MPEXS: A CUDA MonteCarlo of the simulation of electromagnetic interactions

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Introduction

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

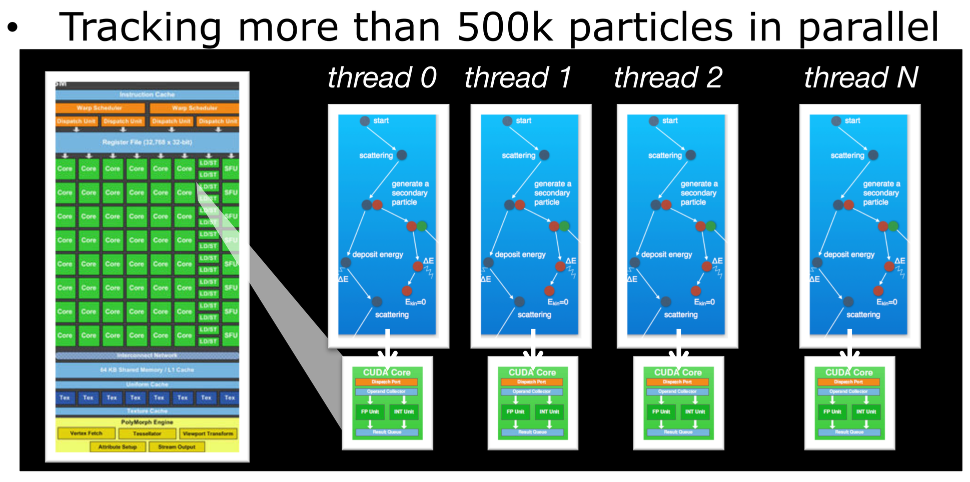
Algorithm details:
- Each CUDA thread tracks an active particle
- Physics processes store secondary particles in thread-local stacks
- Energy is atomically deposited to a global dose array

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 - Collaborators: CENBG (France), KEK (Japan)

Method and Results

Track particles in parallel spreading with many CUDA threads
- Each track is independent
- Tracking more than 500k particles in parallel

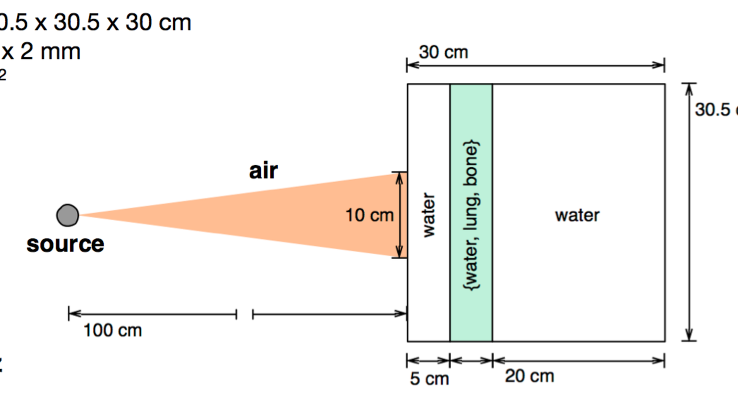


A CUDA thread has
- kinematic information for a particle: position, momentum, energy, energy loss.
- stack storing secondary particles

Verification for Dose Distribution

Dose Distribution of slab phantoms

- phantom size : 30.5 x 30.5 x 30 cm
- voxel size : 5 x 5 x 2 mm
- field size : 10 cm²
- SSD : 100 cm
- slab materials :
  (1) water
  (2) lung
  (3) bone

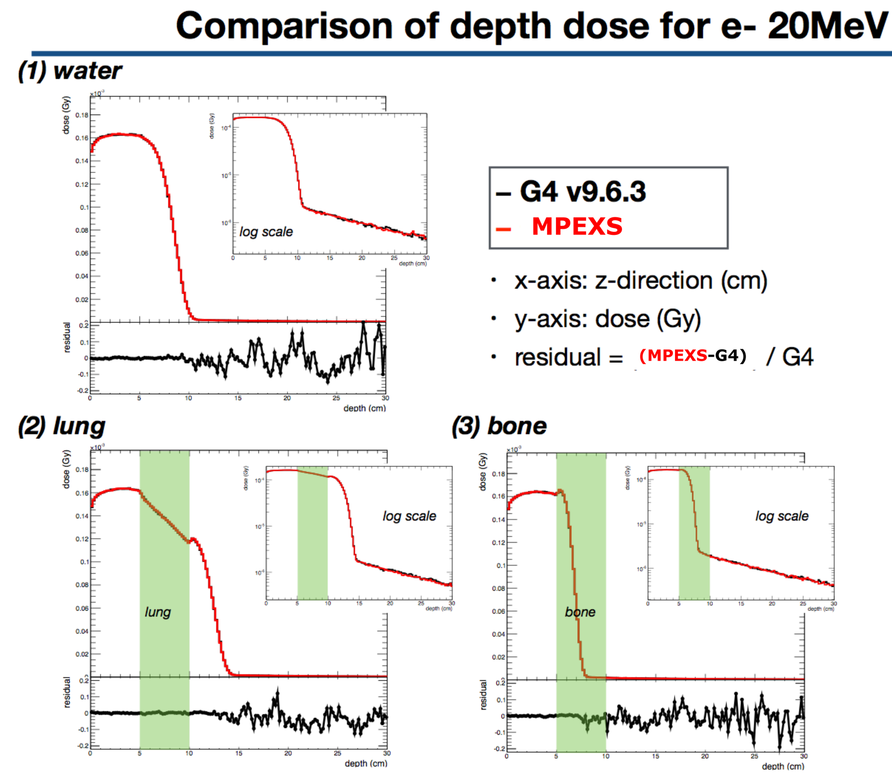


voxel size: 5mm x 5mm x 2mm

Beam particle and its initial kinetic energy:
- electron with 20MeV
- photon with 6MV Linac
- photon with 18MV Linac

	density
water	1.0 g/cm³
lung	0.26 g/cm³
bone	1.85 g/cm³
air	0.0012 g/cm³

Comparison of depth dose for e- 20MeV



Computation Time Performance

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

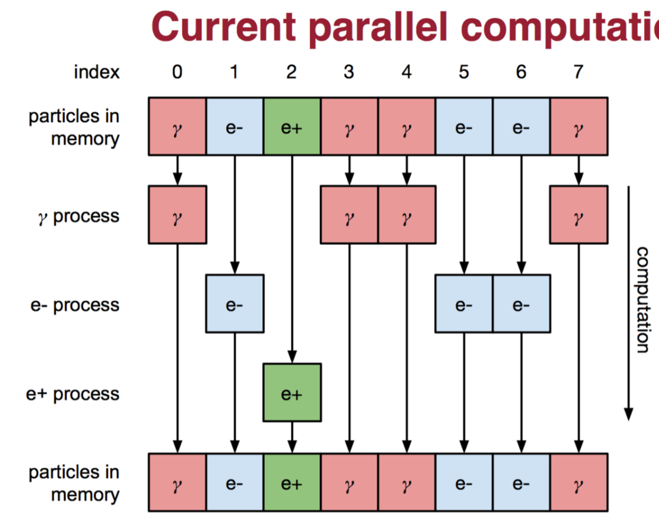
	e- beam with 20MeV		
	(1) water	(2) lung	(3) bone
G4 [msec/particle]	1.84	1.87	1.65
G4CU [msec/particle]	0.00881	0.00958	0.00885
× speedup factor (= G4 / G4CU)	***208***	***195***	***193***

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

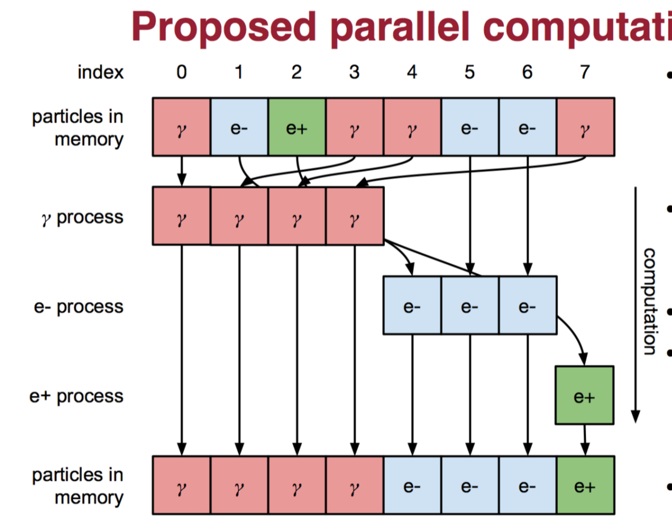
	γ beam with 6MV			γ beam with 18MV		
	(1) water	(2) lung	(3) bone	(1) water	(2) lung	(3) bone
G4 [msec/particle]	0.780	0.822	0.819	0.803	0.857	0.924
G4CU [msec/particle]	0.00336	0.00331	0.00341	0.00433	0.00425	0.00443
× speedup factor (= G4 / G4CU)	***232***	***248***	***240***	***185***	***201***	***208***

Current parallel computation pattern



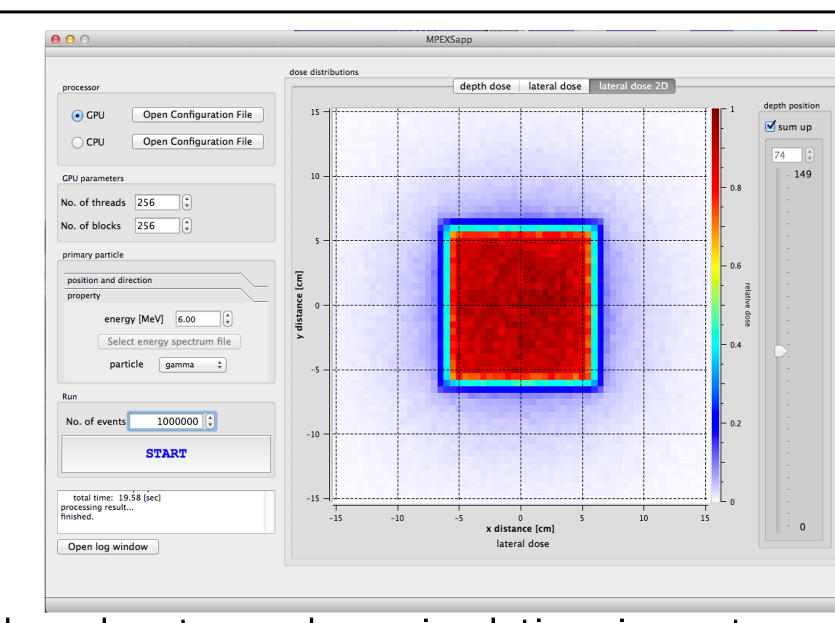
- each index corresponds to a **GPU** thread
- threads diverge based on particle kind for each process called
- thread divergence leads to underutilized **GPU** computational resources
- bad memory access pattern when reading and writing particles from/to global memory

Proposed parallel computation pattern



- sort is performed to group indices corresponding to particles of same kind
- processes called to operate on selected group of particles
- no thread divergence
- bad memory access pattern ***only*** when reading particles from global memory
- particle writes are coalesced

GUI



Qt based: setup and run simulation; inspect results

Conclusions

A CUDA implementation of Geant4 electromagnetic proceses has been created
  Low-energy e/gamma processes
  Voxelized geometry
Extension to Geant4-DNA physics (including chemical phase) available

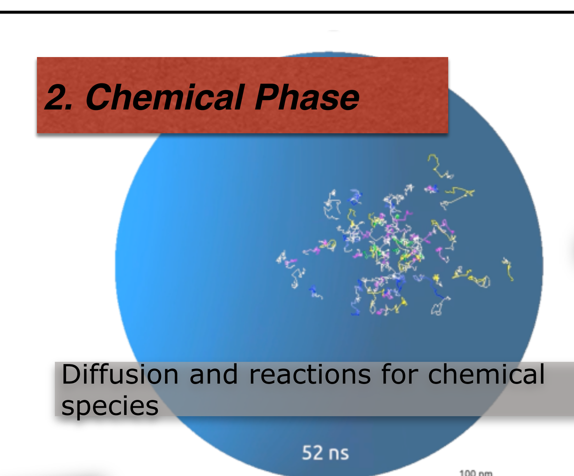
MPEXS:
  same physics quality as Geant4 simulations
  between x150-200 speedup with respect to Geant4

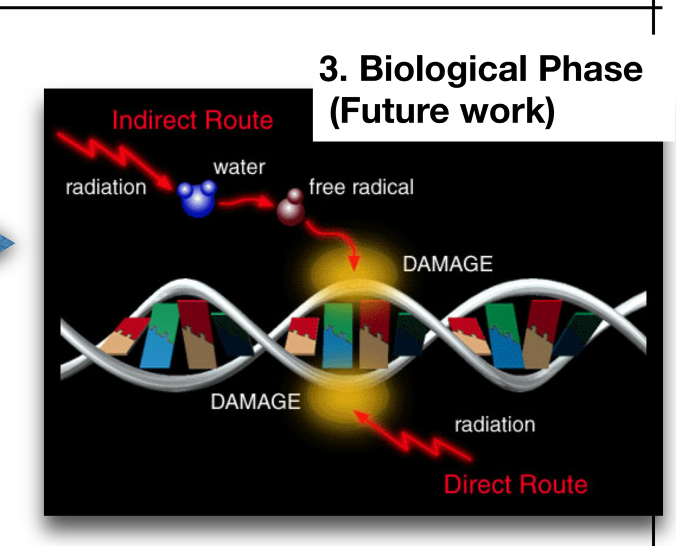
Referecnes

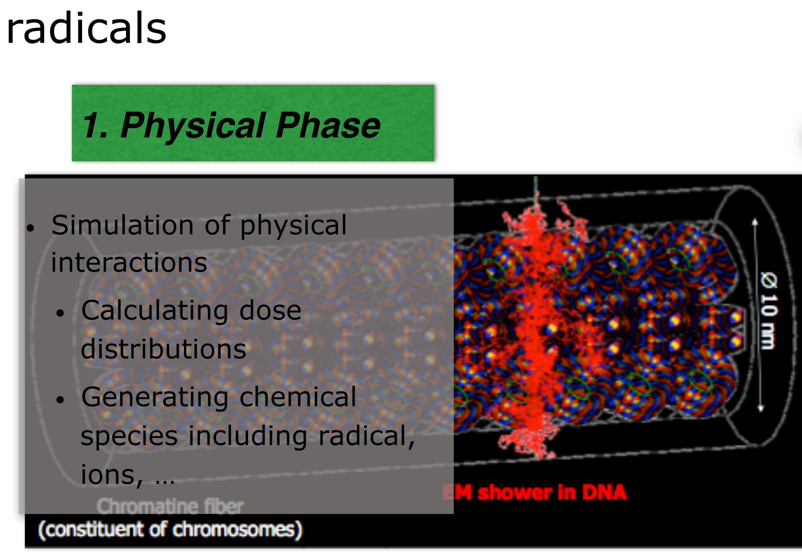
N. Henderson, et al. A CUDA Monte Carlo simulator for radiation therapy dosimetry based on Geant4. <https://dx.doi.org/10.1051/snamc/201404204>
K. Murakami, et al. Geant4 Based simulation of radiation dosimetry in CUDA. <https://dx.doi.org/10.1109/NSSMIC.2013.6829452>
S. Okada, et al. GPU Acceleration of Monte Carlo Simulation at the cellular and DNA levels. <https://dx.doi.org/10.1007/978-3-319-23024-5_29>
S. Agostinelli, et al. Geant4—a simulation toolkit. <https://dx.doi.org/10.1016/S0168-9002(03)01368-8>
M.A. Bernal, et al. Track structure modeling in liquid water: A review of the Geant4-DNA very low energy extension of the Geant4 Monte Carlo simulation toolkit. <https://dx.doi.org/10.1016/j.ejmp.2015.10.087>

Microdosimetry Simulation

Should improve computing performance
  Need days-weeks in CPU simulation
Based on Geant4 10.02 p01
EM Physics for lower energy range
  down to meV
Radiolysis of water
  Diffusion, chemical interaction for radicals







	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	126	347
Process time (Geant4-DNA 10.02 p01)	30.6 sec / event	5.01 sec / event	22.1 sec / event
Process time (MPEXS-DNA)	0.197 sec / event	0.0336 sec / event	0.115 sec / event
Speedup factor	***155x***	***149x***	***192x***

Physical Phase

Particles		Electrons	Protons	Hydrogen atoms	Helium atoms (He^{++}, He^{+}, He^{0})	Gamma
Physics Processes	Elastic scattering	9 eV - 10 keV *Uehara* 10 keV - 1 MeV *Champion*	100 eV - 1 MeV *Hoang*		100 eV - 10 MeV *Hoang*	—
	Excitation	10 eV - 10 keV *Emfietzoglou* 10 keV - 1 MeV *Born*	10 eV - 500 keV *Miller Green* 500 keV - 100 MeV *Born*	10 eV - 500 keV *Miller Green*	1 keV - 400 MeV *Miller Green*	—
	Charge change	—	100 eV - 10 MeV *Dingfelder*	100 eV - 10 MeV *Dingfelder*	1 keV - 400 MeV *Dingfelder*	—
	Ionization	10 eV - 10 keV *Emfietzoglou* 10 keV - 1 MeV *Born*	100 eV - 500 keV *Rudd* 500 keV - 100 MeV *Born*	100 eV - 100 MeV *Rudd*	1 keV - 400 MeV *Rudd*	—
	Vibrational excitation	2 - 100 eV *Michaud et al.*	—	—	—	—
	Disociative attachment	4 - 13 eV *Melton*	—	—	—	—
	Compton scattering	—	—	—	—	100 eV - 1 GeV *Livermore*
	Photoelectric effect	—	—	—	—	100 eV - 1 GeV *Livermore*
	Gamma Conversion	—	—	—	—	100 eV - 1 GeV *Livermore*
	Rayleigh Scattering	—	—	—	—	100 eV - 1 GeV *Livermore*

Deexcitation

Chemical Phase

Electronic state	Process	Dissociation channel	Fraction (%)
Ionization state	Dissociative decay	$H_3O^+ + \bullet OH$	100
Excitation state: A1B1	Dissociative decay	$\bullet OH + H\bullet$	65
	Relaxation	$H_2O + \Delta E$	35
Excitation state: B1A1	Auto-ionization	$H_3O^+ + \bullet OH + e^-_{aq}$	55
	Dissociative decay	$\bullet OH + \bullet OH + H_2$	15
	Relaxation	$H_2O + \Delta E$	30
Excitation state: Rydberg, diffusion bands	Auto-ionization	$H_3O^+ + \bullet OH + e^-_{aq}$	50
	Relaxation	$H_2O + \Delta E$	50
Dissociative attachment: H_2O^-	Dissociative decay	$\bullet OH + OH^- + H_2$	100