The Geant4-DNA project at the Physics-Biology frontier

JFY2015(BIO_02) reports and
JFY2016(APP_01) plan

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2016 Project members

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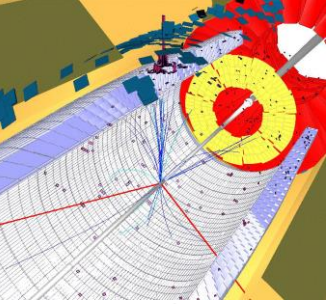
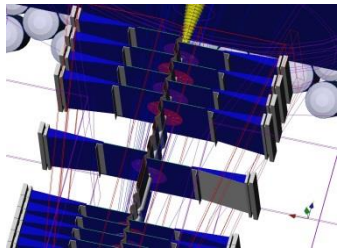
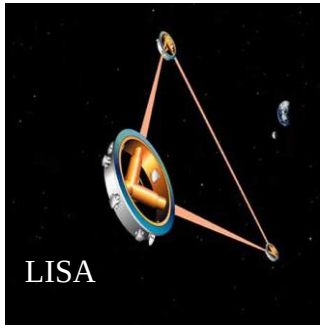
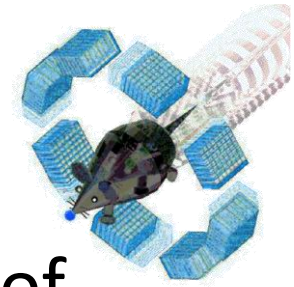


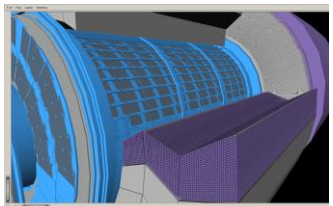


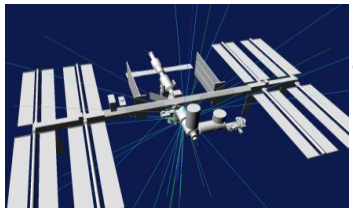
What is Geant4?

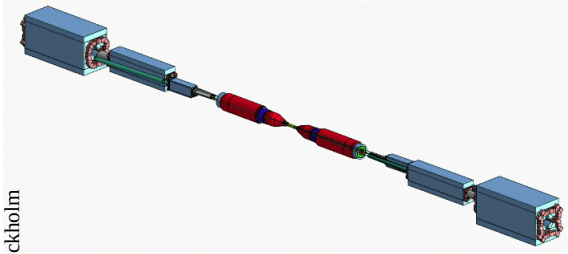
- Geant4 is a software toolkit for simulating interactions between particles and matter
  - Designed based on Japanese efforts
- Developed and maintained by Geant4 Collaboration
  - KEK, SLAC, CERN, FNAL, ESA…….
- Very widely used in many fields, such as HEP, Nuclear Physics, Space, Medicine, Nuclear Engineering and etc.
- All of the ongoing HEP experiments are users of Geant4

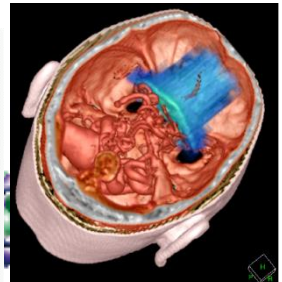












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ckholm

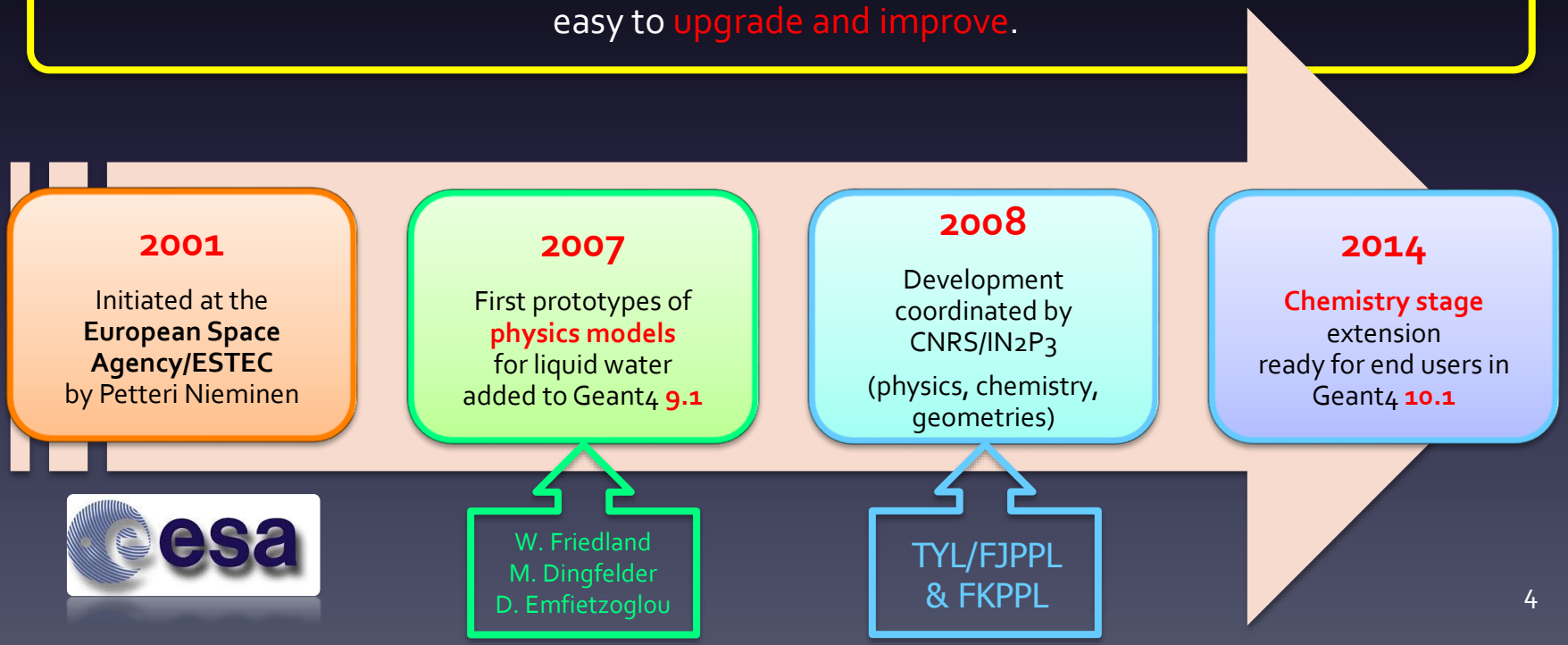
See Int. J. Model. Simul. Sci. Comput. 1 (2010) 157-178 (link)

The Geant4-DNA project

Main objective

Extend the general purpose Geant4 Monte Carlo toolkit for the simulation of interactions of radiation with biological systems at the cellular and DNA level in order to predict early DNA damage in the context of manned space exploration missions (« bottom-up » approach).

Designed to be developed and delivered in a FREE software spirit under Geant4 license, easy to upgrade and improve.



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The Geant4-DNA project

- The code is fully included in Geant4
- It is an independent sub-category of the electromagnetic physics category of Geant4: $G4INSTALL/source/processes/electromagnetic/dna
- An interdisciplinary activity of the Geant4 « low energy electromagnetic physics » working group
- Both are coordinated by CNRS/IN2P3 since 2008
- Integration in Geant4 enables the use of Geant4-DNA physics from inside GATE (2014) and TOPAS (2015)

http://www.topasmc.org

Contact: Joseph Perl @ SLAC

http://www.opengatecollaboration.org

Contact: Irène Buvat @ CNRS

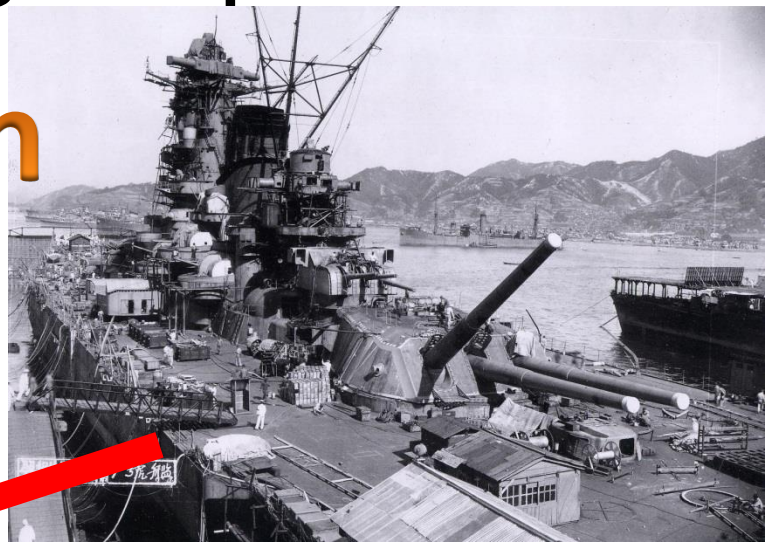
Background of the research

- Parallelism was not taken into account when Geant4 was designed
  - Geant4 is 21 years old
- Emerging new processor architectures require parallelism for efficient resource usage
  - Many-core CPU
  - Large-scale HPC centers(so called super computer centers)
  - GPGPU
- Geant4-DNA is too slow to simulate more complex cases
  - Needs to handle interactions between particles
  - More than Physics processes, e.g. Chemical processes

Paradigm change in processors

Opteron

Xeon



Right decision on the strategy has to be made to win the battle

GPGPU

or

Xeon-Phi

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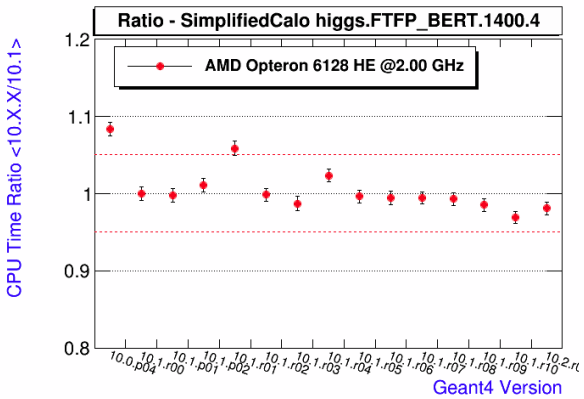
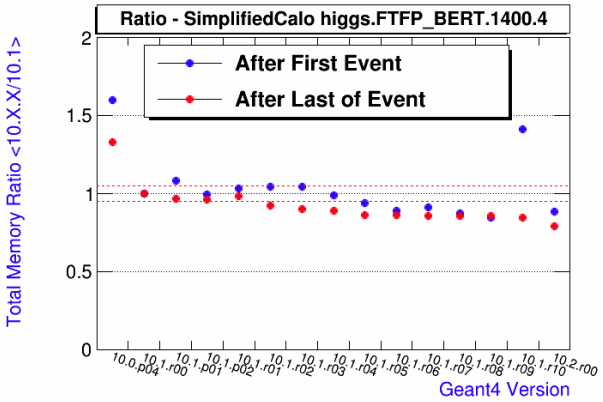
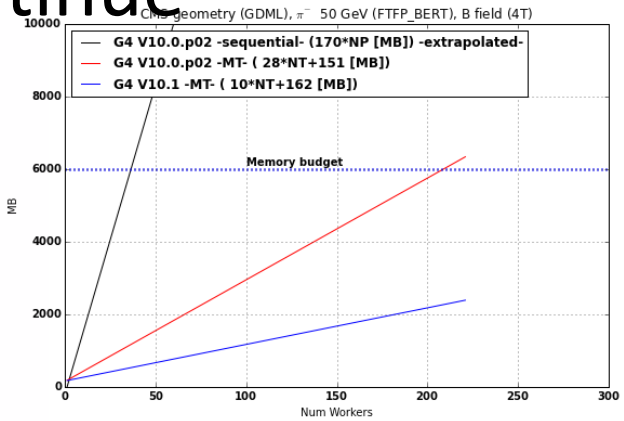
Geant4-MT

- Since version 10.0, Geant4 is multi threaded
  - Share possible information/data among threads to reduce total memory usage
- Runs even on Xeon-Phi more efficiently
- Performance optimizations continue







Highlights in JFY2015

- **MPEXS-DNA: Porting of Geant4-DNA to GPGPU**
  - Up to 280 times faster on GPU than CPU
    - More speedup than the last year
  - Details follows
- **Organization of the 11th Geant4 Space User's Workshop**
  - 11th Geant4 Space User's Workshop in Hiroshima, Japan, on August 26-28th, 2015 (http://nsl.iis.it-hiroshima.ac.jp/geant4/).
  - Geant4-DNA tutorial on August 23-24, 2015 at the same location, and attracted 26 participants, mainly from Japan (https://indico.esa.int/indico/event/82/).
- **Development of Geant4-DNA**
  - Previous Sebastien's talk
  - New accurate alternative Geant4-DNA models were developed in order to simulate the transport of electrons in liquid water, based on the dielectric response function theory. These models include elastic scattering, electronic excitation and ionization.

MPEXS

- Massive Parallel Electro X-ray Simulator *aka* Massive Parallel simulator in EXa Scale
  - The state of the arts radiation transport code for GPU
  - The algorithms and data necessary are taken from Geant4
    - Reproduces the same results completely
  - Not a machine translation
  - Current functionality is limited for EM in water (with different densities)
    - Gradually being enhanced toward HEP detector simulation
- Joint project among SLAC, ICME at Stanford University and KEK
- Funded by *The Japan/US Cooperation Program in the Field of High Energy Physics* and JSPS partly
- Not an open source project

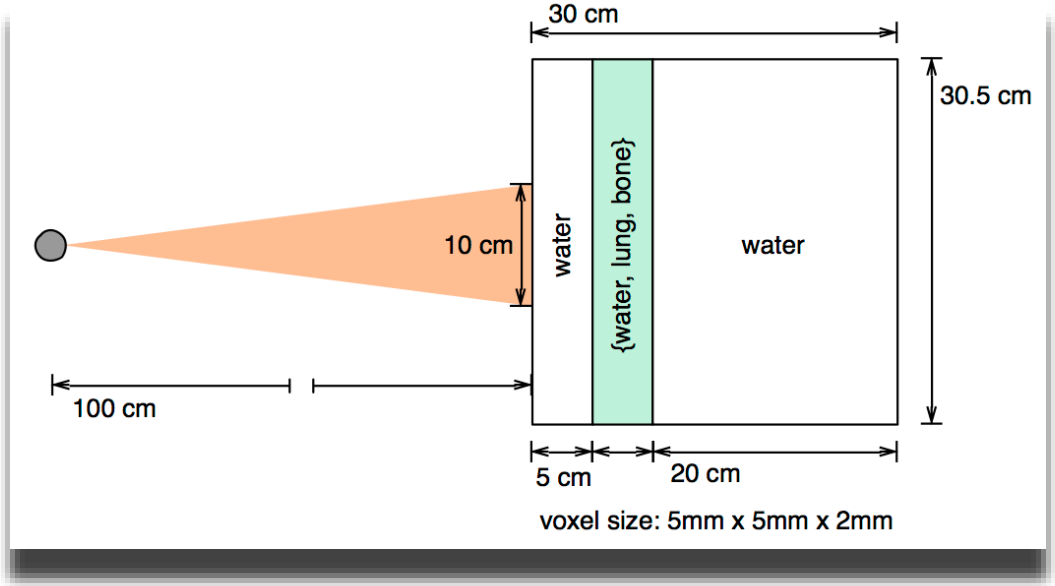
MPEXS Benchmarking

- Phantom size: 30.5 x 30.5 x 30 cm
- Voxel size: 5 x 5 x 2 mm
- Field size: 10 cm^2
- Source surface distance: 100 cm
- Slab materials (30.5 x 30.5 x 5 cm):

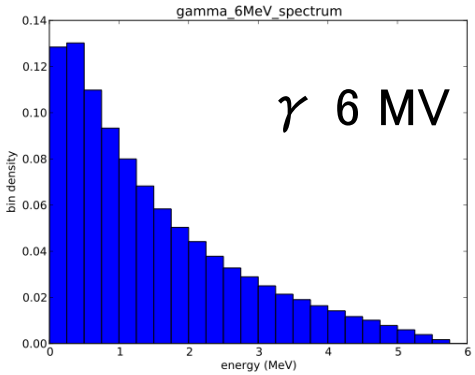
	Density
Water	1.0 g/cm^3
Lung	0.26 g/cm^3
Bone	1.85 g/cm^3
Air	0.0012 g/cm^3

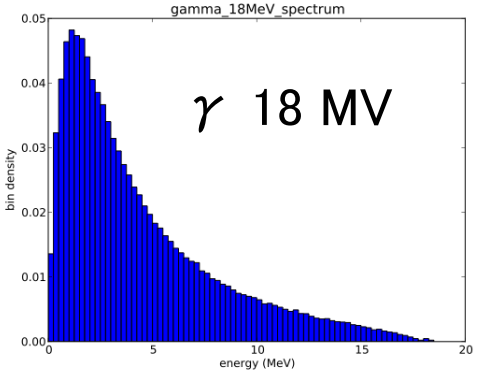
- Beam particles:
  - Electrons (20 MeV)
  - Photons (6, 18 MV)

Simulated geometry setup



Energy spectrums for photons





MPEXS Performance

Up to 250x speedup against single-core CPU

	e- beam with 20MeV		
	Water	Lung	Bone
Geant4 (CPU) [msec/particle]	1.84	1.87	1.65
MPEXS (GPU) [msec/particle]	8.81×10^{-3}	9.58×10^{-3}	8.85×10^{-3}
× speedup factor (= G4 / MPEXS)	*208*	*195*	*193*

	γ beam with 18MV					
	Water	Lung	Bone	Water	Lung	Bone
Geant4 (CPU) [msec/particle]	0.780	0.822	0.819	0.803	0.857	0.924
MPEXS (GPU) [msec/particle]	3.36×10^{-3}	3.31×10^{-3}	3.41×10^{-3}	4.33×10^{-3}	4.25×10^{-3}	4.43×10^{-3}
× speedup factor (= G4 / MPEXS)	*232*	*248*	*240*	*185*	*201*	*208*

- GPU
  - Tesla K20c (*Kepler architecture*)
  - 2,496 CUDA cores, 796 MHz
  - 4096 blocks x 128 threads /block
- CPU
  - Intel Xeon E5-2643 v2 3.50 GHz
- Process time (e- 20 MeV, 50M, water)

~ 25 hr. (single-core CPU) → ~ 7 min. (GPU)

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Cost comparisons (Geant4 vs MPEXS)

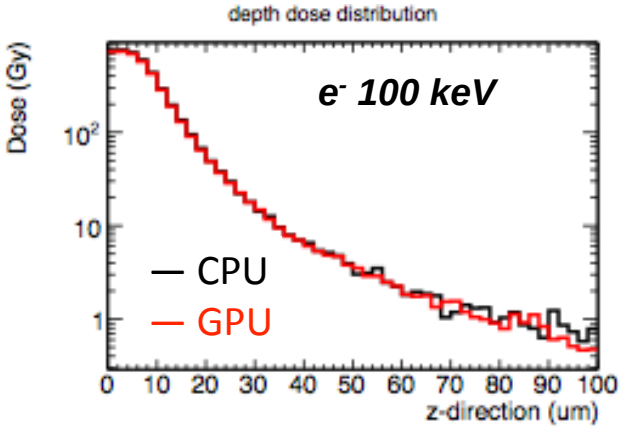
- 1 XCE = One Xeon Core Equivalent Computing power measured by our benchmark software (The same set up with the MPEXS benchmark)
- Rack mount servers with different options
  - Xeon® E5-2690 v3 x 2 (12corex2) 2 socket server (Geant4)
    - ¥1,544,400 /24core 24XCE 77K JPY or 640 USD/XCE
  - Xeon® E5-4650 v3 x 4 (12corex4) 4 socket server (Geant4)
    - ¥5,184,000/48core 48XCE 108K JPY or 900 USD/XCE
  - Xeon E5-2690 v3 x 2 +Xeon Phi 3120P x 4 (Geant4)
    - Computing power of 3120P is equivalent to Xeon 8core
    - ¥3,121,200 56XCE 56K JPY or 470 USD/XCE
  - Xeon E5-2690 v3 x 2 + NVIDIA K40x4 (MPEXS)
    - Computing power of K40 is equivalent to Xeon 250 core
    - ¥4,773,600 1024XCE 4600 JPY or 38 USD/XCE
- Improvements on software results large reduction of hardware procurement costs
- Xeon Phi is much cost effective than Xeon CPU's
- Comparison with GPU is not yet fair enough (MPEXS is a subset of Geant4)

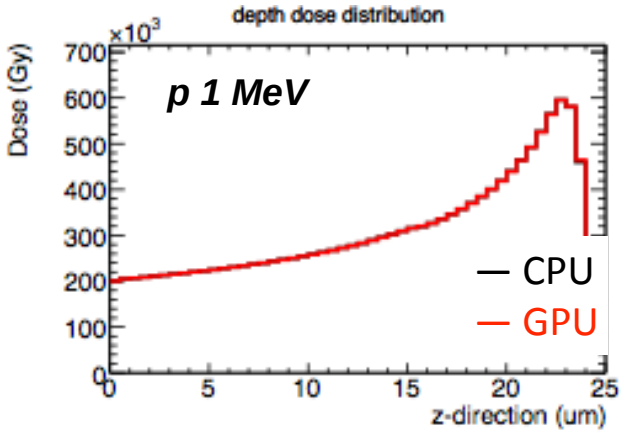
MPEXS-DNA

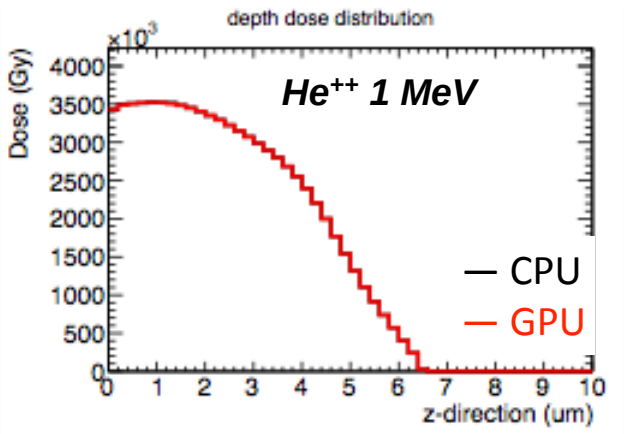
- Based on MPEXS
- Rewrite Geant4-DNA(C++) in CUDA
  - All of functionality in Geant4 10.2 has been available in CUDA
  - Also reproduces the original results completely
  - Corrections and improvements to implementation of Geant4-DNA
- Collaboration between CENBG and Japanese team(KEK and Universities)

Physics Performance for DNA Physics

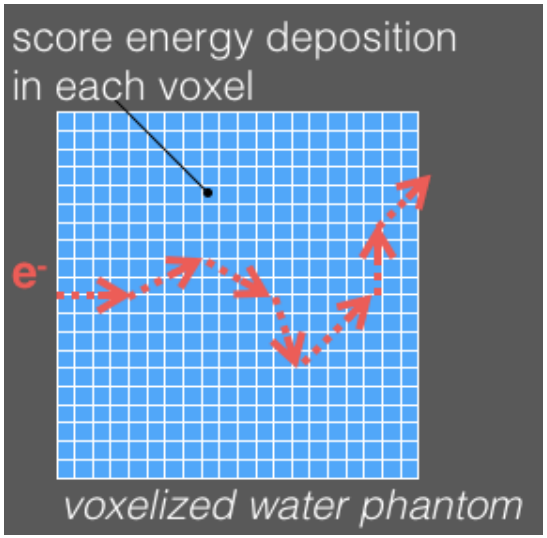
Depth dose curves (CPU vs GPU)







Simulation model



incident particle	initial energy	phantom size	# of voxel cells (voxel size)
e-	100 keV	102 x 102 x 100 um	51 x 51 x 50 (2 x 2 x 2 um)
p	1 MeV	25.5 x 25.5 x 25 um	51 x 51 x 50 (0.5 x 0.5 x 0.5 um)
He++	1 MeV	10.2 x 10.2 x 10 um	51 x 51 x 50 (0.2 x 0.2 x 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	CUDA		Geant4-DNA	speedup factor (=G4/CUDA)
			Total thread numbers (N_{blk} x $N_{thr/blk}$)	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)	4.07×10^{-2}	10.5	***258***
	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)

MPEXS plans(outside of this project)

- Realistic number of materials
- More particle species
- More physics interactions
  - Neutrons and protons
- CAD interface
  - Tessellated solids and tetrahedra
- Applications
  - Calorimeter simulation
  - Medical and etc.

SLAC NATIONAL ACCELERATOR LABORATORY

ICME INSTITUTE for COMPUTATIONAL & MATHEMATICAL ENGINEERING at STANFORD UNIVERSITY

CENBG

2016 MPEXS-DNA plans

- **Continuation of the porting of Geant4-DNA to GPU**
  - Catch up the latest Geant4-DNA implementation
  - Further performance optimizations
  - Benchmark test at CC-IN2P3 in conjunction with COMP_3
    - 20xK80 to be deployed
- **Evaluation of Geant4-DNA accuracy for radiolysis simulation**
  - The effect of physics models on radiolysis (such as effect on radiochemical G yields) will be simulated
- **Application of Geant4-DNA to novel radiotherapy approach**
  - Geant4-DNA new models dedicated to the simulation of radiosensitization effects using nanoparticles internalized in biological cells will be implemented
    - Gold nanoparticle therapy

JFY2015 Publications

- **GPU Acceleration of Monte Carlo Simulation at the Cellular and DNA Levels**, S. Okada, K. Murakami, K. Amako, T. Sasaki, S. Incerti, M. Karamitros, N. Henderson, M. Gerritsen, M. Asai, A. Dotti, Smart Innovation, Systems and Technologies 45 (2016) 323-332

- **Track structure modeling in liquid water: A review of the Geant4-DNA very low energy extension of the Geant4 Monte Carlo simulation toolkit**, M. A. Bernal, M. C. Bordage, J. M. C. Brown, M. Davídková, E. Delage, Z. El Bitar, S. A. Enger, Z. Francis, S. Guatelli, V. N. Ivanchenko, M. Karamitros, I. Kyriakou, L. Maigne, S. Meylan, K. Murakami, S. Okada, H. Payno, Y. Perrot, I. Petrovic, Q.T. Pham, A. Ristic-Fira, T. Sasaki, V. Štěpán, H. N. Tran, C. Villagrasa, S. Incerti, Phys. Medica 31 (2015) 861-874

Summary

- Geant4-DNA has been ported on CUDA/GPU and named as MPEXS-DNA
  - Speedup factor of up to 280 has been achieved against CPU
    - ~ 53 hr. (single-core CPU) -> ~ 12 min. (GPU)
  - Simulated results are agreed very well
  - Further performance optimizations will be done
    - Benchmark tests will be done at CC-IN2P3 with 20xK80
- Gold nanoparticle therapy will be simulated on CUDA/GPU