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

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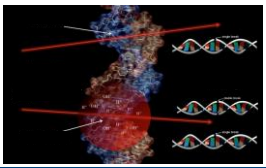
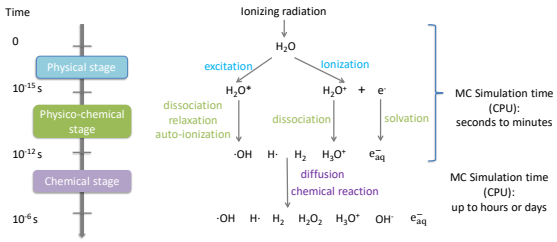
Motivation

- 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



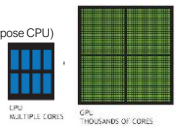
Water radiolysis



- 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

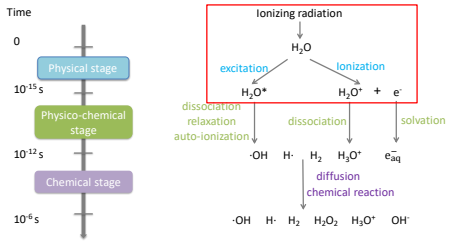
GPU Acceleration

- 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

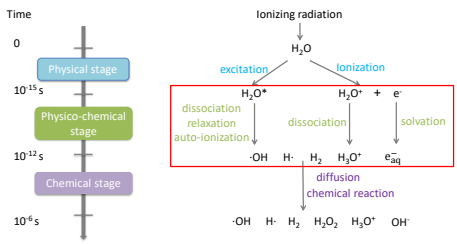
Simulation methods of physical stage



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: $1b_1$, $3a_1$, $1b_2$, $2a_1$, 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: A^1B^1, B^1A^1, 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*)

Simulation methods of physico-chemical stage



Simulation methods of physico-chemical stage

- Decay channels for ionized and excited water molecules

	Process	Decay channel	Fraction (%)
Ionisation (H_2O^+)			
$1b_1$, $3a_1$, $1b_2$, $2a_1$, K	Dissociative decay	$H_2O^+ + {}^{\bullet}OH$	100
Excitation (H_2O^*)			
A^1B_1	Dissociative decay	${}^{\bullet}OH + H^{\bullet}$	65
	Relaxation	$H_2O + \Delta E$	35
B^1A_1	Auto-ionisation	$H_2O^+ + {}^{\bullet}OH + e^-_{aq}$	55
	Dissociative decay	$H_2 + {}^{\bullet}O^{\bullet}$	15
	Relaxation	$H_2O + \Delta E$	30
Ryd. diff bands	Auto-ionisation	$H_2O^+ + {}^{\bullet}OH + e^-_{aq}$	50
	Relaxation	$H_2O + \Delta E$	50

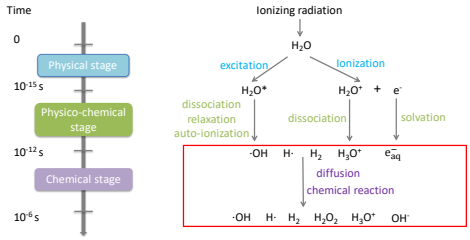
- Thermalization of hot dissociation fragments

$$f(r) = \sqrt{\frac{2}{\pi}}\frac{1}{\sigma^3}r^2\exp\left(-\frac{1}{2}\frac{r^2}{\sigma^2}\right)$$

- Thermalization of sub-excitation electrons

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

Simulation methods of chemical stage



Simulation methods of chemical stage[1]

- **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

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

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

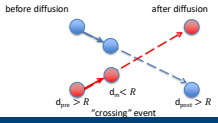
- **Reaction model**: Assuming diffusion-controlled reactions, i.e. a reaction would only occur when the distance of the reactants was no greater than its reaction radius

Reaction[a]
$H^{\bullet} + e^-_{aq} + (H_2O) \rightarrow OH^- + H_2$
$H^{\bullet} + {}^{\bullet}OH \rightarrow (H_2O)$
$H^{\bullet} + H^{\bullet} \rightarrow H_2$
$H_2 + {}^{\bullet}OH \rightarrow H^{\bullet} + (H_2O)$
$H_2O_2 + e^-_{aq} \rightarrow {}^{\bullet}OH + {}^{\bullet}OH$
$H_3O^+ + e^-_{aq} \rightarrow H^{\bullet} + (H_2O)$
$H_3O^+ + {}^{\bullet}OH \rightarrow (^3H_2O)$
${}^{\bullet}OH + e^-_{aq} \rightarrow OH^-$
${}^{\bullet}OH + {}^{\bullet}OH \rightarrow H_2O_2$
$e^-_{aq} + e^-_{aq} + (2H_2O) \rightarrow 2OH^- + H_2$

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

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



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

GPU Implementation

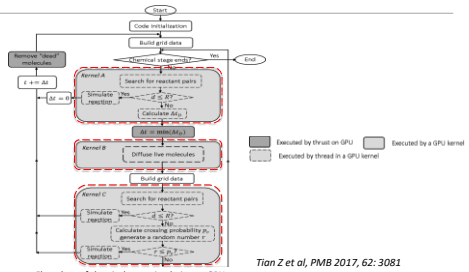
- **Physical stage**
  - Each GPU thread was responsible for simulating the transport of one incident radiation particle
  - The generated ionized and excited water molecules were recorded using atomic operation to avoid GPU writing conflict
  - Secondary particles generated during the simulation were stored in a stack temporally
  - 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

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

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

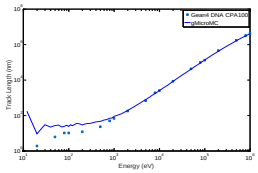


Flow chart of chemical stage simulation on GPU

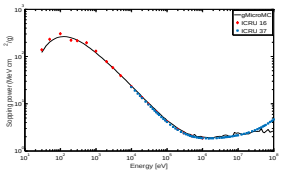
Tian Z et al, PMB 2017, 62: 3081

Results

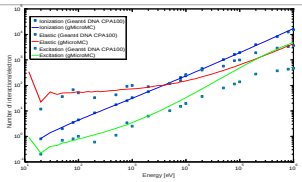
- Physical stage:



Comparison results of track length of electrons of different energies



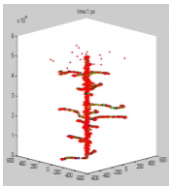
Comparison results of stopping power of electrons of different energies



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

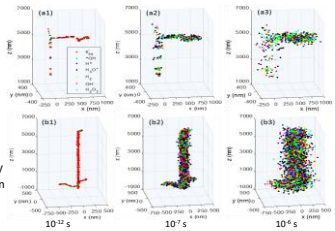
- GPU acceleration of physical stage: simulating electron of 750 keV

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



750keV electron

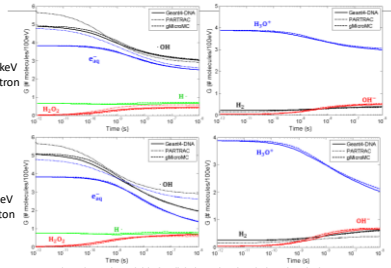
5MeV proton



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

750keV electron

5MeV proton



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

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 3mm diameter) and 5 MeV proton (depositing ~0.5MeV in a sphere of 50 μm).

		e^-_{aq}	·OH	H_3O^+	H·	H_2	OH^-	H_2O_2
750 keV electron	Geant4-DNA	2.51	3.03	3.00	0.66	0.49	0.39	0.45
	gMicroMC	2.51	3.07	3.06	0.72	0.53	0.36	0.41
	Difference (%)	0.00	1.32	2.00	9.09	8.16	7.69	8.89
5MeV proton	Geant4-DNA	1.38	1.97	2.05	0.73	0.63	0.66	0.70
	gMicroMC	1.40	1.97	2.15	0.80	0.60	0.70	0.67
	Difference (%)	1.45	0.00	4.88	9.59	4.76	6.06	4.29

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	599.2	171.1
5MeV proton	56122	96446.5	489.0	197.2

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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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