Monte Carlo Simulation of Dose Enhancement Around Gold Nanoparticles for the Development of a Nanoparticle-Doped Dosimetric Gel

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Enhancing Sensitivity with Gold Nanoparticles

Goal: Increase the dose received by the gel by increasing photoelectric interaction [1]

$$Photoelectric \sim Z^3$$

$Compton$ independent of Z

Dose Enhancement Factor (DEF):
Depends on:

- Atomic mass of the heavy element used
- Concentration of heavy elements
- Radiation energy

$$DEF = \frac{Dose\ with\ High\ Z\ element}{Dose\ without\ High\ Z\ element}$$

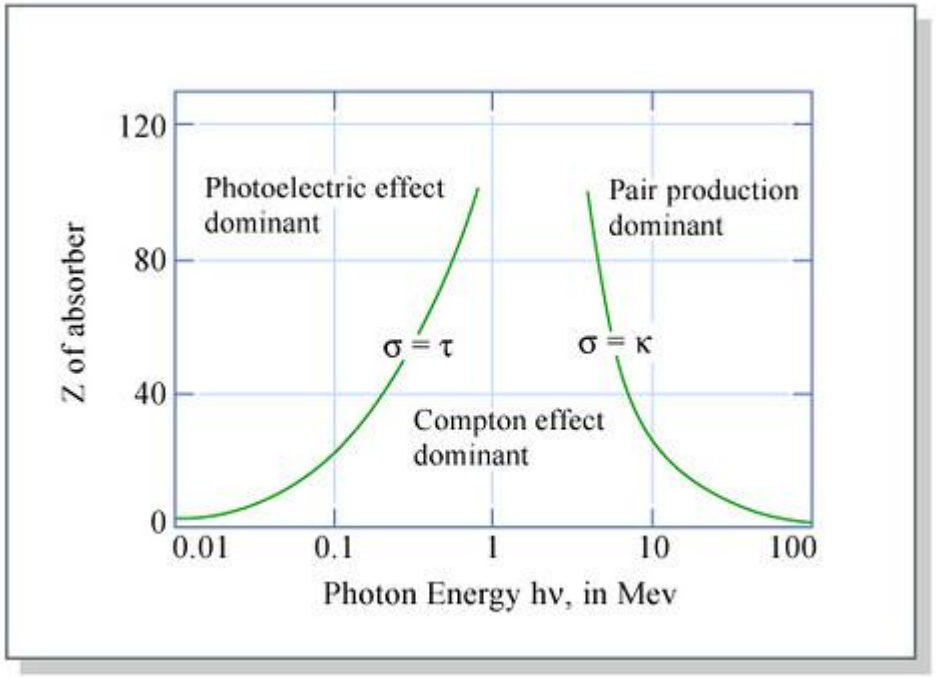


Figure 2: Photoelectric effect is dominant for lower energies and high Z of the absorber[1]

Gel dosimetry

- Made of polymers

- Tool for determining absorbed doses

- Oxidation reactions modifying the gel's appearance

- Visualization of the trace left by radiation in gels

- 3D dose reconstruction to control doses deposited during treatments

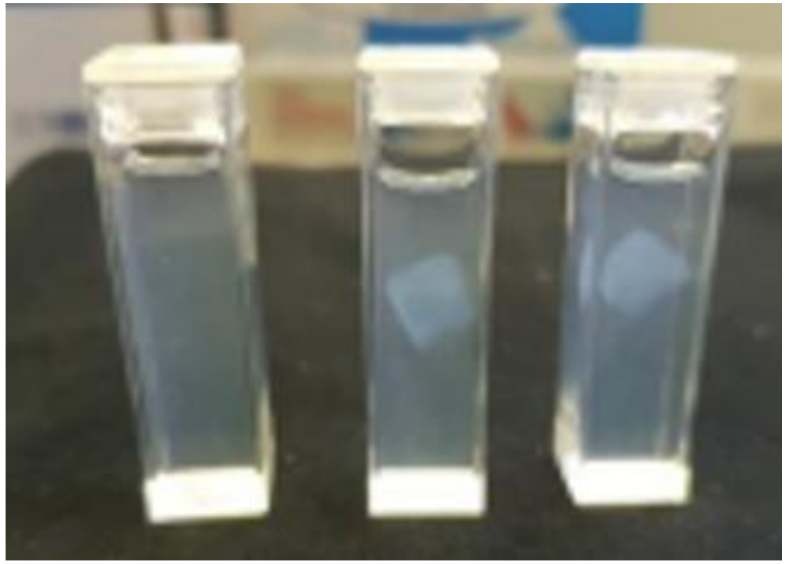


Figure 1: Dosimetric gel vials. The two on The right are irradiated

De Deene, Y., & Jirasek, A. (2024) [2]

AuNP-Doped Gel detector

- Novel idea to increase gel sensitivity
- Mesured dose in gel is oxydation dependent
- Coupling with metal nanoparticles (NPs) to increase absorption and ROS creation
- Multiple parameters to optimize

Irradation beam parameters	Gel parameters	Nanoparticle parameters
• **Particle type** • **Energy dependance** • Dose dépendance	• Reading sensitivity • Saturation	• **Elemental composition** • **Concentration** • **Size** • Impact on lecture

Vlastou, E.(2022)[3]

Monte Carlo dosimetry

- Experimentally varying all parameters is time- and resource-intensive.
- Nanoparticle dose distribution is different than with homogeneous composition
- Nanometric scale simulations using GEANT4-DNA physics list implemented in GATE.

Incerti, S., et al. (2018) [4]
Sarrut D, et al. (2022) [5]

From nanoscale to macroscale

- Objective : obtain a macroscopic equivalent dose that takes into account the nanoparticle distribution in a determined voxel

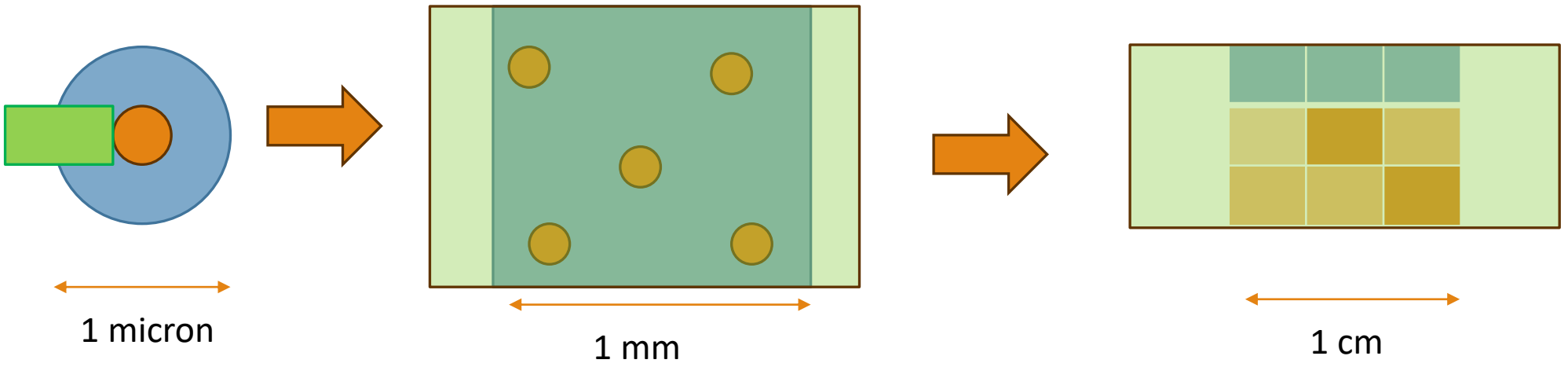


Figure 2 : Workflow of the modélisation of macroscopic dose enhancement of nanoparticle

Nanometric study

- Simulation Setup :
  - 50 nm gold NP embedded in 1 micron water sphere.
  - 50 nm Water NP embedded in 1 micron water sphere
- Measurement of
  - electron production
  - Radial dose distribution
    - Dosemap of 1 nm3 voxel size over a distance up to 100 nm from the center, then (10 nm)3 up to 1000 nm.

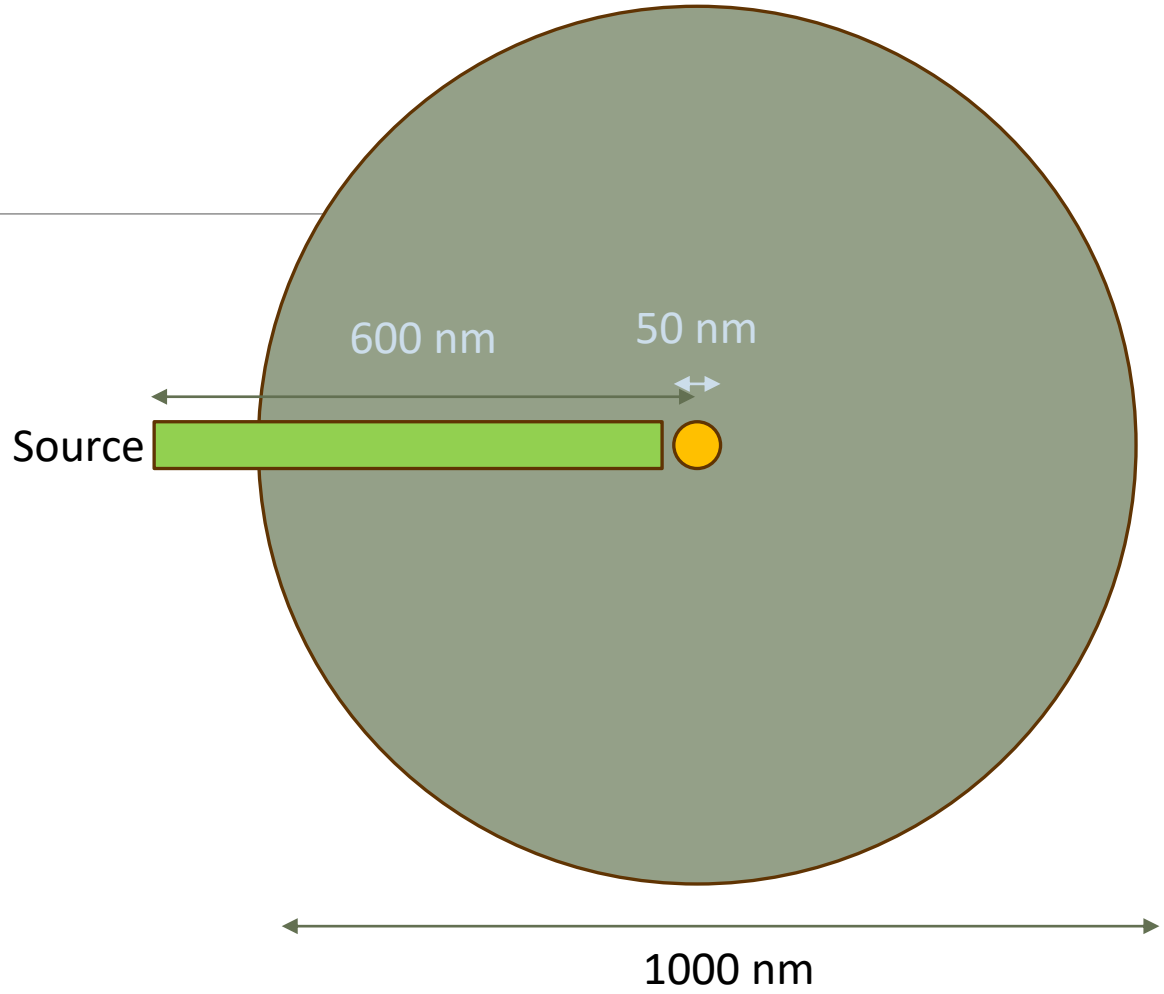
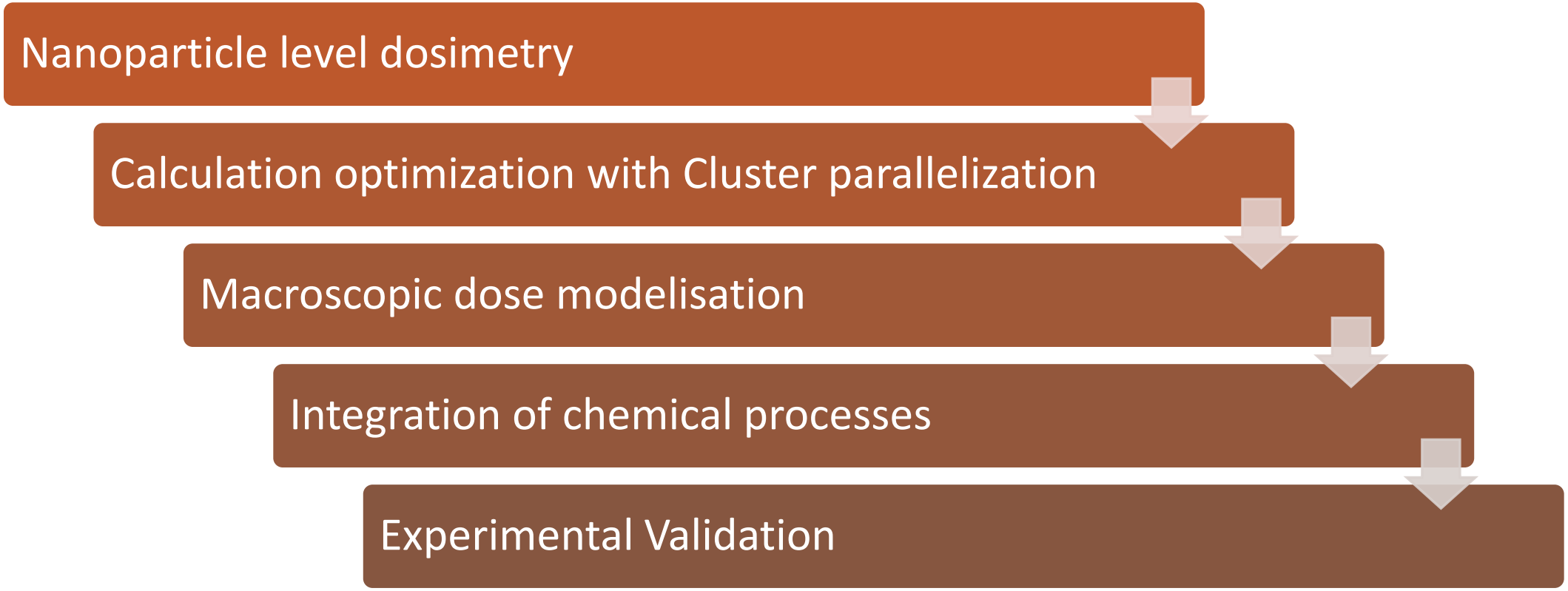


Figure 3: Geometry of the nanoscale setup. A 50 nm nanoparticle is at the center of a 1000 nm water sphere. The beam is 100 keV and is the same size as the nanoparticle

Workflow


Nanoparticle level dosimetry
Calculation optimization with Cluster parallelization
Macroscopic dose modelisation
Integration of chemical processes
Experimental Validation

Preliminary results

X-ray energy	FLUKA GNP	FLUKA WNP	PENELOPE GNP	PENELOPE WNP	PHITS 3.02 GNP	PHITS 3.02 WNP	Gate G4DNA GNP	Gate G4DNA WNP
50 keV	$1,2.10^{-3}$	$1,4.10^{-6}$	$5,7.10^{-4}$	$3,9.10^{-6}$	$6,1.10^{-4}$	$1,2.10^{-5}$	$2,26.10^{-3}$	$1,42.10^{-4}$
100 keV	$1,0.10^{-3}$	$1,58.10^{-6}$	$3,9.10^{-4}$	$6,9.10^{-6}$	$5,0.10^{-4}$	$4,0.10^{-6}$	$1,59.10^{-3}$	$1,02.10^{-4}$
150 keV	$3,1.10^{-4}$	$1,52.10^{-6}$	$1,6.10^{-4}$	$7,0.10^{-6}$	$1,6.10^{-4}$	$1,6.10^{-6}$	$5,82.10^{-4}$	$9,23.10^{-5}$
200 keV	$1,5.10^{-4}$	$1,6.10^{-6}$	$1,0.10^{-4}$	$6,4.10^{-6}$	$8,3.10^{-5}$	$1,7.10^{-6}$	$3,14.10^{-4}$	$8,39.10^{-5}$
250 keV	$9,0.10^{-5}$	$1,4.10^{-7}$	$6,4.10^{-5}$	$6,5.10^{-6}$	$4,3.10^{-5}$	$3,6.10^{-6}$	$2,19.10^{-4}$	$7,66.10^{-5}$

Number of electron per incident photon – GNP = 50 nm diameter

Preliminary results
Dose measurement in droplet

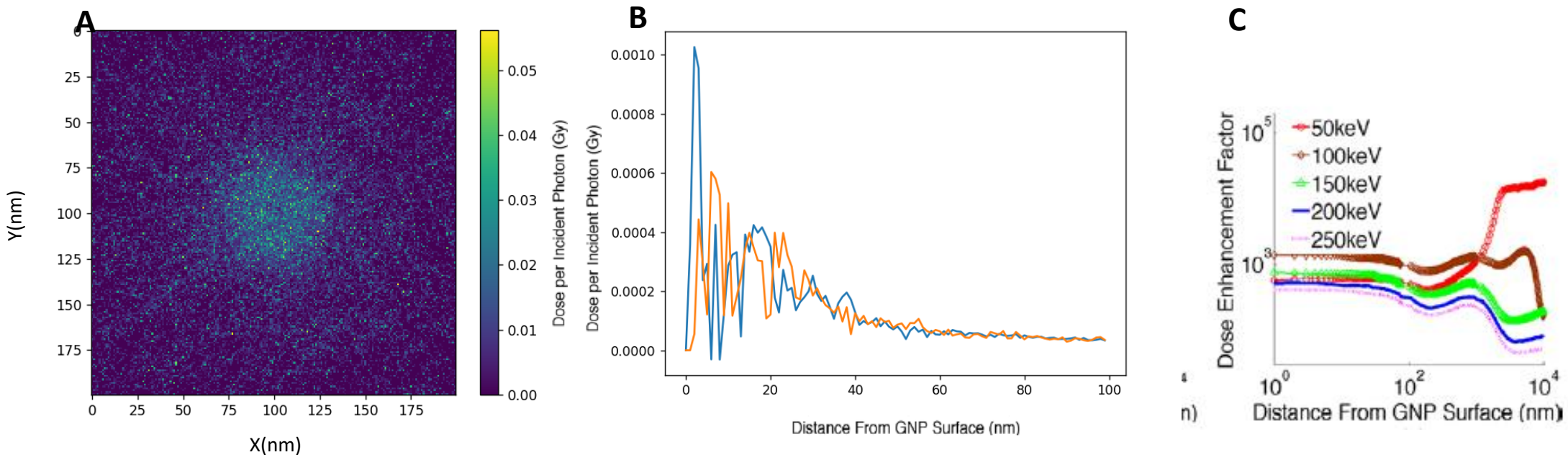


Figure 4: A. Dose map at the central slice around a 50nm diam. NP irradiated with a beam of 100 keV. B. Radial dose distribution up to 100 nm distance. C. Dose enhancement factor calculated by Lin et al. (2014) [6]

Discussion and perspective

- Different code algorithms lead to different results
- Importance of the choice physics processes
- Separation of the modelisation of the beam interacting with the nanoparticle and the dose enhancement with phase space files
- Adapt the code for changing parameters easily and parallelize calculation
- Potential development of a NanoDoseActor for GATE

Thank you for your attention

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