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OpenDNA
An OpenCL-based Monte Carlo simulation code

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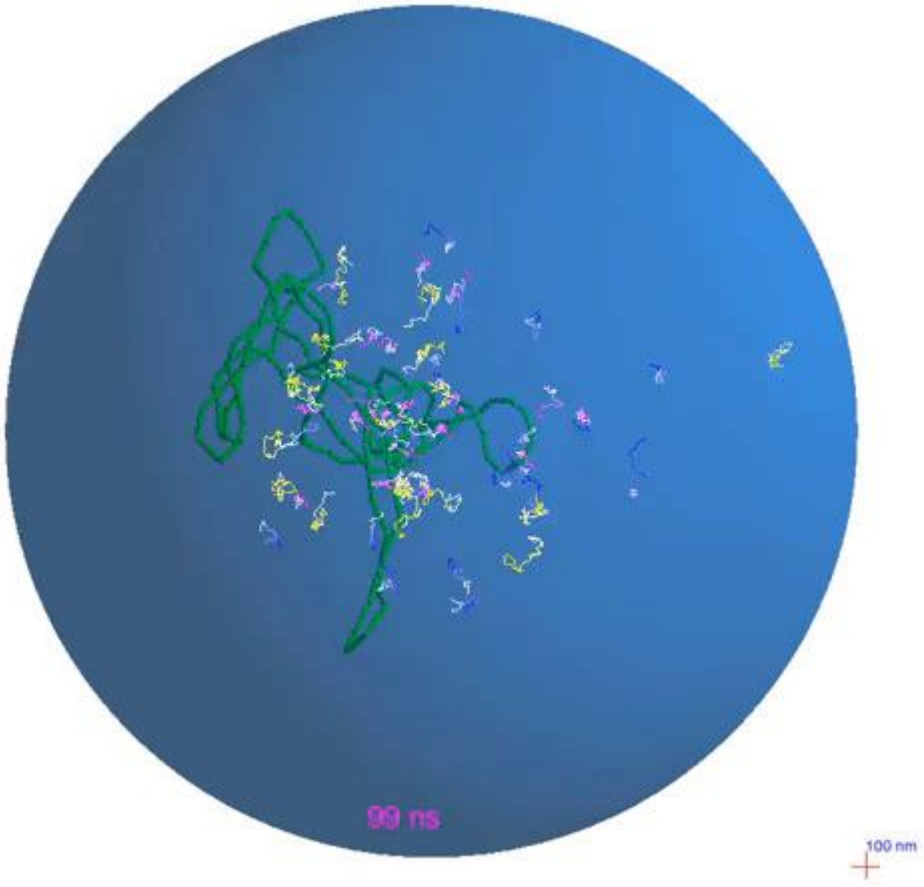
Outline

- Background & introductory
- Benchmarking
  - Proton simulation
  - Alpha particle simulation
  - Radial energy distribution
- Summary

Introduction: Geant4-DNA

- An Analogue MC Code
  - Microdosimetry simulation

- Physical process
- Chemical species
- Spatial & temporal resolutions

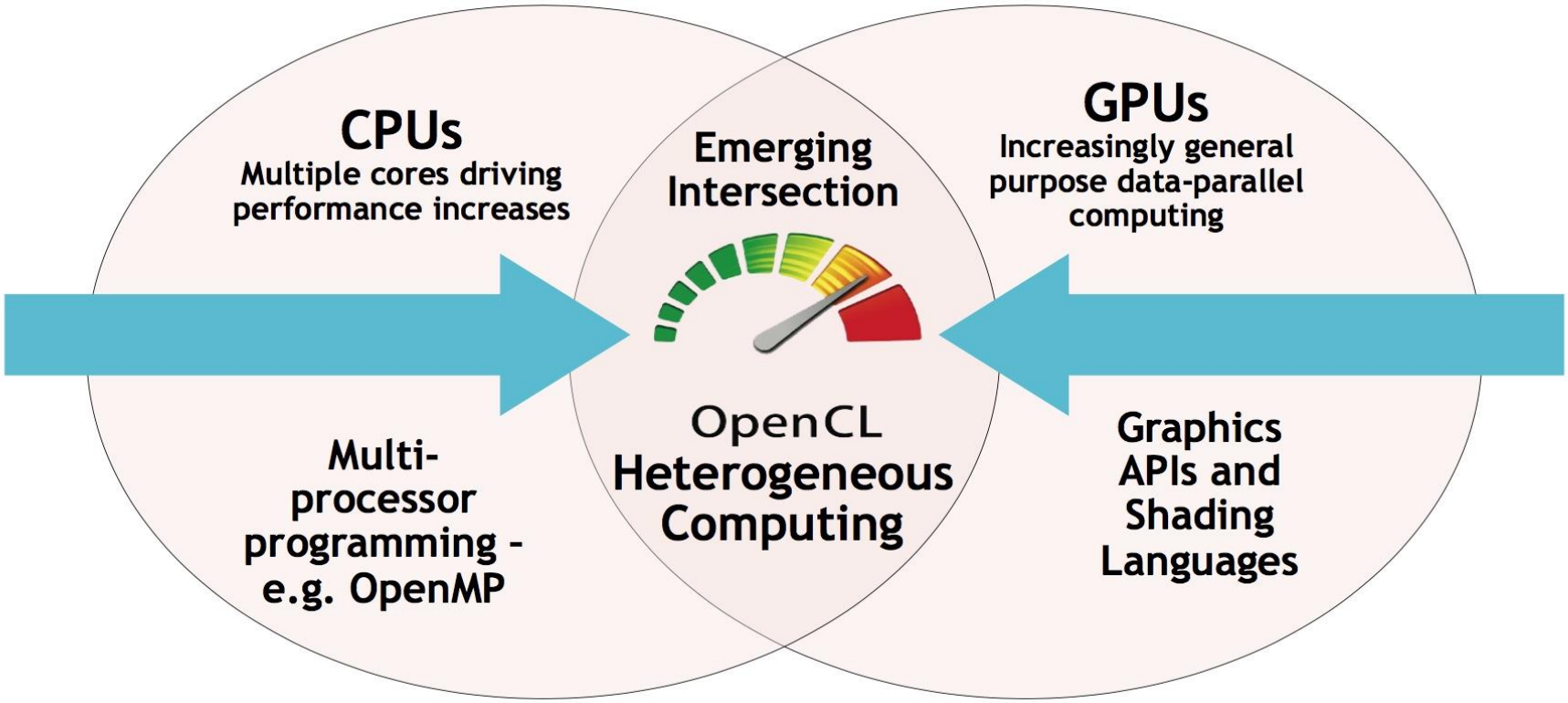


Ref: http://geant4-dna.org

Introduction: OpenDNA

- What is OpenDNA
  - OpenDNA is an OpenCL-based track structure simulation code based on Geant4-DNA's xs data which runs on multiple devices and heterogeneous compute environment.
- And why & how?
  - To create a fast yet portable track structure simulation code
  - **OpenCL** offers both high performance and portability

Introduction: OpenCL

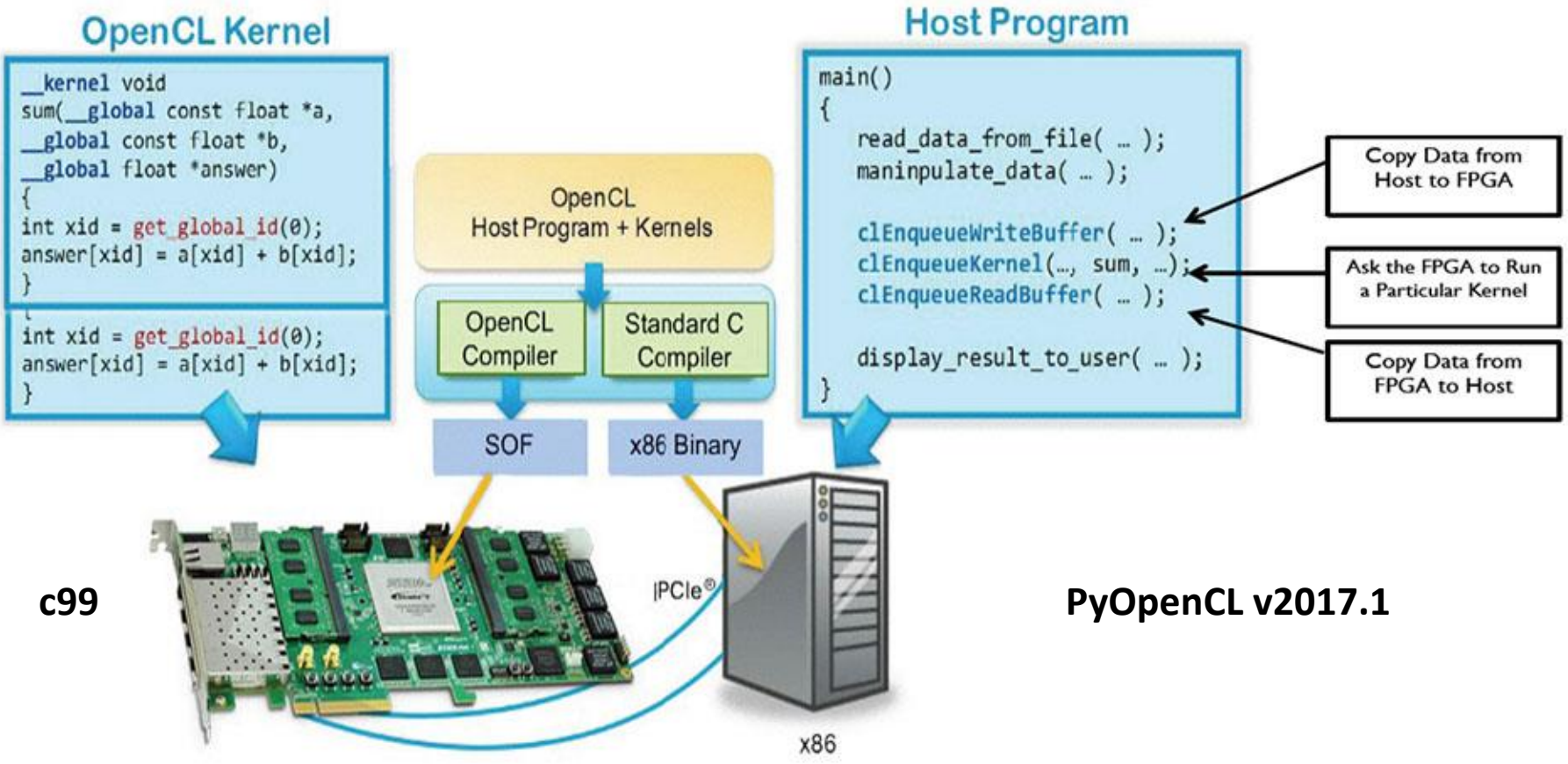


OpenCL – Open Computing Language

Open, royalty-free standard for portable, parallel programming of heterogeneous parallel computing CPUs, GPUs, and other processors

Introduction: OpenCL

Introduction: OpenCL



c99

PyOpenCL v2017.1

M&M – Electron

Models: e- (electron)

Electron process	Model used	Min Energy	Max Energy
Elastic scattering	Screened Rutherford Model	9 eV	1 MeV
Excitation	Emfieltzoglou, Born Models	9 eV	1 MeV
Ionisation	Emfieltzoglou, Born Models	11 eV	1 MeV
Vibration excitation is not considered.			

M&M – Proton

Models: P (proton, H+), H (hydrogen)

Common processes	Model used	Min Energy	Max Energy
Nuclear elastic	Screened Rutherford Model	100 eV	1 MeV
Excitation	Miller Green Model	10 eV	100 MeV
Ionisation	Born, Rudd Models	100 eV*	100 MeV
Particle-dependant process	Model used		
Charge increase, H	Dingfelder Model	1 keV	100 MeV
Charge decrease, P	Dingfelder Model	1 keV	100 MeV

M&M - Alpha particle

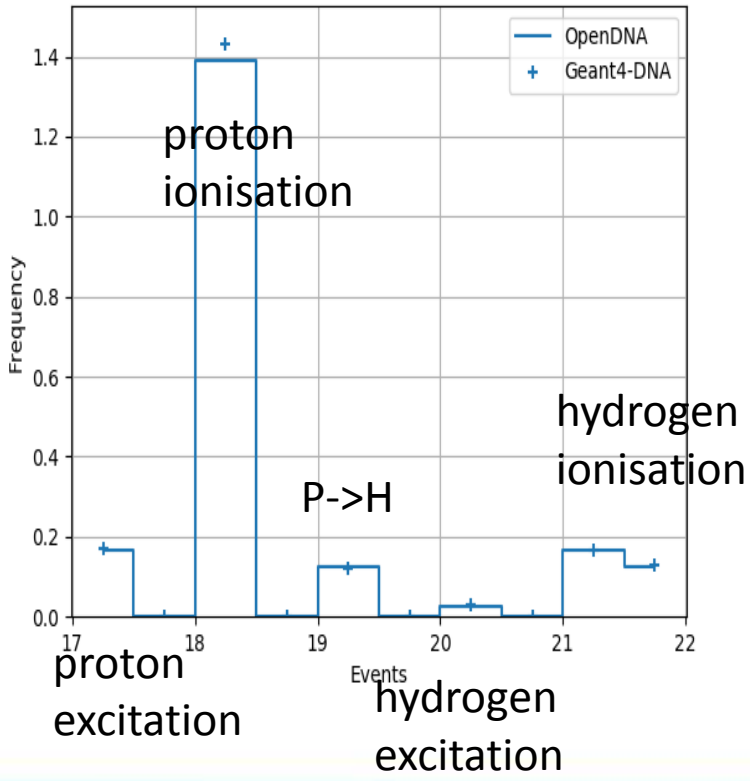
Models: Alpha particle (He++), He+, He

Common processes	Model used	Min Energy	Max Energy
Nuclear elastic	Screened Rutherford Model	100 eV	1 MeV
Excitation	Miller Green Model	1 keV	400 MeV
Ionisation	Rudd Model	1 keV*	400 MeV
Particle-dependant process	Model used		
Charge increase, He, He+	Dingfelder Model	1 keV	400 MeV
Charge decrease, He+, He++	Dingfelder Model	1 keV	400 MeV

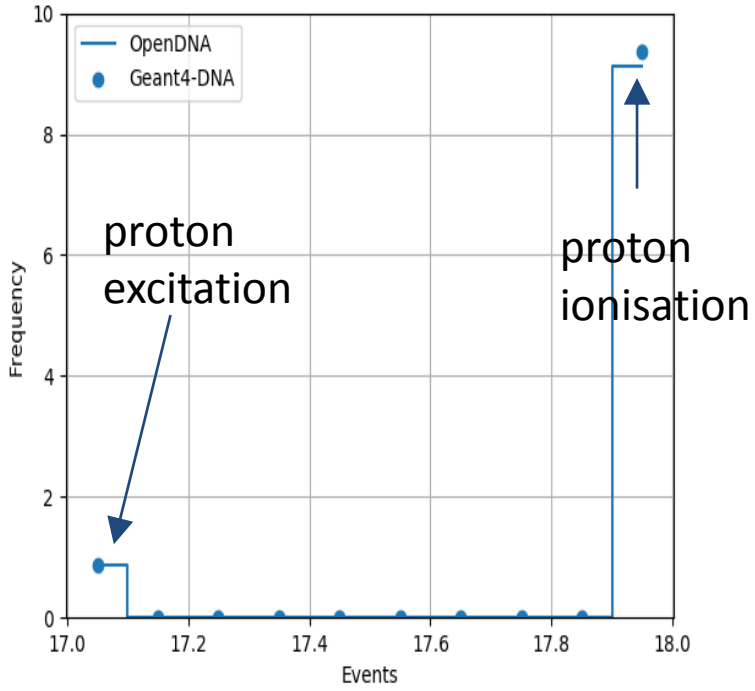
Results - proton

1.Events

E = 1 MeV



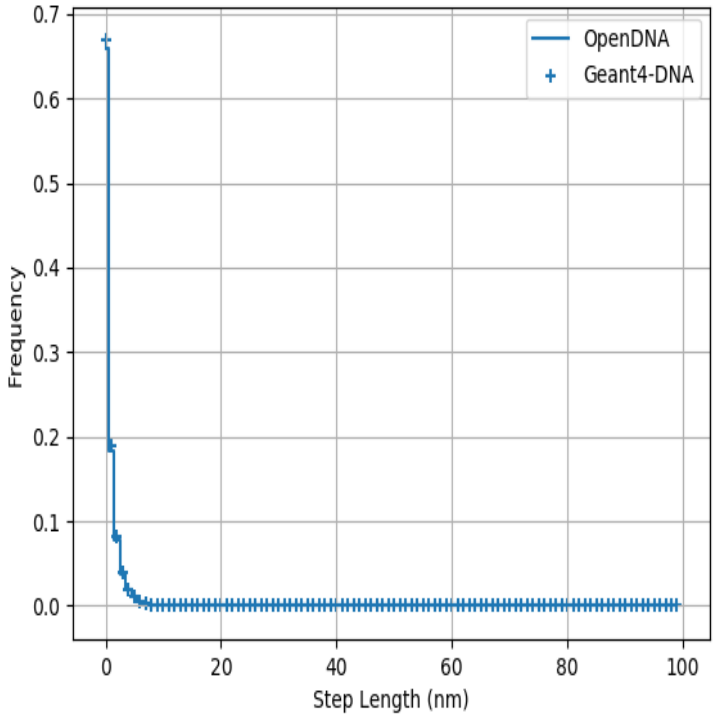
E = 10 MeV



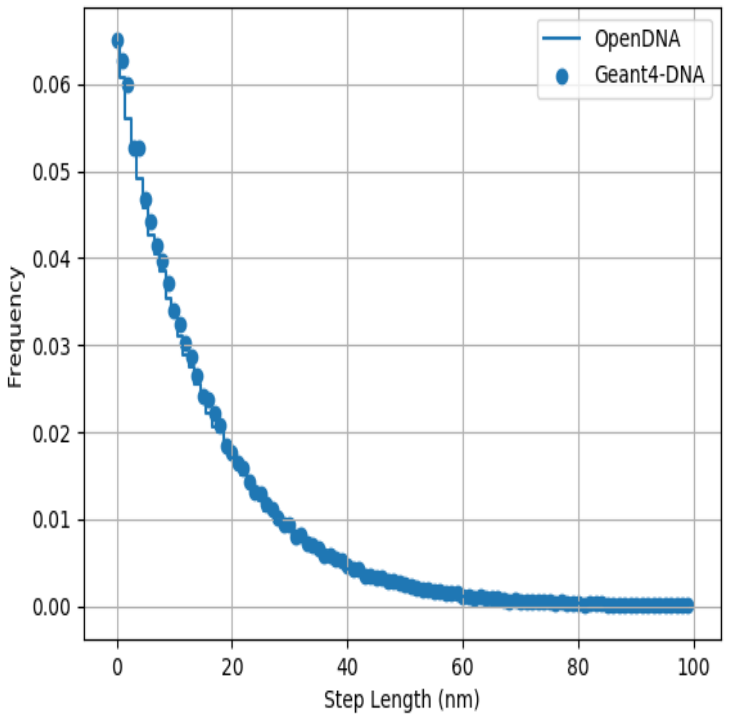
Results - proton

2. Step length

E = 1 MeV



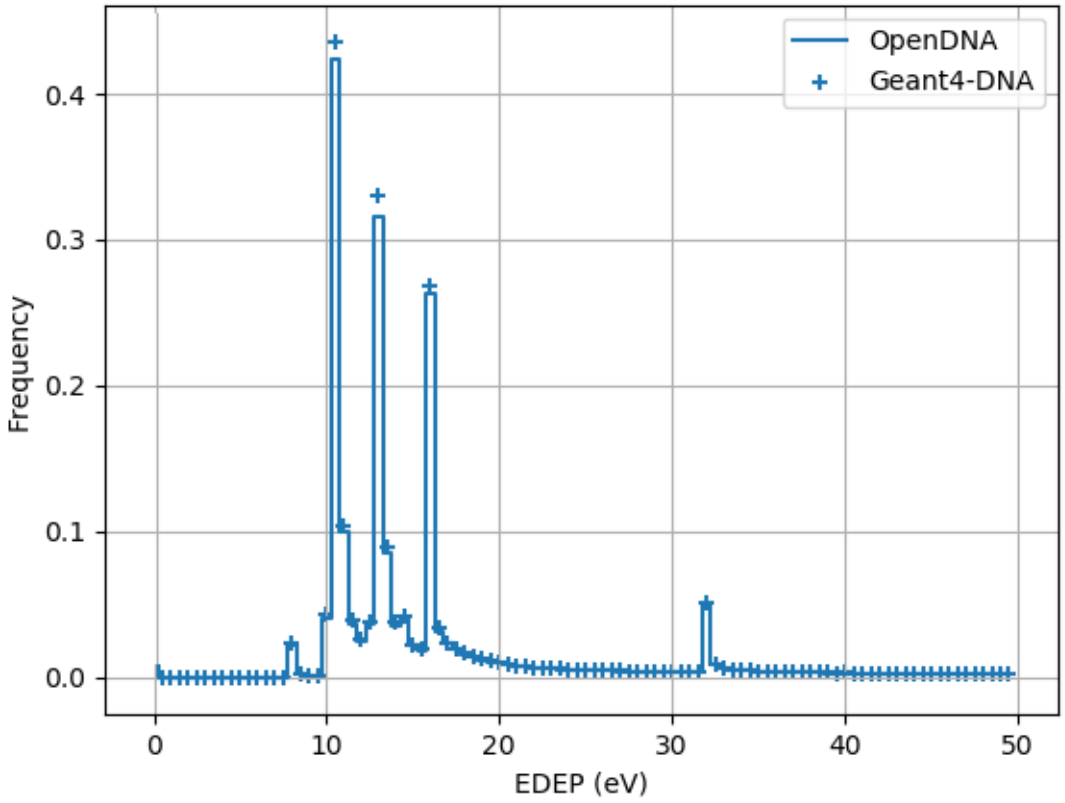
E = 10 MeV



Results - proton

3. Edep

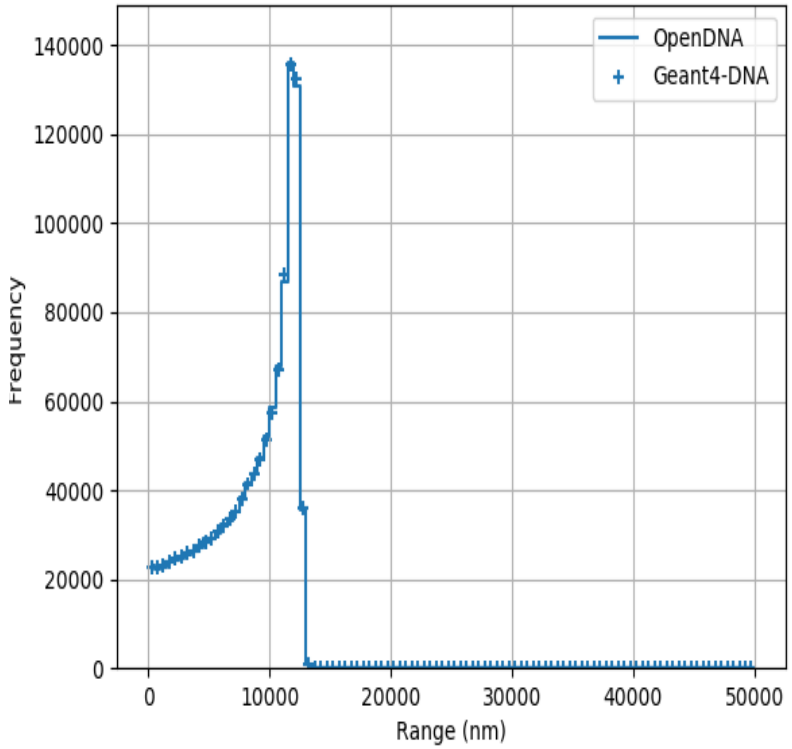
E = 1 MeV



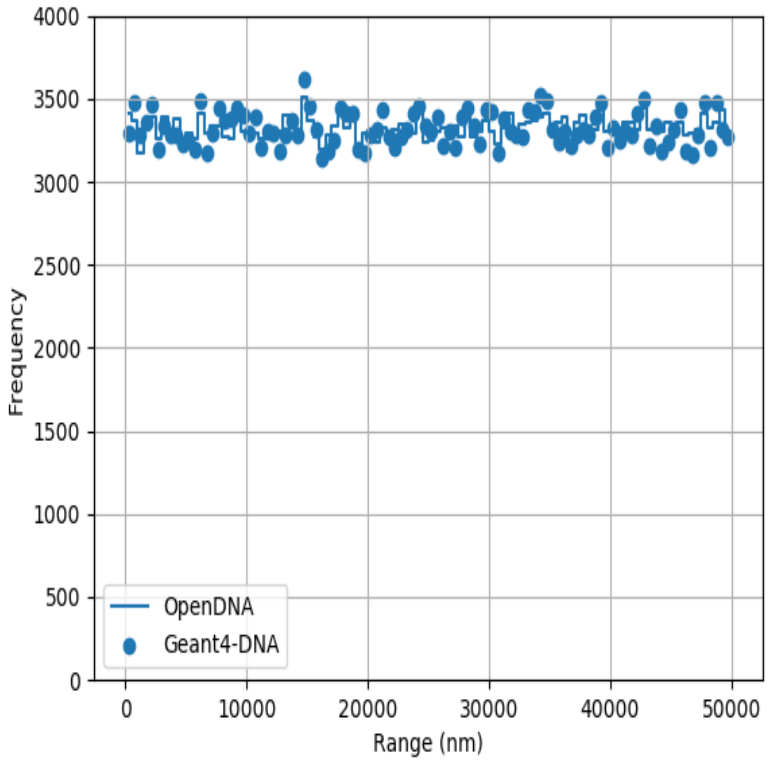
Results - proton

4. Range

E = 1 MeV



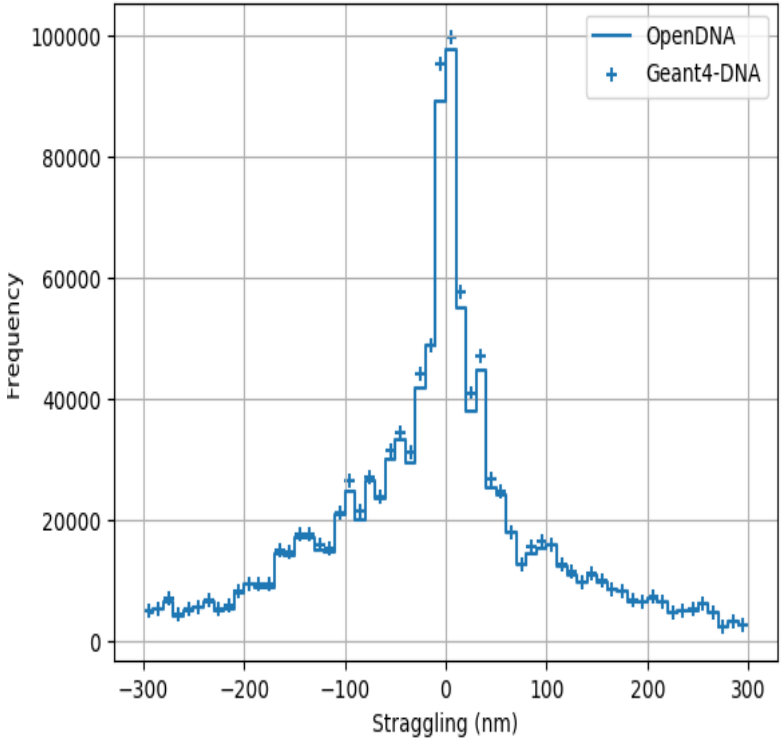
E = 10 MeV



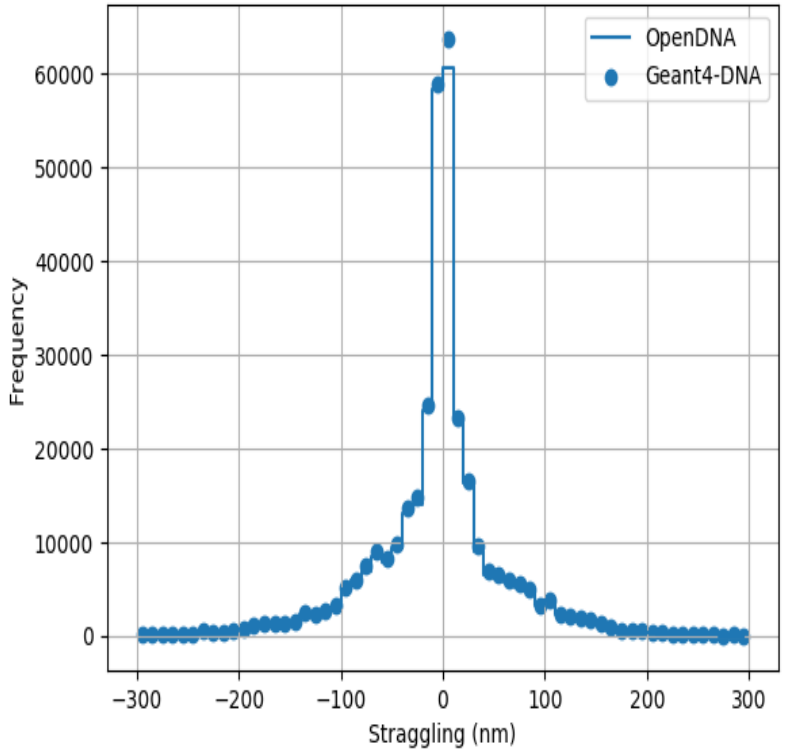
Results - proton

4. Straggling

E = 1 MeV

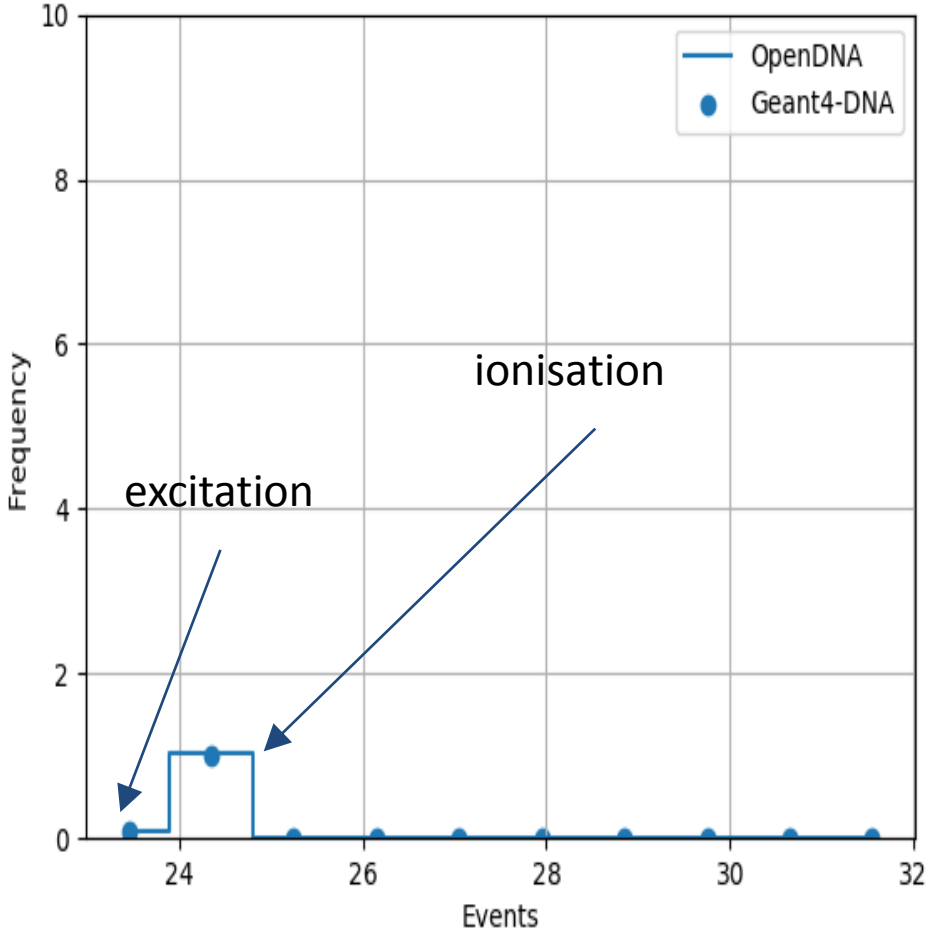


E = 10 MeV



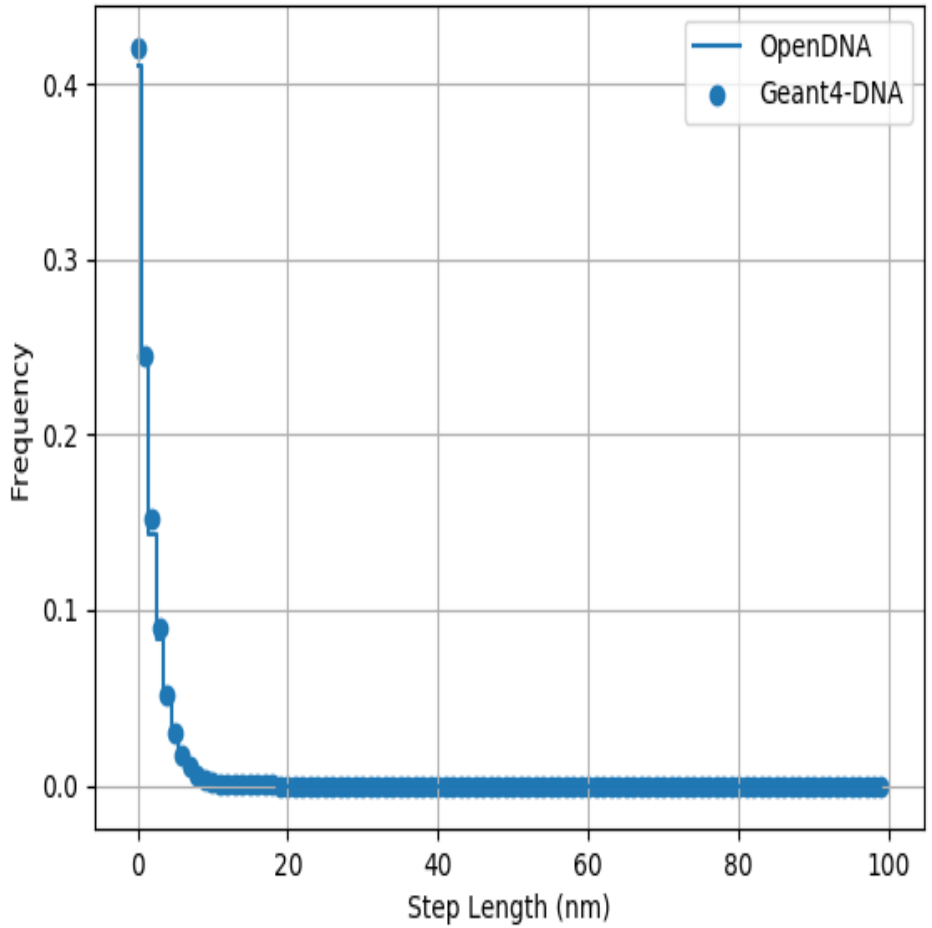
Results - 20 Mev alpha particle

1.Events



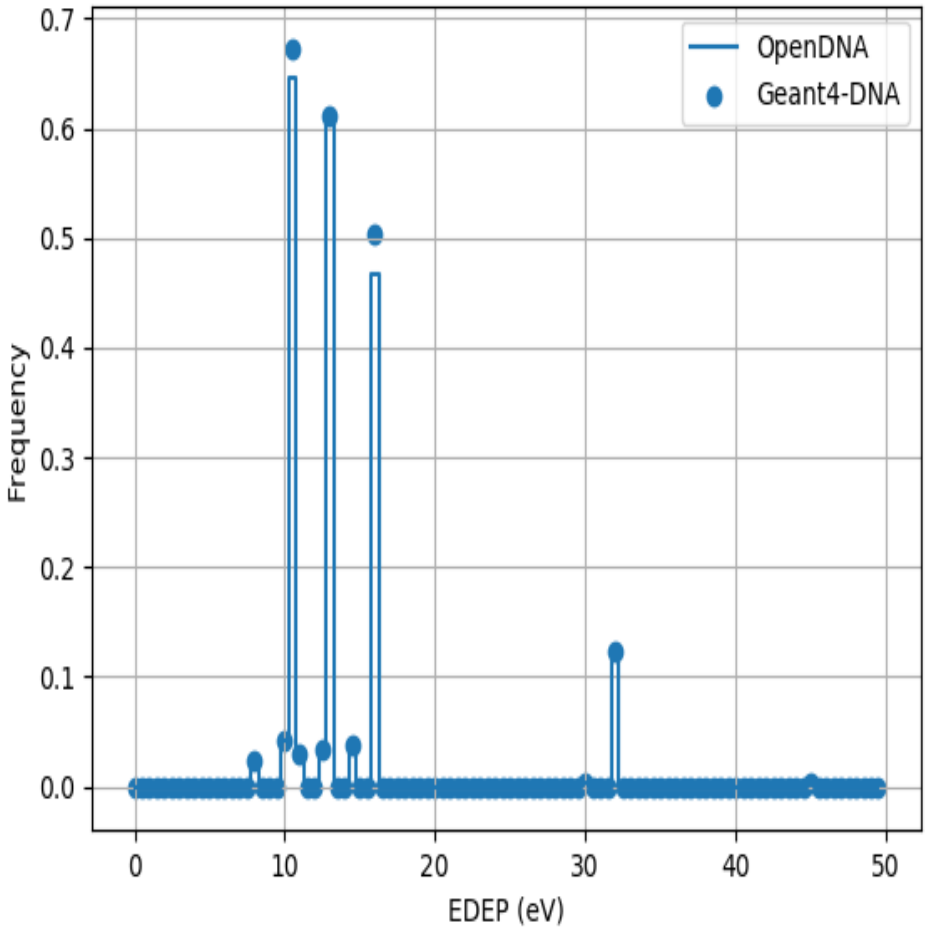
Results - 20 Mev alpha particle

2. Step length



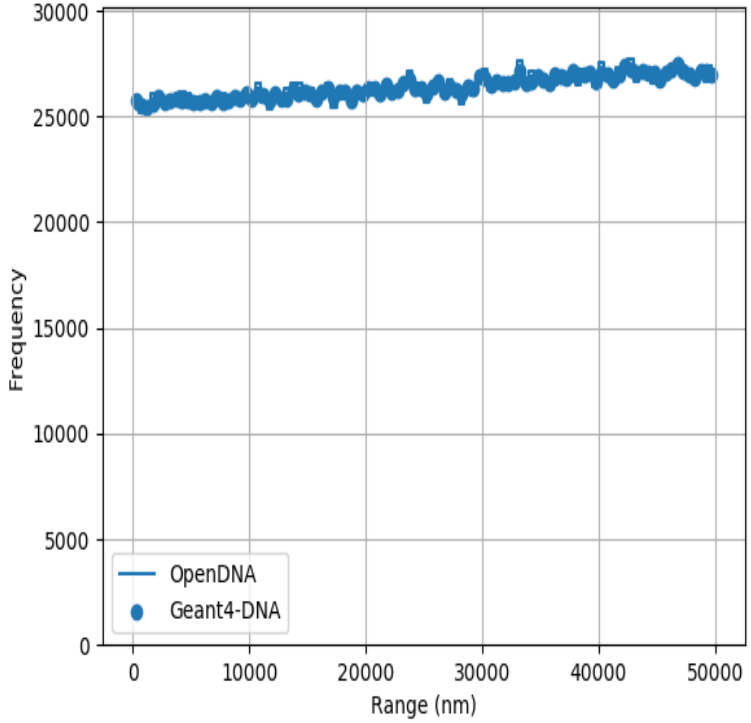
Results - 20 Mev alpha particle

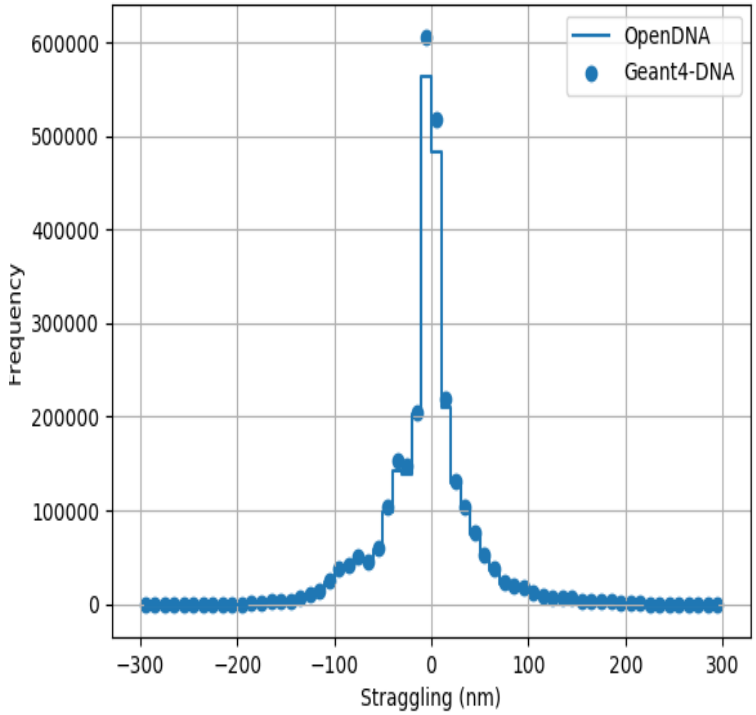
3. Edep



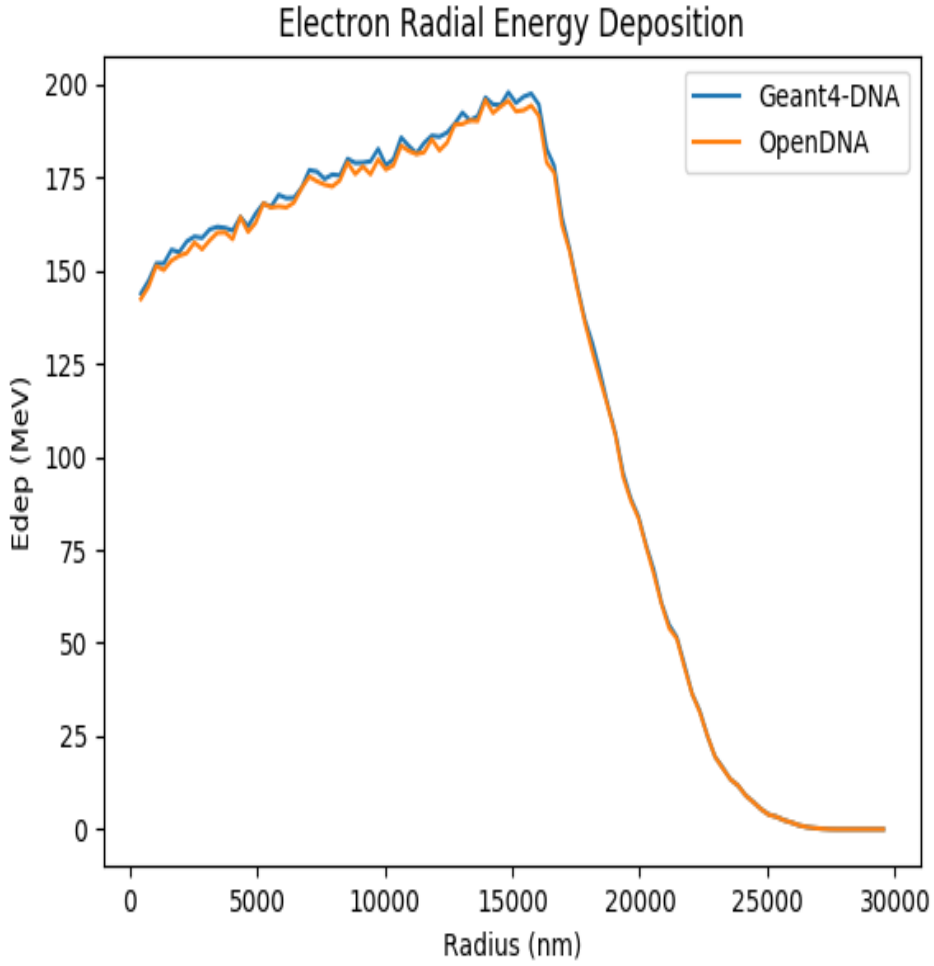
Results - 20 Mev alpha particle

4. Range & straggling





Results - 100 keV Electron - RED

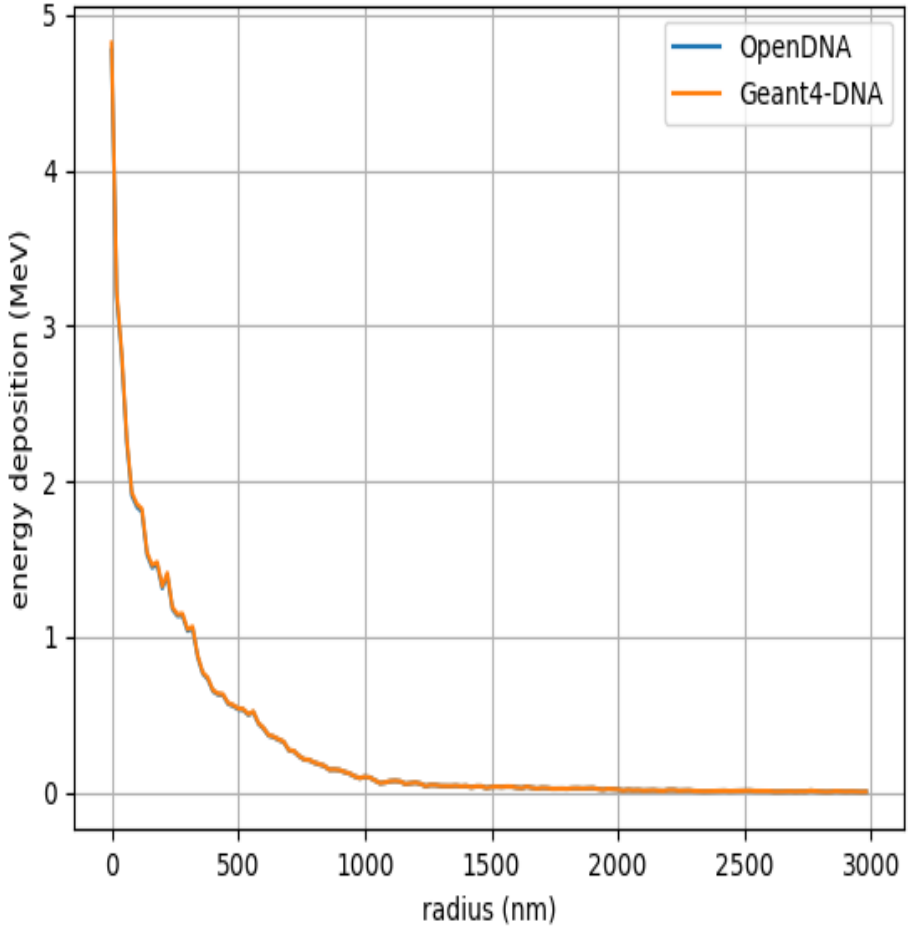


Mac Pro (Late 2013)
CPU for Geant4-DNA
Intel Xeon E5

GPU for OpenDNA
AMD FirePro D700

Time	
Geant4-DNA	50 min
OpenDNA	18 min

Results - 10 MeV proton - RED

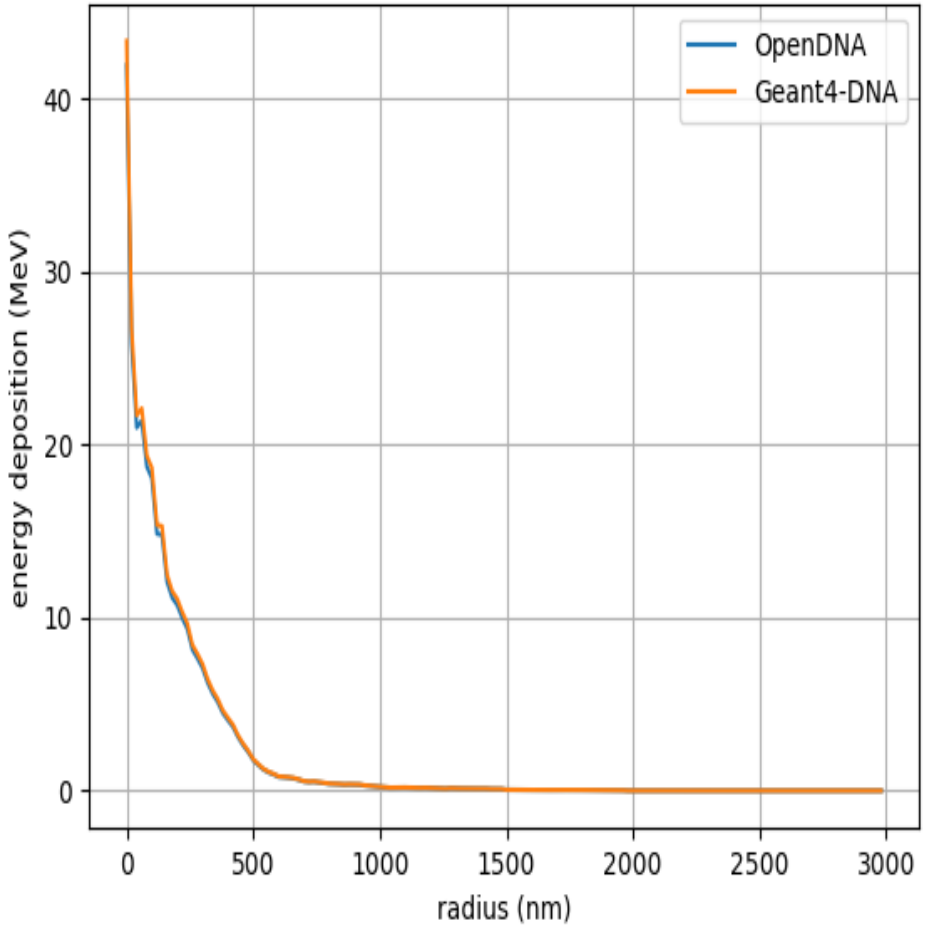


Mac Pro (Late 2013)
CPU for Geant4-DNA
Intel Xeon E5

GPU for OpenDNA
AMD FirePro D700

Time	
Geant4-DNA	18 min
OpenDNA	8 min

Results - 20 MeV alpha particle - RED



Mac Pro (Late 2013)
CPU for Geant4-DNA
Intel Xeon E5

GPU for OpenDNA
AMD FirePro D700

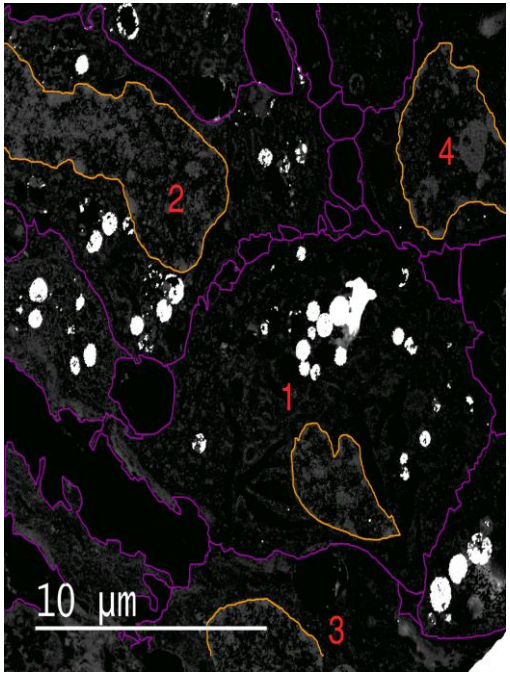
Time	
Geant4-DNA	38 min
OpenDNA	12 min

Summary

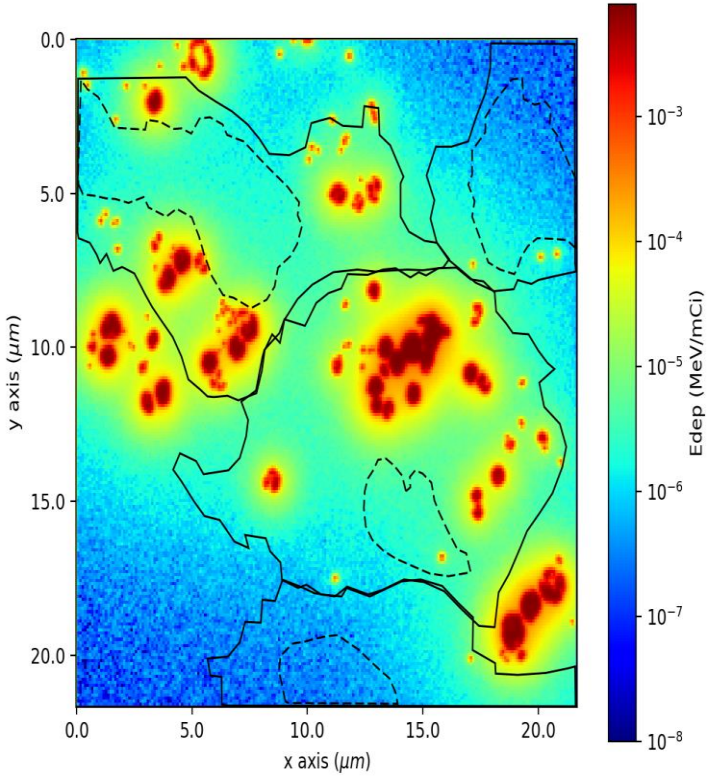
- An openCL based track structure code was
  - Created for electron, proton & alpha particle
  - Preliminarily tested

- Perspectives:
  - OpenCL tuning & optimization
  - Comprehensive benchmarking
  - Microdosimetry applications
  - Add chemical processes

Application - ^{103}Pd@AuNP dosimetry



TEM image



Geant4-DNA

To be done

OpenDNA

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Thank you for your attention!

Questions? Comments?