Simulating Muon-Induced DNA Damage in Geant4-DNA

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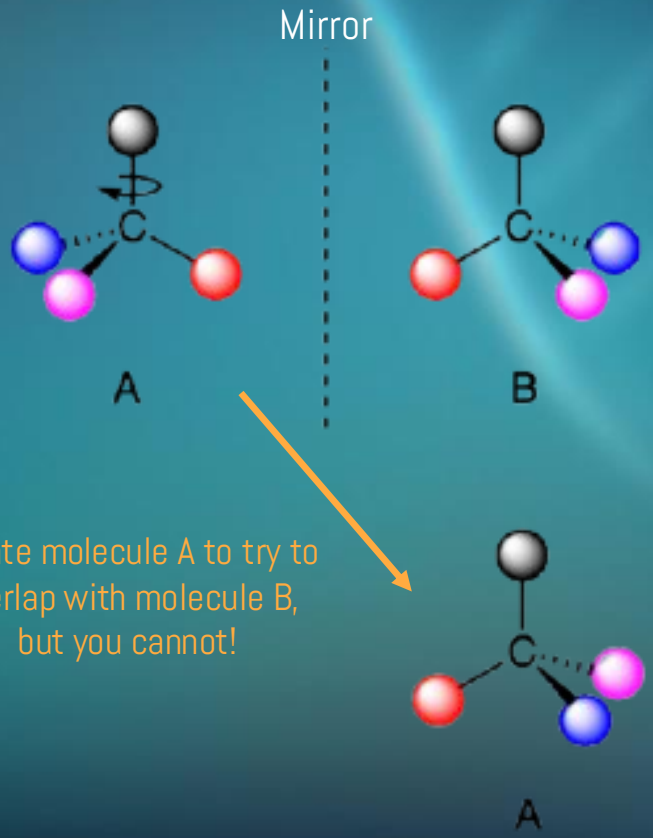
01
Background

Chirality

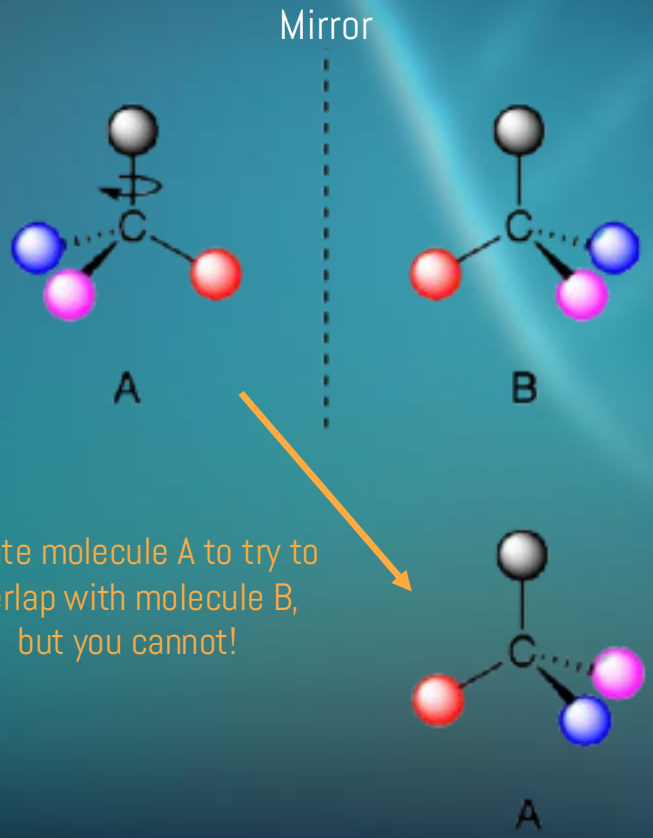


A **chiral** molecule cannot be superimposed over its mirror image.

Enantiomers are chiral molecules that are mirror images of each other.

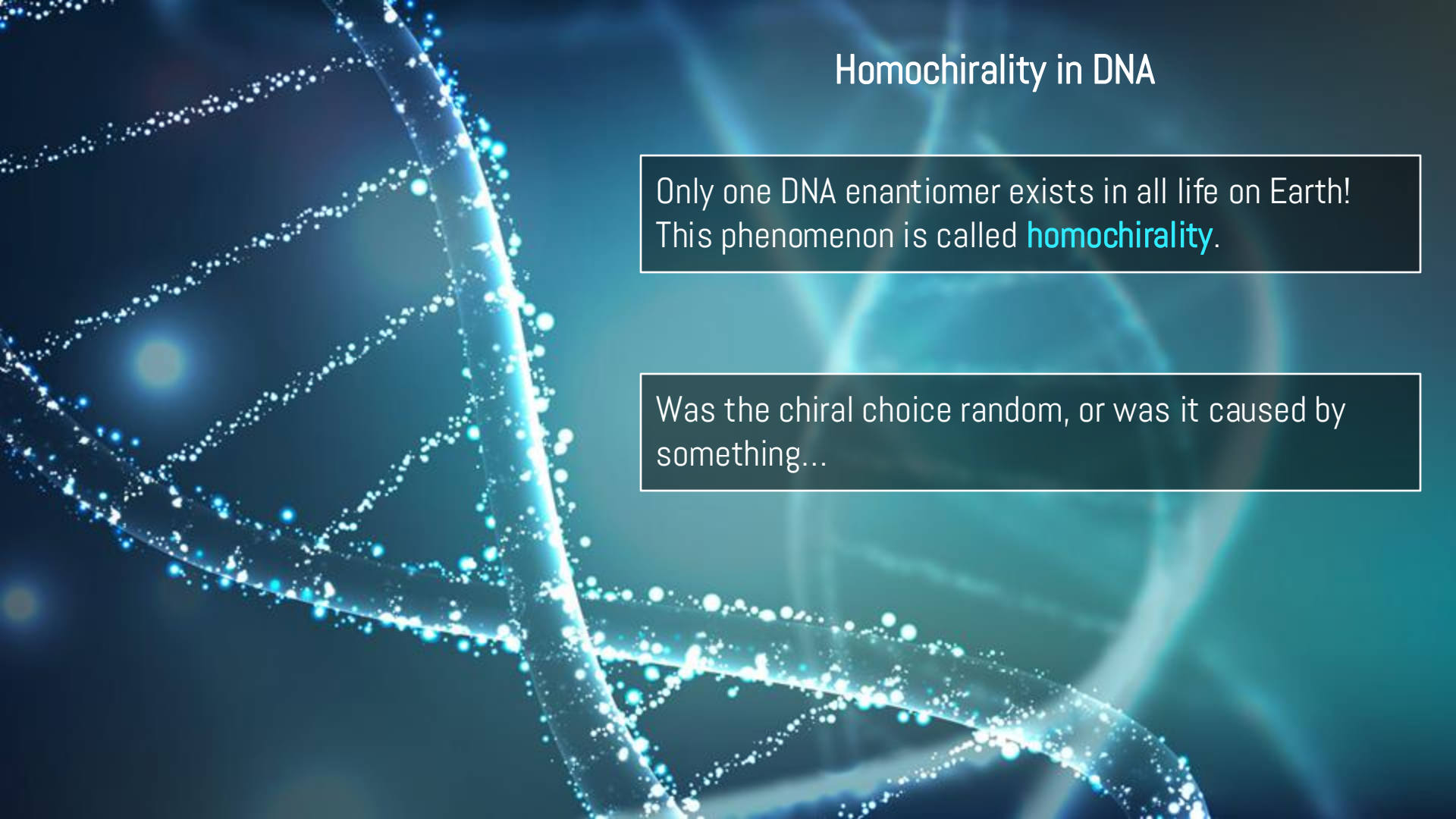
LibreTexts. (n.d.). *Illustration of chiral molecules* [Image]. LibreTexts Chemistry. https://chem.libretexts.org/

Chirality



In chiral environments, the chirality of the enantiomers will affect their interactions.

LibreTexts. (n.d.). *Illustration of chiral molecules* [Image]. LibreTexts Chemistry. https://chem.libretexts.org/



Homochirality in DNA

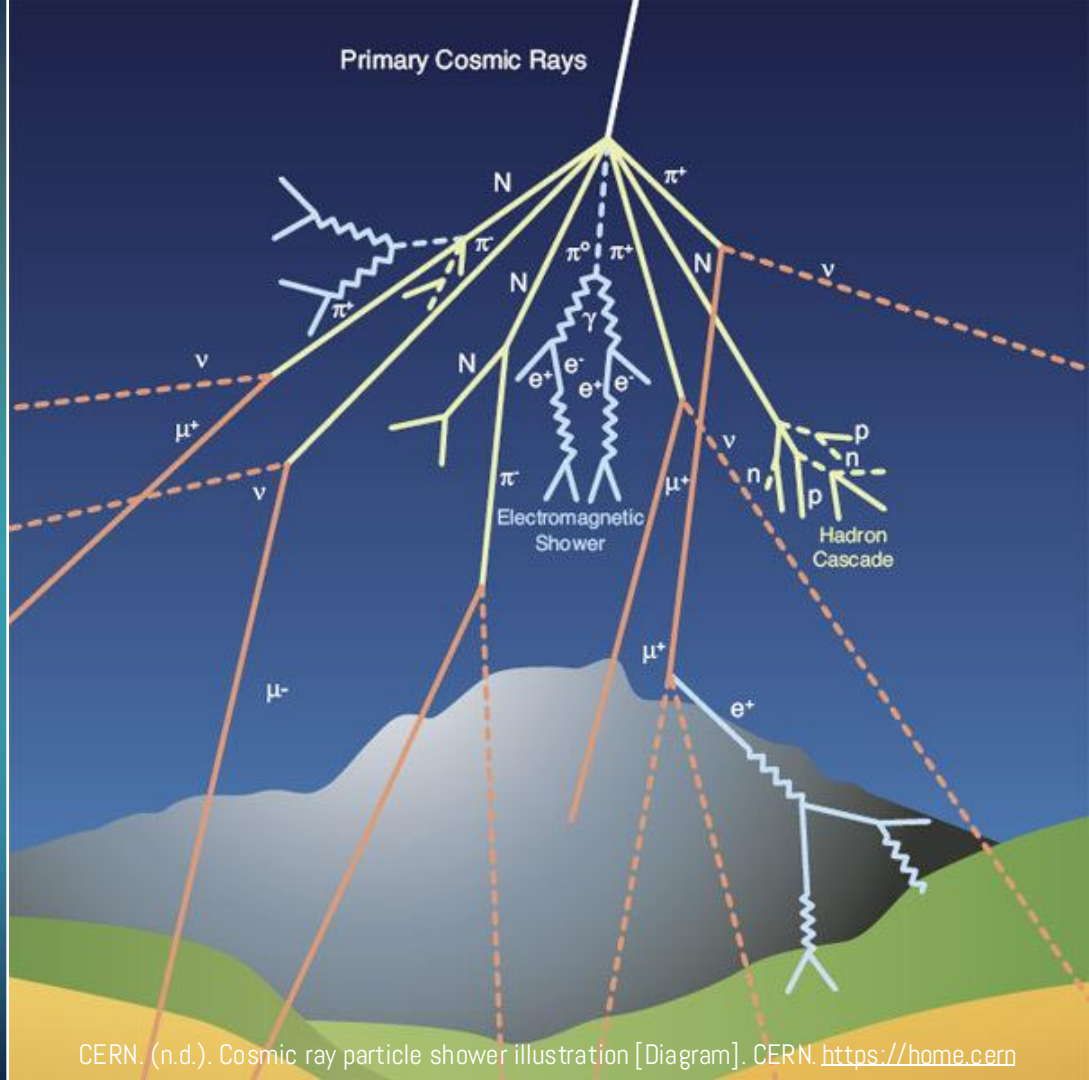
Only one DNA enantiomer exists in all life on Earth! This phenomenon is called **homochirality**.

Was the chiral choice random, or was it caused by something…

Cosmic Ray Showers

At Earth's surface, muons dominate!

Why else are these muons interesting?



CERN. (n.d.). Cosmic ray particle shower illustration [Diagram]. CERN. https://home.cern

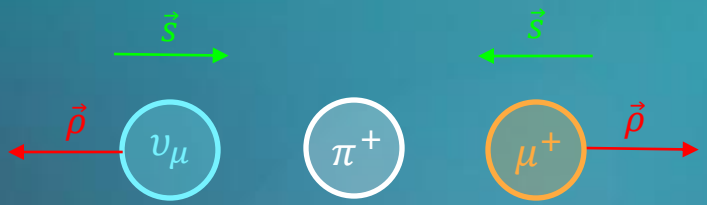
Parity Violation

Parity Transformation

$(x, y, z) \longrightarrow (-x, -y, -z)$

$\vec{\rho} \longrightarrow -\vec{\rho}$

$\vec{s} \longrightarrow \vec{s}$



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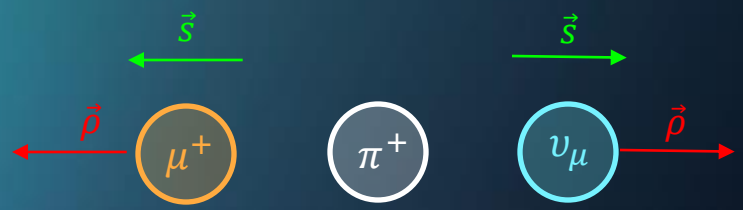

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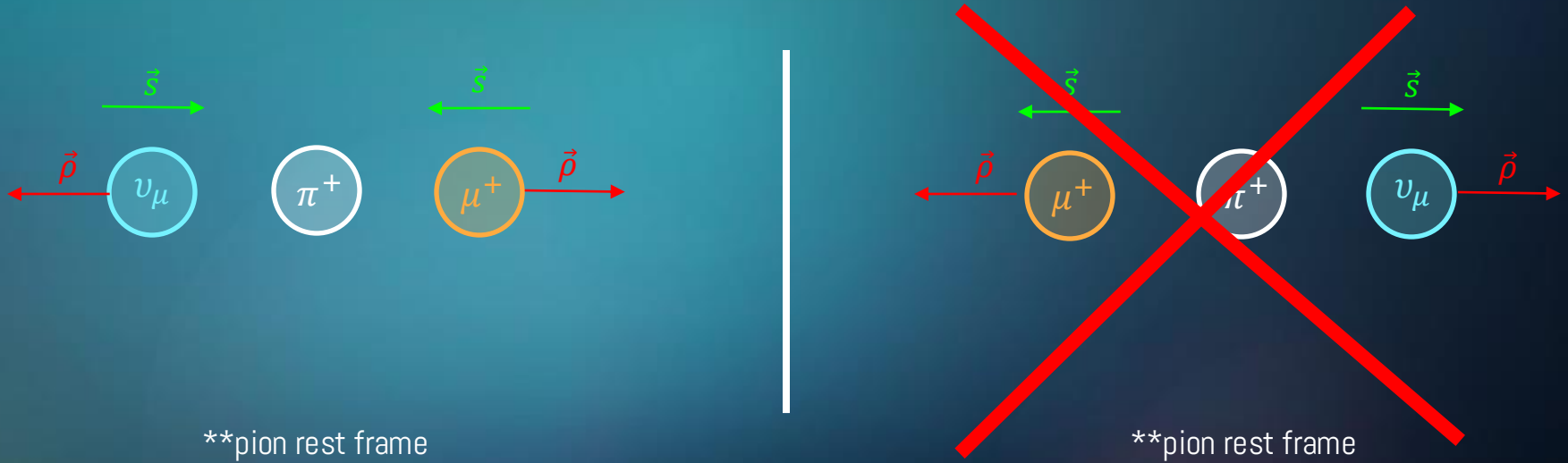

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Spin Polarization

$$P = \frac{N_{\uparrow\uparrow} - N_{\uparrow\downarrow}}{N_{\uparrow\uparrow} + N_{\uparrow\downarrow}}$$

$N_{\uparrow\uparrow}$: number of muons with spin parallel to momentum

$N_{\uparrow\downarrow}$: number of muons with spin antiparallel to momentum

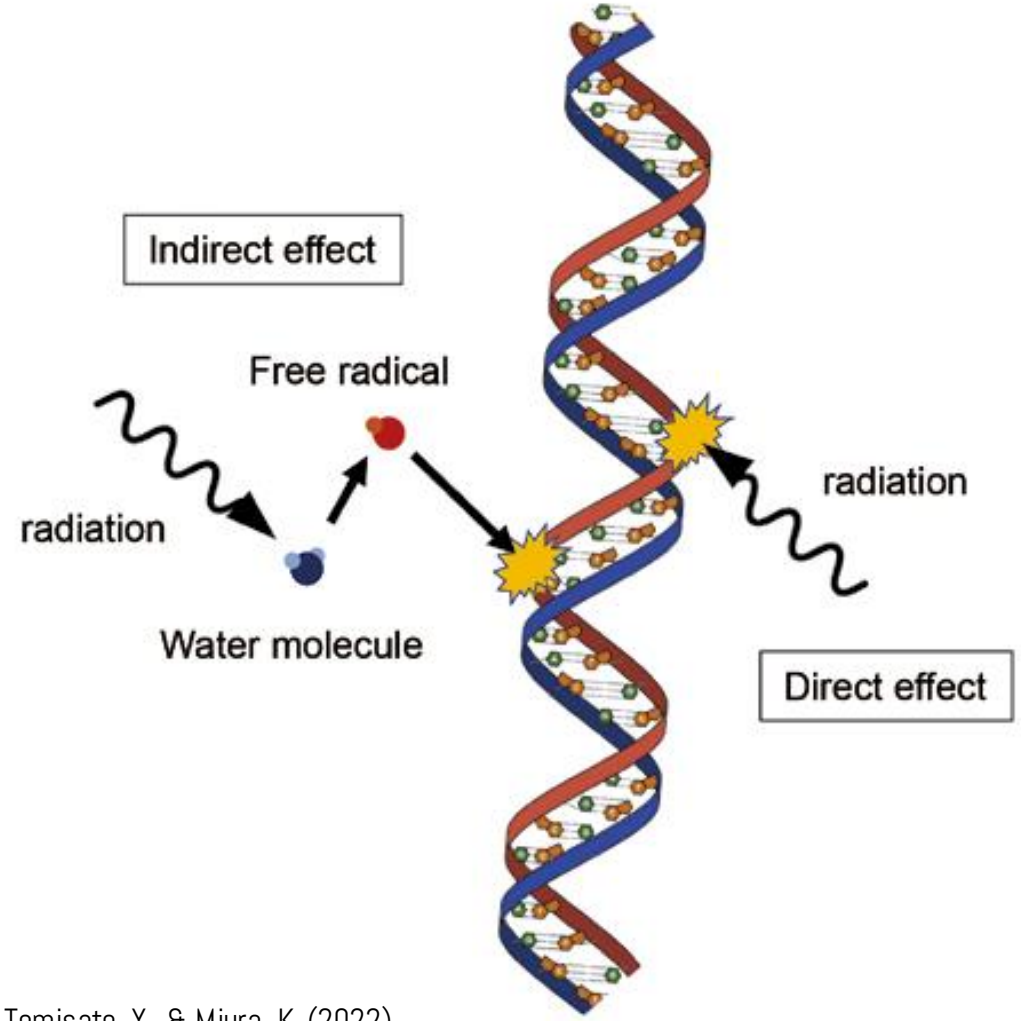
Cosmic ray muons are spin-polarized.

Muons retain their polarization.

DNA Damage

Muon radiation primarily damages DNA through ionization.

Indirect Damage vs Direct Damage



Tomisato, Y., & Miura, K. (2022)

Hypothesis

Premise 1

Cosmic ray muons cause DNA mutations which played a significant role in the evolution of life.

de Groen, P. C. (2022)

Premise 2

The spin polarization introduces a chiral environment that is relevant to chiral chemical reactions.

Globus, N., Fedynitch, A., & Blandford, R. D. (2021)

Hypothesis

The spin polarization of cosmic ray muons is directly responsible for the chiral choice observed in DNA today.

Globus, N., & Blandford, R. D. (2020)

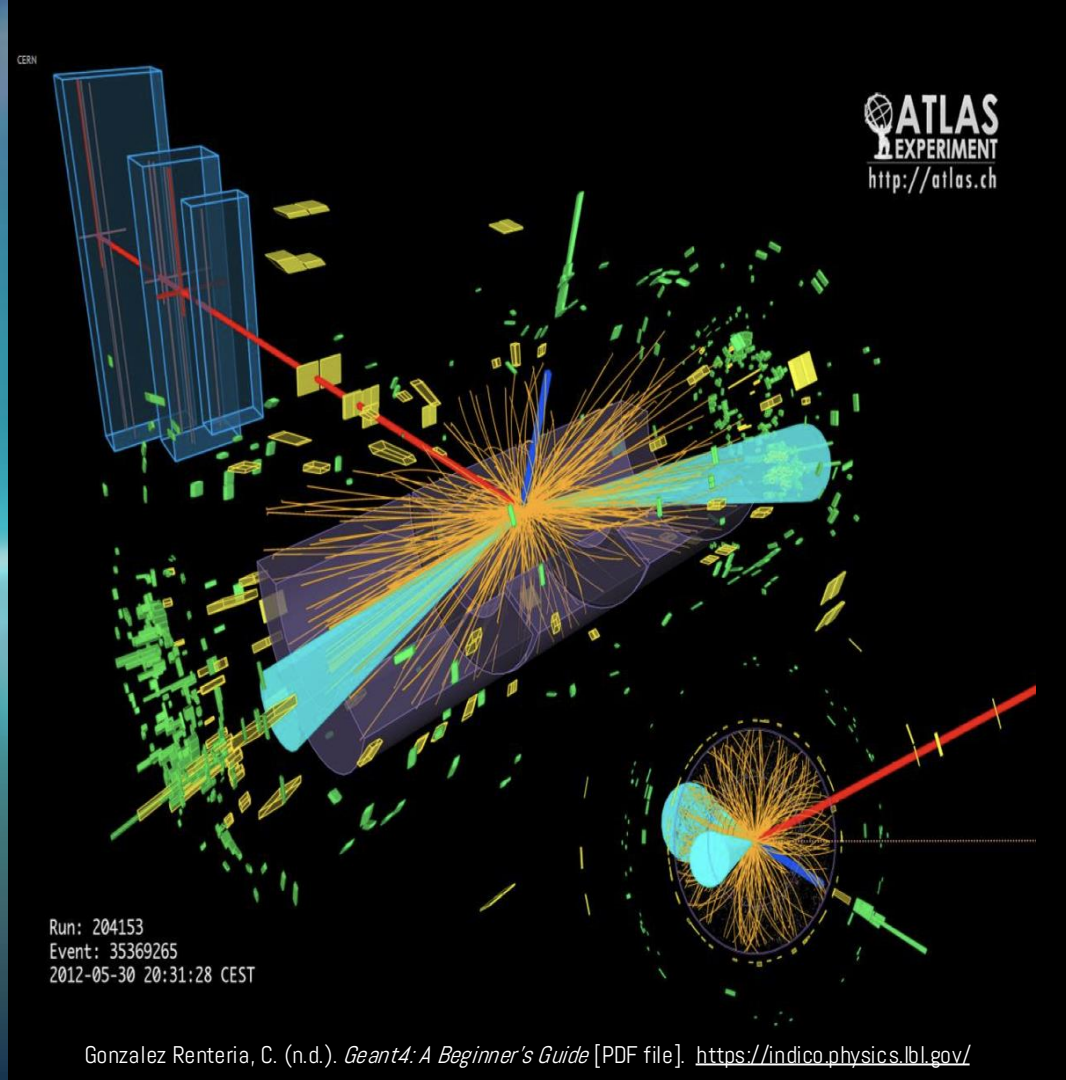
02
Methods

Geant4

Monte Carlo simulation toolkit created by CERN.

Passage of particles and radiation through matter.

Low accuracy, fast performance.



Gonzalez Renteria, C. (n.d.). *Geant4: A Beginner's Guide* [PDF file]. https://indico.physics.lbl.gov/

Geant4-DNA

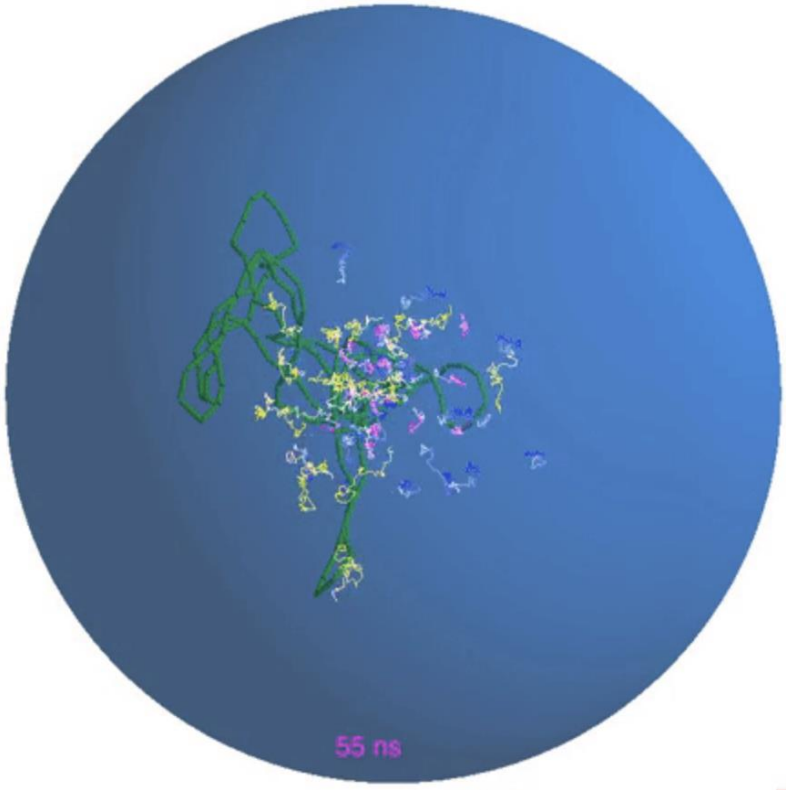
Extension of the Geant4 toolkit.

Models for lower energies.

Includes chemistry models.

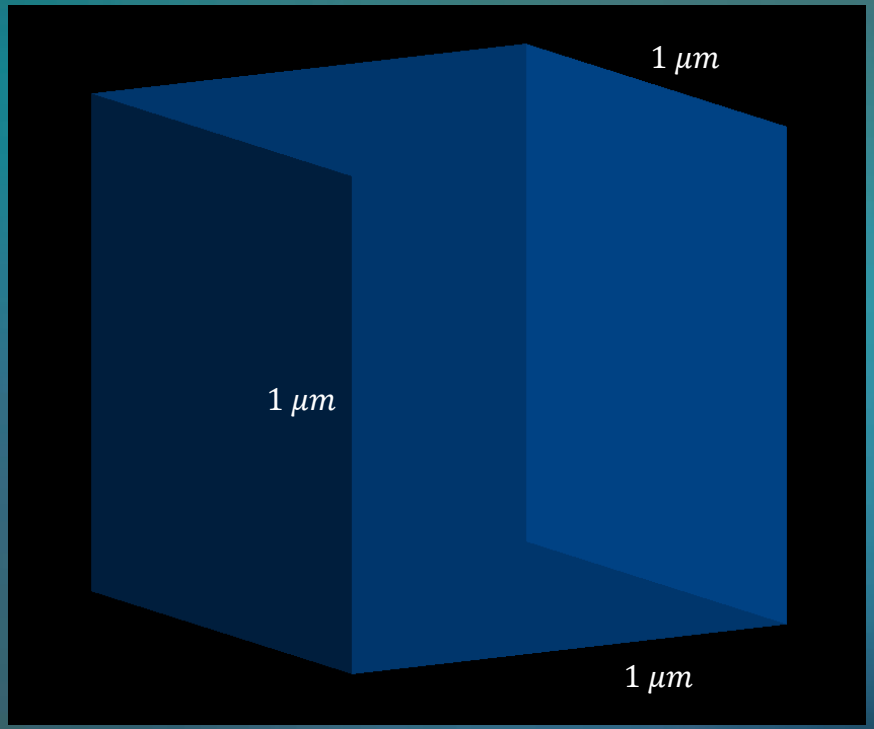
High accuracy, slow performance.

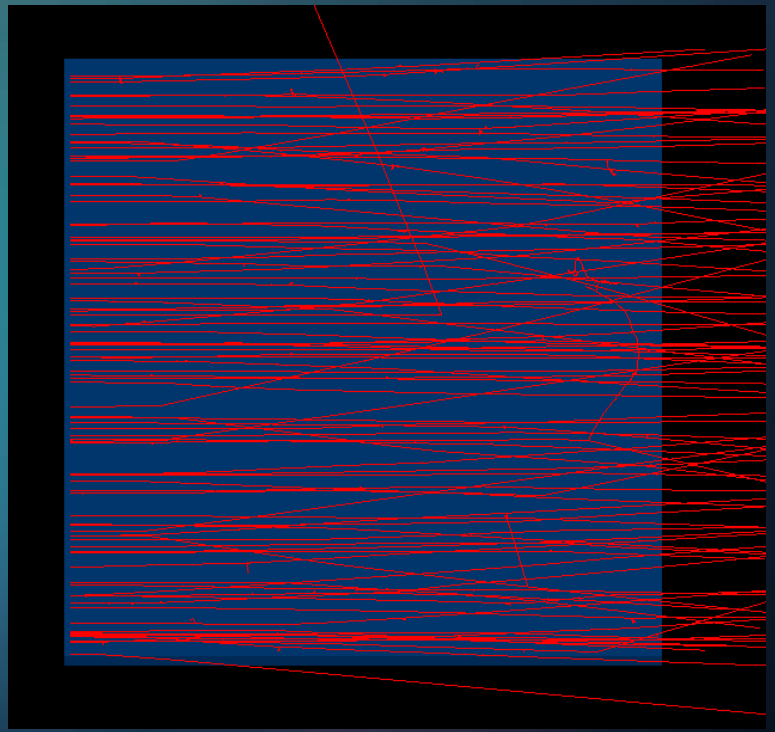
Unfortunately, no muons.



Stepan, V. (n.d.). *Geant4-DNA chemistry stage* [Image]. Geant4-DNA. https://geant4-dna.in2p3.fr

Our Geant4-DNA Simulation





Approximating 65 MeV/c Muons as Electrons

$\boldsymbol{\beta\gamma}$ *factor*

We simulate electrons with equivalent stopping power as muons. This means using equivalent $\beta\gamma$.

$$\rho = \gamma m v$$

$$\frac{\rho}{mc} = \beta\gamma, \quad \text{where } \beta = \frac{v}{c}$$

Experimental Muon Beam

$$\beta\gamma = \frac{65\frac{MeV}{c}}{\left(105.7\frac{MeV}{c^2}\right)*c} = 0.61$$

Simulated Electrons

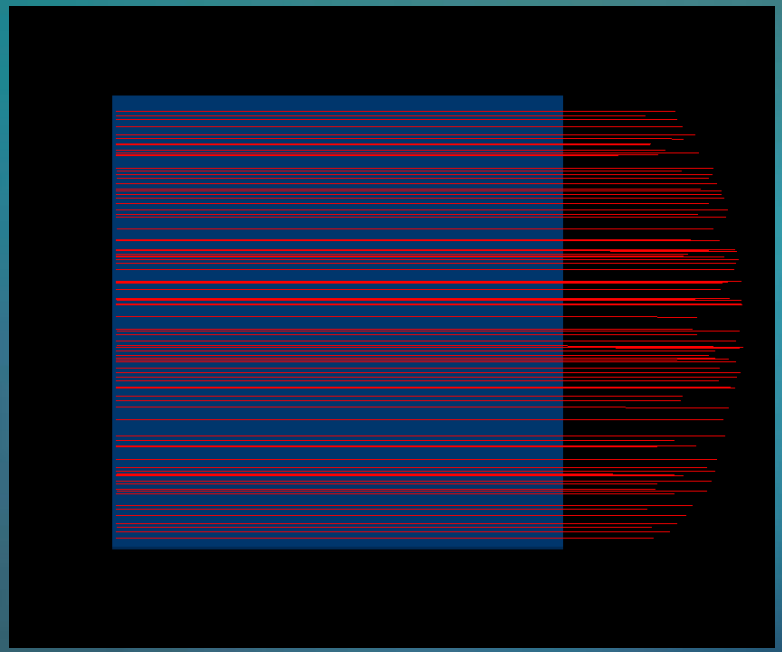
$$\rho_e = \beta\gamma mc$$

$$\rho_e = (0.61)\left(0.511\frac{MeV}{c^2}\right) * c$$

$$\boldsymbol{\rho_e = 0.31\ \frac{MeV}{c}}$$

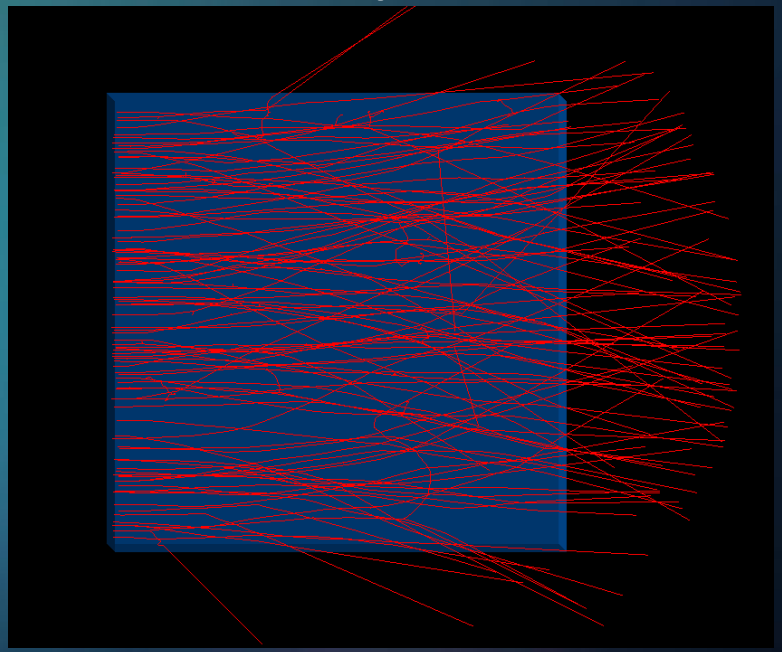
Approximating 65 MeV/c Muons as Electrons

Scattering



$\rho_e = 65\ MeV/c$

Cube side length: $\mathbf{10}\ \boldsymbol{\mu m}$



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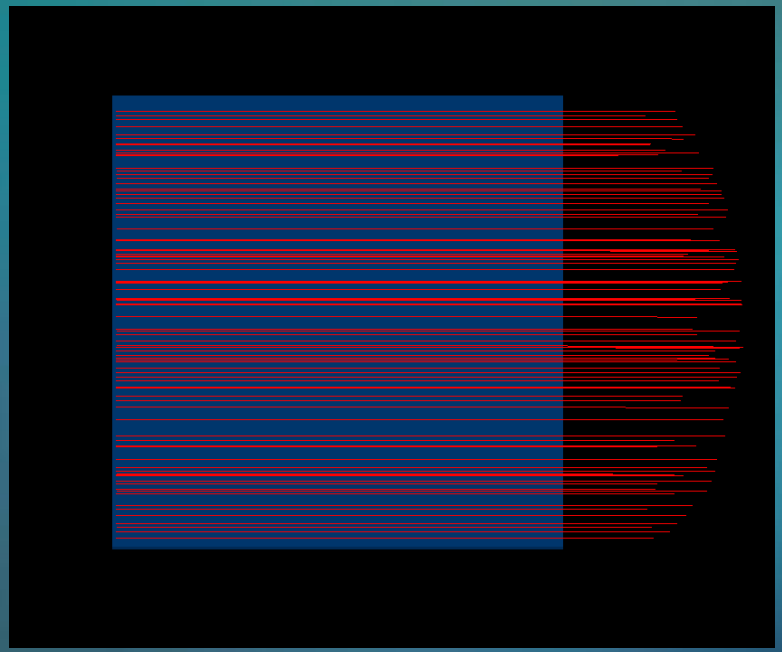
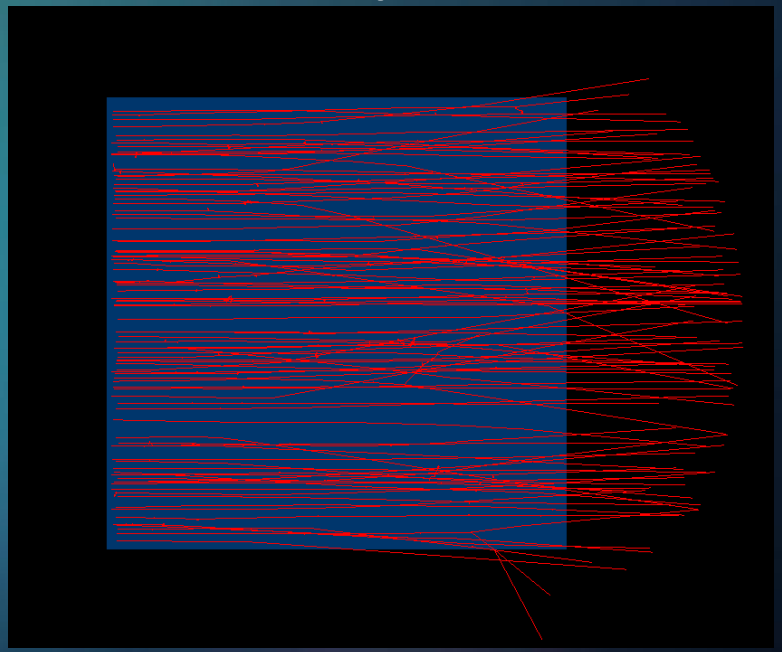
Approximating 65 MeV/c Muons as Electrons

Scattering



$\rho_e = 65\ MeV/c$

Cube side length: $1\ \mu m$



$\rho_e = 0.31\ MeV/c$

03
Results

Radiochemical Yields

$$G = \frac{molecules}{100\ eV}$$

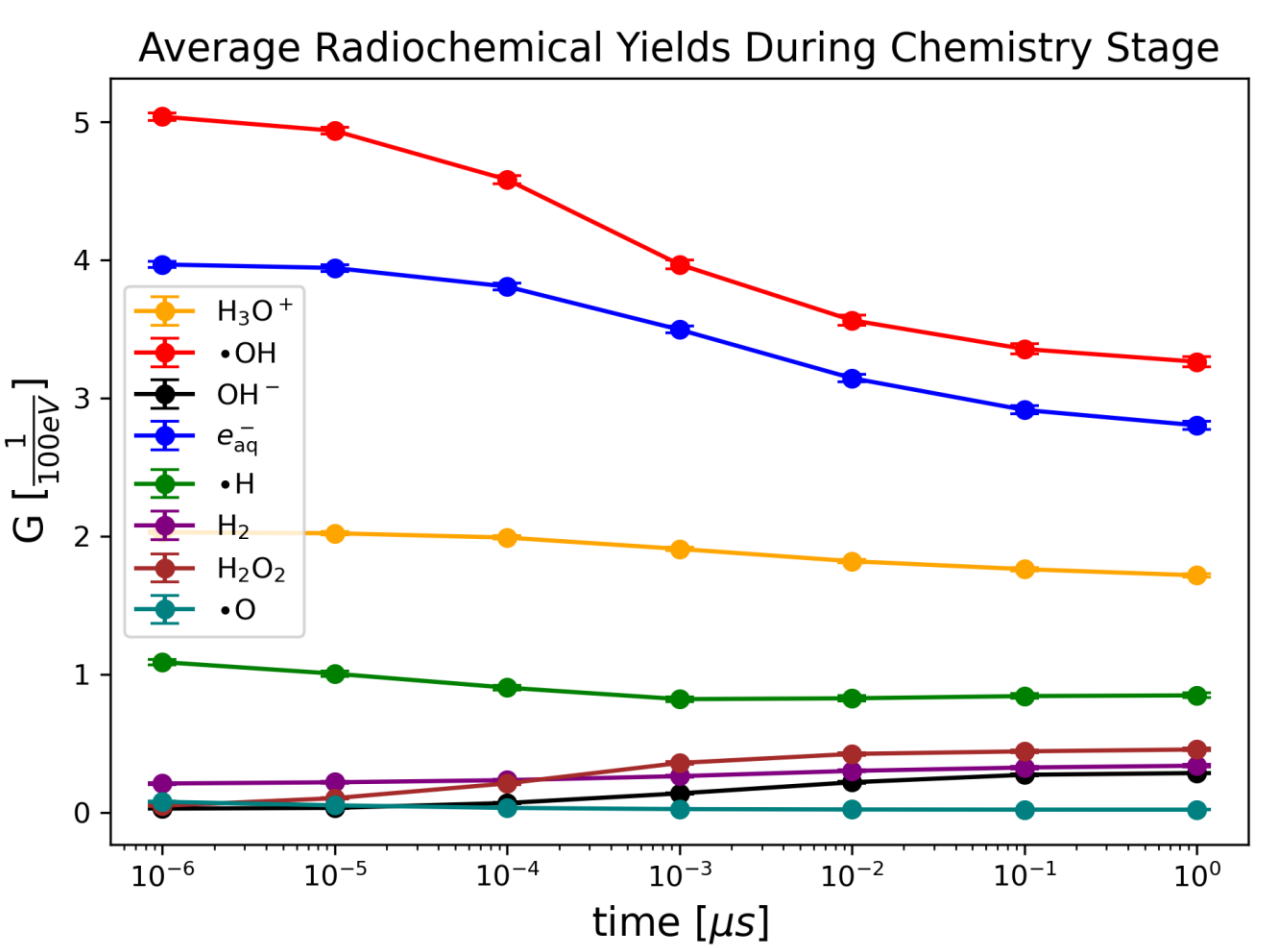


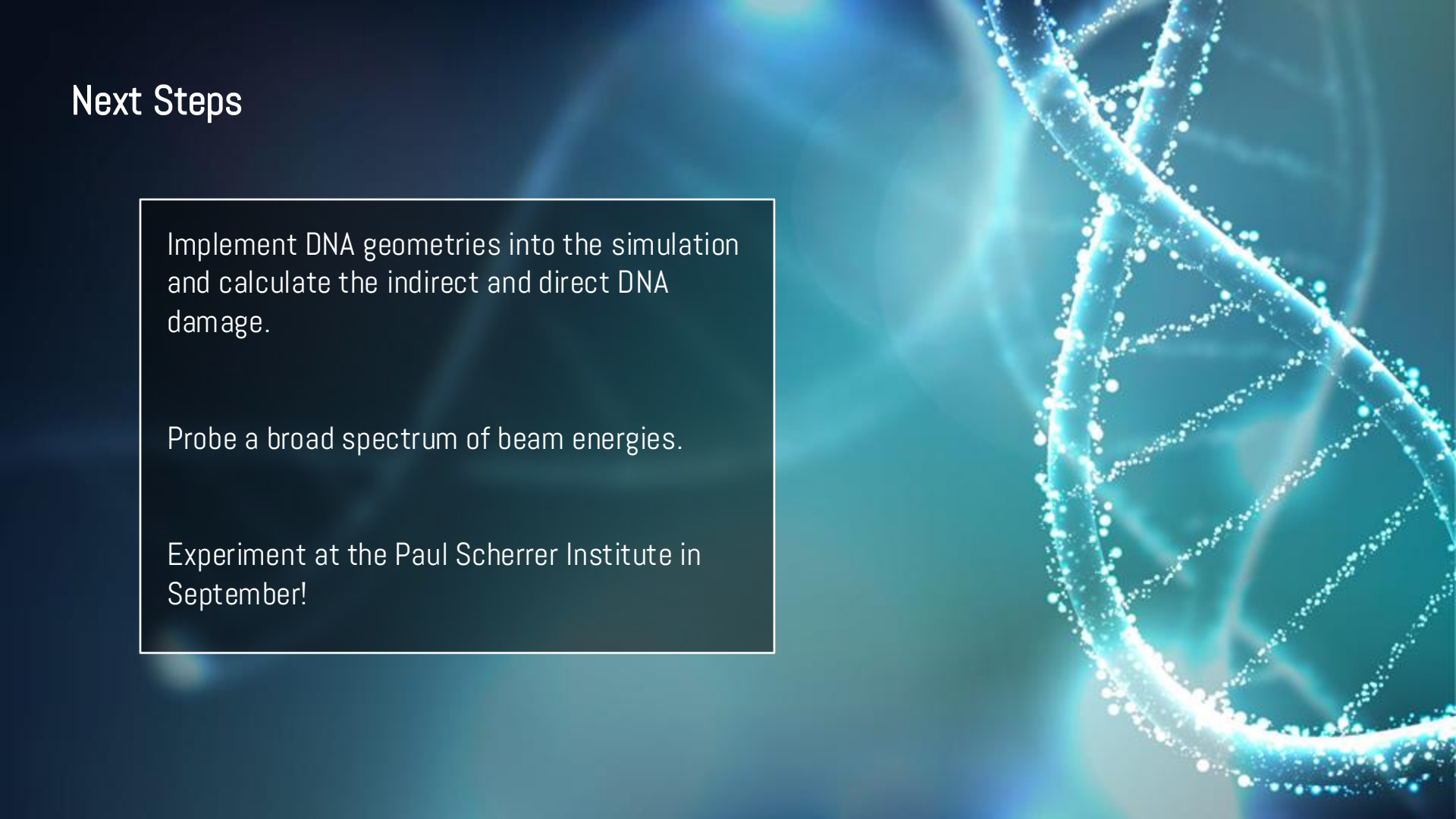
Figure 1: Radiochemical yields of water radiolysis products, for a 0.31 MeV/c uniformly distributed electron beam through a water cube of side length 1 μm.

Next Steps

Implement DNA geometries into the simulation and calculate the indirect and direct DNA damage.

Probe a broad spectrum of beam energies.

Experiment at the Paul Scherrer Institute in September!



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Globus, N., Blandford, R. D., & Fedynitch, A. (2021). Polarized muons and the origin of biological homochirality. *arXiv preprint arXiv:2110.01975*

Tomisato, Y., & Miura, K. (2022). Chromosome spread after Giemsa staining [Figure]. In Cytogenetic biodosimetry in radiation emergency medicine: 3. The basics of chromosomes for biodosimetry. *Radiation Emergency Medicine, 11(2), 82–86.*

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SIMONS FOUNDATION

Stanford University

STONY BROOK UNIVERSITY
SIMONS STEM SCHOLARS

THANKS

Does anyone have any questions?

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Backup Slides

Our Geant4-DNA Simulation