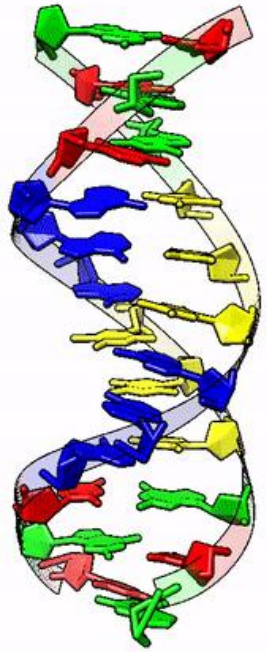

Recent developments on ion transport simulation in Geant4

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Matthew Vologzhin
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22/08/2025

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Data Analysis
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State
University

Preliminaries

(Relevance | Purposes | Tasks)

Relevance

In the coming decades, many space missions are planned, including some with human participation and some without. Despite the differences in their goals, each mission faces the challenge of cosmic radiation. This radiation can cause various types of breakdowns, from **single event effects in microcontrollers** to **breaks in the DNA chain**. As we know, developing these missions is costly and time-consuming, so it is essential to assess the risks to both human life and technology in space projects.

Purposes

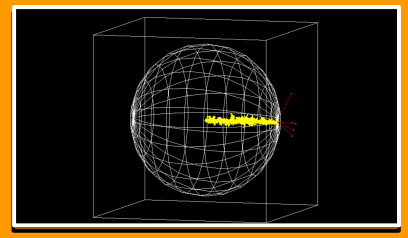
I. Create new DNA-model of ionization losses
II. Validation modeling Geant4 data using ICRU90

Tasks

I. Develop test-ground using Geant4
II. Develop model of ionization losses based on «*physical*» charge
III. Test physical configuration: DNA and EM Standard Physics
IV. Realize python-script for visualization data

Plan

START
- **Preliminaries**
- Why the water?
- Geant4-application



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- DNA *11.3*
- Rudd Ion models *11.3*

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- Detour factor
- Range
- Computation time
- SKIF Cyberia

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- New plans

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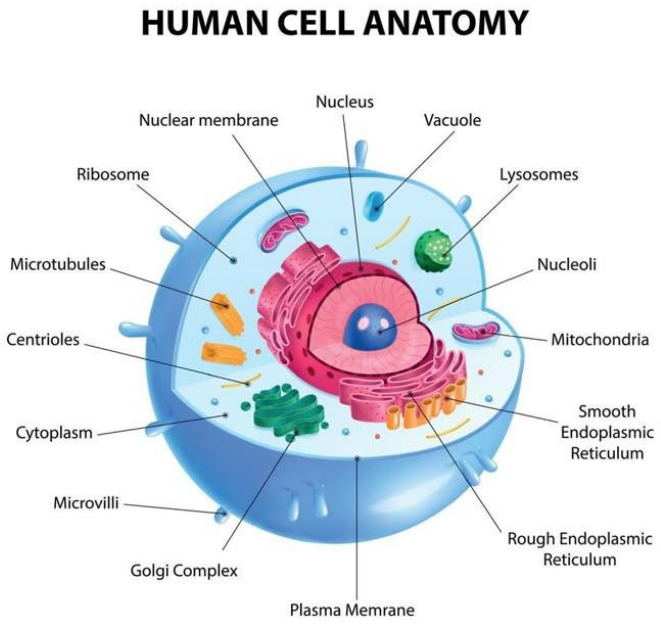
Preliminaries: Why the water?

A cell is composed of approximately **60-80%** water

If we can model the interaction between ionizing radiation and water, we can also effectively simulate medical procedures & cosmic missions

For example,
effects of **Van Allen radiation belts** or **galactic cosmic radiation** on cells



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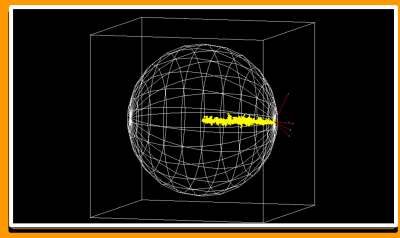

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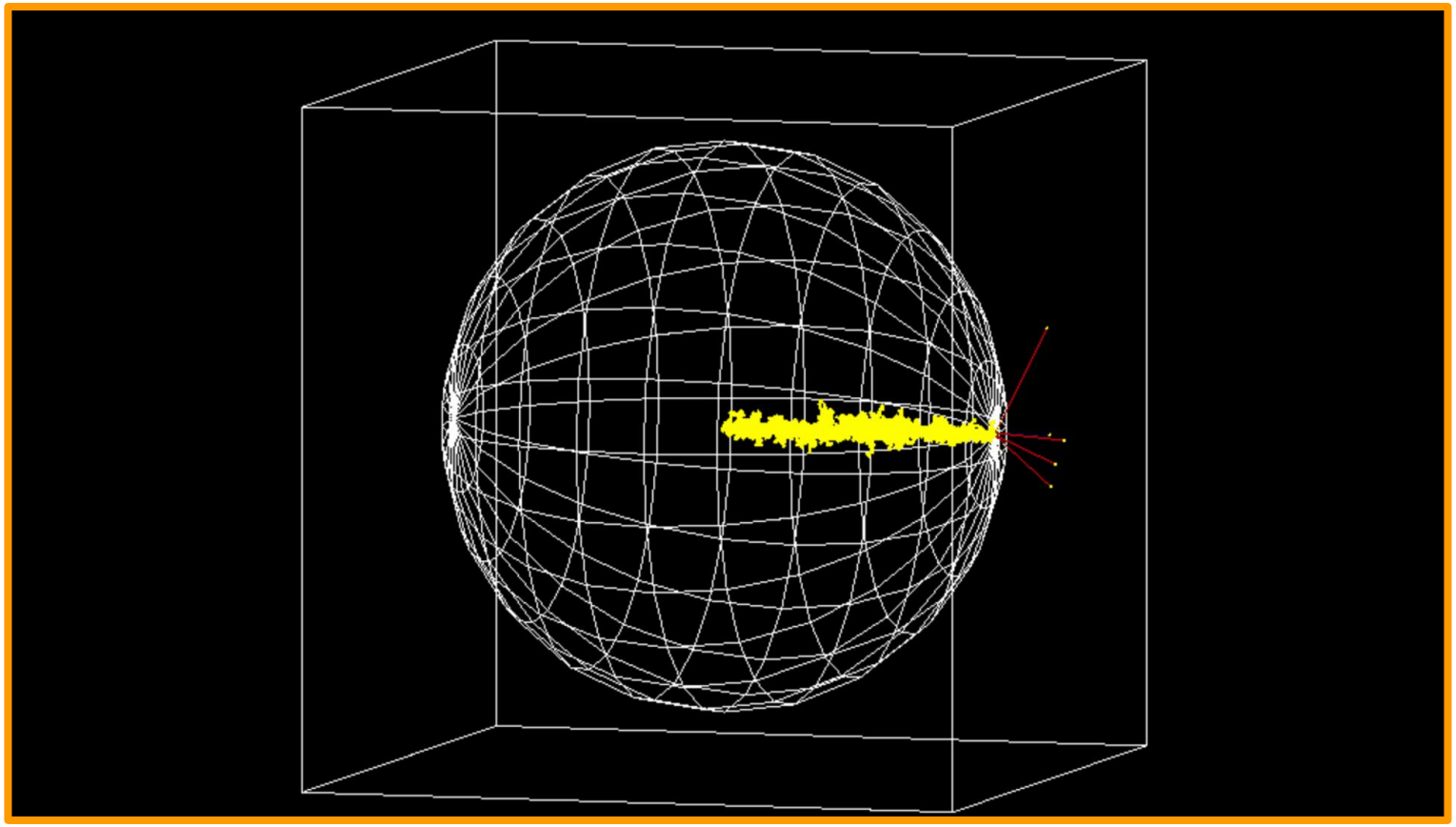
Preliminaries: Geant4-application



«Test-ground for Ion ranges: The water sphere & Incoming particle»

Plan

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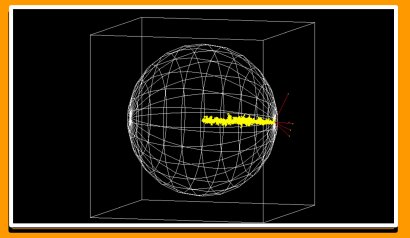

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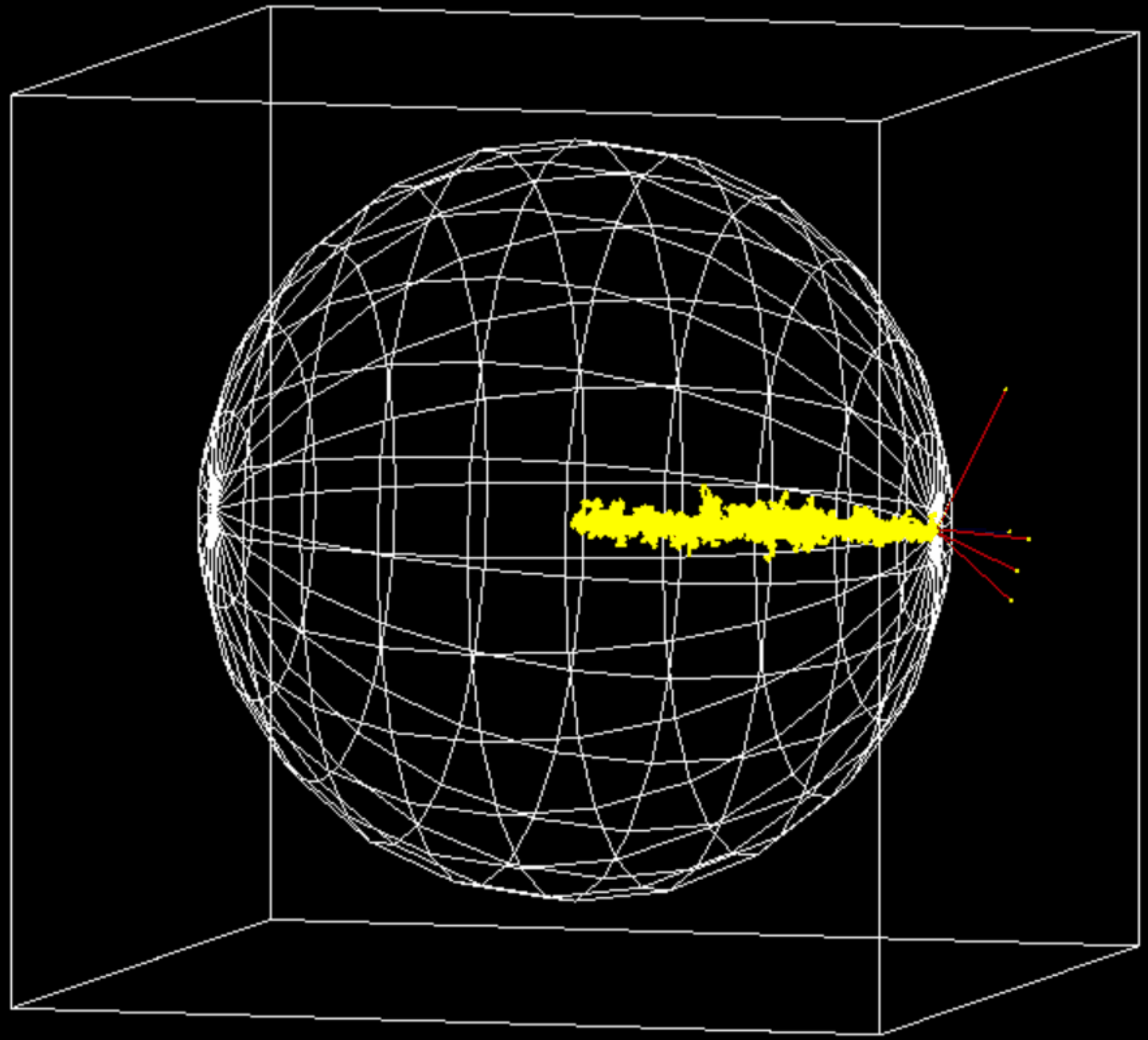


Part I

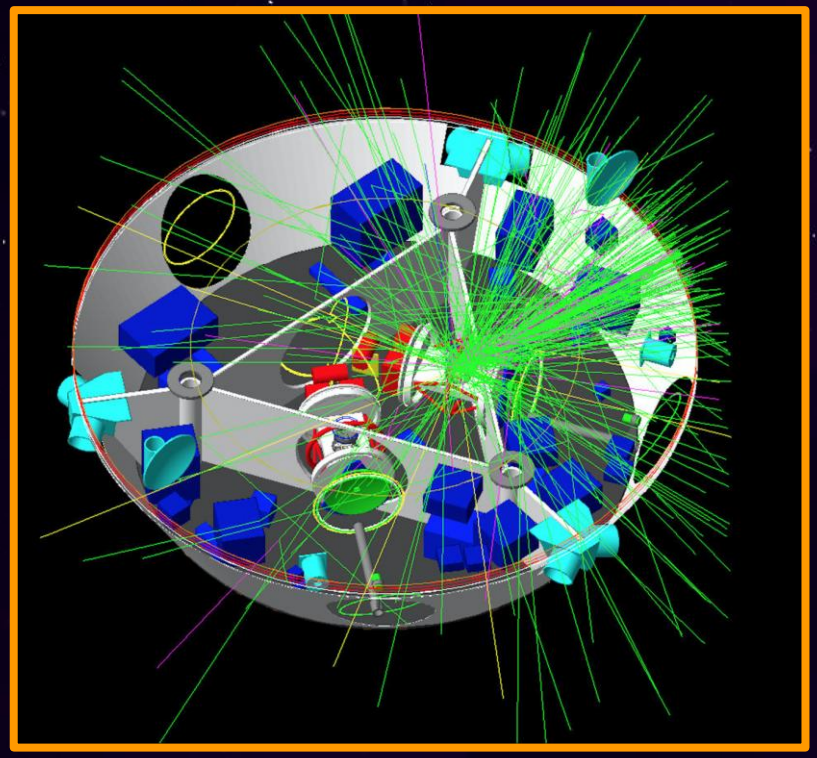
EM PHYSICS LISTS

What is Geant4?

- **Geant4** is **Monte-Carlo toolkit** for passage of the particles through matter simulation (Last version: *11.3*)
- Geant4 provides modeling a both **high energy physics** (astroparticles, accelerated particles) and **low energy physics** (DNA breaks, radiation effects)
- Yon need answer to three question to create Geant4 application:

What? Where? How?

Particle. Geometry. Models



«Example of using Geant4 application»

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What is Physics List?

- **Physics List** is a set of particles and physical models which uses to describe processes relate to particles
- **The existing Physical Lists:** transportation, electromagnetic, decay, hadronic(elastic/inelastic) lists etc.
- **Standard EM & DNA** are lists that uses to modeling electromagnetic process but at various *energies* and *geometry scales*

  Condensed-history approach = Standard EM
  Detailed-track structure approach = DNA
- **Option** is the configuration of the specific Physical List

G4EmStandardPhysicsList_option4

"G4" – Geant4

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Plan

EM Physics Lists: Standard 11.3

- **G4EmStandardPhysicsList** uses for simulation of high energy particles which participate in electromagnetic interaction

- Standard EM Physics List consist of models:

1) *G4BetheBlochModel*
   default high-energy model for heavy particles
2) *G4LindhardSorensenModel*
   using for ions $Z > 2$
   using: ICRU73 & ICRU90
3) *G4BraggModel*
   for protons, backup for all ions, effective charge for ions
   using: ICRU90 & PSTAR
4) *G4BraggIonModel*
   for alpha-particles
   using: ICRU90 & ASTAR

High-energy MODELS

Low-energy MODELS

- It's based on ***Condensed-History approach***

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Plan

EM Physics Lists: DNA 11.3

- **DNA Physics list** uses to modeling low-energy particles based on ***Detailed-Track structure approach***
- Main configurations:
  option 2 (*precisest*)
  option 4 (*worst*)
  option 6 (*CPA100-models*)
  option 8 (*dynamic charge*)

- It consist from models:

1) *G4DNABornIonisationModel* for protons
2) *G4DNARPWBAIonisationModel* for protons
3) *G4DNARuddIonisationExtendedModel* for ions
4) *G4DNARuddIonisationDynamicModel* for ions

Energy	Particle		
	Protons	Alpha-type	Other Ions
$E < 0.5$ MeV/u	*Rudd model*	*Rudd model*	
$0.5 < E < 100$ MeV/u	*Born model*		
$100 < E < 300$ MeV/u	*RPWA model*		
$E > 300$ MeV/u	*Standard models*		

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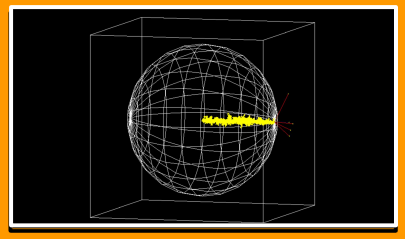

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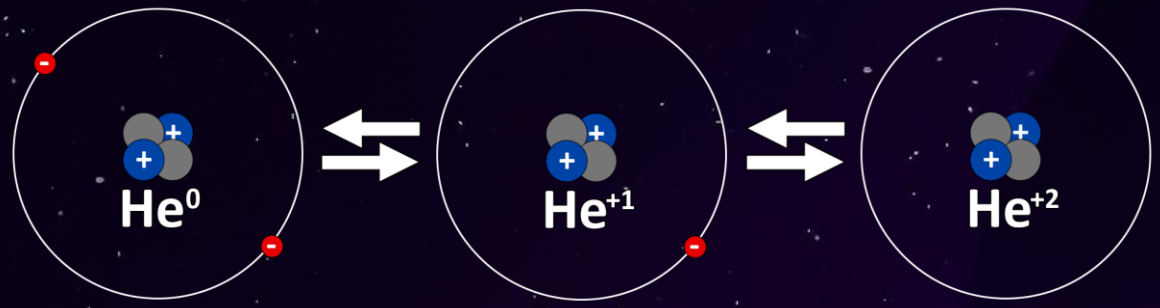
Rudd Ion models 11.3

- **Rudd model** (*Nucl. Track Rad. Meas. 16 (1988) 219*) provides sampling of electron emission in proton or electron collision with water molecule
- Three flavors of the model:
  1. G4DNARuddIonisationModel – **DNA Option #4**
     (*The effective charge*)
  2. G4DNARuddIonisationExtendedModel – **DNA Option #2**
     (The effective charge)
  3. G4DNARuddIonisationDynamicModel – **DNA Option #8**
     (The dynamic charge = charge exchange with the media)



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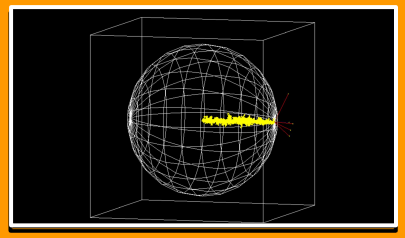

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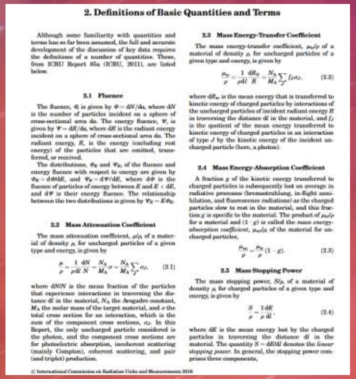
Part II
PLOTS

Comparison **Geant4** VS **ICRU90**

- **ICRU90** - the report of the International Commission on Radiation Units and Measurements (*ICRU*), published in October 2016


2. Definitions of Basic Quantities and Terms

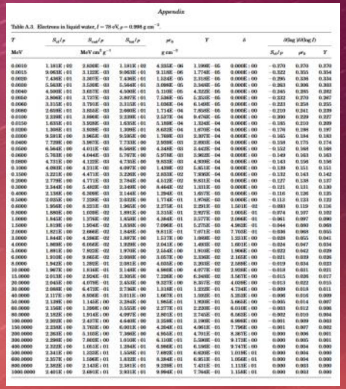
2.1 Fluence

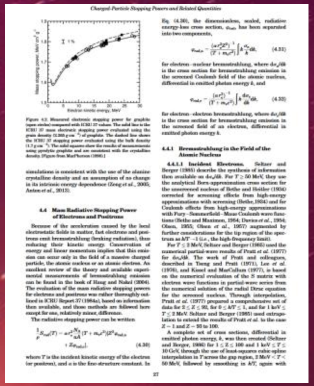
2.2 Mass Attenuation Coefficient

2.3 Mass Energy-Transfer Coefficient

2.4 Mass Energy-Absorption Coefficient

2.5 Mass Stopping Power


Appendix


Charged-Particle Stopping Powers and Related Quantities

- **ICRU90** consists Ranges, Detour factors, and Stopping power in the water media for:
  electron, positron, proton, alpha, carbon

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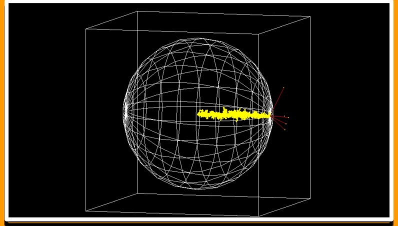

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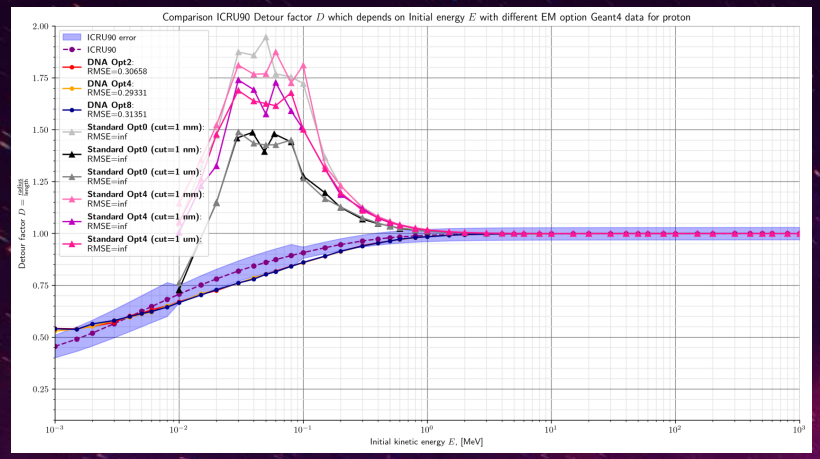
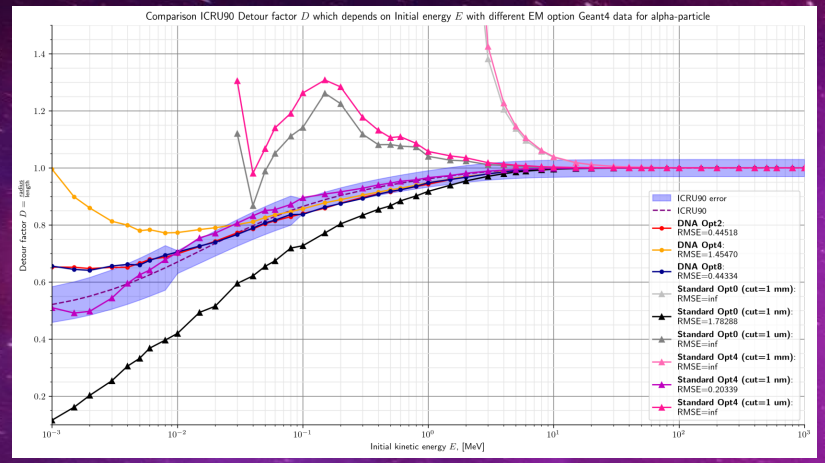
Geant4 VS ICRU90: Detour factor

Detour factor is the ratio of the penetration depth to the actual path length

$$\text{Detour factor} = \frac{\text{radius}}{\text{length}}$$





It characterizes the scattering of the particles

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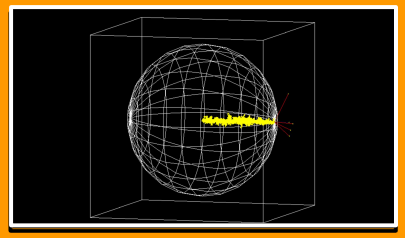
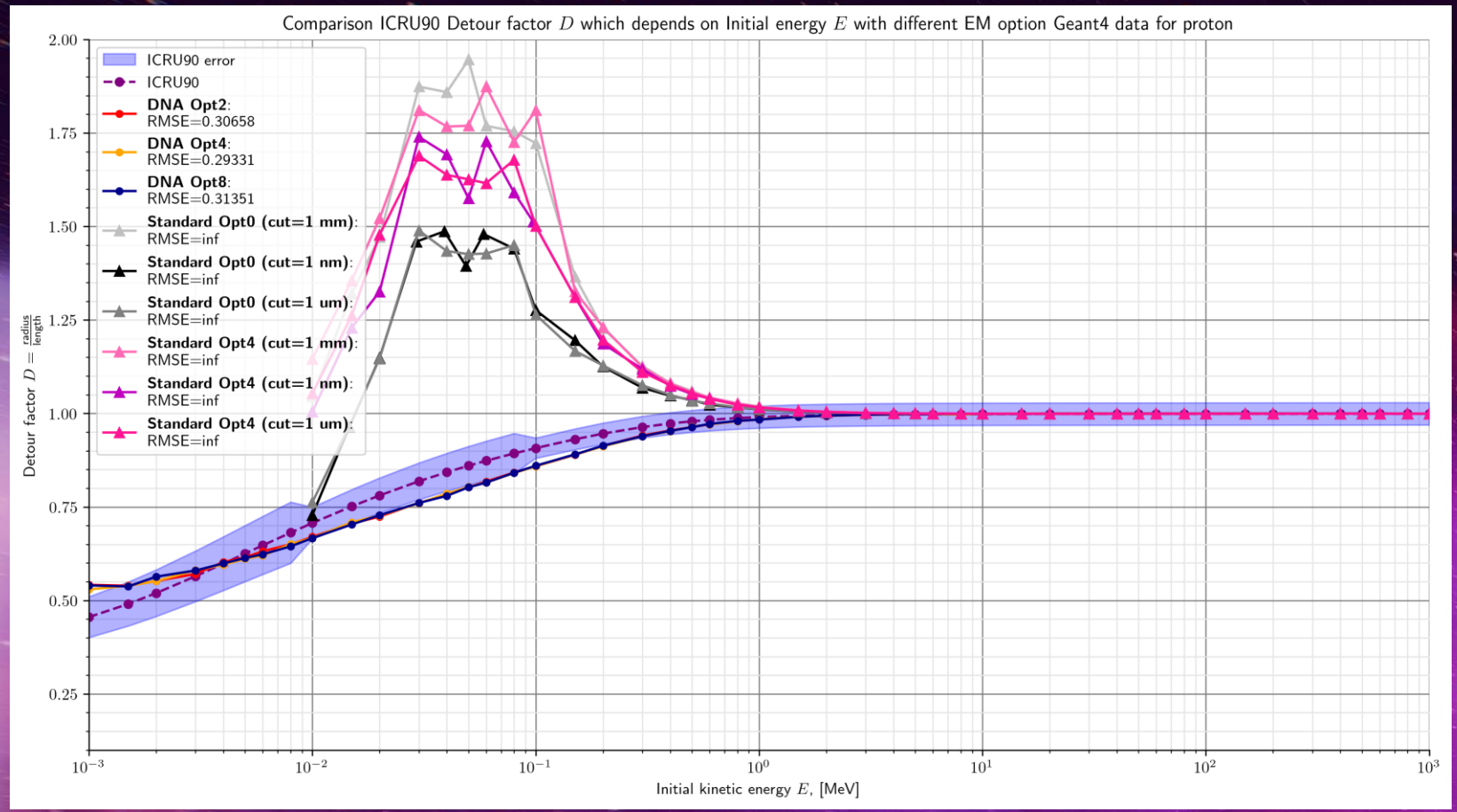


Geant4 VS ICRU90: Detour factor



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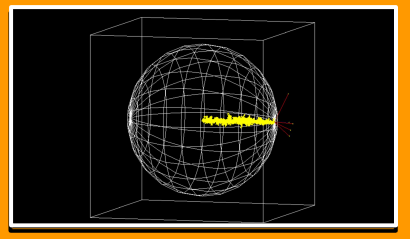

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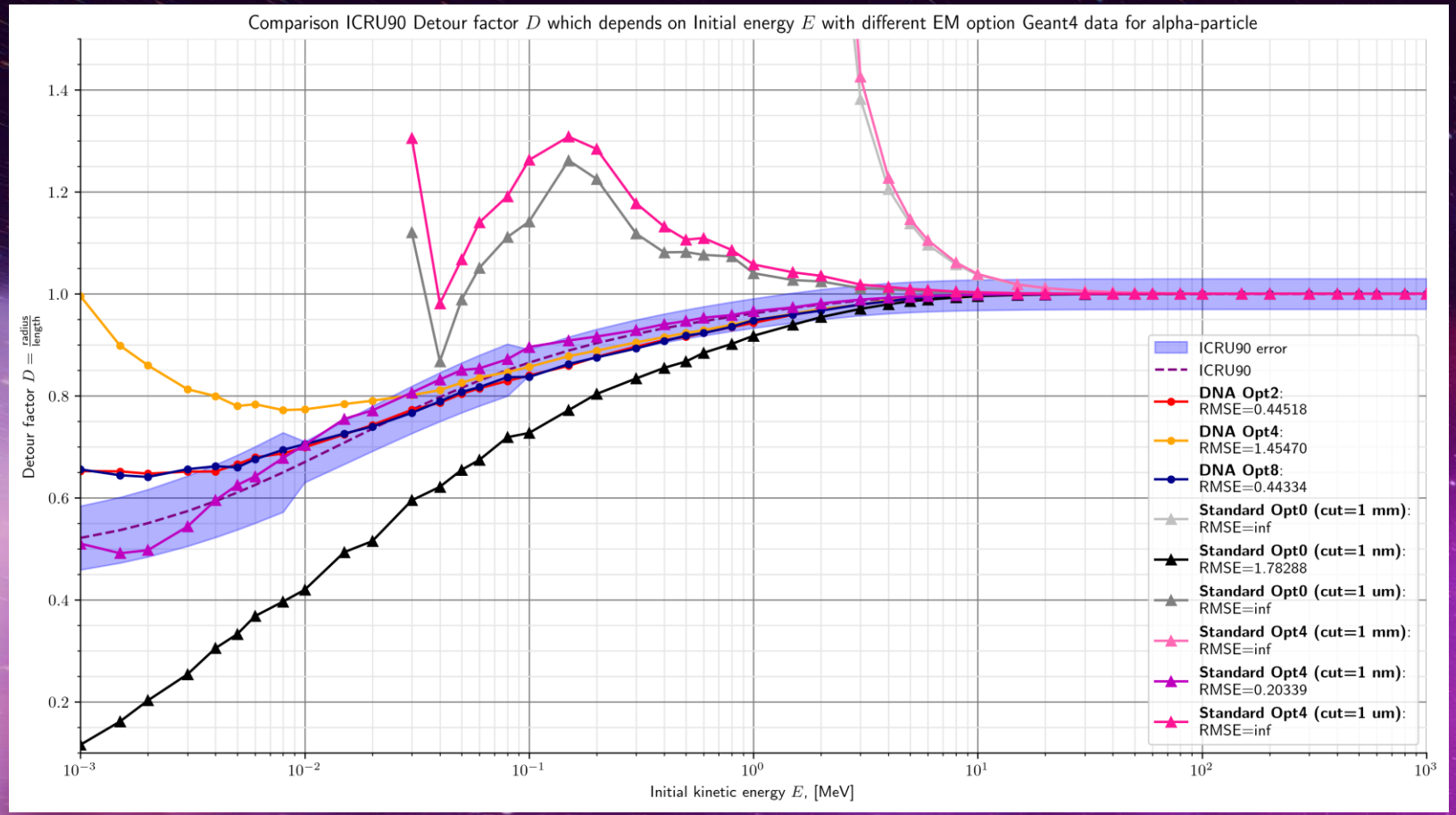
Geant4 VS ICRU90: Detour factor



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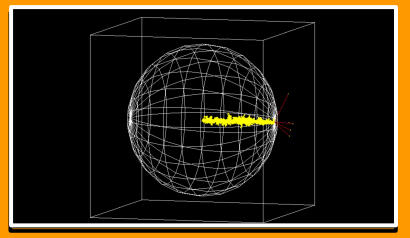

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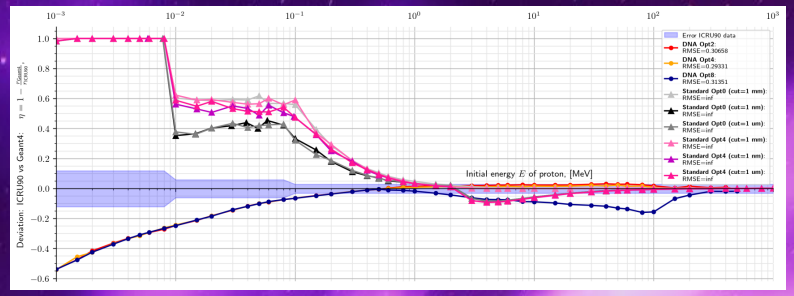
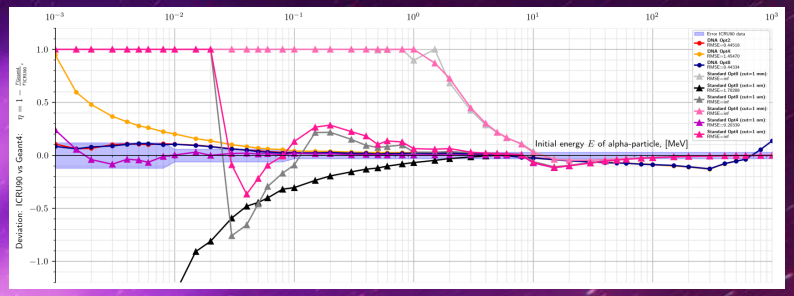
Geant4 VS ICRU90: Range



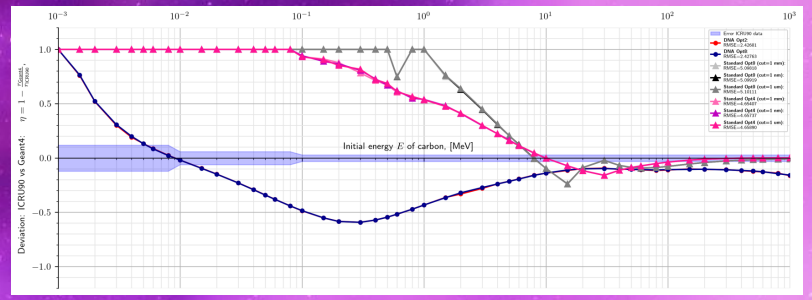


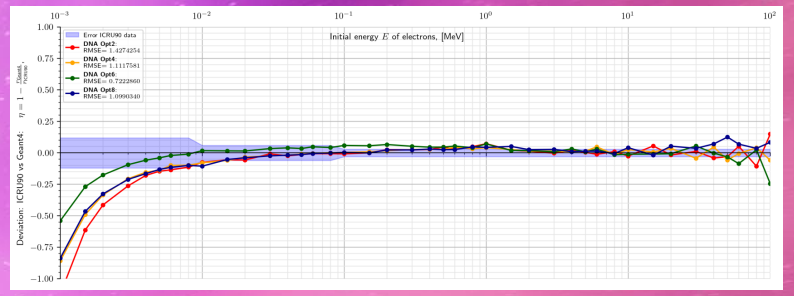
Range is the path length of some particle in some material

Dynamical charge

$$He^0 \leftrightarrow He^{+1} \leftrightarrow He^{+2}$$

$$\text{Deviation} = 1 - \frac{\text{Range}_{\text{Geant4}}}{\text{Range}_{\text{ICRU90}}}$$





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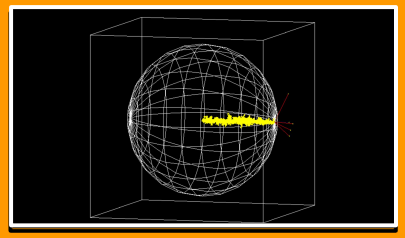

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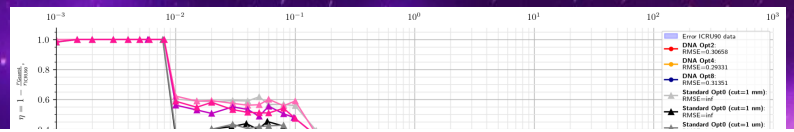

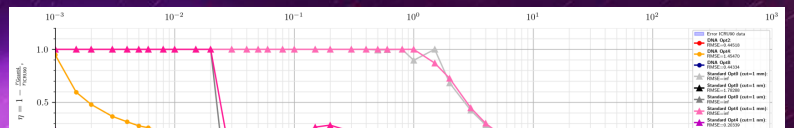

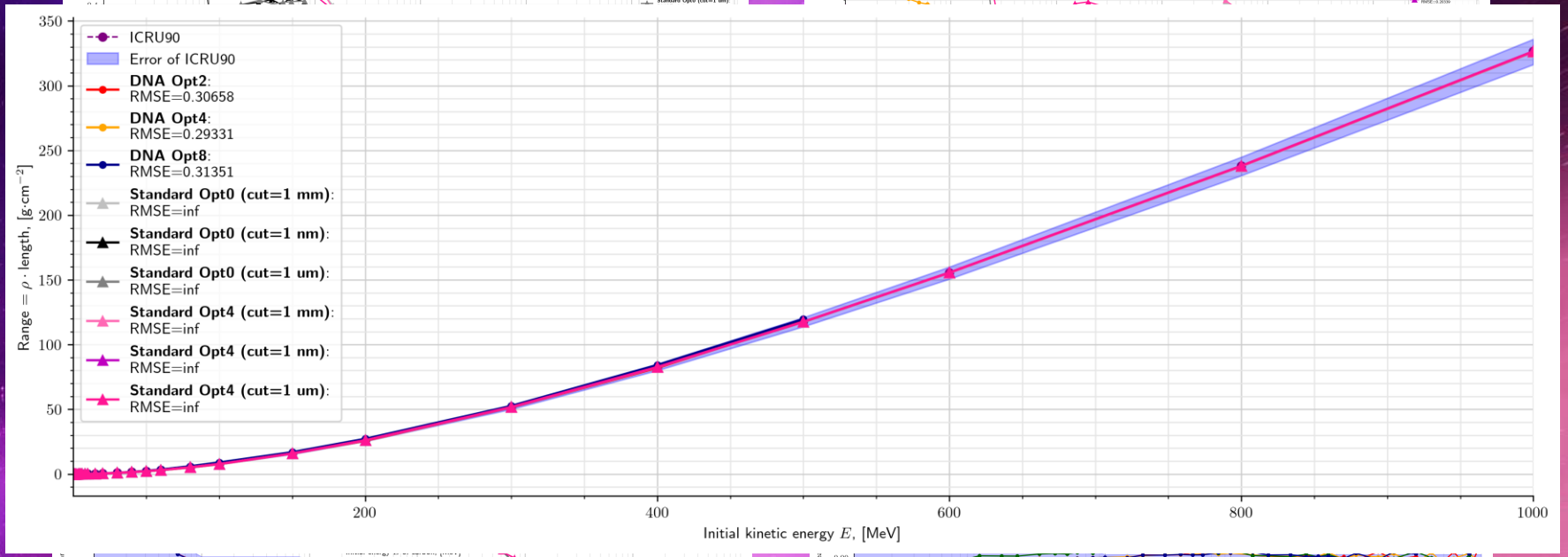

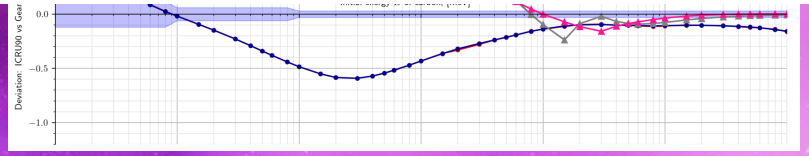

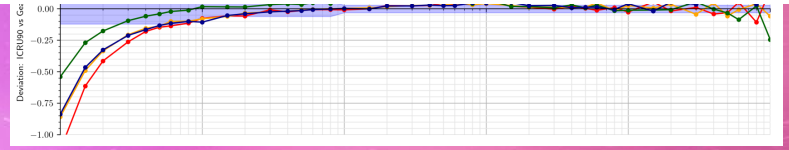

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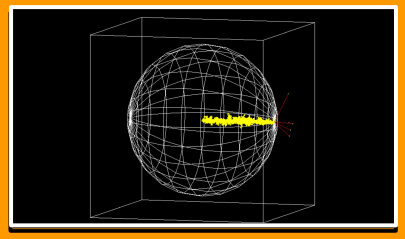

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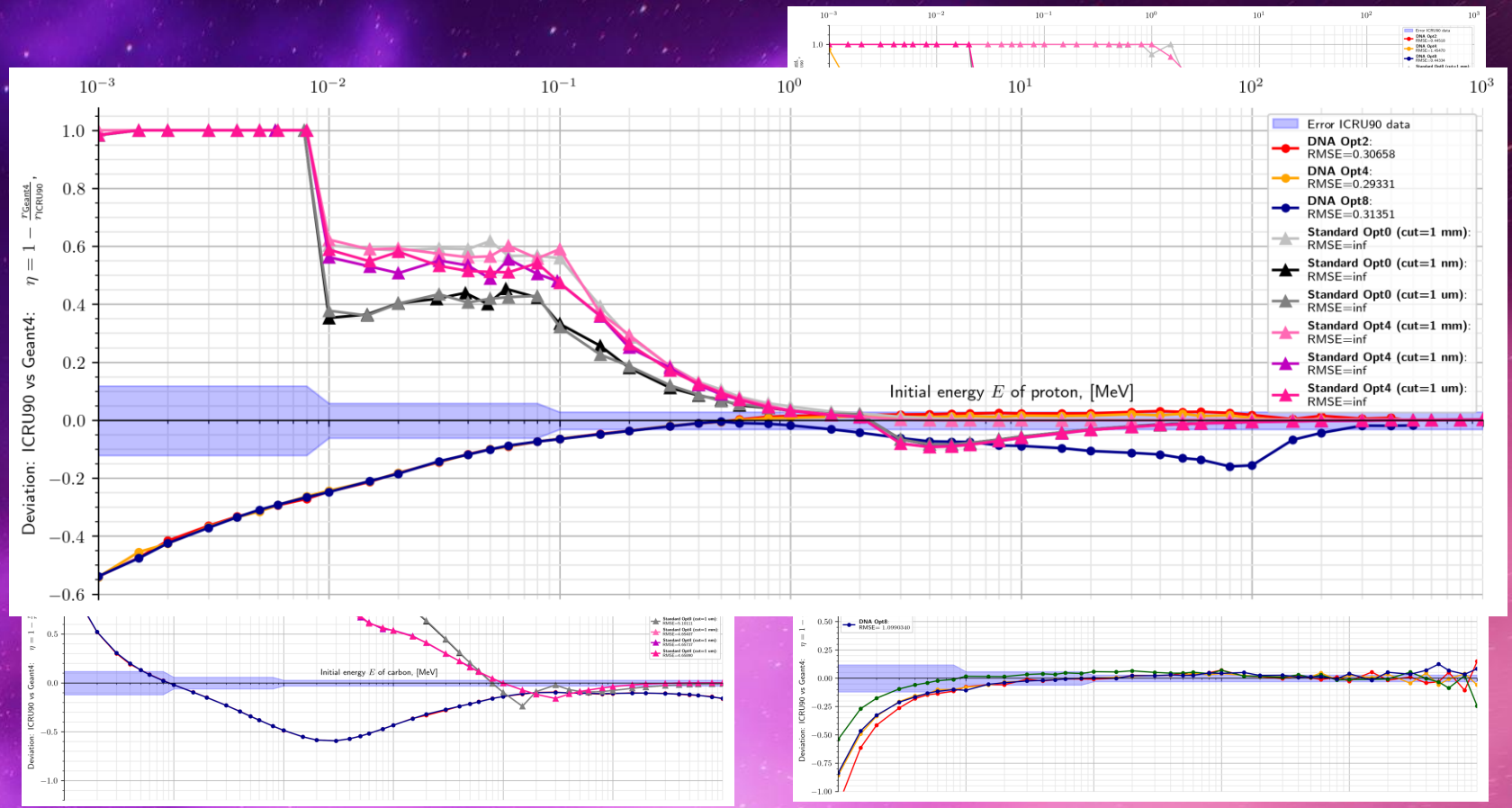
Geant4 VS ICRU90: Range



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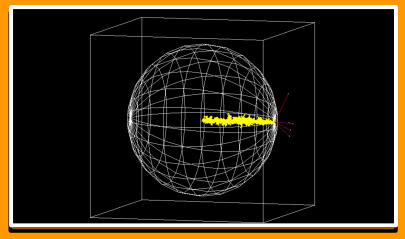

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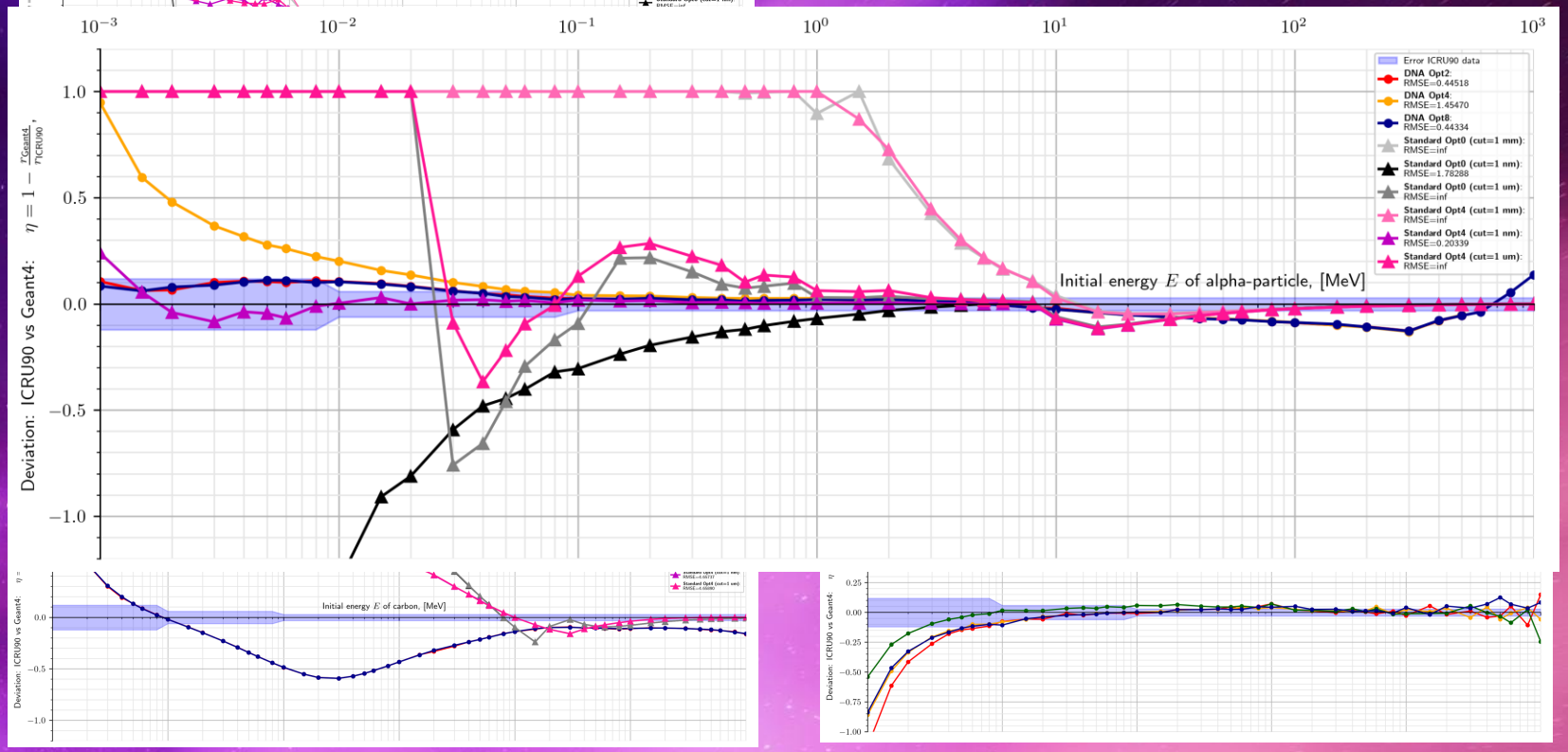

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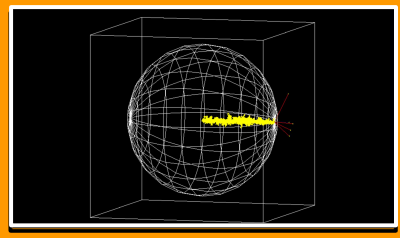

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- **Range**
- Computation time
- SKIF Cyberia

END
- General conclusion
- New plans

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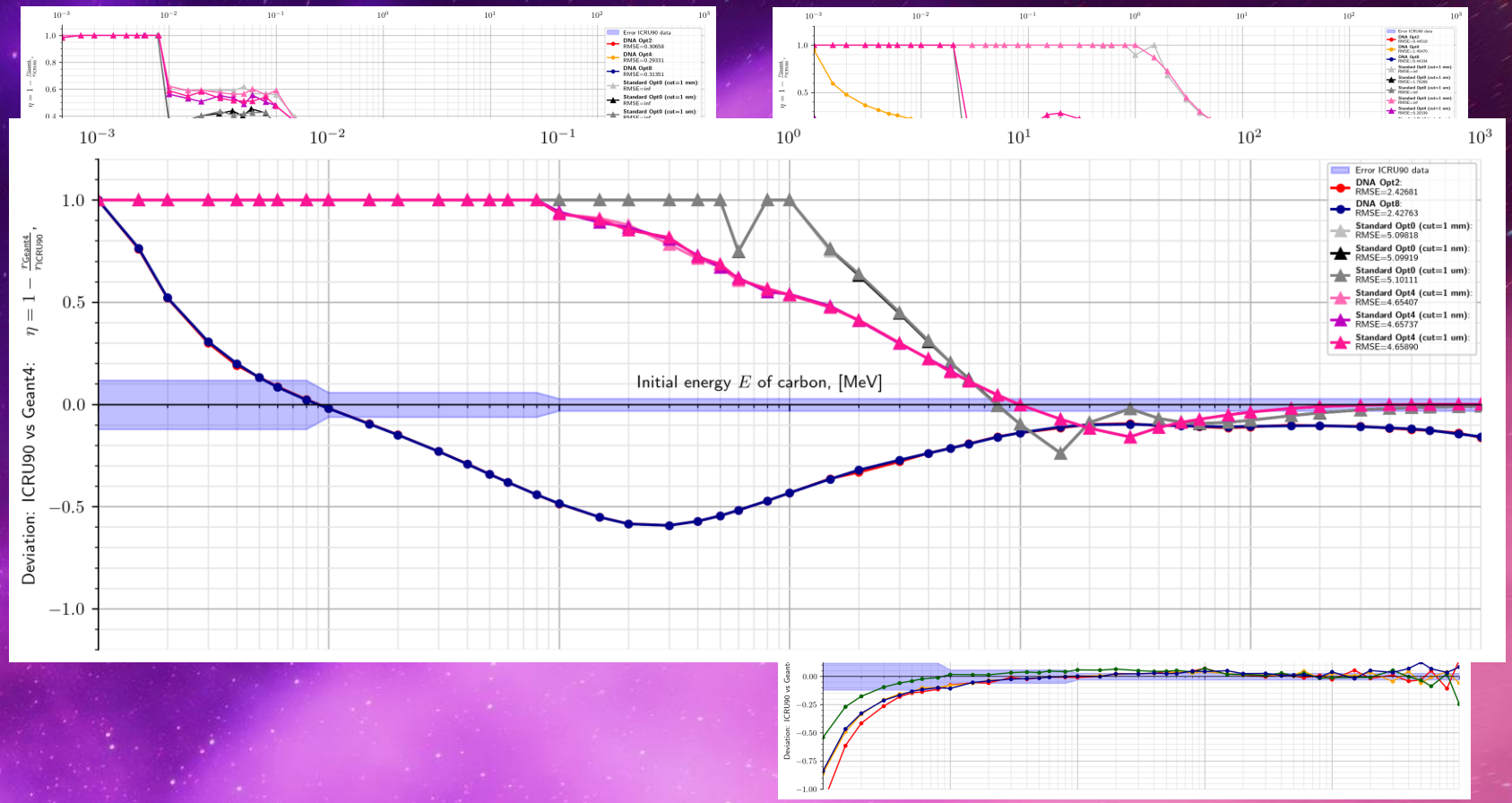
Geant4 VS ICRU90: Range



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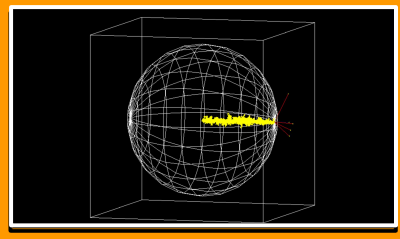

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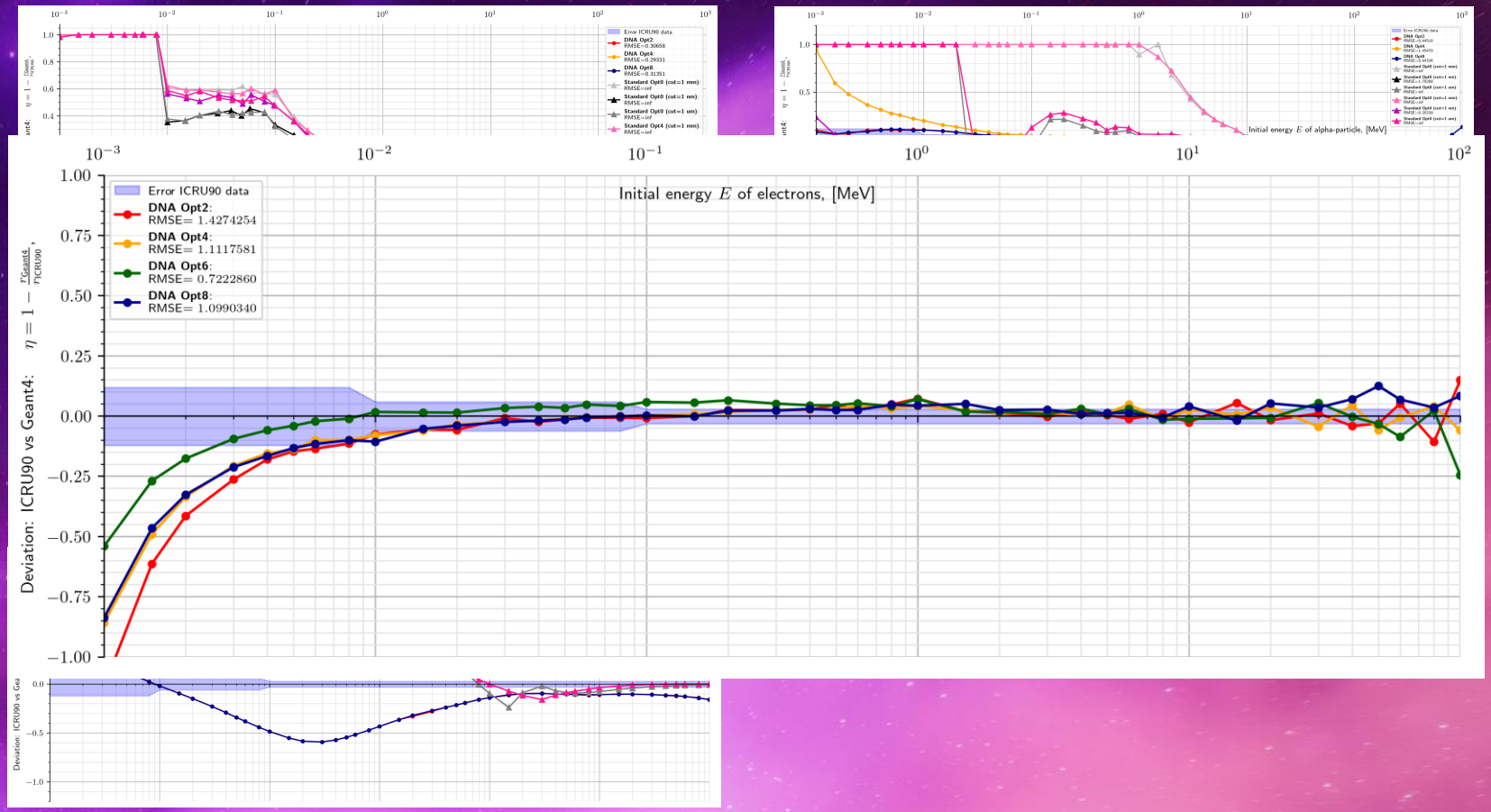

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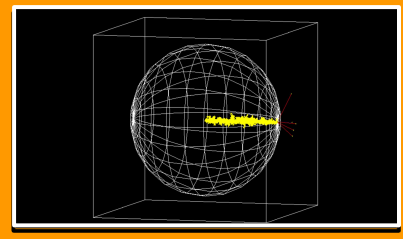

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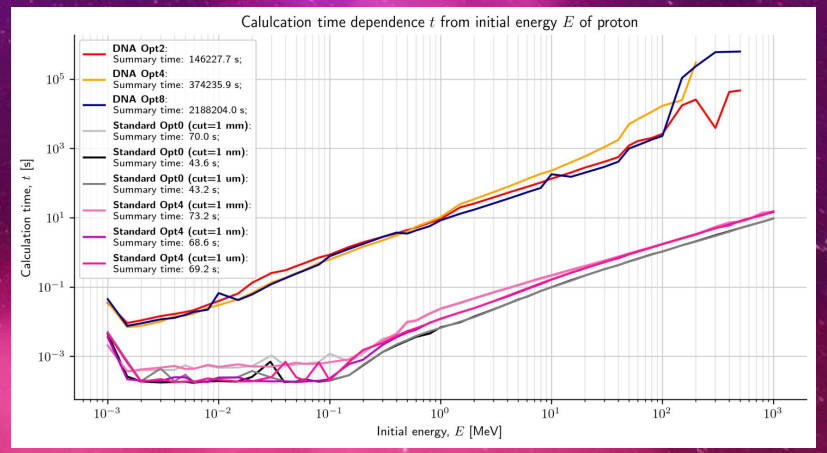

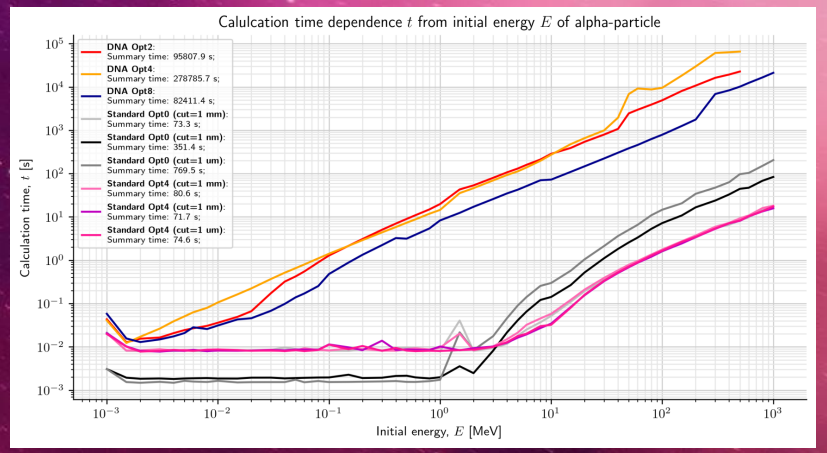

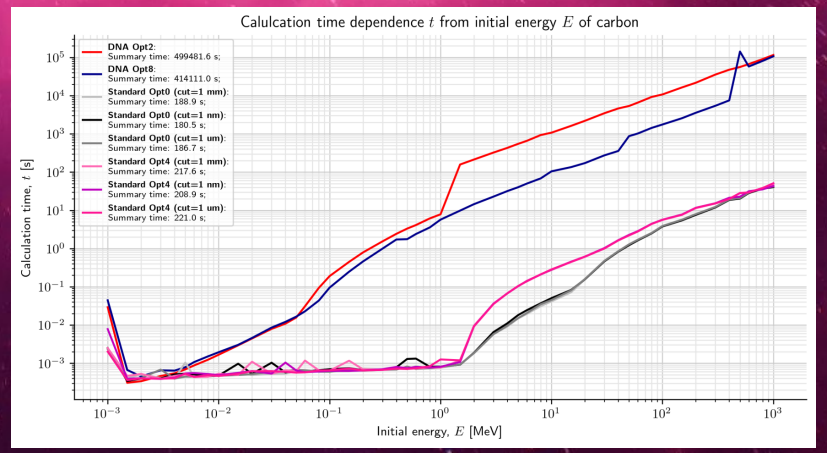

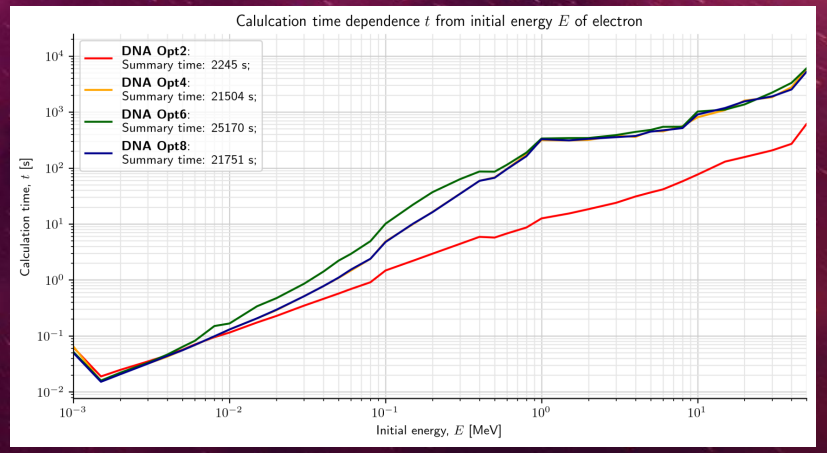

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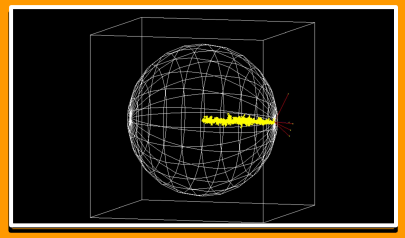

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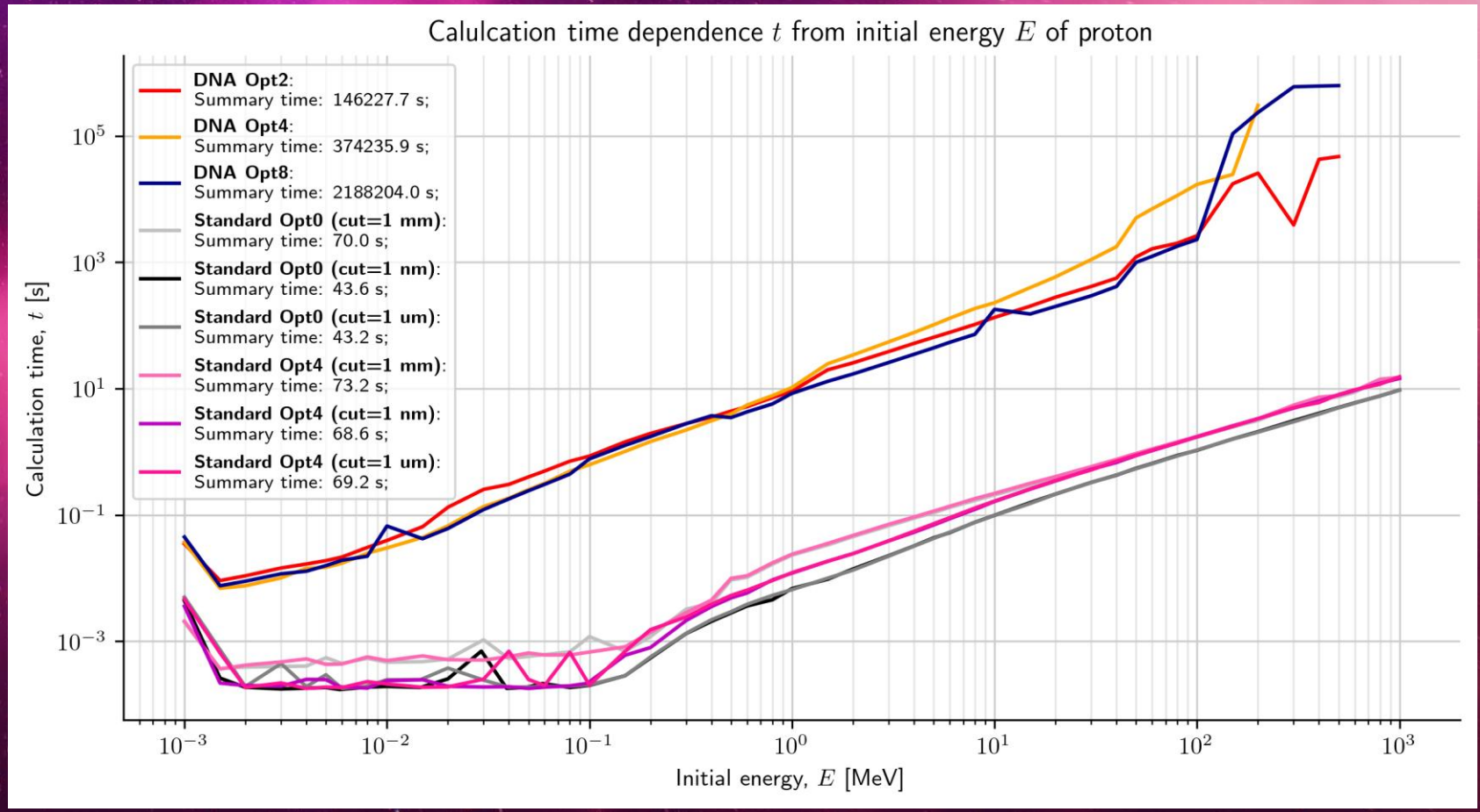

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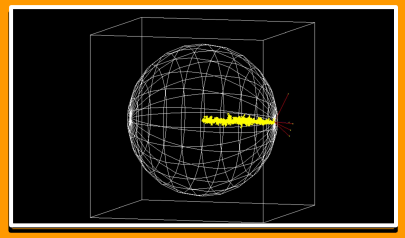

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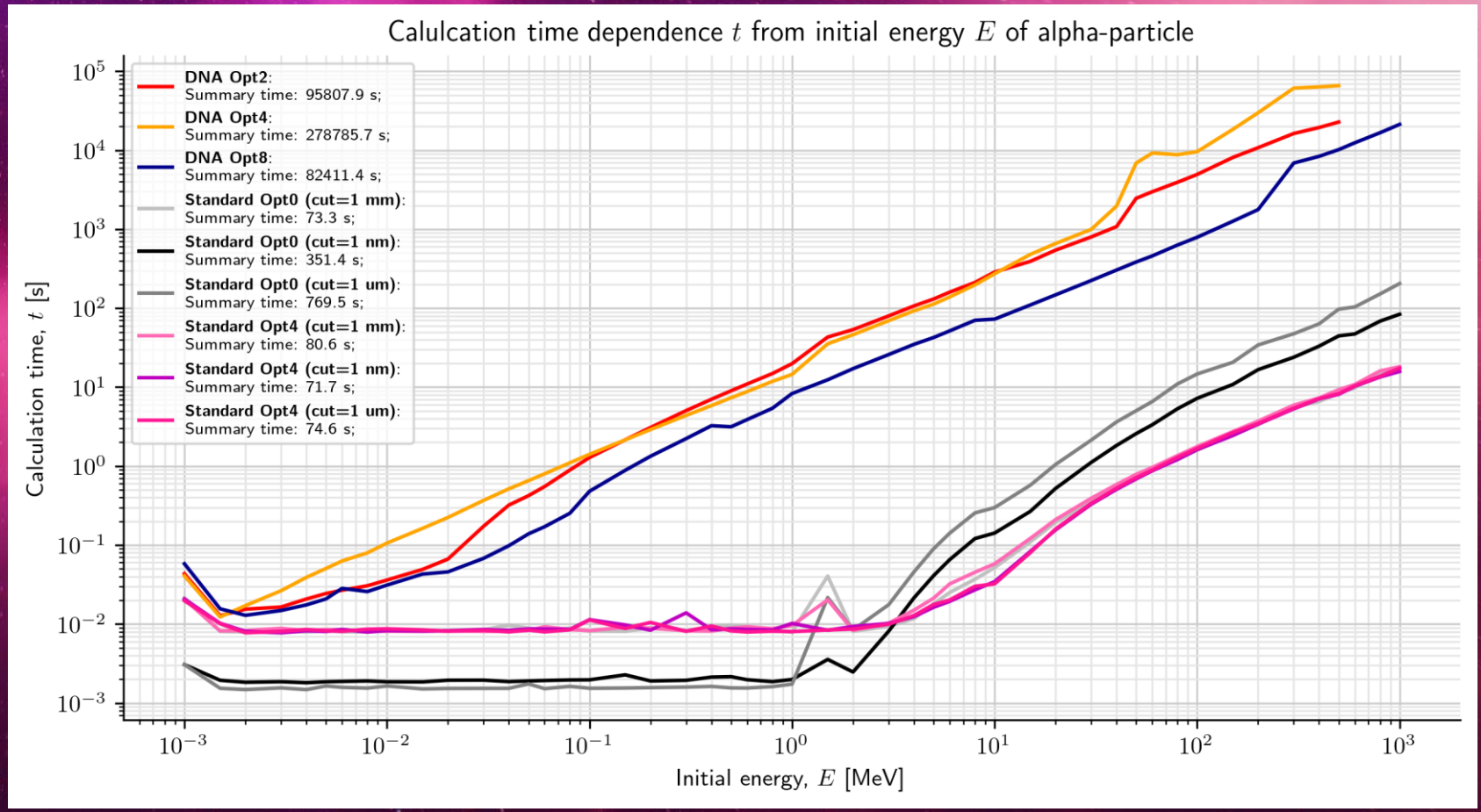

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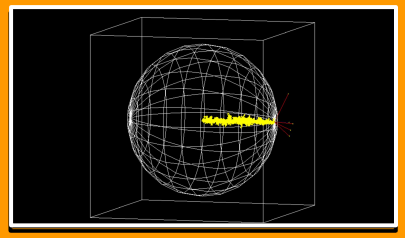

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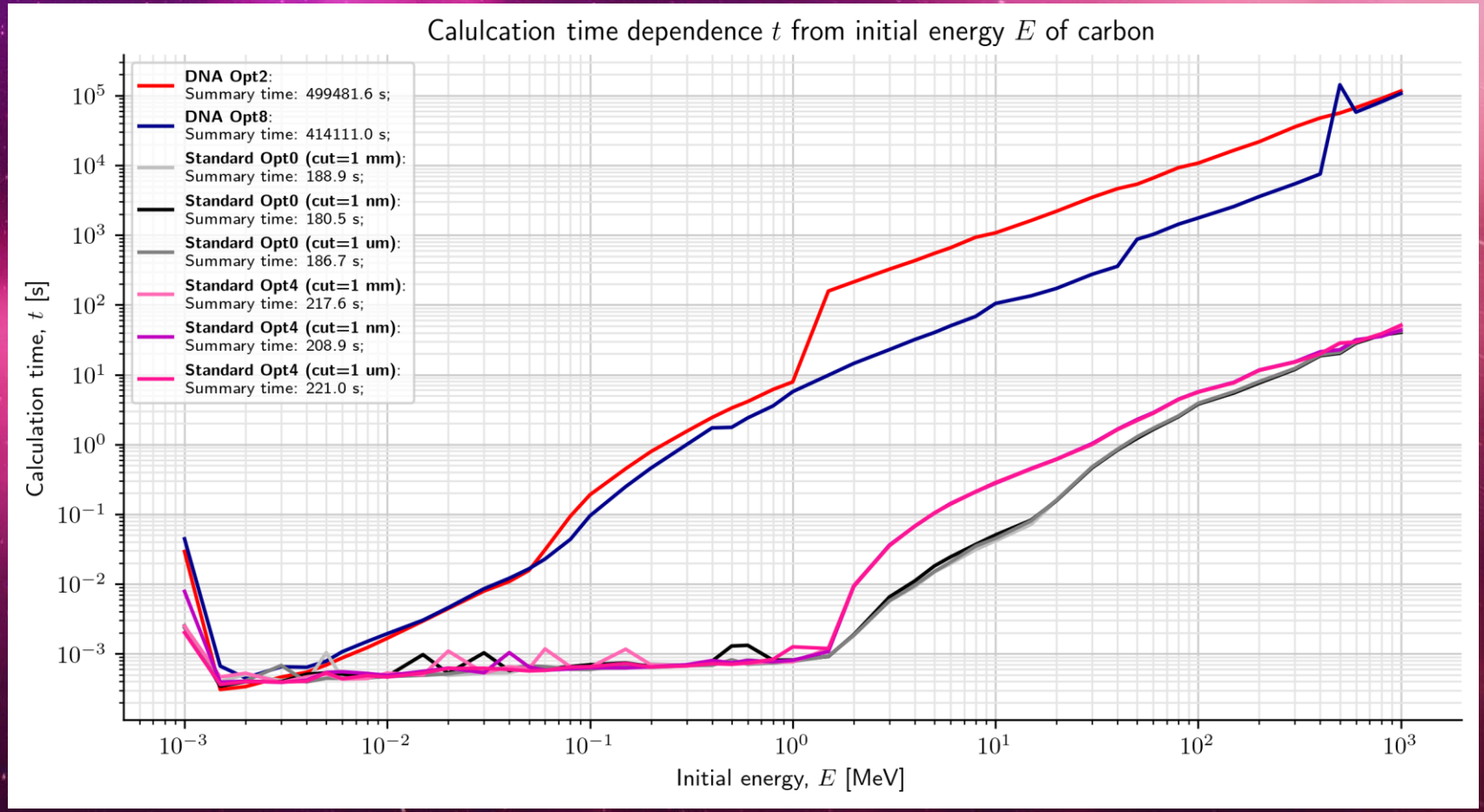

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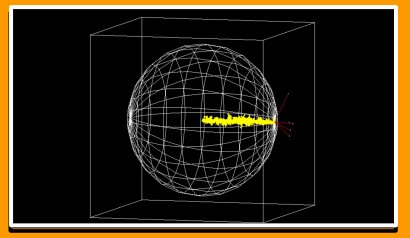

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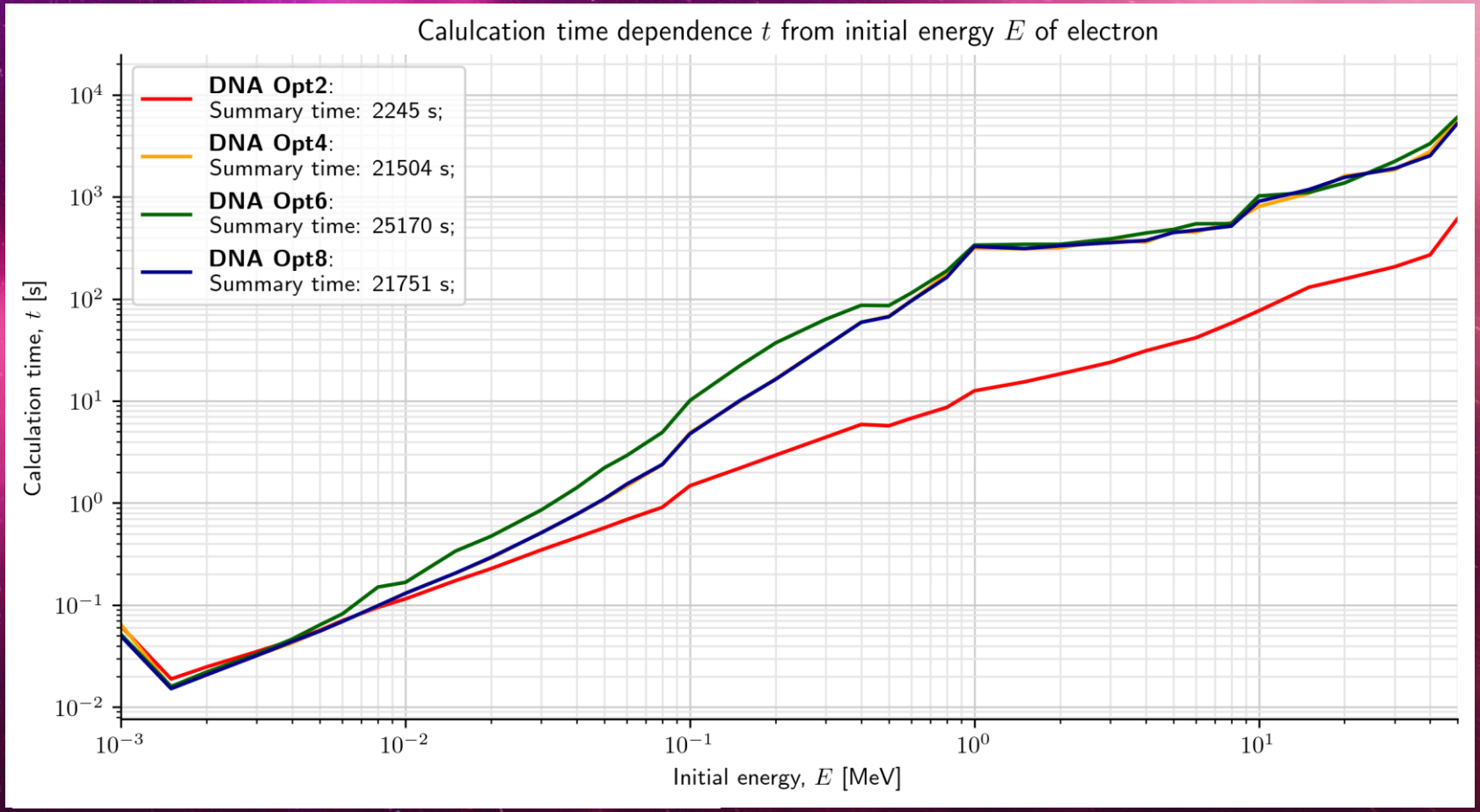

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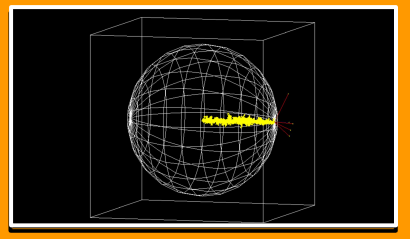

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Geant4 VS ICRU90: SKIF Cyberia

«Director of the TSU SKIF Cyberia Supercomputing Center demonstrates new equipment for Vladimir Ivanchenko»

Processor: Intel Xeon Silver 4114T
(40 threads with a maximum PROCESSOR clock speed of 3 GHz)
RAM: 93 GB

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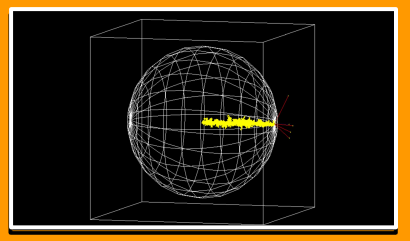

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The END

Conclusion & Plans

Conclusion

- **New ionization losses** model was developed:
it uses "*dynamic charge*" concept (*G4DNARuddIonisationDynamicModel.cc*)

- Geant4 EM Physics Lists (*Standard & DNA*) **validation** was performed based on the result of ICRU90 review:

- Proton
  1) **Detour factor** isn't described by EM Standard Physics Lists up to 1 MeV
  2) **DNA Opt4** is the best for **Range**
  3) **DNA Opt2** is the **fastest option**
- Alpha-particle
  1) **Detour factor** isn't described by EM Standard Physics Lists up to 1 MeV
  2) **EM Standard Opt4 (cut = 1 nm)** is the best for **Range** among All Physics Lists
  3) **DNA Opt2** & **DNA Opt8** are the best for **Range** among DNA Physics Lists
  4) **DNA Opt8** is the **fastest option** among DNA Physics Lists
- Carbon
  1) **DNA Opt2** & **DNA Opt8** are the best for **Range**
  2) **DNA Opt8** is the fastest option among DNA Physics Lists
- Electron
  1) **DNA Opt6** is the best for **Range**
  2) **DNA Opt2** is the **fastest option**

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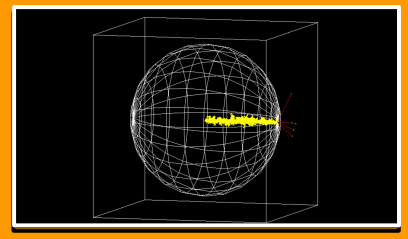
Plan



New plans

- Developing new *G4ChargeIncrease.cc* and *G4ChargeDecrease.cc* classes for heavy ions. For example: B10, C12, Fe56 etc.

- Developing new methods to use Chemistry Lists for modeling alpha-particles using EM Standard Option 4 – It provides possibility to modeling **brachytherapy**, **targeted alpha-therapy** much faster than any DNA Physics Lists

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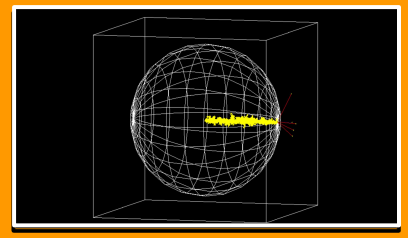
Plan



Thank you for your attention!

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Laboratory
of High Energy Physics
Data Analysis

Tomsk
State
University

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the Government of the Russian Federation (Agreement No. 075-15-2025-009 of 28 February 2025)

I’m ready to answer your questions!

matvey.vologzhin@mail.ru