

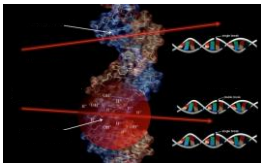
gMicroMC: Accelerating Microscopic Monte Carlo Simulation Using Rapid Parallel Processing Platforms

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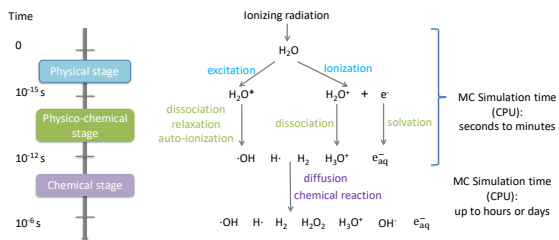


Motivation

- Ionizing radiation causes damage through **water radiolysis**, with DNA as the primary target of the generated radiolytic molecules.
- Accurate modeling of water radiolysis is essential to understand the radiobiological mechanisms and quantitatively test the related hypotheses



Water radiolysis



- Physical and physico-chemical stage:
 - Computationally acceptable
- Chemical stage is **highly time-consuming** on conventional CPU because:
 - Simulation of a dynamic process over several orders of magnitude in time (10^{-12} s ~ 10^6 s)
 - An ionizing particle can generate a large number of radiolytic molecules in water
 - A highly correlated many-body simulation problem due to the mutual chemical reactions: **algorithm complexity $O(N^2)$**
- This time limitation hinders a number of related research studies, particularly cell-level simulations

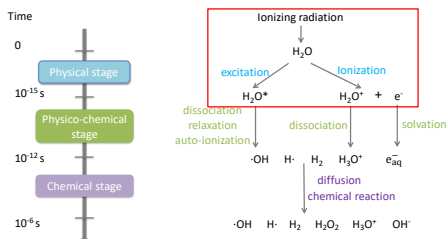
GPU Acceleration

- A huge boost of GPU application in scientific computing
- What is GPU?
 - Graphics Processing Unit, co-processor, needs a host (General-purpose CPU)
 - Originally developed for accelerating 2D or 3D graphics rendering
- GPU vs CPU:
 - CPU: a few cores optimized for sequential serial processing
 - GPU: thousands of smaller, more efficient cores designed for handling multiple tasks simultaneously
 - Data level parallelism: Single Instruction, Multiple Data



- We have successfully applied GPU in radiotherapy problems:
 - Image reconstruction
 - Treatment planning
 - Monte Carlo Dose Calculation (external radiotherapy, brachytherapy, proton, carbon)
- GPU is also known to successfully accelerate the simulation of fluid system, contacting particle system, cell biological system
- We initiated the development on a GPU-based fast microscopic MC simulation package, named gMicroMC

Simulation methods of physical stage



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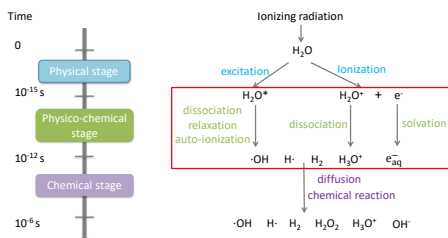
Simulation methods of physical stage

- Currently, our physical stage simulation only supports electron transport in water (1 eV-10 MeV)
- **Ionization**
 - Considered five ionization shells: 1b₁, 3a₁, 1b₂, 2a₁, K-shell
 - Relativistic binary-encounter-Bethe model (BEB) (*Phys Rev A* 2000, 62: 052710-52711)
 - Energy loss: Composition sampling method (*Physica Medica* 2016, 32:1833-1840)
- **Excitation**
 - Considered five excited states: A¹B¹, B¹A¹, Ryd A+B, Ryd C+D, diffuse bands
 - A semi-analytic model (*Journal of Geophysical research*, 1972, 77(25): 4797-4811)
- **Elastic scattering**
 - <200 eV: a semi-empirical parameterization method (*Brenner, D.J. & Zaider, M. Phys. Med. Biol.* (1983), 29:443-447)
 - >200 eV: Rutherford cross section with a screening parameter (*Uehara, S et al Phys. Med. Biol.* (1992) 37, 1841-1858)

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Simulation methods of physico-chemical stage



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Simulation methods of physico-chemical stage

- Decay channels for ionized and excited water molecules

Process	Decay channel	Fraction (%)	
Ionization (H ₂ O ⁺)			
H ₂ , Du, D ₂ , D ₂ , K	Dissociative decay	H ₂ O ⁺ + *OH	100
Excitation (H ₂ O [*])			
A ¹ h	Dissociative decay	*OH + H ⁺	65
	Relaxation	H ₂ O + M	35
B ¹ A'	Auto-ionization	H ₂ O ⁺ + *OH + e _{aq} ⁻	35
	Dissociative decay	H ₂ + *O [*]	15
	Relaxation	H ₂ O + M	30
Ryd. diff bands	Auto-ionization	H ₂ O ⁺ + *OH + e _{aq} ⁻	30
	Relaxation	H ₂ O + M	50

- Thermalization of hot dissociation fragments

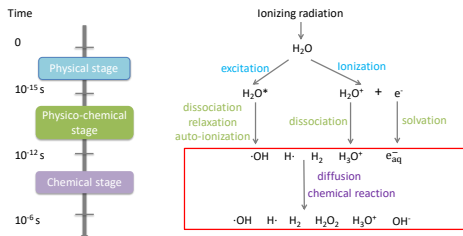
$$f(r) = \sqrt{\frac{2}{\pi}} \frac{1}{\sigma^2} \exp\left(-\frac{1}{2\sigma^2} r^2\right)$$

- Thermalization of sub-excitation electrons

$$f(r) = 4r \exp(-2r)$$

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Simulation methods of chemical stage



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Simulation methods of chemical stage¹

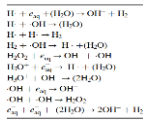
- Step-by-step method:** Dividing the dynamic chemical stage into small consecutive time steps
- Diffusion model:** Each molecule was considered as an individual Brownian object with random and independent motion, following a 3D Gaussian distribution

$$P(x,y,z)dx dy dz = \frac{1}{(4\pi D\Delta t)^{3/2}} \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2}{4D\Delta t}\right) dx dy dz$$

- D: diffusion coefficient of the molecule;
- Δt: step size of time step

- Reaction model:** Assuming diffusion-controlled reactions, i.e. a reaction would only occur when the distance of the reactants was no greater than its reaction radius

Reaction¹



1. M. Karamitos, et al. Journal of Computational Physics 274 (2014) 841–882

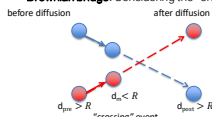
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Simulation methods of chemical stage

- **Dynamic time step:**

- Prefer small time step in order not to miss any interactions, but results in longer simulation time
- Dynamic time step is to improve simulation efficiency without sacrificing accuracy
- For each potential reactant pair, we calculated a time interval during which the reaction would not occur with a 95% confidence interval
- The step size was set as the minimum step size between all the pairs at the current step

- **Brownian bridge:** Considering the "crossing" event and estimate the probability of crossing



$$P_c = \exp\left(-\frac{(d_{sep} - R)(d_{blue} - R)}{D_p \Delta t}\right)$$

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GPU Implementation

- **Physical stage**

- Each GPU thread was responsible for simulating the transport of one incident radiation particle
- The generated ionized and excited water molecules were recorded using atomic operation to avoid GPU writing conflict
- Secondary particles generated during the simulation were stored in a stack temporarily
- Once the simulation of the incident radiation particles were finished, the secondary particles were simulated, one particle per thread

- **Physico-chemical stage**

- Each GPU thread was responsible for simulating the decay and thermalization of one molecule

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GPU Implementation

- **Chemical stage:**

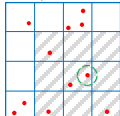
- Each GPU thread was responsible for simulating the diffusion and chemical reactions of one molecule
- A molecule array was allocated to record the evolution (species, spatial locations) of the radiolytic molecules during chemical stage
- A buffer array was also allocated to record the third product of the reactions if existed
- A tag array was used to inform the GPU regarding the status of each molecule ("alive"/"dead") during simulation to avoid reaction conflicts

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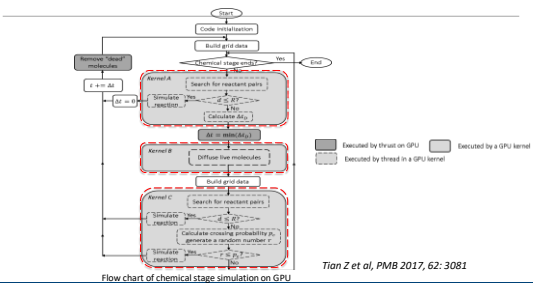
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Grid data approach

- **Grid data approach:** reduce algorithm complexity in the simulation of the chemical stage
 - Divide the volume of interest into a grid of uniformly sized cells
 - Cell size: the largest reaction radius out of all the reaction types considered in our simulation
 - Rearrange the molecules in the molecule array according to their cell IDs
 - A non-empty-cell array storing cell IDs of the non-empty cells, and an associated start-position array indicating the index of each cell's first molecule in the sorted molecule array
 - For each molecule, only search for its potential reactants within the same cell and the neighboring cells



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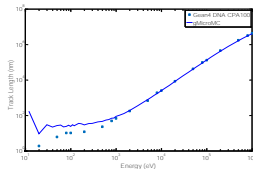


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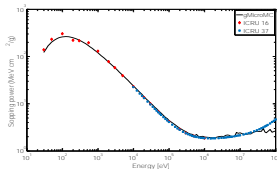


Results

- Physical stage:



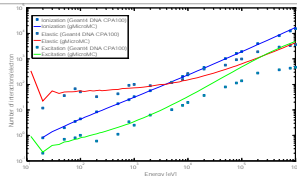
Comparison results of track length of electrons of different energies



Comparison results of stopping power of electrons of different energies

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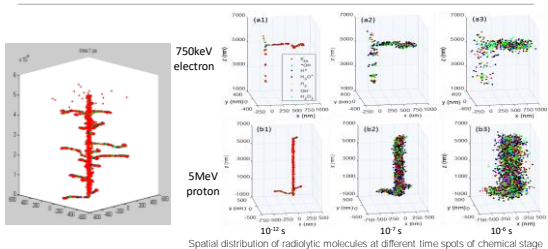


Comparison results of number of interactions occurred for electrons of different energies

GPU acceleration of physical stage: simulating electron of 750 keV

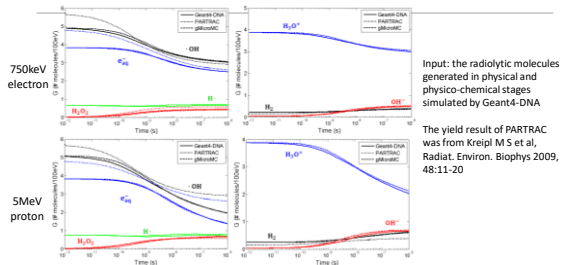
	CPU	GPU	Speed-up factor
1 electron	5 sec	10.5 sec	0.5
2048 electrons	116 min	12 min	9.3

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Spatial distribution of radiolytic molecules at different time spots of chemical stage

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Input: the radiolytic molecules generated in physical and physico-chemical stages simulated by Geant4-DNA

The yield result of PARTRAC was from Kreipl M S et al, Radiat. Environ. Biophys 2009, 48:11-20

Time-dependent yield of radiolytic molecules during chemical stage

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Table 1. Yield values (molecules/100 eV) of radiolytic species present at the end of chemical stage for 750 keV electron (depositing all its energy in a sphere of 3nm diameter) and 5 MeV proton (depositing -0.5MeV in a sphere of 50 μm).

	e_{aq}^-	$\cdot\text{OH}$	H_2O^+	$\text{H}\cdot$	H_2	OH^-	H_2O_2
750 keV electron	Geant4-DNA	2.51	3.03	3.00	0.66	0.49	0.39
	gMicroMC	2.51	3.07	3.06	0.72	0.53	0.36
	Difference (%)	0.00	1.32	2.00	9.09	8.16	7.69
5MeV proton	Geant4-DNA	1.38	1.97	2.05	0.73	0.63	0.66
	gMicroMC	1.40	1.97	2.15	0.80	0.60	0.70
	Difference (%)	1.45	0.00	4.88	9.59	4.76	6.06

Table 2. Efficiency test results, including the amount of radiolytic molecules at the beginning of the chemical stage in the two cases, denoted as N(t), t=1ps; total simulation time taken by Geant4-DNA on CPU and our gMicroMC on GPU; the speed-up factor achieved by our package compared to the Geant4-DNA.

	Simulation time [s]		Speed-up factor
	Geant4-DNA (CPU)	gMicroMC (GPU)	
750 keV electron	101829	102865.4	171.1
5MeV proton	56122	96446.5	197.2

Summary

- We have validated the simulation of each individual stage implemented in gMicroMC
- End-to-end test to validate gMicroMC as an entire package is ongoing
- Simulation of DNA damage will be implemented into our package
- Fast simulation of the water radiolysis will facilitate many radiobiology related research:
 - Cell-level simulation of radiation damage
 - Effect of nano-particle in radiotherapy
 - Mechanism of ultrahigh dose rate FLASH irradiation
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