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LIDINE 2025: LIght Detection In Noble Elements

A Comprehensive Monte Carlo Simulation Tool on Electron Transport in Noble Gases and Liquids

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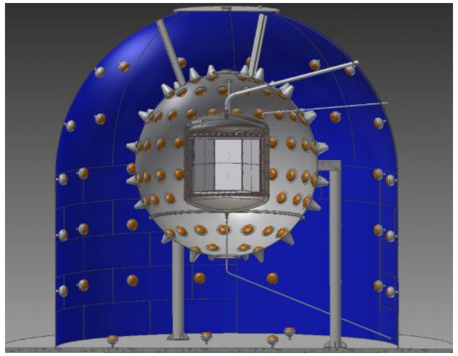
PART 01 **Introduction**

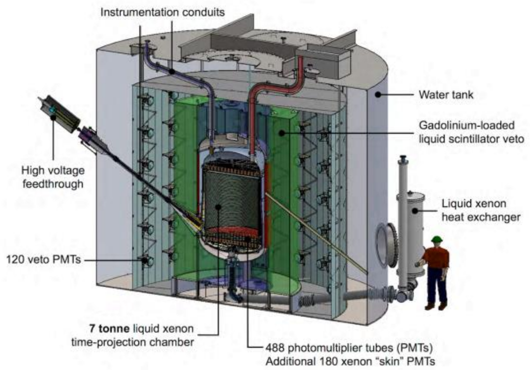
1. introduction

The micro-physics study of electron transport in noble gases and liquids holds significance for particle detection technologies.

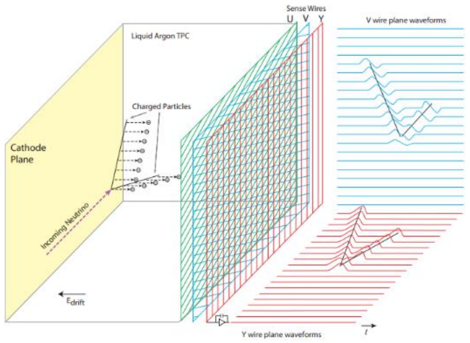
■ Neutrino/dark matter detection



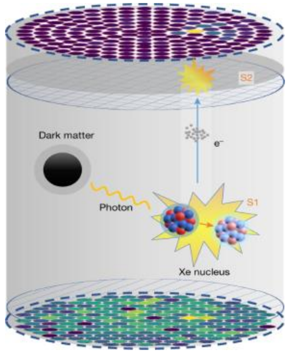
DarkSide-50 (dual-phase LAr)



LUX-ZEPLIN(LXe)



MicroBooNE(LAr)



Pandax(LXe)

■ Electron transport simulation tools available

Mainly for gas and solid:

Type	Name	Application
for gas and solid	MagBoltz /PyBoltz…	Garfield++
For liquid	TRASLATE	gas/liquid Ar
For liquid	*Yj Xie et al.*	liquid Ar/Xe

■ Research gap

- ☐ **The MC tools for electron transport in noble gases and liquids remain incomplete.**
- ☐ **More accurate or optimized liquid simulation model.**

1 introduction

■ Objectives

- □ This work aims to establish a comprehensive Monte Carlo tool for noble gases He/Ne/Ar/Kr/Xe and liquids Ar/Kr/Xe in electric field from 10 V/cm- 2000 V/cm.
- □ validating the key electron swarm parameters: drift velocity and diffusion coefficients

■ Research Value

- □ Predict the electron properties that are poorly measured or not measured, eg. the diffusion in LAr /LKr.
- □ Potential applications ranging from microscopic mechanism studies to macroscopic detector performance analysis using the parameters evaluated herein .

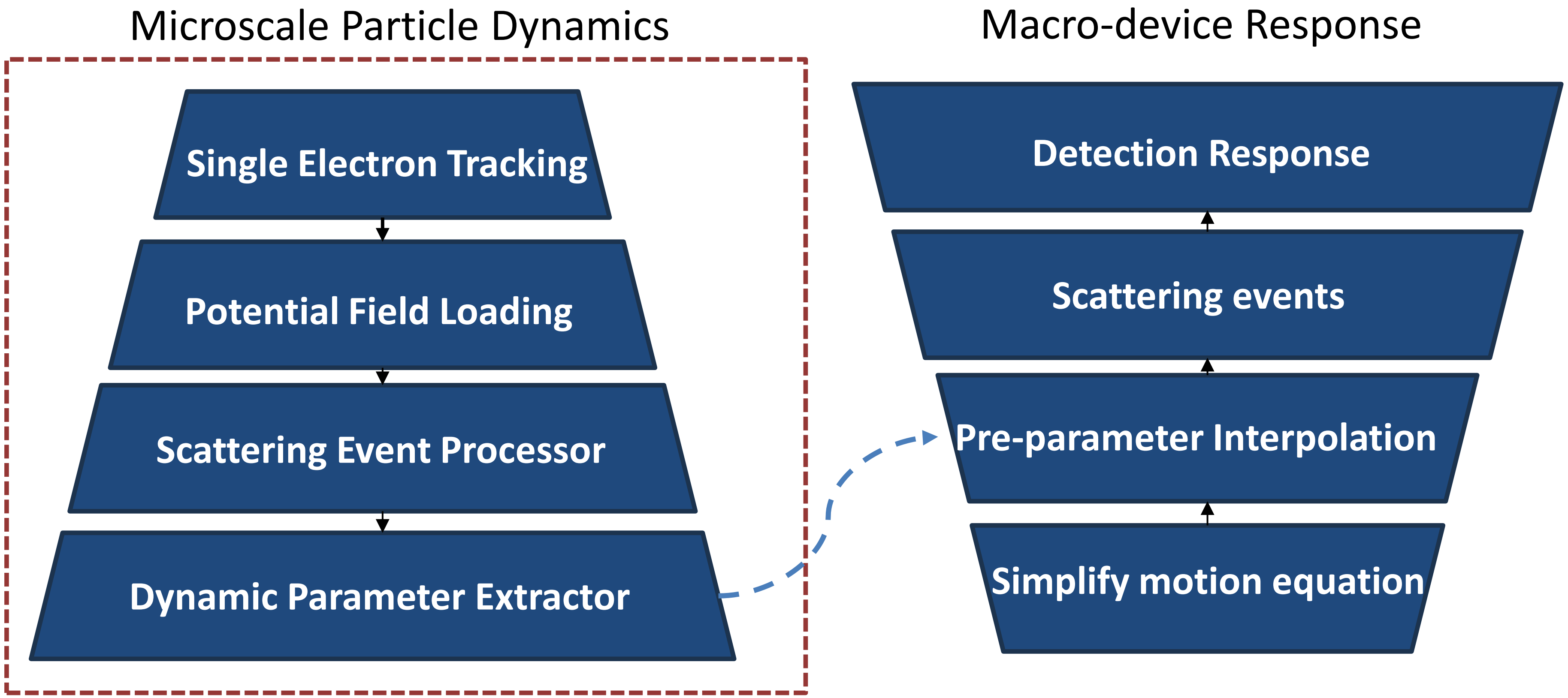
PART 02 **Simulation framework**

2.1 simulation approach

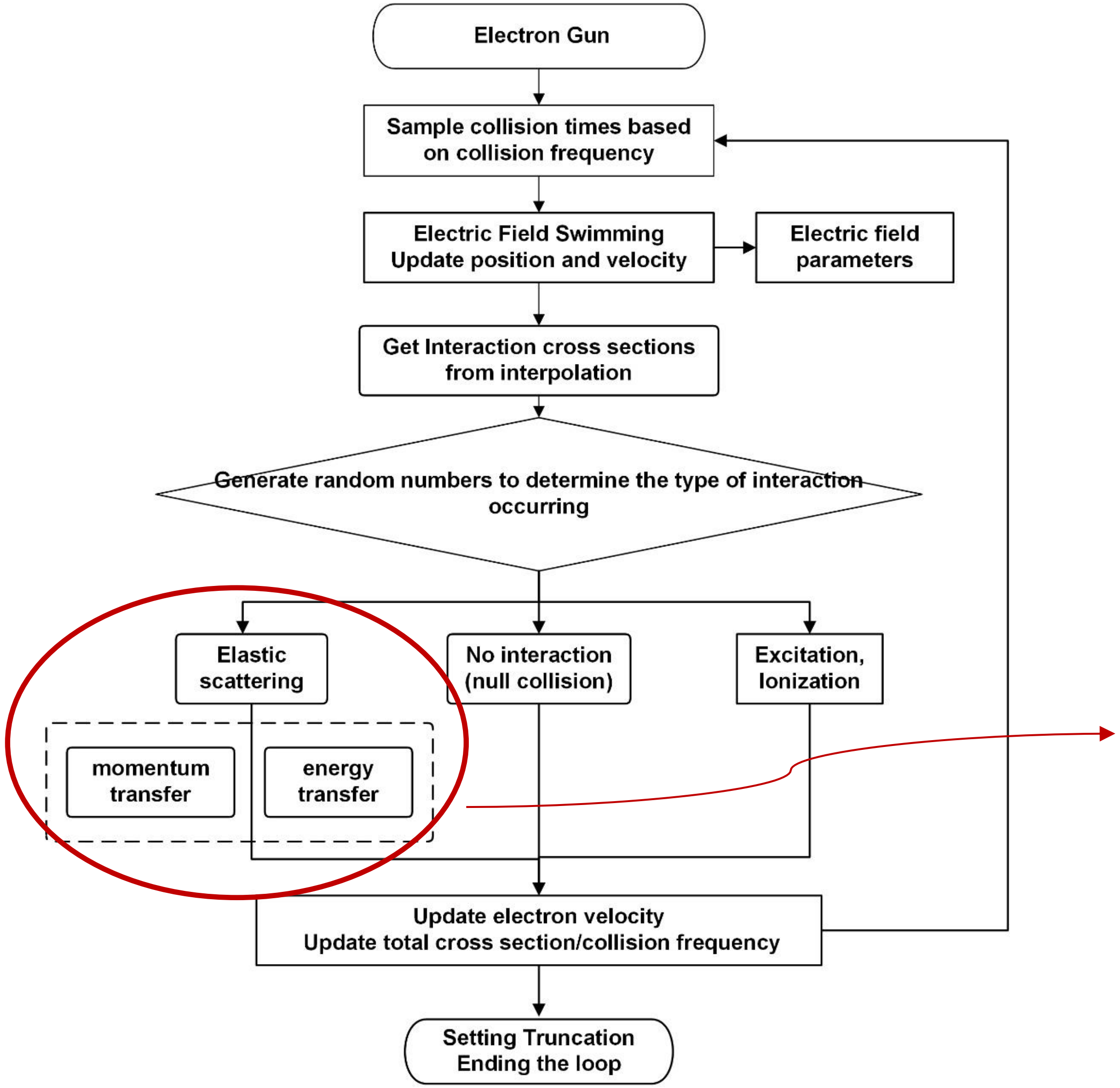
Electron transport simulation methodologies are primarily categorized into two approaches:

(1) High-fidelity simulation for microscopic mechanism

(2) Parameterized simulation for macroscopic detector systems.



2.1 Basic simulation framework



The framework of the MC simulation for electron transport

- Electron-atom collisions.
- Elastic scattering, excitation, ionization.
- For electric field: null collision technique.

  2x, 5x, and 10x collision frequencies are implemented.
- C++.

The difference between electron transport in liquid and gas

- the increase in atom density from gas to liquid phase
- the low energy region of interest for electrons

the electron wavelength is comparable to the atom distance.

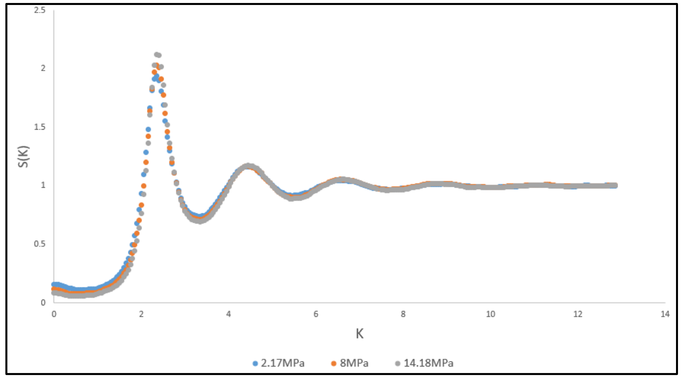
coherent scattering

2.2 liquid phase simulation model

- Electron is considered not only as a single particle, but more as waves interacting with multiple scattering centers.
- The positions of the atoms are spatially correlated

  liquid structure factor S(k)

- Cohen and Lekner theory [Cohen M.H., et al. (1967)], the mean free path of electron elastic collisions in liquids is divided into two types:



structure factor of liquid neon [L. A. de Graaf,et al. (1971)]

energy transfer

- change the electron’s energy without changing the direction

$$\Lambda_0(\epsilon)^{-1} = N2\pi \int_0^{\pi} \sigma(\theta,\epsilon)(1 - P_i(\cos\theta)) \sin\theta d\theta$$
$$= N\sigma(\epsilon)$$

momentum transfer

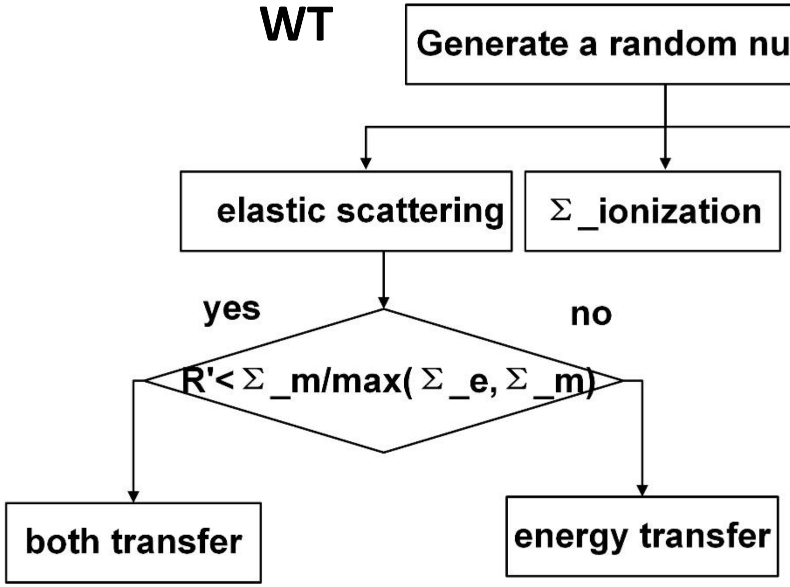
- change the direction of the electron without changing the energy

$$\Lambda_1(\epsilon)^{-1} = N2\pi \int_0^{\pi} \sigma(\theta,\epsilon)(1 - P_i(\cos\theta))S(K) \sin\theta d\theta$$
$$= N\sigma(\epsilon)S(K)$$

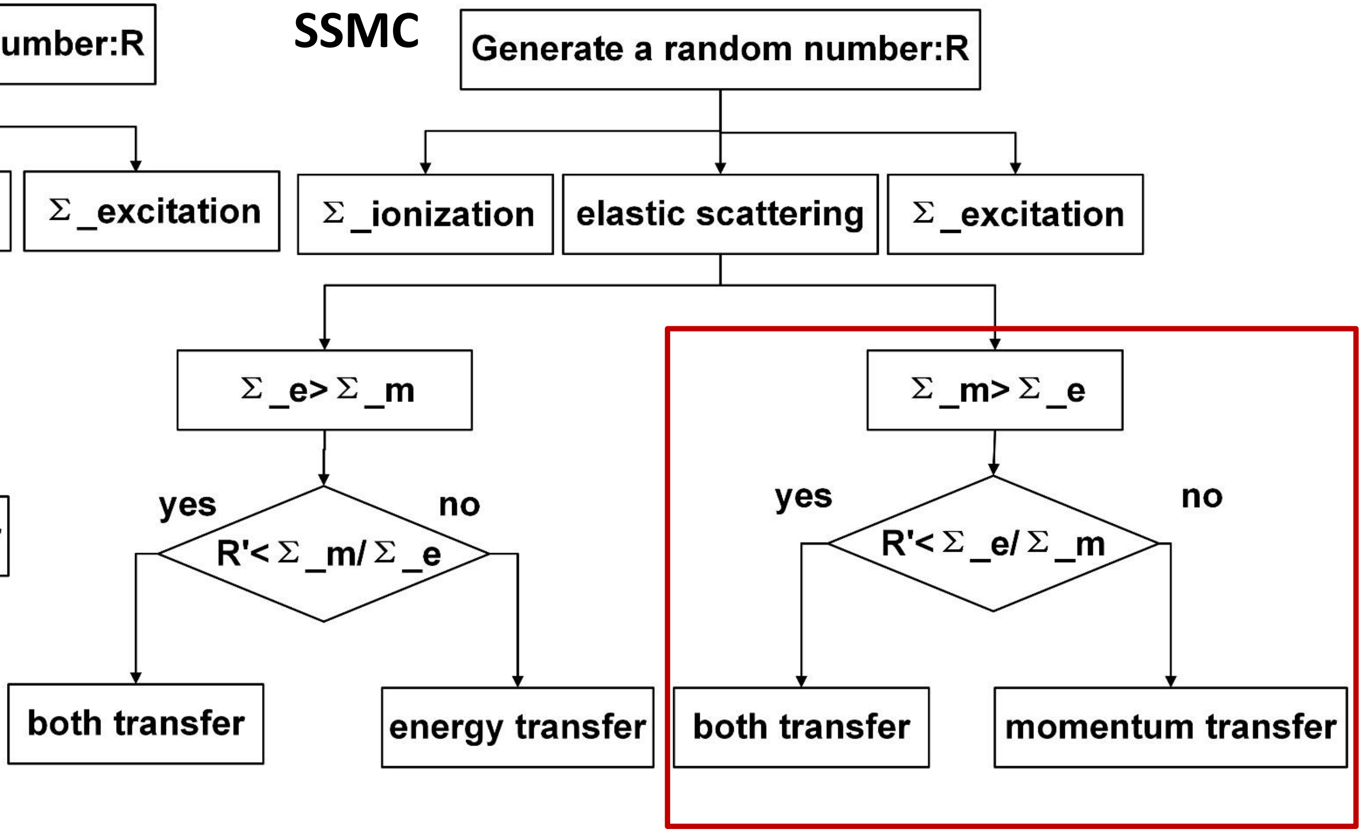
2.2 liquid phase simulation framework

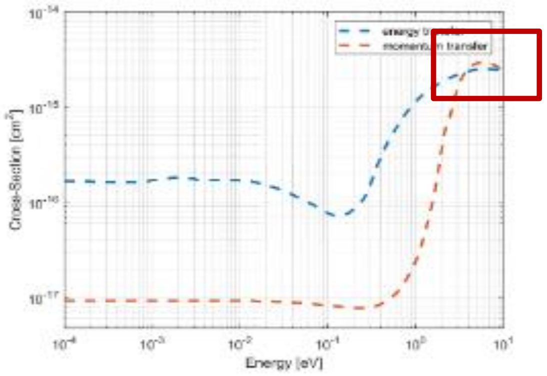
WT(Tattersall,W) and SSMC(State Structure MonteCarlo) models for electron elastic scattering simulation in liquids.

WT



SSMC





energy transfer and momentum transfer cross sections from Y.Sakai

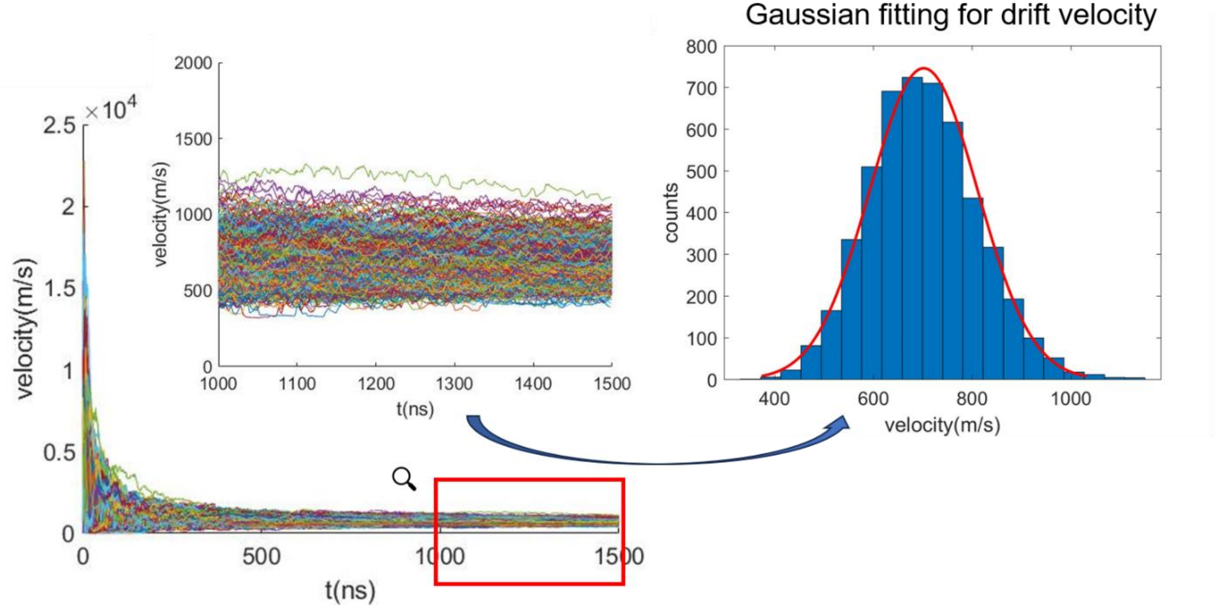
PART 03 **Result and Discussion**

3.1 swarm parameters in simulation

How to verify the tool？

drift velocity

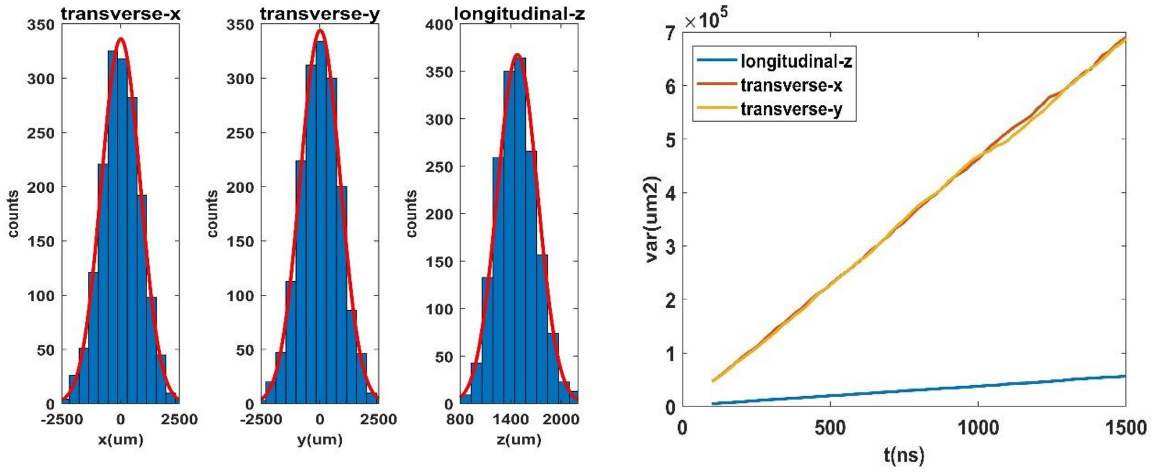
Taking electrons with the initial energy of 1 eV at 295K as an example.



electron drift velocity over time in 100V/cm, with demonstrated local zoom details and Gaussian fit to drift velocity

diffusion coefficient

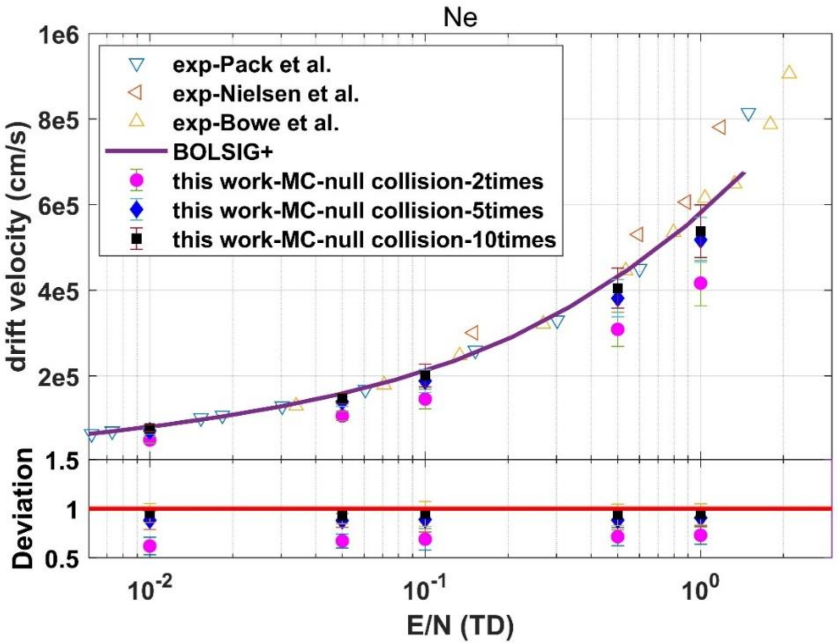
$$f(r,t)=\frac{N}{4\pi Dt}\exp\frac{-r^2}{4Dt}\qquad D=\frac{\sigma^2}{2t}$$

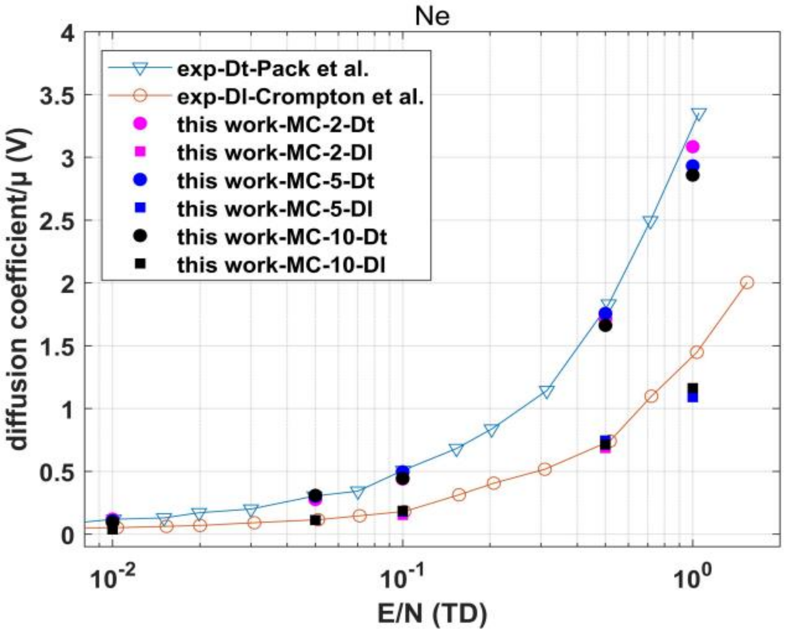


transverse and longitudinal diffusion of electrons

3.2 gas phase

□ drift velocity and diffusion coefficient in gas phase

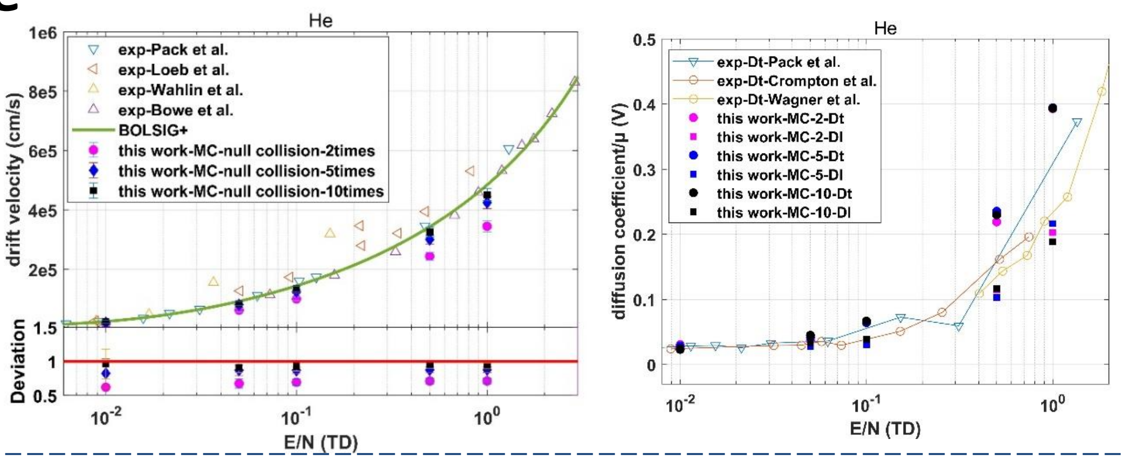




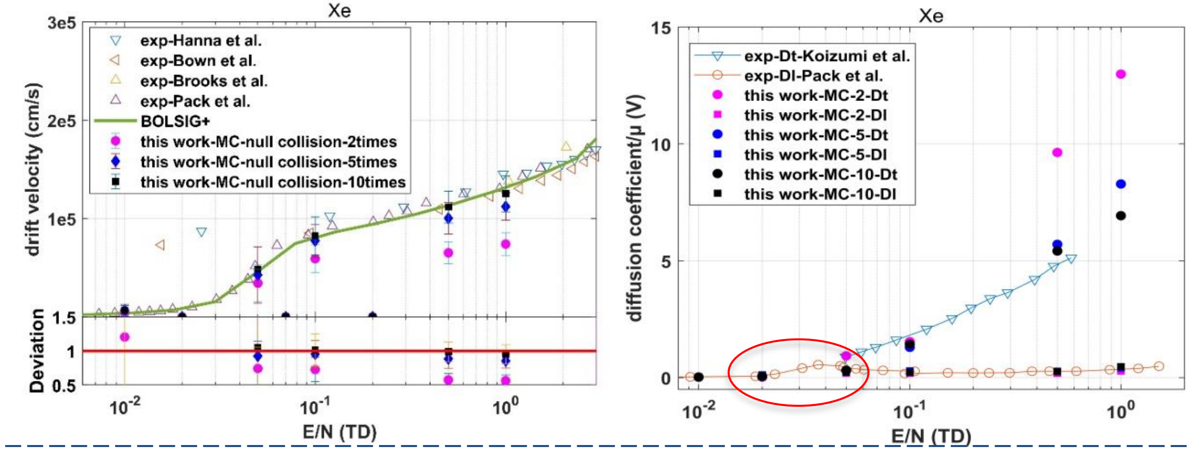
- Null collision technique : Opting for a collision frequency of 10x strikes a balance between simulation efficiency and accuracy.
- The effect of the electric field on the longitudinal diffusion coefficient is related to the trend of momentum transfer cross section with the change of energy.

3.2 gas phase

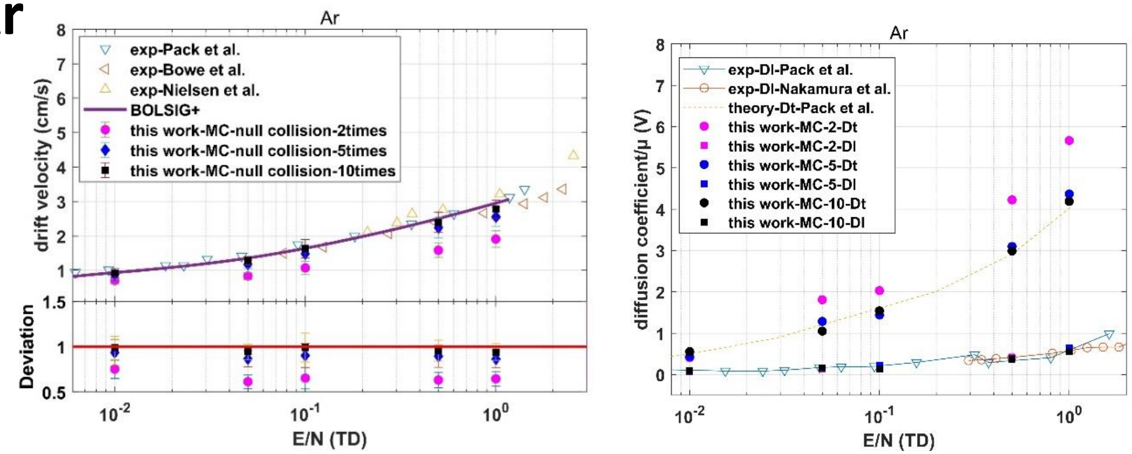
He



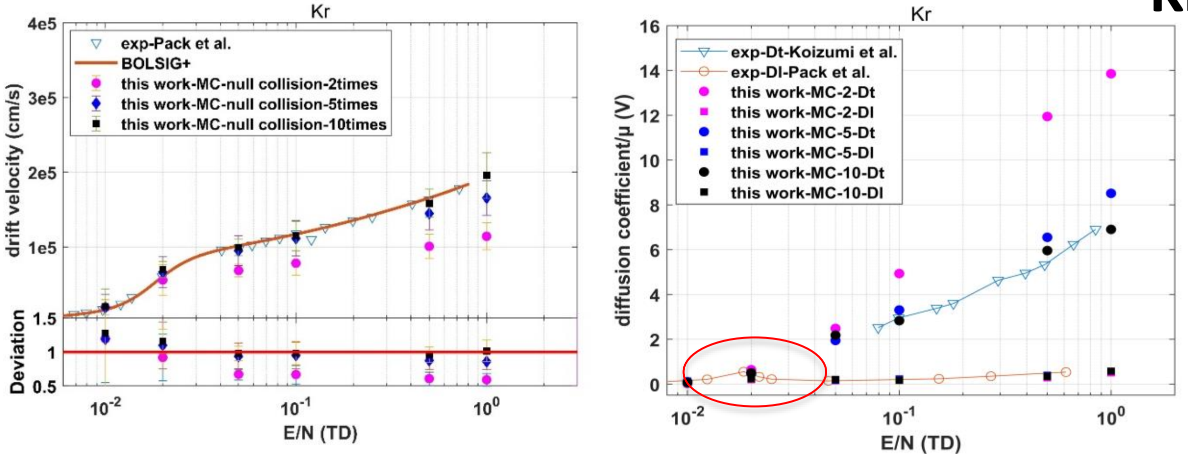
Xe



Ar



Kr

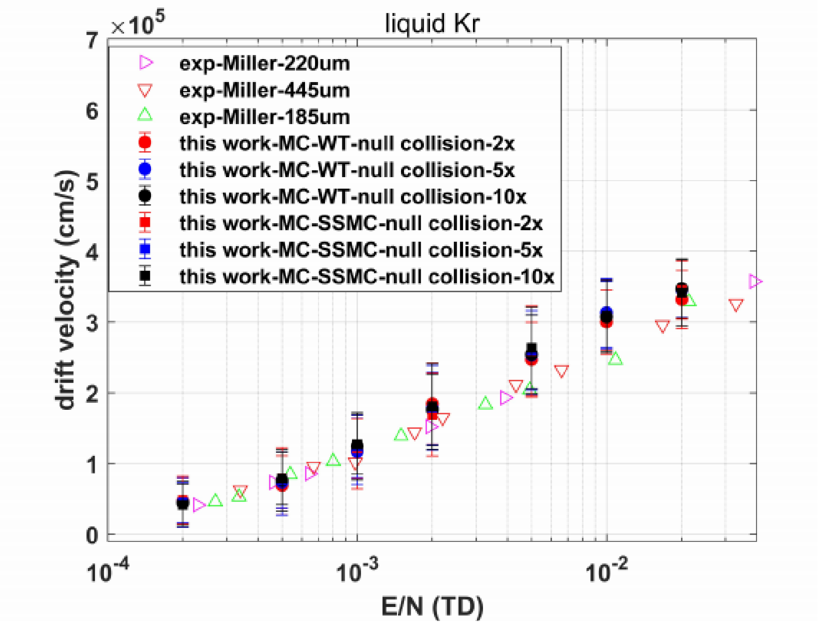


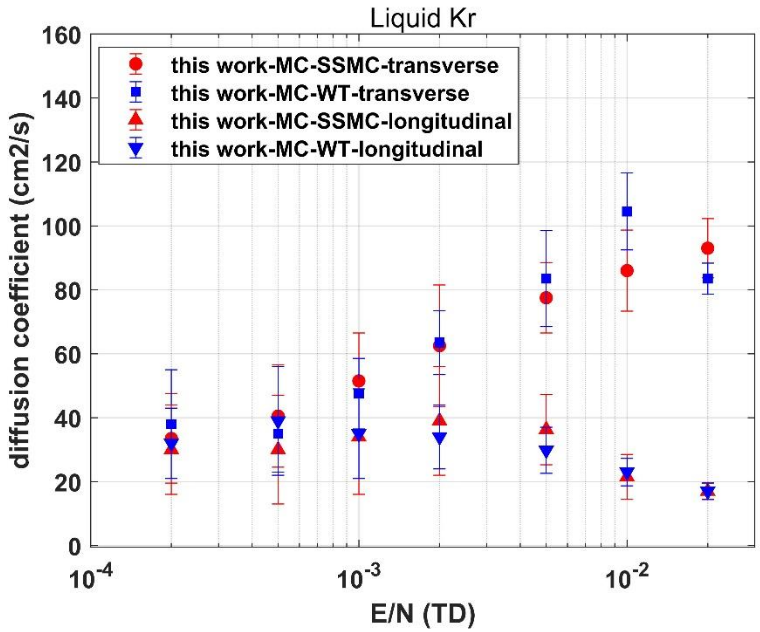
- For Ar, the transition point is below 0.01td (10V/cm).
- For Kr and Xe, the transition points for *Dl* occur at approximately 0.02td and 0.04td.

3.3 liquid phase

☐ drift velocity and diffusion in noble liquids

liquid Kr





- The simulated drift velocity in the WT and SSMC model exhibits a high level of consistency, which is as expected.
- Opting for a collision frequency of 2x .
- The reason for discrepancy between simulation results and the experimental data ：

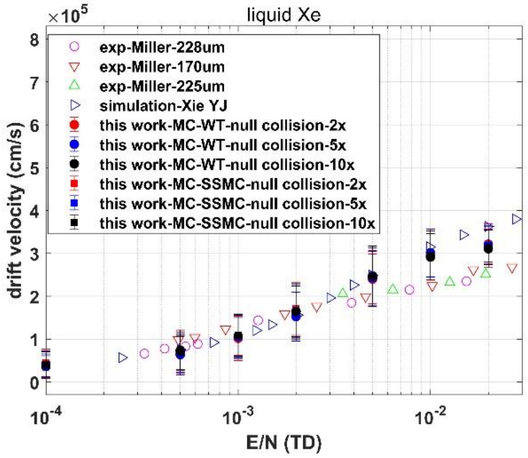
  The absence of electron recombination processes in the simulation.

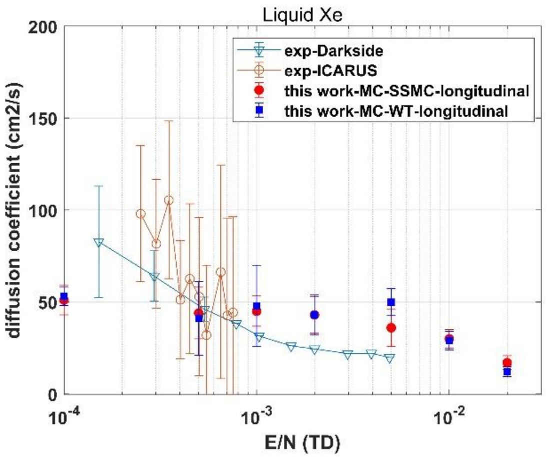
  The assumption of a pure environment in the simulation, whereas experimental setups may contain trace impurities.

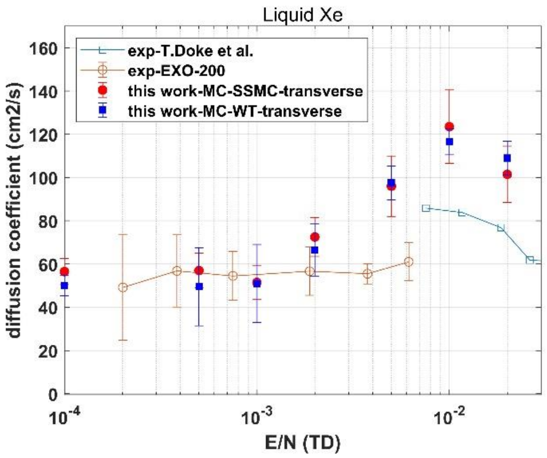
3.3 liquid phase

□ drift velocity and diffusion in noble liquids

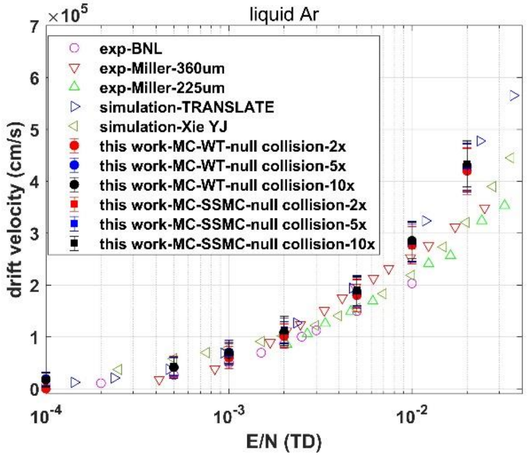
Liquid Xe

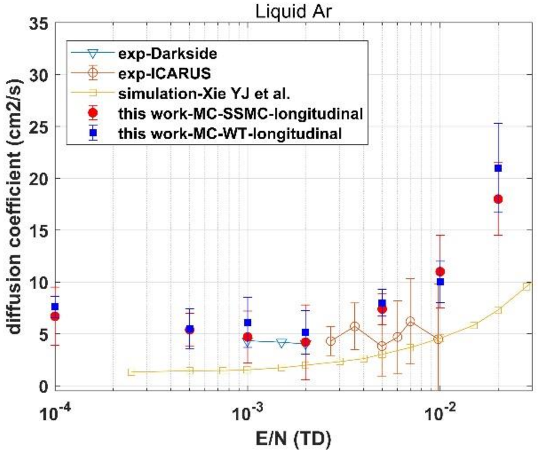


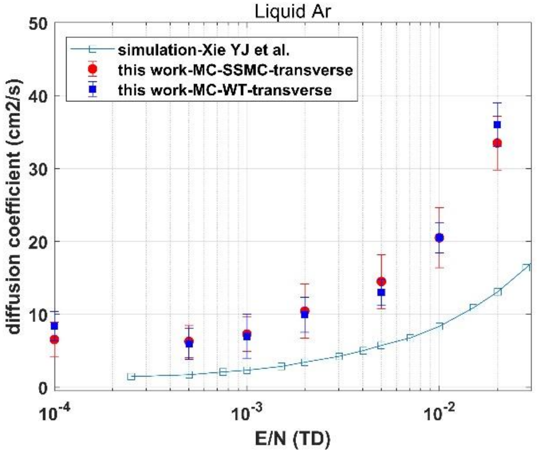




Liquid Ar







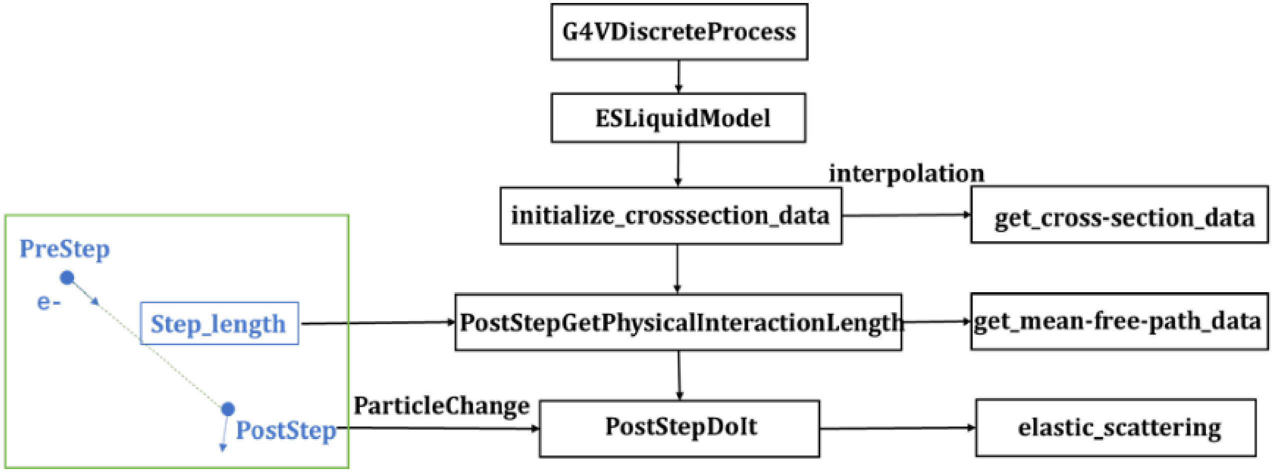
- The simulated drift velocity and diffusion coefficients in liquids show good agreement with experimental publications.

4 Implementation in Geant4

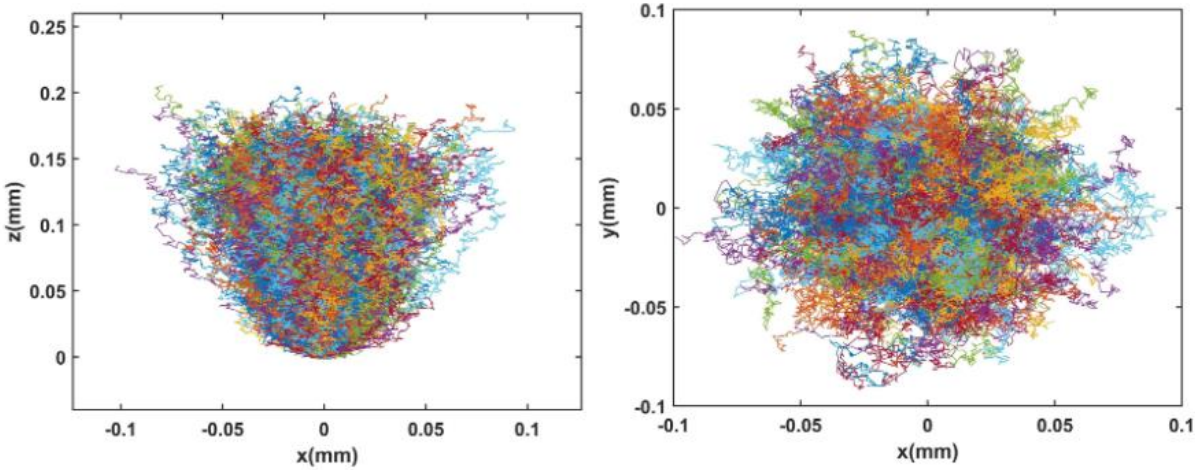
☐ Add electron coherent scattering model in Geant4

Geant4 encompasses an extensive library of physical processes including:
- electromagnetic interactions,
- optical interactions,

  ……
- **lack of coherent scattering in noble liquids**.



Schematic diagram of the electron scattering model in noble liquids in G4



Three-dimensional of electron trajectories in 1000V/cm electric field.

PART 04 **Conclusion**

4 Conclusion

Conclusion

- A comprehensive MC simulation tool designed for electron transport in noble gases He/Ne/Ar/Kr/Xe, and liquids Ar/Kr/Xe.
- The validation of the tool underscores the reliability and accuracy of the electron transport for noble gases and liquids.
- Open source. a standalone simulation tool or combined with Geant4.

https://doi.org/10.1016/j.nima.2025.170666

https://github.com/huahua440/noble-gas-liquid/tree/main

Prospects

- Gas and liquid mixture.
- Liquid neon and liquid helium.
  - a localized state known as ”eBubble”.
  - no suitable Monte Carlo model available.

THANK YOU！

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