decay channel	Fraction (%)
Ionization state	Dissociative decay	$\text{H}_3\text{O}^+ + \bullet\text{OH}$	100
Excitation state: A1B1	Dissociative decay	$\bullet\text{OH} + \text{H}\bullet$	65
	Relaxation	$\text{H}_2\text{O} + \Delta E$	35
	Auto-ionization	$\text{H}_3\text{O}^+ + \bullet\text{OH} + \text{e}^-_{\text{aq}}$	55
Excitation state: B1A1	Dissociative decay	$\bullet\text{OH} + \bullet\text{OH} + \text{H}_2$	15
	Relaxation	$\text{H}_2\text{O} + \Delta E$	30
	Auto-ionization	$\text{H}_3\text{O}^+ + \bullet\text{OH} + \text{e}^-_{\text{aq}}$	50
Excitation state: Rydberg, diffusion bands	Relaxation	$\text{H}_2\text{O} + \Delta E$	50

Chemical Phase

58

The strategy for chemical simulation

(1) Calculate intermolecular distance (d) for all pairs

- If find pairs within reaction radius ($d < R$), make reactions

$$R = \frac{k}{4\pi N_A D}$$

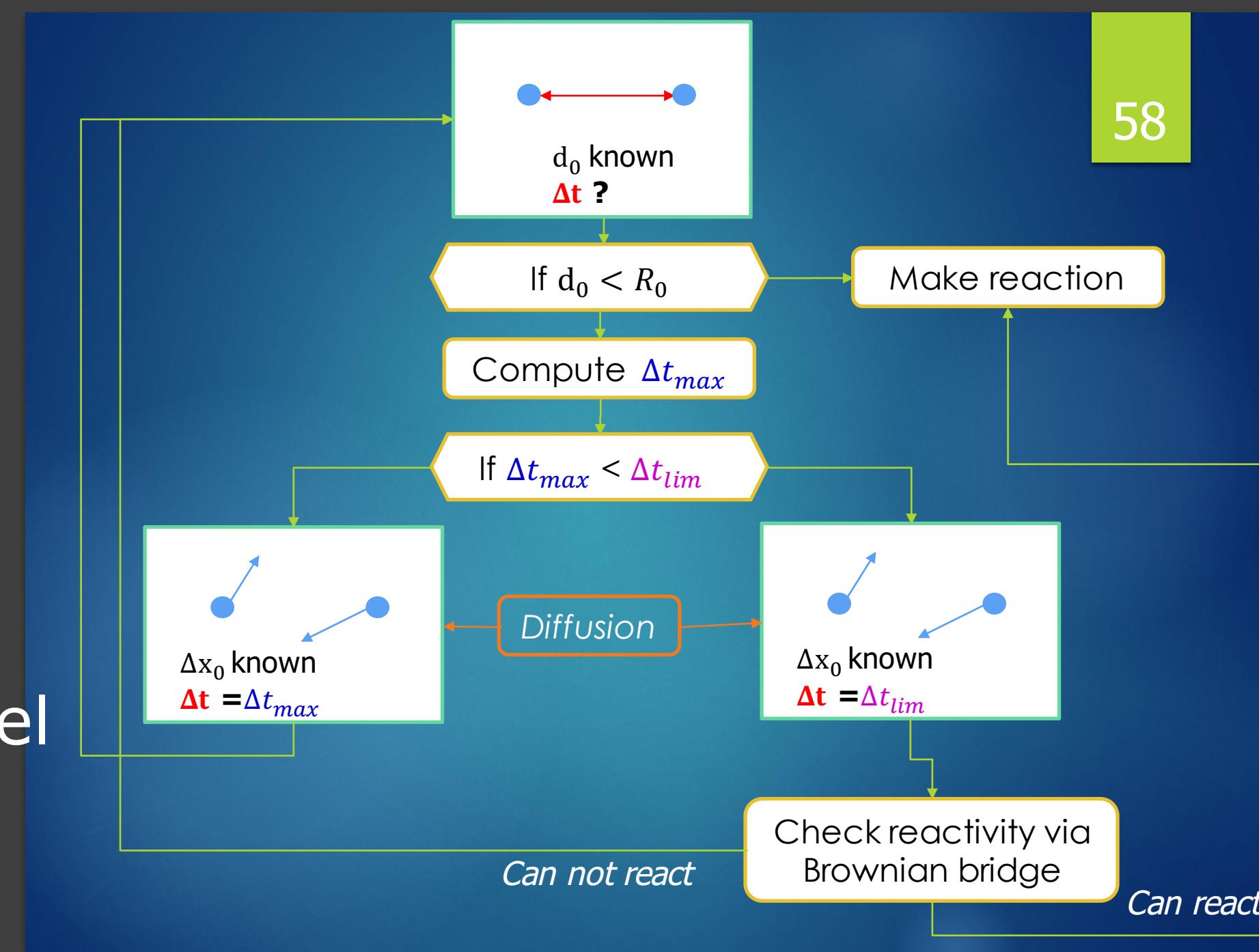
Smoluchowski model

(2) Find minimum distance within pairs and calculate time step

(3) Diffuse molecules

(4) Loop (1) ~ (3) until time reaches 1 μ s

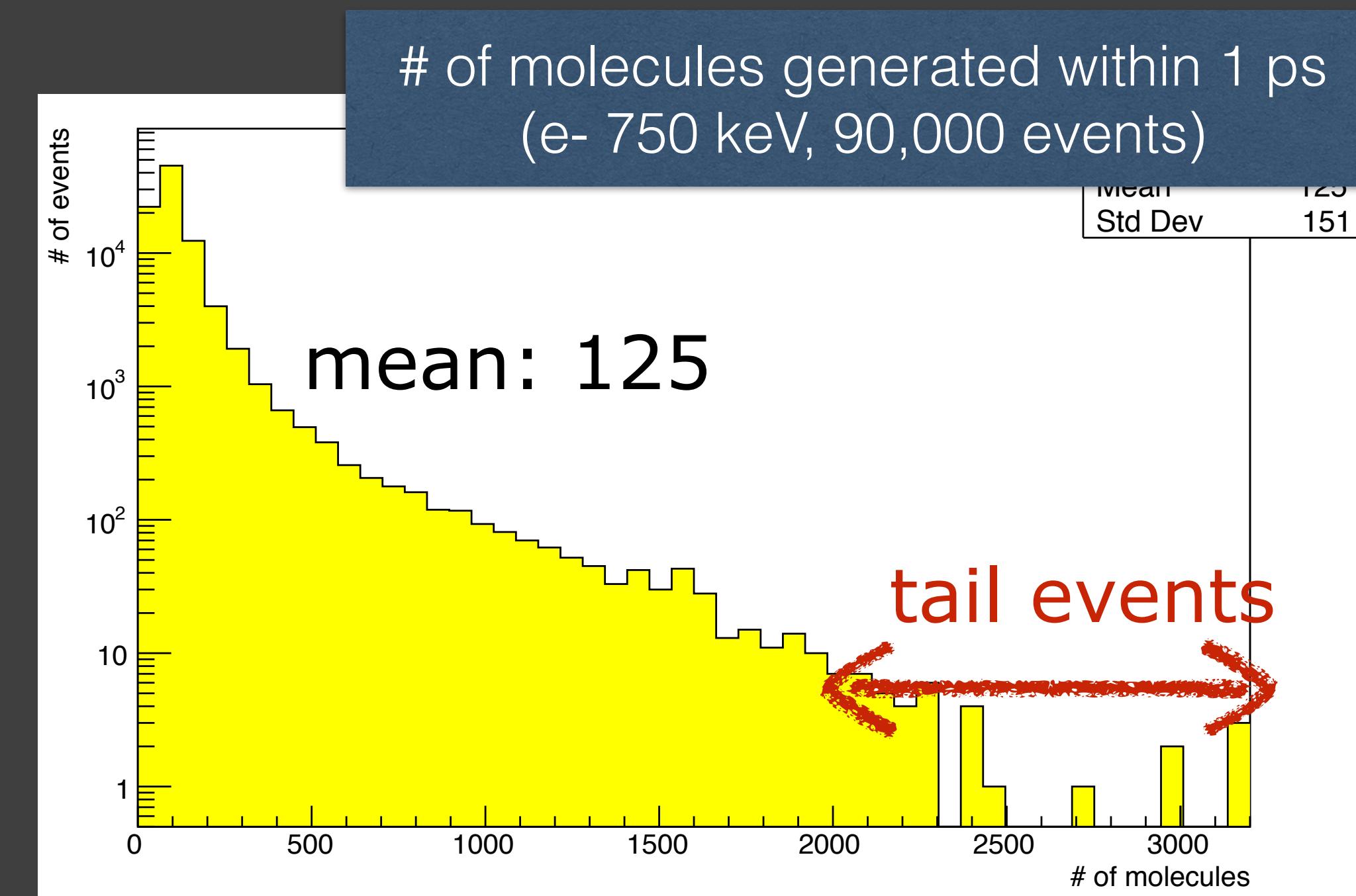
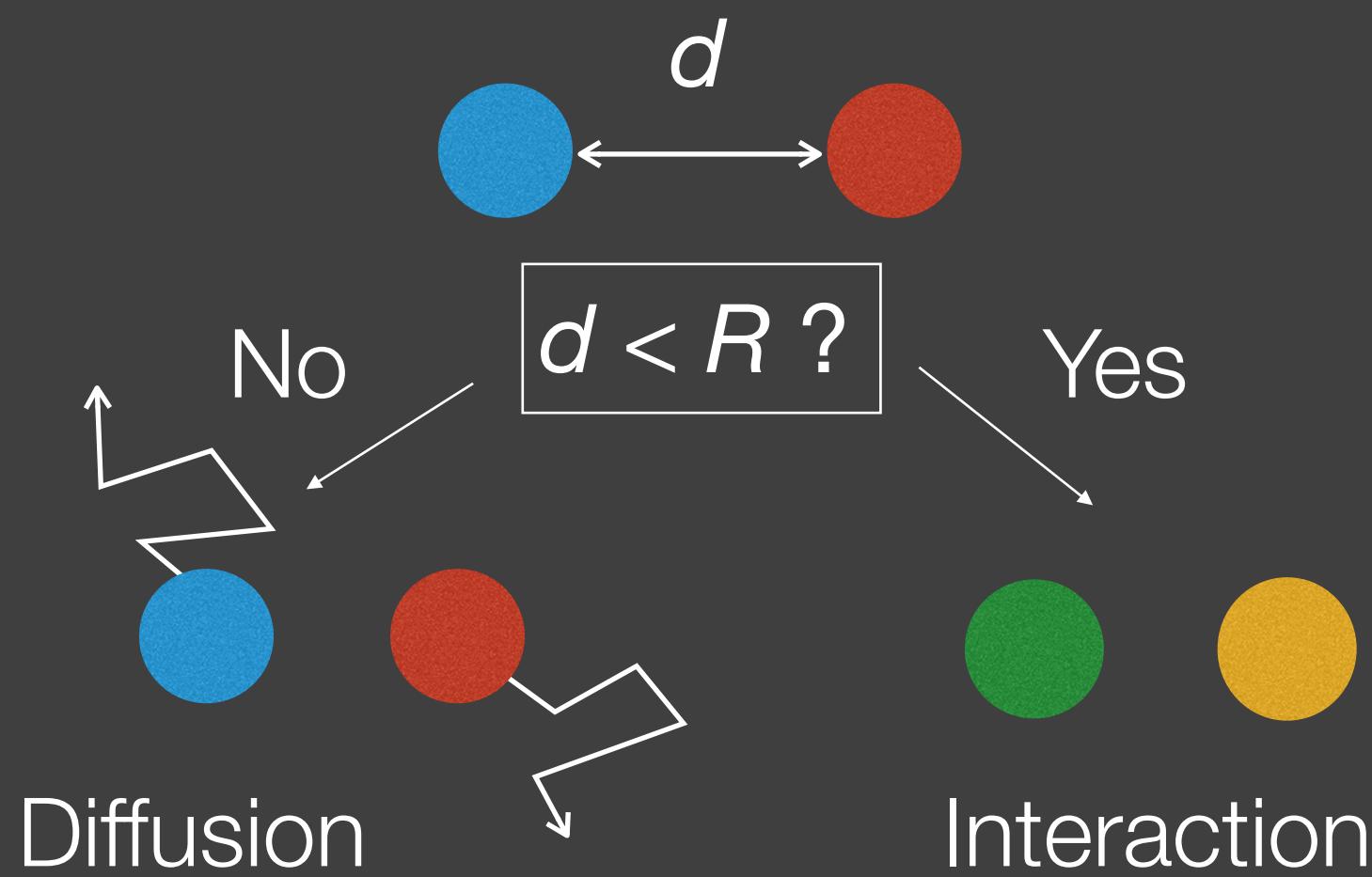
Species	Diffusion coefficient ($\times 10^{-9} \text{ m}^2/\text{s}$)
H_3O^+	9.0
$\text{H}\bullet$	7.0
OH^-	5.0
e^-_{aq}	4.9
H_2	4.8
$\bullet\text{OH}$	2.8
H_2O_2	2.3



Reaction	Reaction rate ($\times 10^{10} \text{ M}^{-1}\text{s}^{-1}$)
$2e^-_{\text{aq}} + 2\text{H}_2\text{O} \rightarrow \text{H}_2 + 2\text{OH}^-$	0.50
$e^-_{\text{aq}} + \bullet\text{OH} \rightarrow \text{OH}^-$	2.95
$e^-_{\text{aq}} + \text{H}\bullet + \text{H}_2\text{O} \rightarrow \text{OH}^- + \text{H}_2$	2.65
$e^-_{\text{aq}} + \text{H}_3\text{O}^+ \rightarrow \text{H}\bullet + \text{H}_2\text{O}$	2.11
$e^-_{\text{aq}} + \text{H}_2\text{O}_2 \rightarrow \text{OH}^- + \bullet\text{OH}$	1.44
$\bullet\text{OH} + \bullet\text{OH} \rightarrow \text{H}_2\text{O}$	0.44
$\bullet\text{OH} + \text{H}\bullet \rightarrow \text{H}_2\text{O}$	1.44
$\text{H}\bullet + \text{H}\bullet \rightarrow \text{H}_2$	1.20
$\text{H}_3\text{O}^+ + \text{OH}^- \rightarrow 2\text{H}_2\text{O}$	1.43

An issue of Chemical Phase

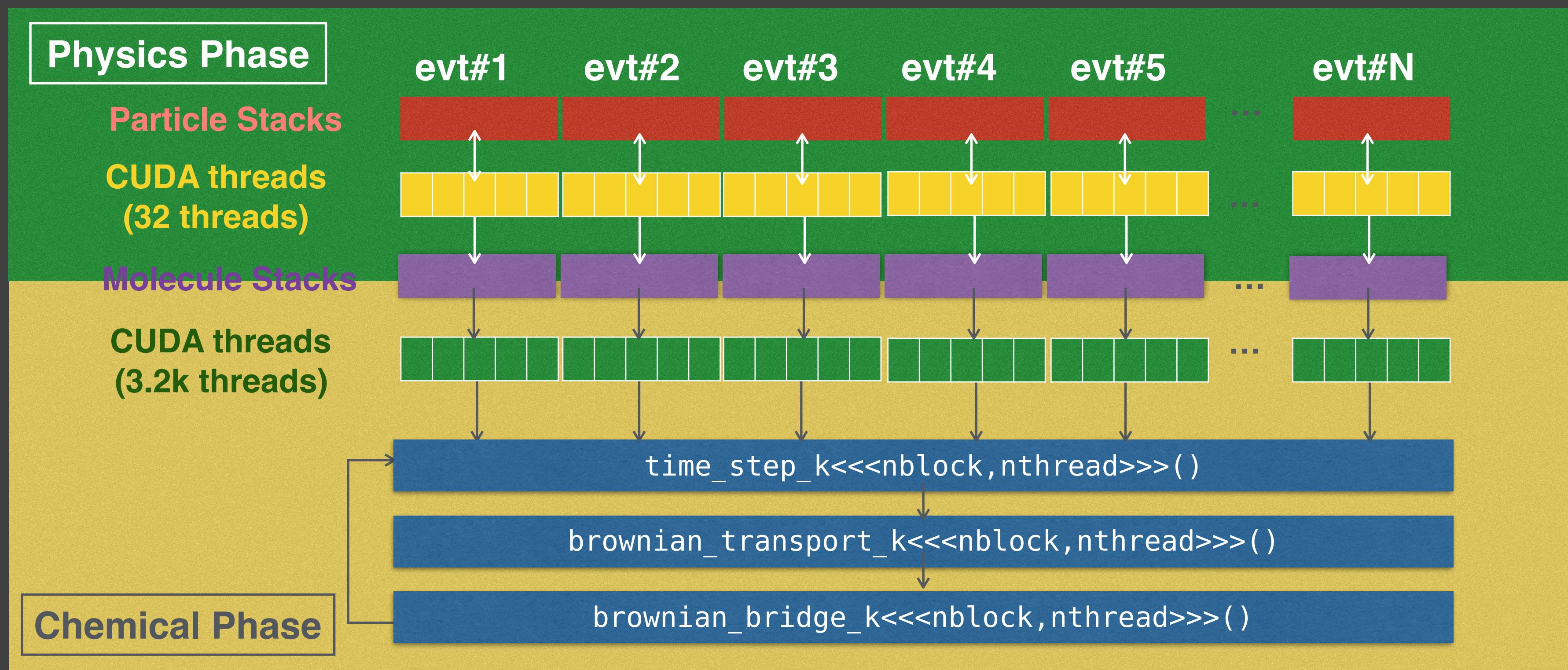
Process time for calculating intermolecular distance for all possible pairs increases by $O(N^2/2)$ -> **Need longer time**



- Tail events cause long duration. Ignoring rare events may allow for reducing simulation time. But we don't know
 - How much rare events contribute to DNA damage?
 - How biological scientists focus on rare events?

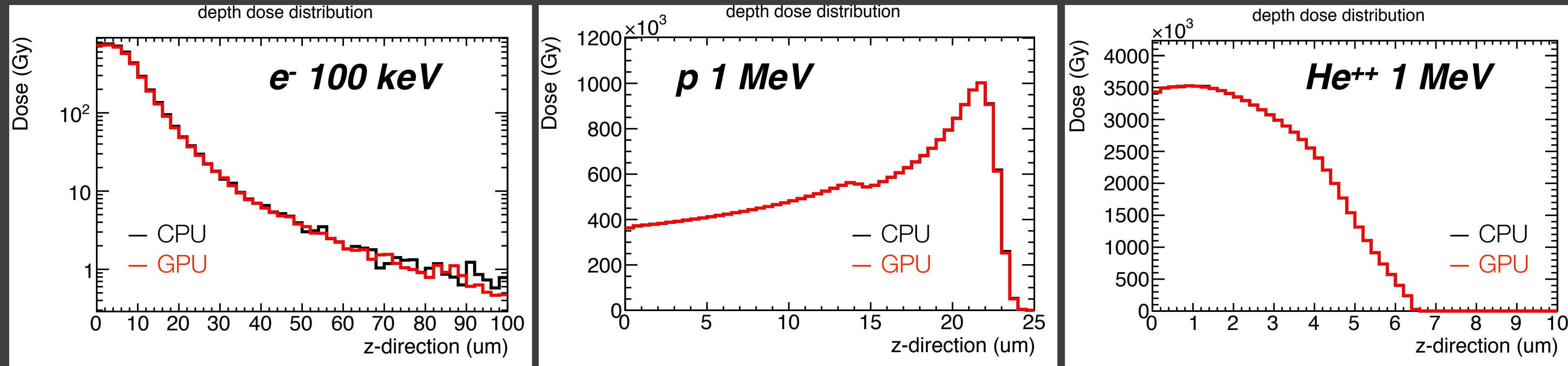
MPEXS-DNA Physics and Chemical Simulation

- Simulating up to ~10k events in parallel processing
 - MPEXS-DNA performs physics simulation
 - Allocate new stack storing molecules generated by physical interactions
 - Switch to chemical simulation after all events finish physics simulation
 - Assign 3.2k CUDA threads per event to calculate intermolecular distance for all pairs, make reactions, compute time step, and transport molecules



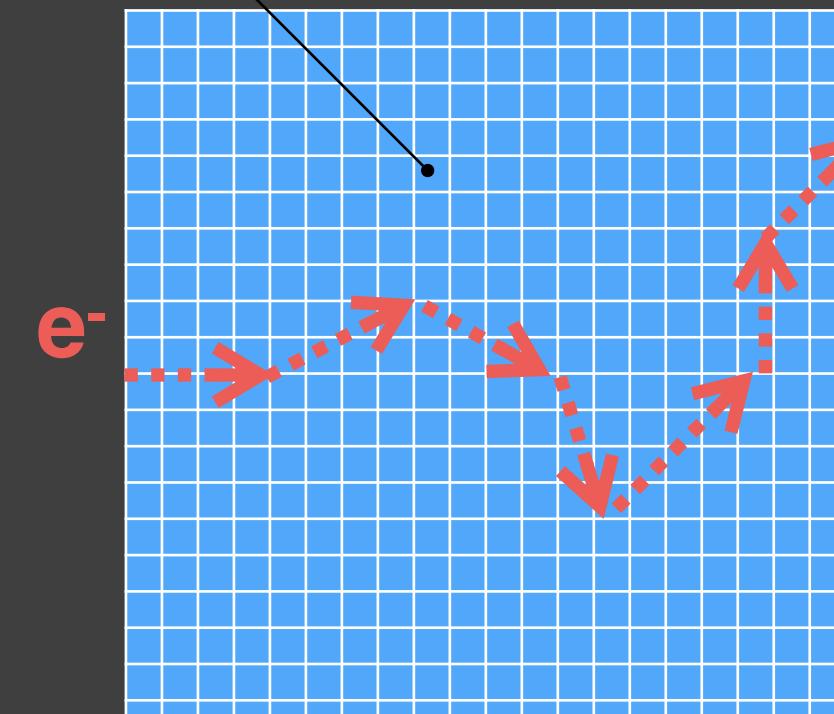
Physics Performance for DNA Physics

Depth dose curves (CPU vs GPU)



Simulation model

score energy deposition
in each voxel



voxelized water phantom

incident particle	initial energy	phantom size	# of voxel cells (voxel size)
e^-	100 keV	$102 \times 102 \times 100$ um	$51 \times 51 \times 50$ ($2 \times 2 \times 2$ um)
p	1 MeV	$25.5 \times 25.5 \times 25$ um	$51 \times 51 \times 50$ ($0.5 \times 0.5 \times 0.5$ um)
He^{++}	1 MeV	$10.2 \times 10.2 \times 10$ um	$51 \times 51 \times 50$ ($0.2 \times 0.2 \times 0.2$ um)

Computing Performance for Physics Simulation by MPEXS-DNA

- ~ 280 times speedup against single-core CPU
 - ex.) Process time (~ 16k protons with 1 MeV)
 - ~ 53 hr. (single-core CPU) -> **~ 12 min.** (GPU)

	Incident particle	Initial energy	MPEXS-DNA		Geant4-DNA	speedup factor (=G4/MPEXS)
			Total thread numbers ($N_{blk} \times N_{thr/blk}$)	Process time (sec/particle)	Process time (sec/particle)	
DNA Physics	e-	100 keV	524,288 (4,096 x 128)	3.53×10^{-3}	0.764	277
	p	1 MeV	524,288 (4,096 x 128)	5.97×10^{-2}	11.8	265
	He ⁺⁺	1 MeV	524,288 (4,096 x 128)	6.10×10^{-2}	12.3	269
Standard EM Physics	e-	20 MeV	524,288 (4,096 x 128)	8.81×10^{-6}	1.84×10^{-3}	208

- GPU (NVIDIA, Tesla K20c, 2496 cores, 706 MHz)
- CPU single core (Intel, Xeon E5-2643 v2, 3.50 GHz)

GPU Performance of MPEXS-DNA for Physics and Chemical Simulation

- up to **210 times** speedup against single-core CPU
 - ~ 4 days (single-core CPU) -> **~ 30 min.** (e- 10 keV, 10k events)
 - ~ 12 hr. (single-core CPU) -> **~ 6 min.** (e- 750 keV, 10k events)
 - ~ 3 days (single-core CPU) -> **~ 20 min.** (p 20 MeV, 10k events)

Computing Performance including physical phase (Geant4-DNA vs MPEXS-DNA)

	e- 10 keV	e- 750 keV	p 20 MeV
Water phantom size	1 x 1 x 1 um	5 x 5 x 5 um	1 x 1 x 1 um
Average # of molecules generated at 1 ps	419	125	366
Process time (Geant4-DNA)	34.6 sec / event	4.99 sec / event	27.5 sec / event
Process time (MPEXS-DNA)	0.201 sec / event	0.0343 sec / event	0.129 sec / event
Speedup factor	172x	146x	213x

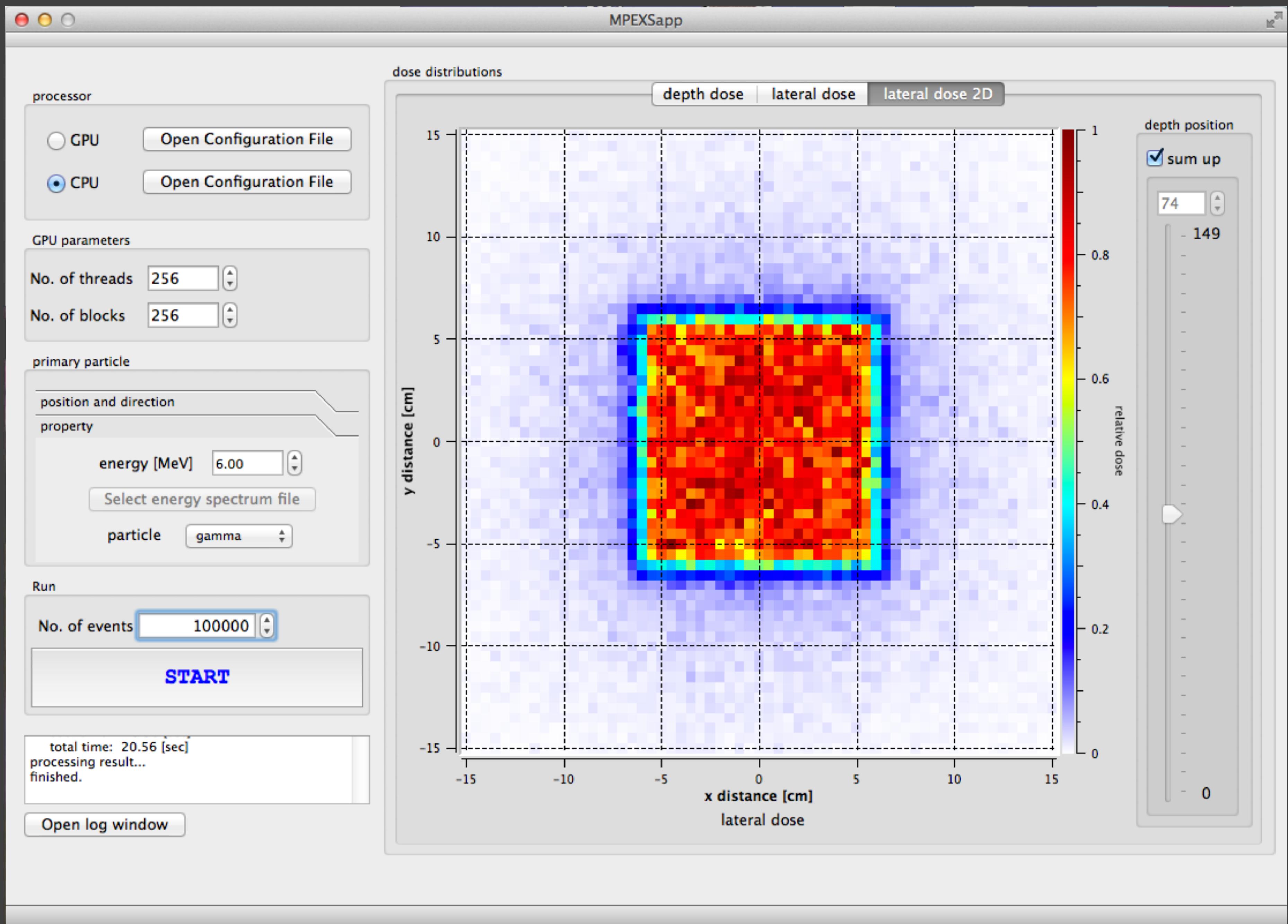
- GPU (NVIDIA, Tesla K20c, 2496 cores, 706 MHz)
- CPU single core (Intel, Xeon E5-2643 v2, 3.50 GHz)

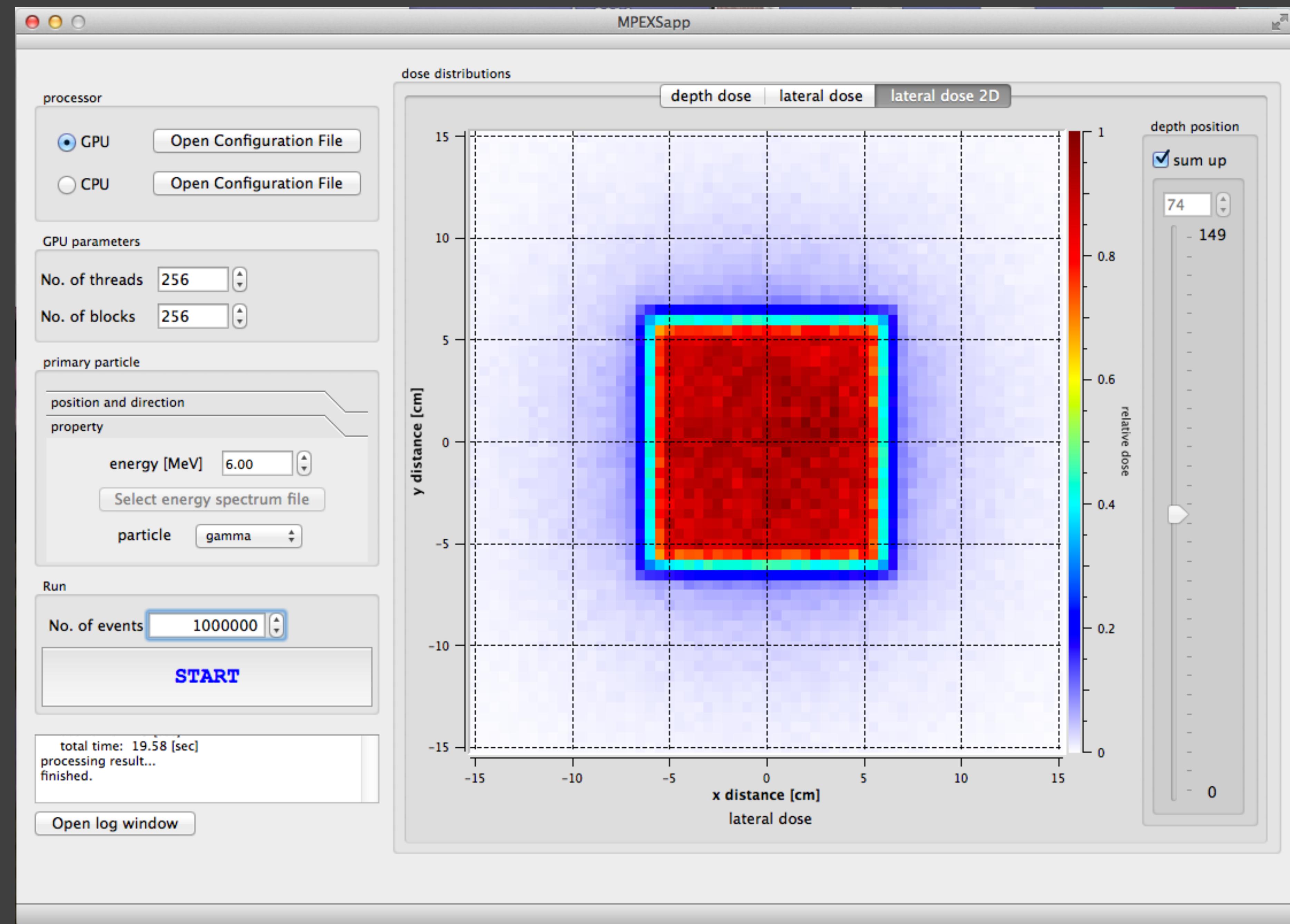
MPEXS-DNA Summary

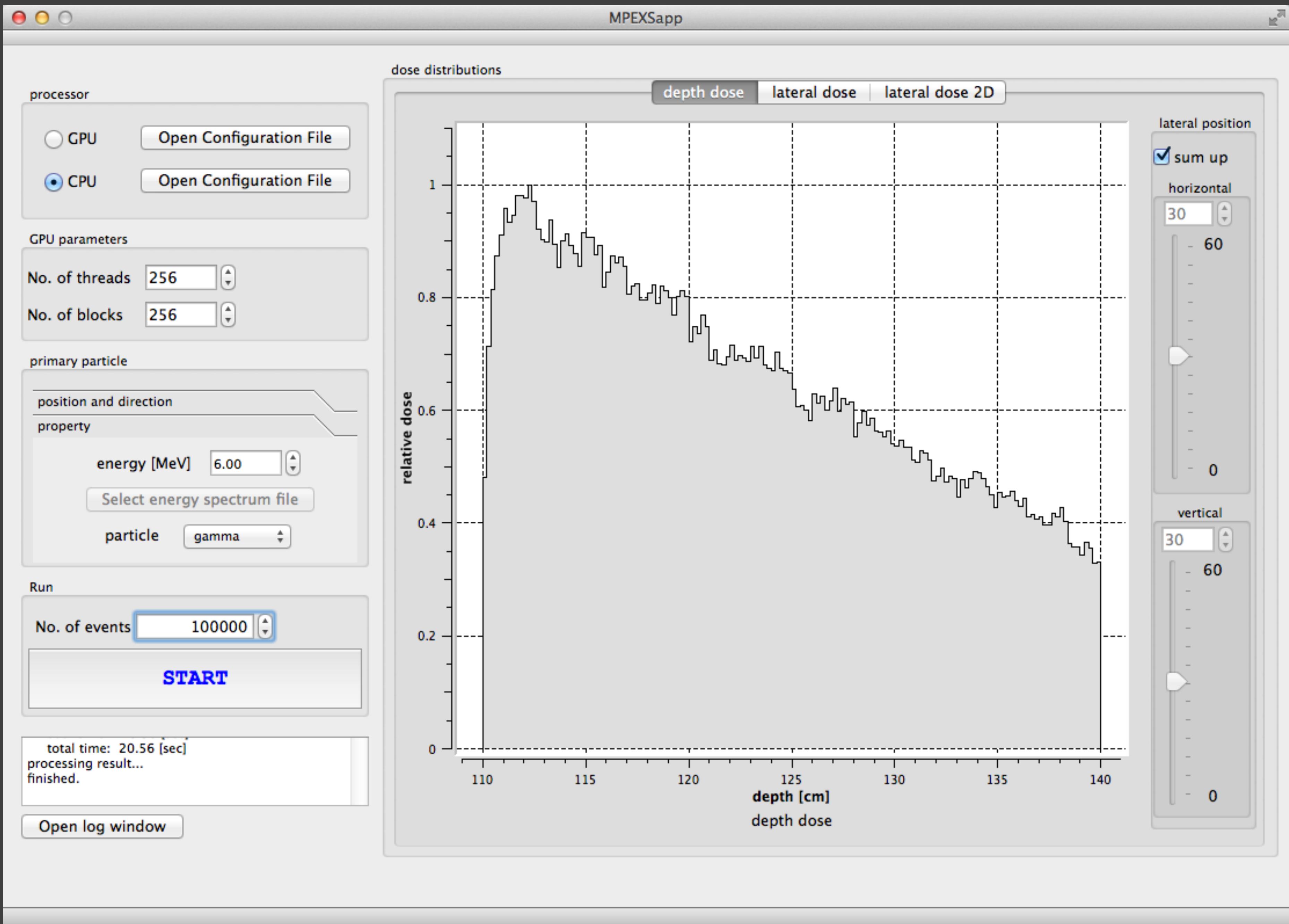
- MC approach for estimating biological effects of radiation at DNA scale
- DNA physics simulation can be run on GPU
 - DNA physics processes are implemented in CUDA
 - MPEXS-DNA has the same accuracy as Geant4-DNA
 - **Achieve up to 280 times speedup with GPU**
- Chemical processes have also been implemented
 - TODO: detailed verifications
 - **Up to 210 times speedup in physics and chemical simulations**

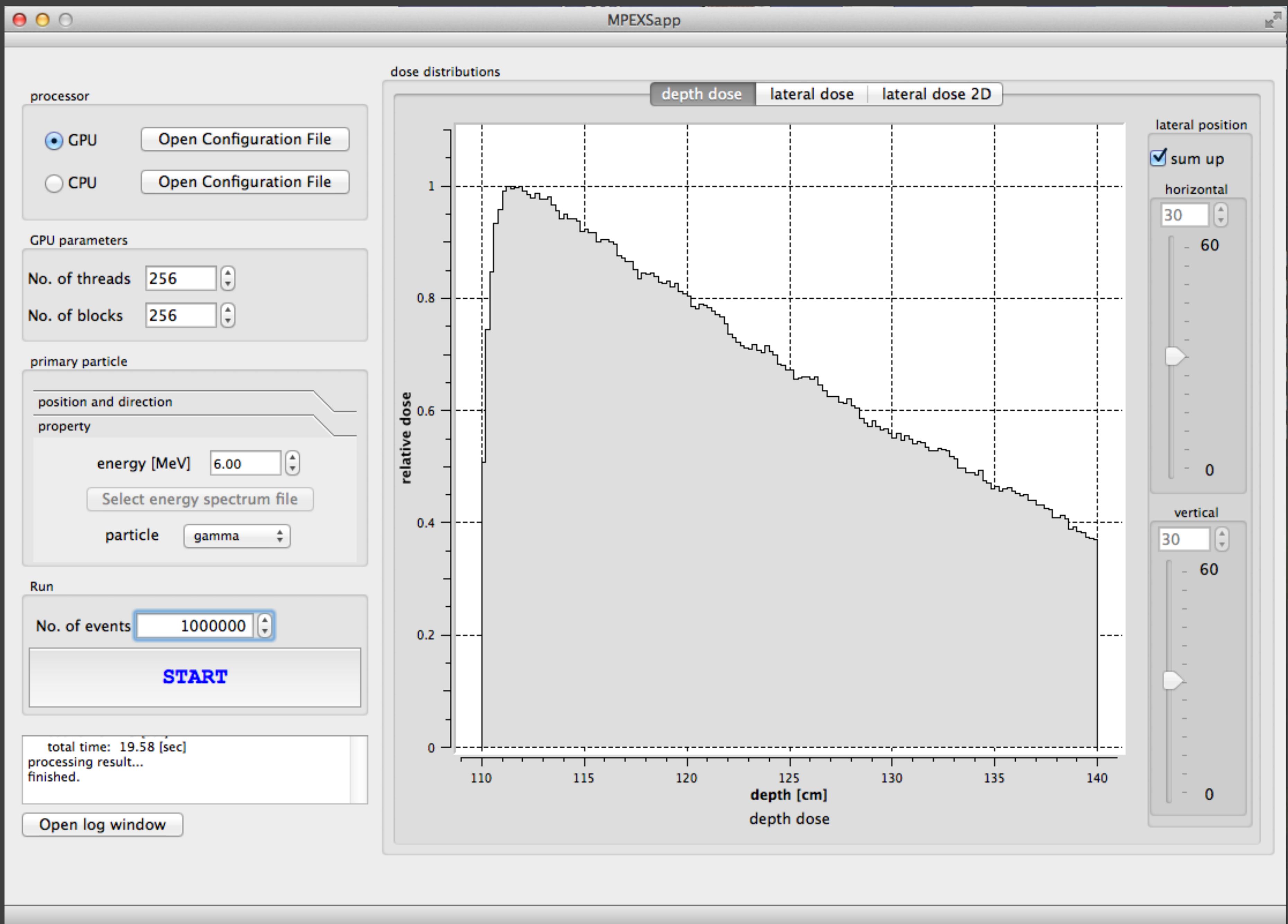
MPEXS – GUI

- QT GUI for MPEXS for demonstration purposes
- Developed by Akinori Kimura, Ashikaga Institute of Technology
- 100K events of 6 MeV gamma on single core of CPU (Intel i7, 2.6 GHz)
- 1M events of 6 MeV gamma on 256*256 GPU threads (NVIDIA GeForce GT 750M)
- It takes about the same time (~20 sec) for 100K events on single core of CPU and 1M events on GPU.









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