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IV GEANT4 INTERNATIONAL USER CONFERENCE

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University of New South Wales (UNSW)

GEANT4-Gamma Diffraction Code Based on Laue lens Modelling: Design Foundation and Implementation of the First Set of Models in GEANT4

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GEANT4 A SIMULATION TOOLKIT

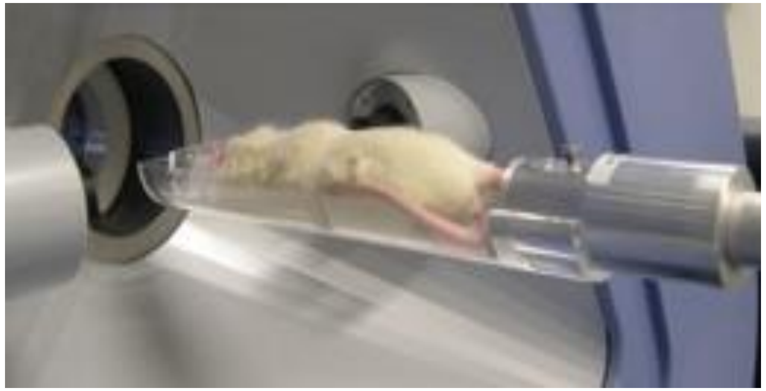
Italy, October 24-26, 2022

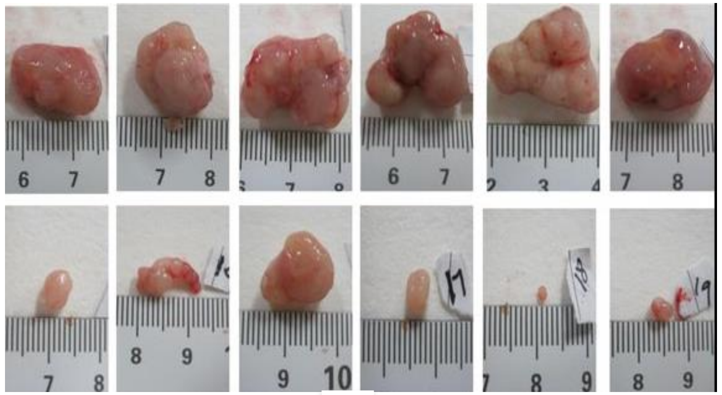
OUTLINE

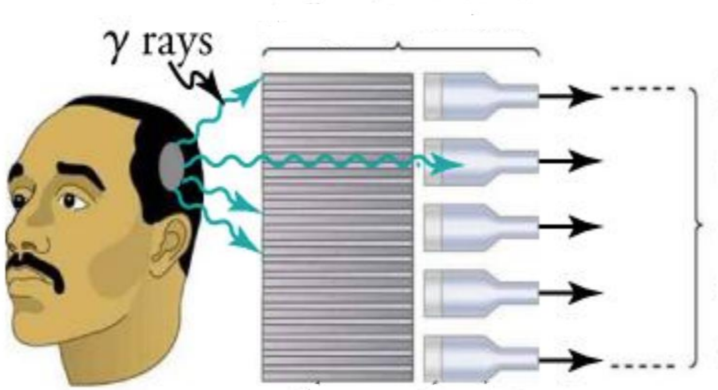
Introduction → Motivation → Proposed Laue lens Design → Laue lens Diffraction Example → Validation Study and Results → Conclusion

INTRODUCTION: Research Story !

Why We Need a Paradigm Shift in SPECT Imaging ?







❌ **Submillimeter** Resolution

❌ Detect tumours at **Submicron Volumes** with 3D information

❌ **Decouple sensitivity and resolution**

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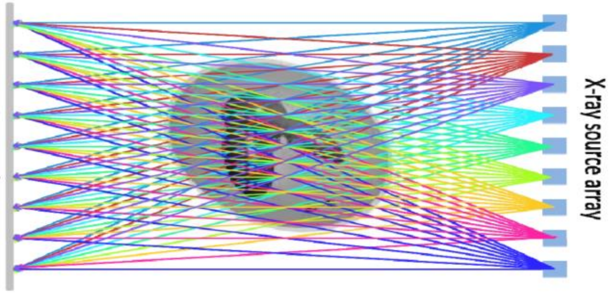
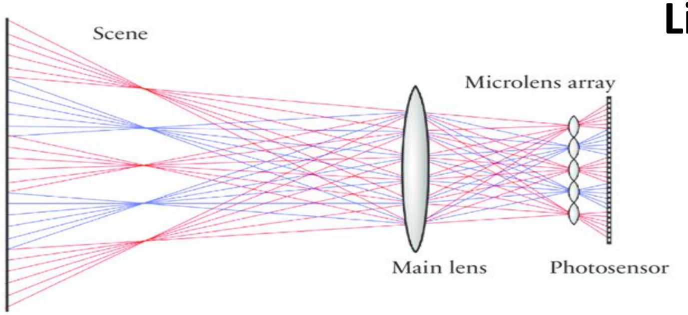
INTRODUCTION: Research Story!

Dr. Murat Tantali's patent



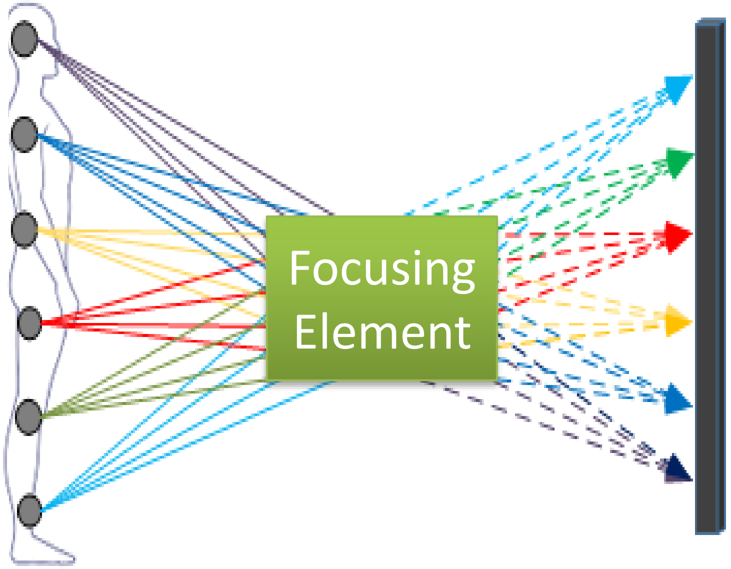
Light Filed Concept in CT Imaging

A multiple pinhole camera, akin to optical light field imaging.



Light Field Concept in SPECT Imaging

Optical elements ✗ Gamma Rays



Research Question 1
Is it possible to apply the concept Light field imaging in SPECT ?

Research Question 2
Can we focus Gamma Rays on the Energy Range of 140.5 keV

LITERATURE
SPECT Design Optimization

Motivation
Problem

No	Reference, Year	Research Objective	Methodology	Comments
1	[6], 2010	Design SPECT collimator with different pinholes prototypes	Developed and validated an efficient Monte Carlo simulation tool for studying multi-pinhole	Results have shown potential for the optimization of multi-pinhole design; however, the final designed system suffers from low sensitivity and the small field of view (FOV).
2	[7],2010	Investigate the effect of multiplexing on the reconstructed image quality	Simulations based on three digital phantoms. Compare the reconstructed images for different degrees of multiplexing	It was shown that having mixed (Multiplexed and non-multiplexed) data improved the SNR due to the reduced noise level in the reconstructed images.
3	[8],2015	This study investigated a parallel-hole collimator with cone-shaped holes, to limit penetration	Monte Carlo and a prototype PC collimator was used in an experimental phantom	Study showed reduced collimator penetration reduced in once shaped collimator compared to parallel
4	[9],2013	Increase SPECT resolution	Designed a static full-ring multi-pinhole brain SPECT	The target spatial resolution is very low and did not result in an unambiguous improvement.
5	[10],2017	Design an MPH collimator Enhanced spatial resolution and employ multiplexing	Mechanical design of the MPH with shutter mechanism to allow multiplexing was developed using the SolidWorks. GATE simulations	MPH collimator assembly is modelled in SolidWorks. Did not suggest multiplexing reconstitution solutions.
6	[11],2017	Design collimator for high spatial resolution and sensitivity imaging - Parkinson's disease	Mechanical design used in constructing a multi-pinhole collimator. SolidWorks simulation & GATE Monte Carlo package to simulate brain imaging	Despite having the optimized number of pinholes for brain SPECT been determined, some of the reconstructed images showed artefacts that were likely caused by the overlap of projections or multiplexing effect on detector plane

LITERATURE:
Gamma Focusing in Astronomy

Motivati
on
Problem

No	Reference, Year	Research
1	[20],1967	Astrophysics began exploring the possibility of detecting gamma rays and energetic x-rays from distant astrophysics
2	[21],1968	A crystal lens with NaCl covering energy band of 20-140 Kev were proposed. However, the designed lens did not improve the signal to noise ratio. Hence, was not improved by the astrophysics community
3	[22-25],1980s	Seven papers were published by the Argonne group discussing different designs for Laue lens crystals for focusing energetic photons in the astrophysics field
4	[26],2003 [27],2006	Exploring Laue Lenses applications as a solution with great potential to overcome the limitations in non-focusing detection methods

RESEARCH PROBLEM : Explore the Literature

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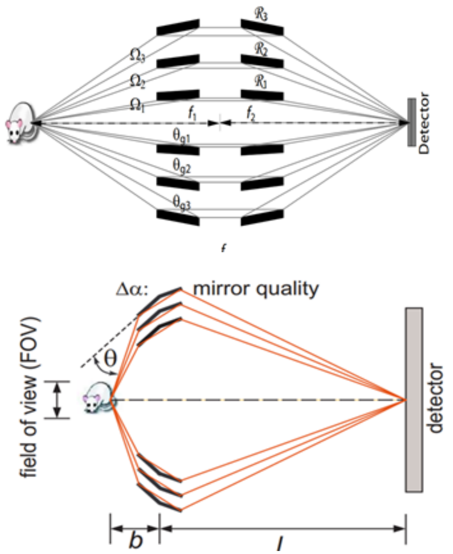

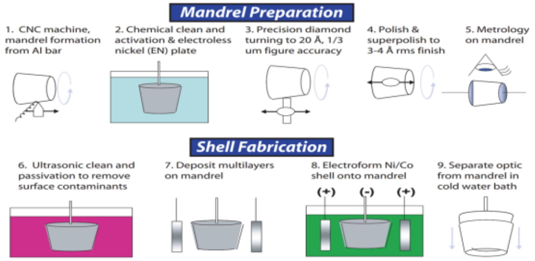

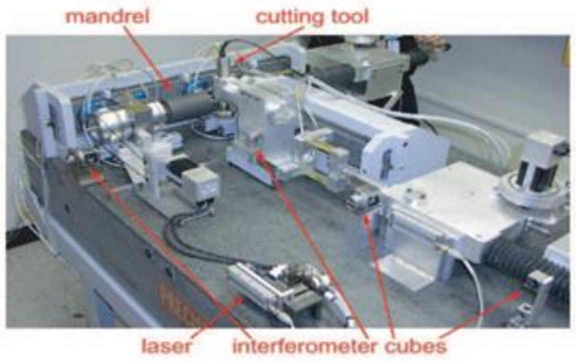

Achieved 0.1 mm Resolution in small animal imaging

Not suitable for studies with energy gamma application.

27.5 keV

90-200 keV

RESEARCH PROBLEM : Explore The Literature

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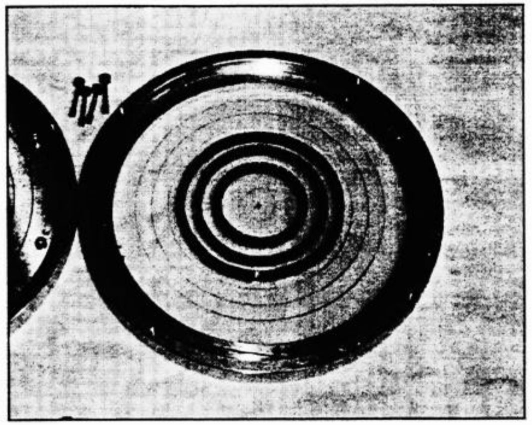
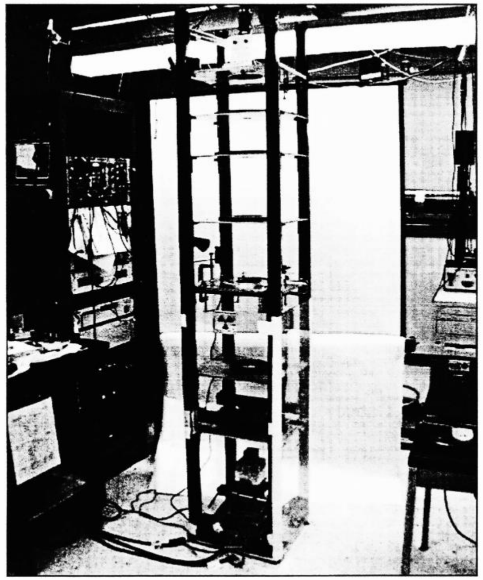
Throughout the 1980s, the Argonne group began seven research projects examining various designs for Laue lens crystals to focus gamma-rays the range of 140.5 Kev





PATENT : Gamma Focusing using Laue lens

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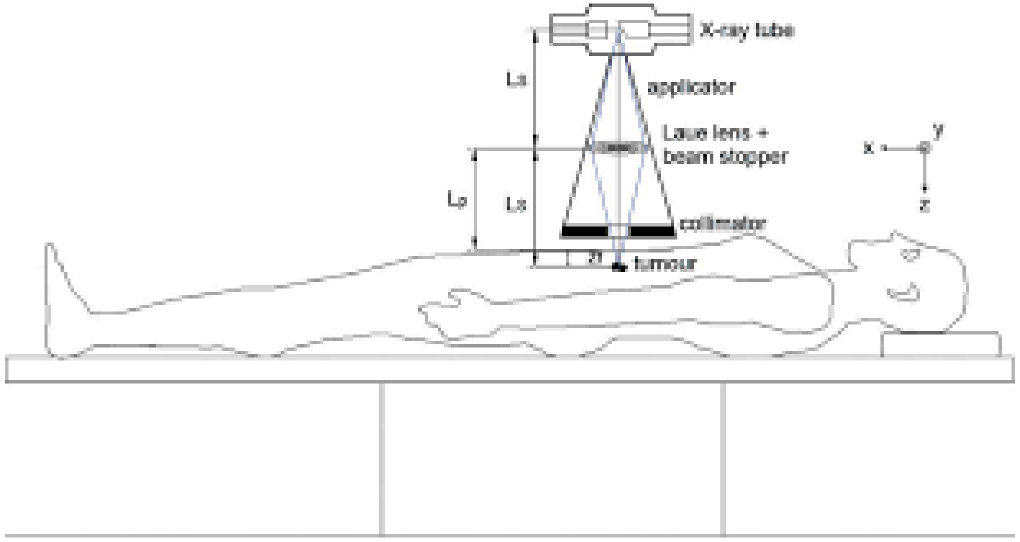
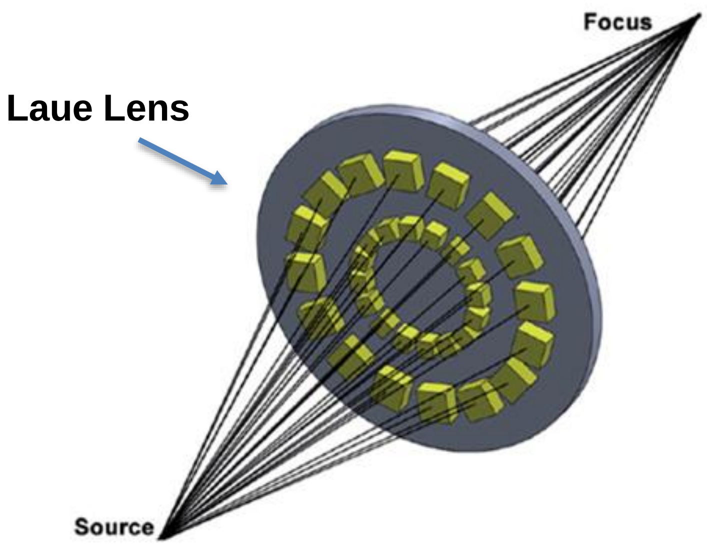
RESEARCH PROBLEM : Explore The Literature

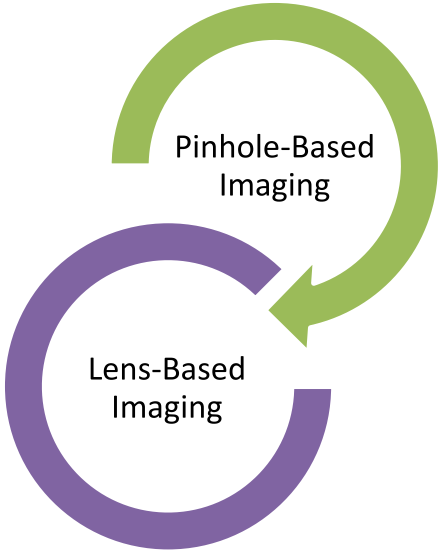


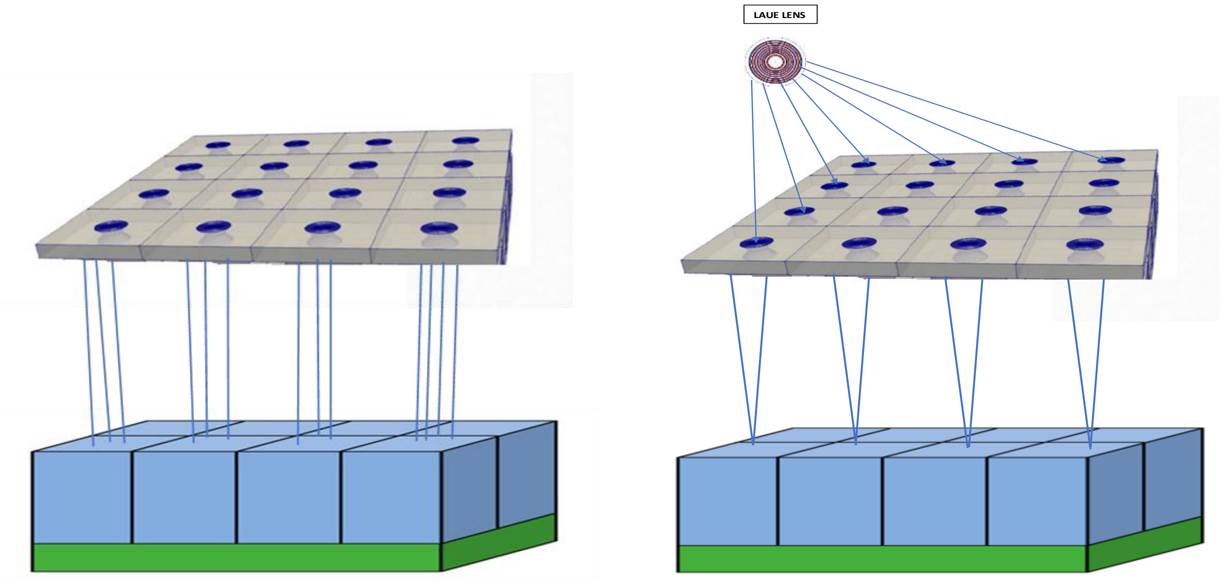
Radiotherapy : Gamma Focusing using Laue lens

What is the Laue lens?

- Laue lens is an aggregate of crystals having the ability to focus high energy photons through diffraction.



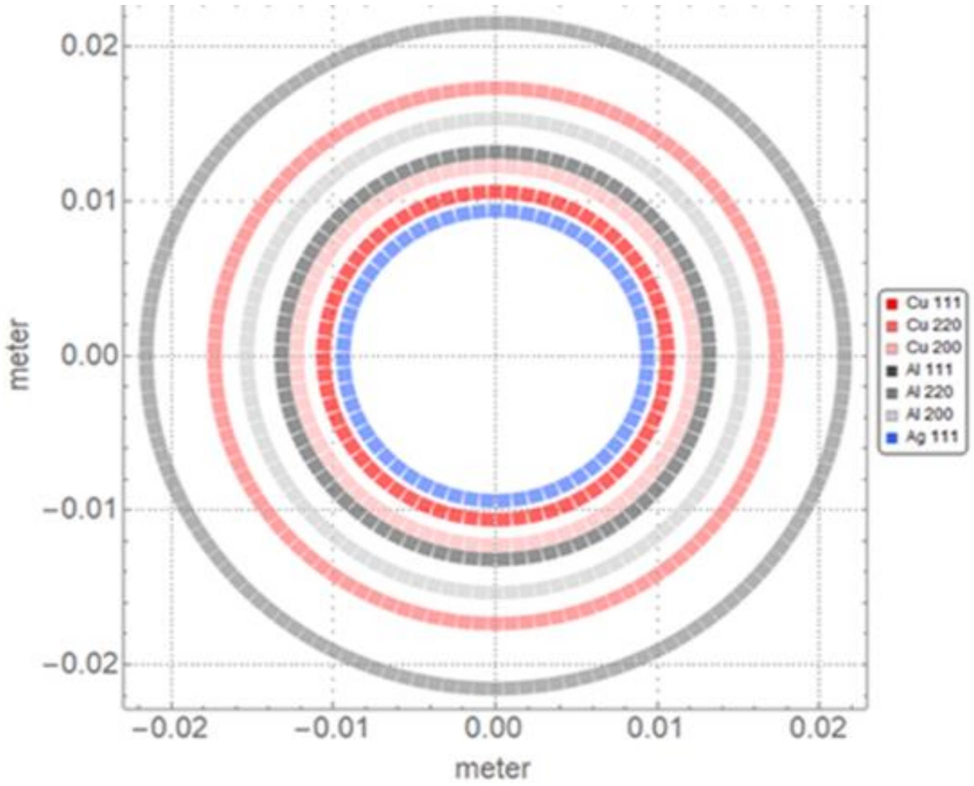




Proposed Design

Laue Lens Design

This research aims to investigate the performance of a **novel Lens-Based SPECT** imaging system proposed for small animal and brain imaging.



Material	Reflectivity	Absorption	Thickness (mm)	Ring radius (mm)	Number of crystals	Bragg angle
Al (111)	37.42%	19.04%	5.50	9.47	53	0.01894
Al (200)	35.50%	21.68%	6.36	10.94	62	0.02187
Cu (200)	26.96%	32.86%	1.81	12.25	70	0.02450
Al (220)	29.64%	29.44%	9.08	15.47	90	0.03093
Cu (220)	24.30%	36.17%	2.04	17.23	102	0.03465
Al (311)	26.14%	33.89%	10.77	18.35	108	0.03627
Cu (311)	22.44%	38.45%	2.20	20.33	121	0.04064

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MONTE CARLO SIMULATIONS

MATLAB

Single Lens-Based SPECT

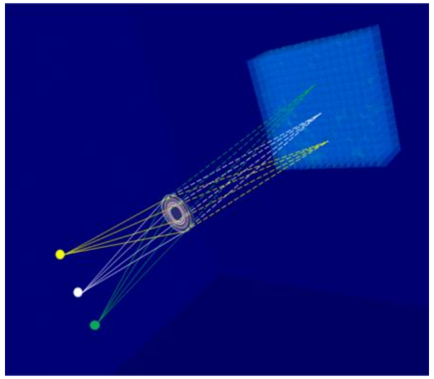
- Developed a dedicated Monte Carlo Environment
- Developed a 3D reconstruction algorithm
- Validation Study: depth and shift
- Conducted a comparative study

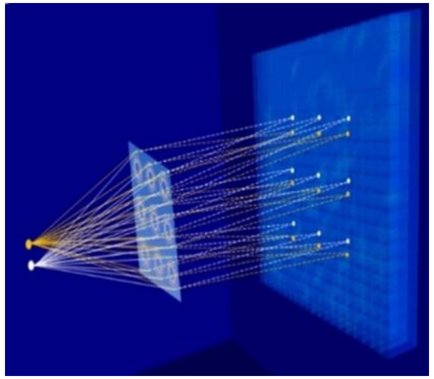
Modular Lens-Based SPECT

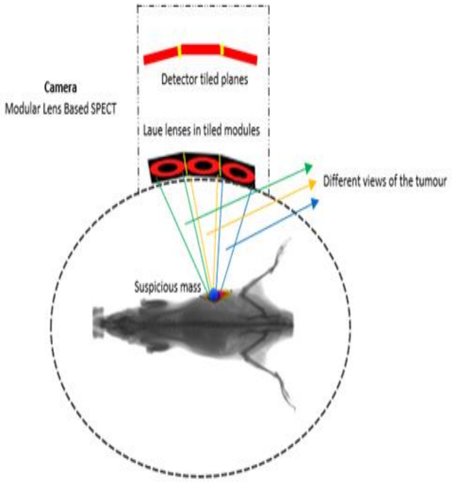
- Developed a dedicated Monte Carlo Environment
- Developed a 3D reconstruction algorithm
- Validation Study: Mapping the sensitivity throughout the FOV.
- Conducted a comparative study

Multi Lens-Based SPECT

- Developed a dedicated Monte Carlo Environment
- Developed a novel 3D reconstruction algorithm
- Validation Study: depth and shift
- Conducted a comparative study







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Forward Projection and 3D Reconstruction

MATLAB

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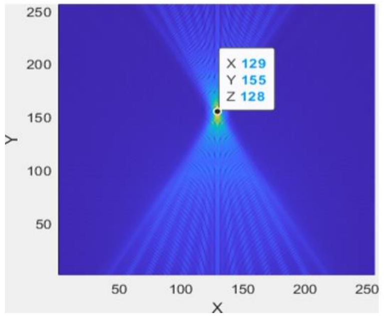

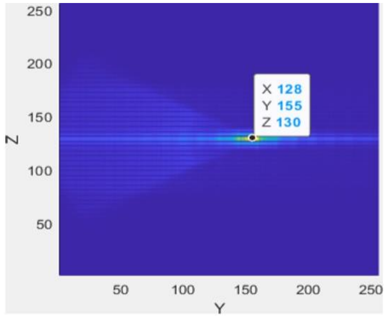

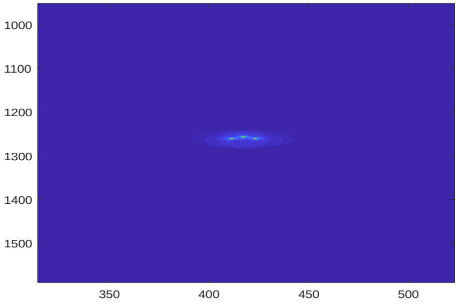

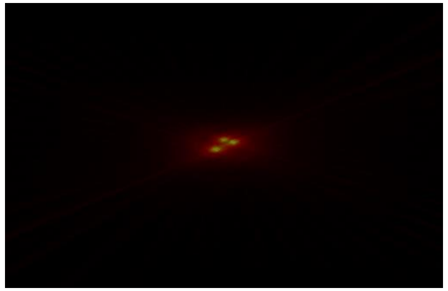

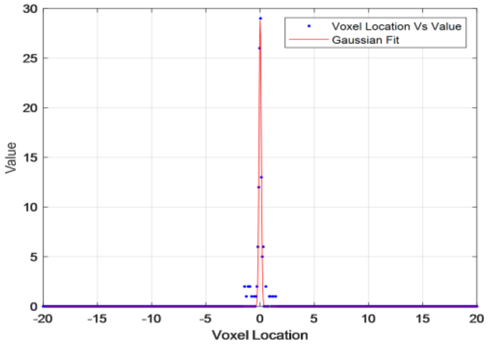

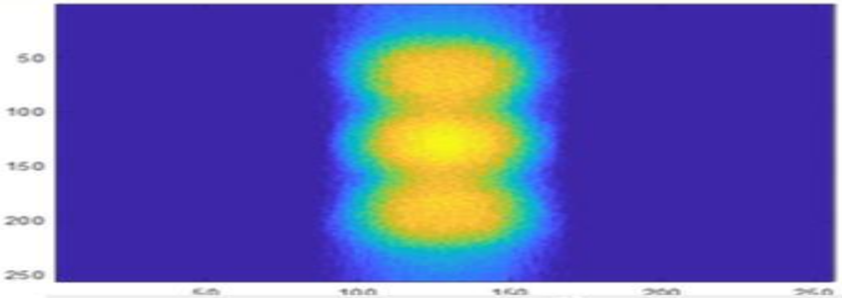

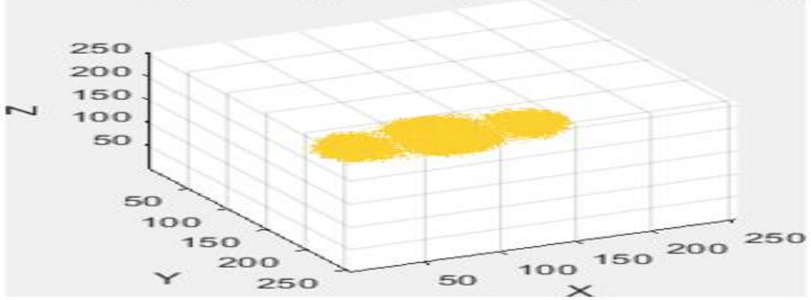

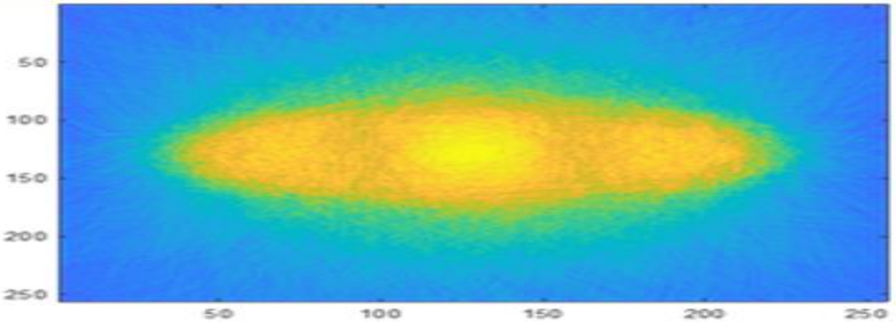

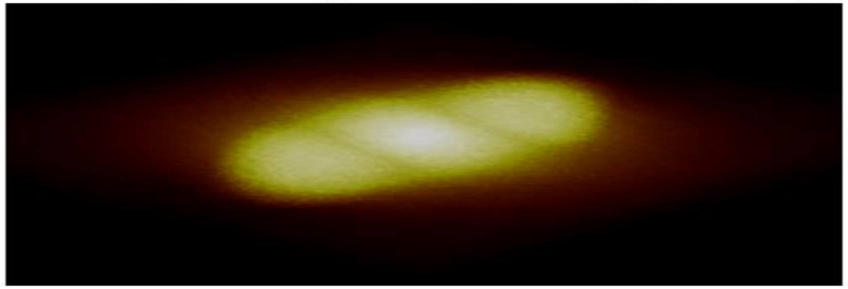

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VALIDATION AND COMPARATIVE STUDY

MATLAB

Axial shift of the source	Efficiency of Module 1	Efficiency of Module 2	Efficiency of Module 3	Efficiency of the three Modules	Sensitivity hits/emitted
X=+0.1, Y=0.	2.2%	2%	1.98%	6.2%	$7.8 \cdot 10^{-5}$
X=+0.3, Y=0	1.96%	1.91%	1.85%	5.72%	$7.2 \cdot 10^{-5}$
X=+0.5, Y=0	1.86%	1.81%	1.8%	5.47%	$6.9 \cdot 10^{-5}$
X=+0.7, Y=0	1.78%	1.76%	1.669%	5.21%	$6.6 \cdot 10^{-5}$
X=+0.9, Y=0	1.67%	1.66%	1.63%	4.95%	$6.2 \cdot 10^{-5}$
X=0, Y=+1.5	1.56%	1.5%	1.4%	4.46%	$5.7 \cdot 10^{-5}$
X=0, Y=+2	1.39%	1.36%	1.32%	4.07%	$5.2 \cdot 10^{-5}$
X=+2.5, Y=0	1.23%	1.2%	1.09%	3.52%	$4.6 \cdot 10^{-5}$
X=+3, Y=0	0.98%	0.92%	0.9%	2.8%	$3.8 \cdot 10^{-5}$

*The efficiency is calculated based on the percentage of the diffracted photon to the emitted ones by the source.

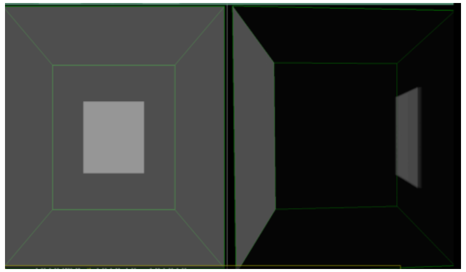
*The sensitivity is approximated based on the Monte Carlo simulation of an isotropic point source.

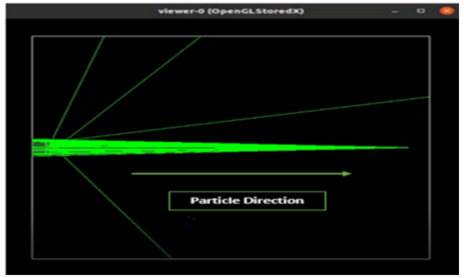
Source	Phantom Depth Z [mm]	Pixel Location	Voxel Size	Max & Min Bounds [mm]	Estimated Depth of The Reconstructed Phantom [mm]
1 sphere	1	155	10/256	-5, -5	1.005
1 sphere	5	254	10/256	-5, -5	5
1 sphere	10	252	20/256	-10, 10	9.97
1 sphere	15	252	30/256	-15, 15	14.967
1 sphere	30	252	30/256	-15, 15	29.966

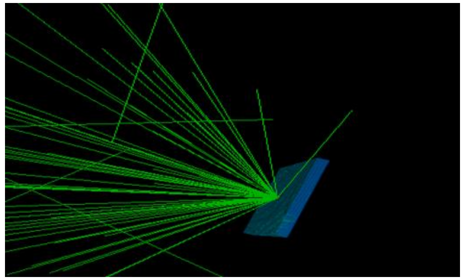
Source	The Shift from The Lanes Axis [mm]	Pixel Location	Voxel Size	Max & Min Bounds [mm]	Estimated X Y Shift of The Reconstructed Phantom [mm]
3 Spheres	X=0.1, Y=0.1	131	10/256	-5, -5	0.103
3 Spheres	X=-0.1, Y=-0.1	126,126	10/256	-5, -5	-0.098
3 Spheres	X=0.05, Y=0.05	129,129	10/256	-5, -5	0.047
3 Spheres	X=-0.05, Y=-0.05	127,127	10/256	-5, -5	-0.0481

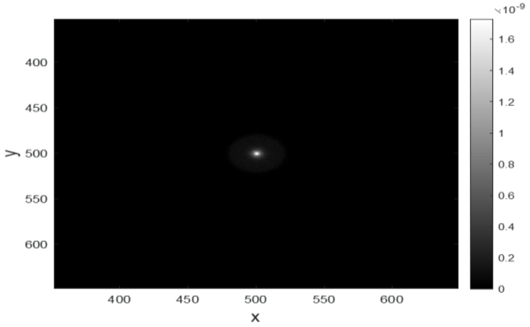
MONTE CARLO SIMULATIONS

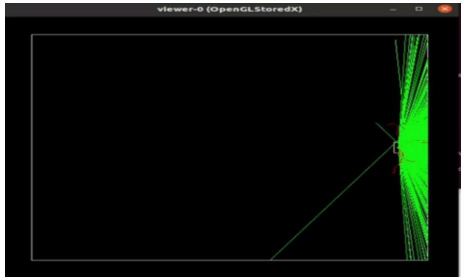
GAMOS Toolkit

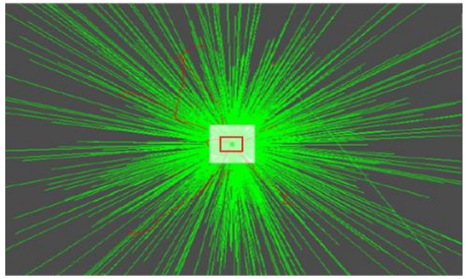


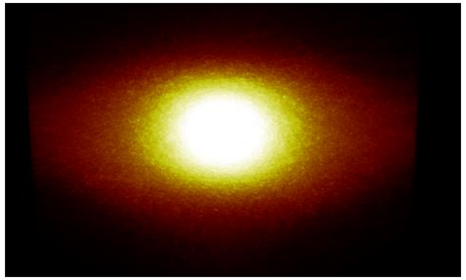


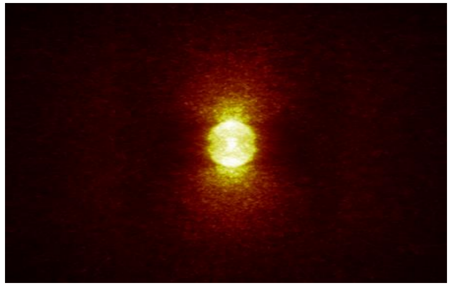






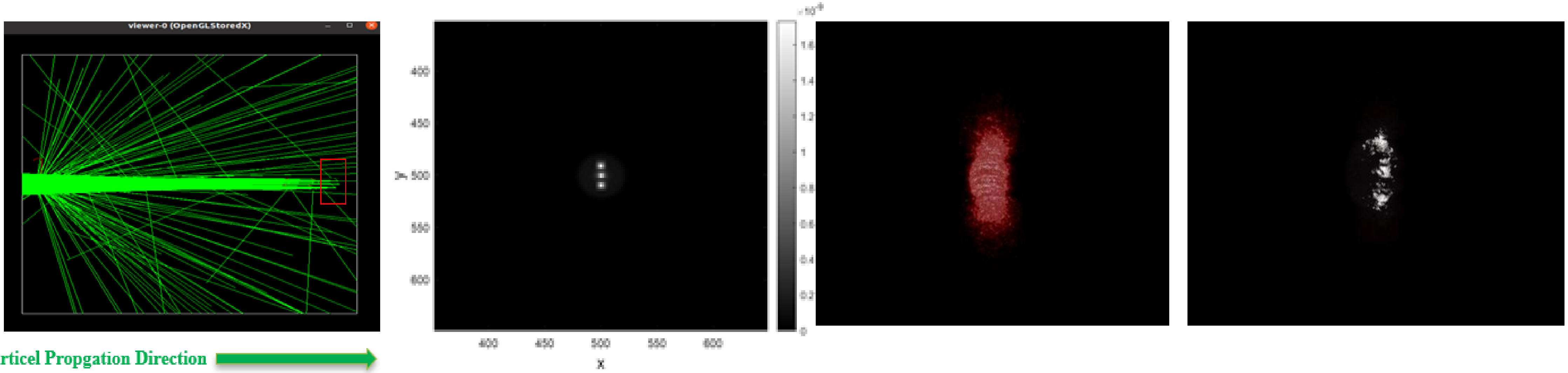






MONTE CARLO SIMULATIONS

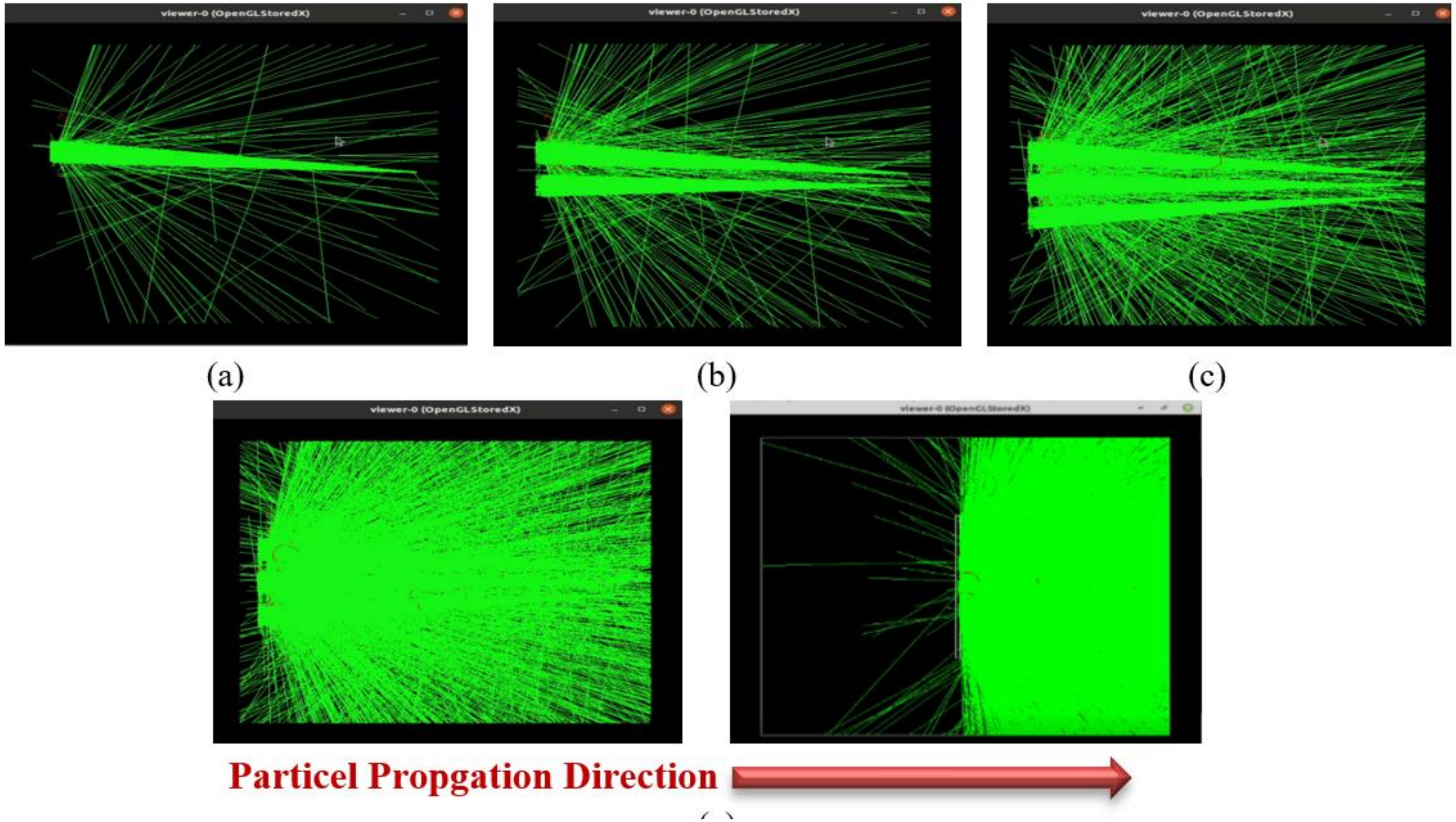
GAMOS Toolkit

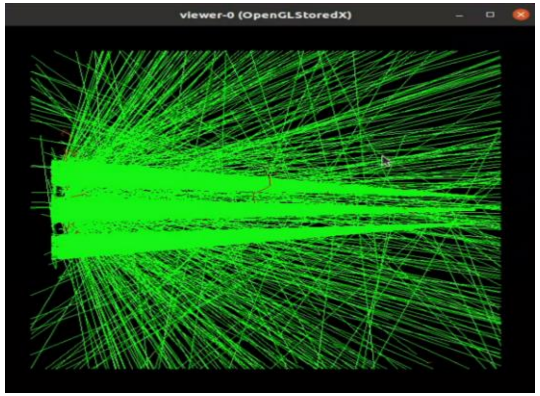


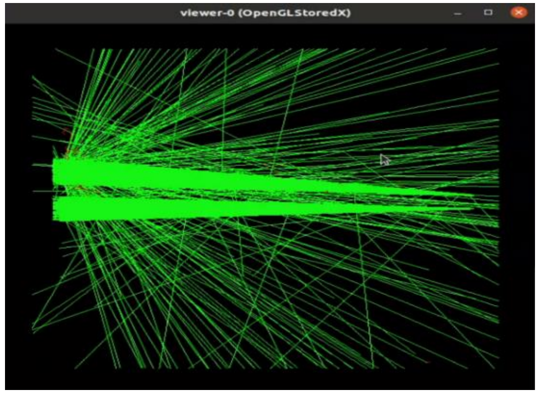
Particel Propgation Direction

MONTE CARLO SIMULATIONS

GAMOS Toolkit







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MONTE CARLO SIMULATIONS

MATLAB-Multi, Single and Modular Lens-Based SPECT

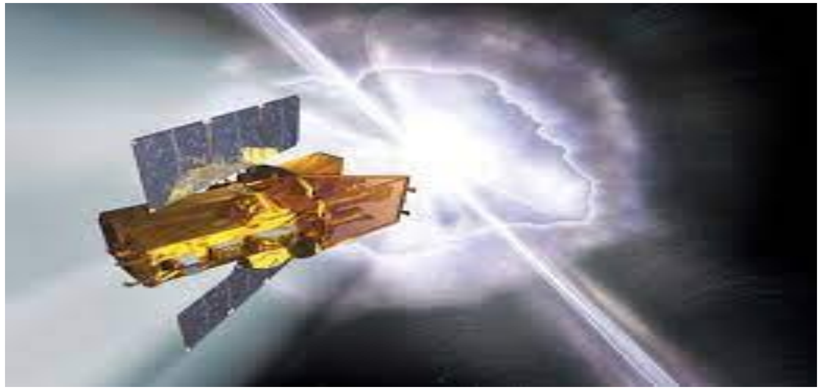
System	Configuration	Resolution (mm)	Sensitivity $(hits/emitted)$
***Parallel SPECT (LEHR) 39x39 Pinholes**	Pinhole diameter 1.2 mm, septal thickness 0.2 mm, pinhole depth 35 mm, source-to-collimator distance 25 mm.	1.9	$3 . 10^{-5}$
***Parallel SPECT (LEHR) 39x39 Pinholes**	Pinhole diameter 1.2 mm, septal thickness 0.2 mm, pinhole depth 30 mm, source-to-collimator distance 20 mm.	2.5	$3.2 . 10^{-5}$
Single Lens-Based SPECT	Laue lens radius 20.83 mm, thickness 1 mm, source-to-lens distance 500 mm	0.1	$2.9 . 10^{-5}$
Modular Lens-Based SPECT	Three modules, each module consists of a Laue lens radius 20.83 mm, thickness 1 mm, source-to-lens distance 500 mm.	0.1	$9 . 10^{-5}$
Multi Lens-Based SPECT	9 Laue lenses, array of 3x3, each Laue lens radius 20.83 mm, thickness 1 mm, source-to-lens distance 500 mm.	0.1	$7 . 10^{-5}$

***Collimator set is simulated in present study.**

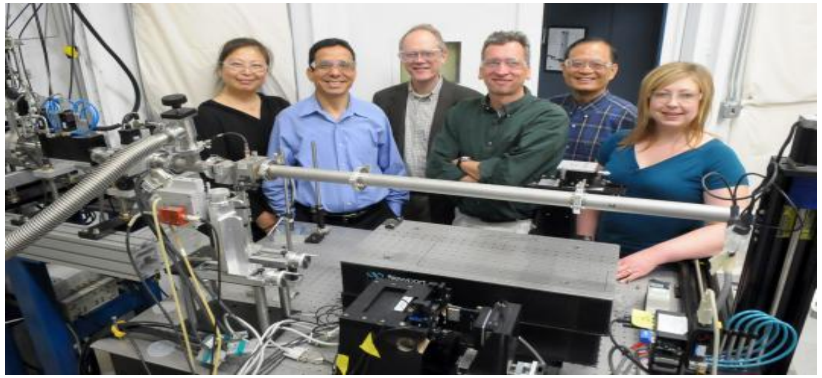
The GEANT4 Developed Advanced Example

WHY?

- Presently, great interest and scientific expertise are available to push forward new technologies in Gamma-ray lenses.



- Laue gamma diffraction has recently attracted considerable attention as a powerful method for developing a high energy-rays focuser.



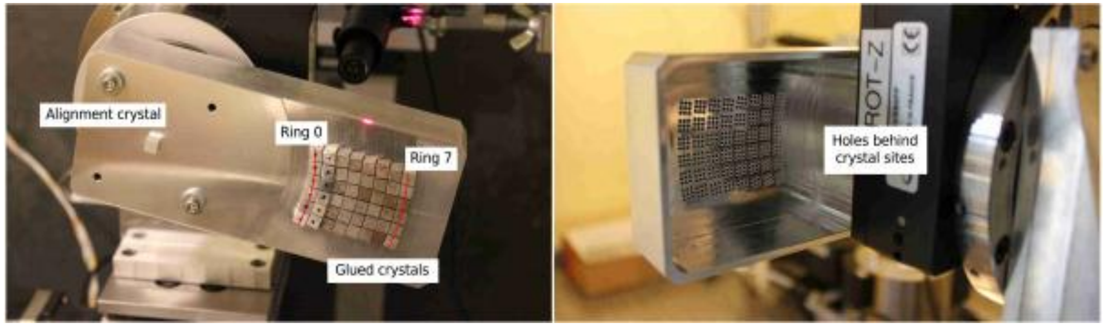
- Conducting physical experiments on Laue lens behaviour seems to be a fundamental tool for understanding the physical issue and elucidating the main concept in gamma diffraction.

The GEANT4 Developed Advanced Example

- However, Laue lens manufacture is quite challenging as it requires high precision to position and align diffractive crystals of various elements.

- A readily feasible alternative to physical experiments is computer simulations of the Laue lenses in a stable state-of-the-art high-energy physics simulation environment such as GEANT4.

- However, the Laue diffraction process has not been implemented in any of the available Monte Carlo simulation platforms so far.



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The GEANT4 Laue Lens Advanced Example

THIS WORK

- This is one of the primary obstacles researchers encounter in their attempts to model the Laue lens in a realistic particle tracking environment.

- **This work aims to present the first attempt to model the X-ray and gamma rays focusing based on Laue diffraction in the GEANT4 toolkit using an advanced example in its early conception.**

- The necessary practical knowledge for developing and running the developed application that will be utilized in real experiments was acquired from the user's guide for Application Developers, Rev 6.0: Geant4 Release 11.0, 10th December 2021.

The GEANT4 Laue Lens Advanced Example

TO Make it WORK

1. **Set the Mean Free Path**: But our code doesn't give the mean free path and it must be set to a value to make it G4 process.

In our work: The Mean Free Path: We set the mean free path to a very large number (DBL_MAX: DBL_MAX is the maximum valid double value) and put the logic as to whether a particle interacts in the PostStepDoIt.

Laue Lens Example:

The code executes if the material has the LaueLens properties defined.

```
G4double G4LaueLensProcess::GetMeanFreePath(const G4Track&, G4double,
                                            G4ForceCondition* condition)
{
  *condition = StronglyForced;
  return DBL_MAX;
```

The GEANT4 Laue Lens Advanced Example

TO Make it WORK

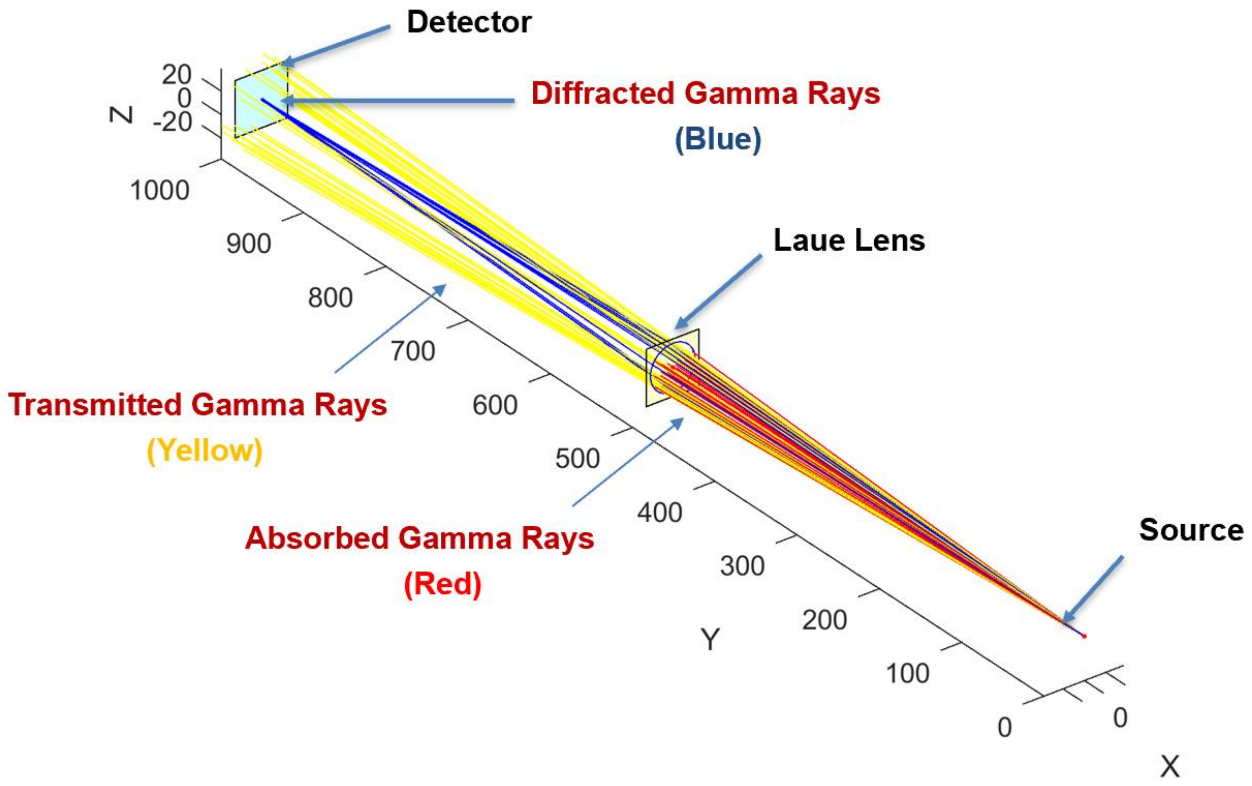
2. The code changes the primary or generate secondaries:

Laue Lens Example: The code changes primary, it is similar to optical processes.

3. Geometry.

Laue Lens Example: The process will run if you set the Laue lens properties to the material.

GEANT4 Laue Lens Advanced Example
Laue Lens Diffraction



- The rays will be emerging from various directions from the object under study and will be focused by the Laue lens via diffraction.
- Depending on the intersection point in the lens volume, the algorithm determines the three different possibilities: transmission, absorption, or diffraction at the Laue lens plane.
- A detector is placed at the focus plane, perpendicular to the lens axis. The absorbed rays will be halted by the code, while diffracted and transmitted photons will arrive at the detector plane at different places.
- Thus, adequate Laue lens shielding is critical for preventing the sensor from detecting the transmitted photons.

GEANT4 Laue Lens Advanced Example

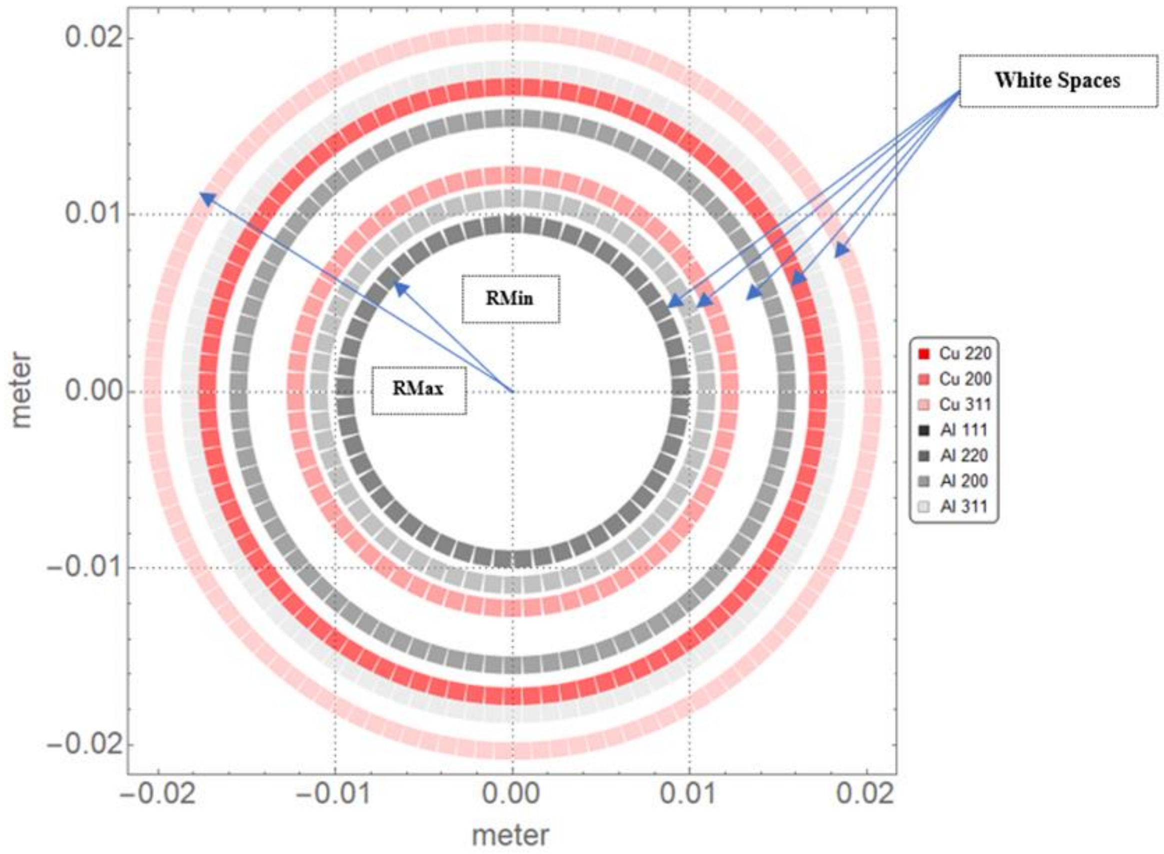
Laue Lens Diffraction

- For the diffracted photons, the code uses the interaction point in the Laue lens to calculate the direction towards the detector, and the hit point on the detector plane as (XD, YD, ZD).

- The resulting position of a diffracted photon at the focal plane depends on the source position, the photon direction , the photon energy, and the interaction point inside the single crystal.

- The photon distribution—due to the entire Laue lens—on a plane at a given distance from the lens results to be the sum of the contributions of all the crystals that constitute the lens.

SIMPLIFICATIONS AND ASSUMPTIONS

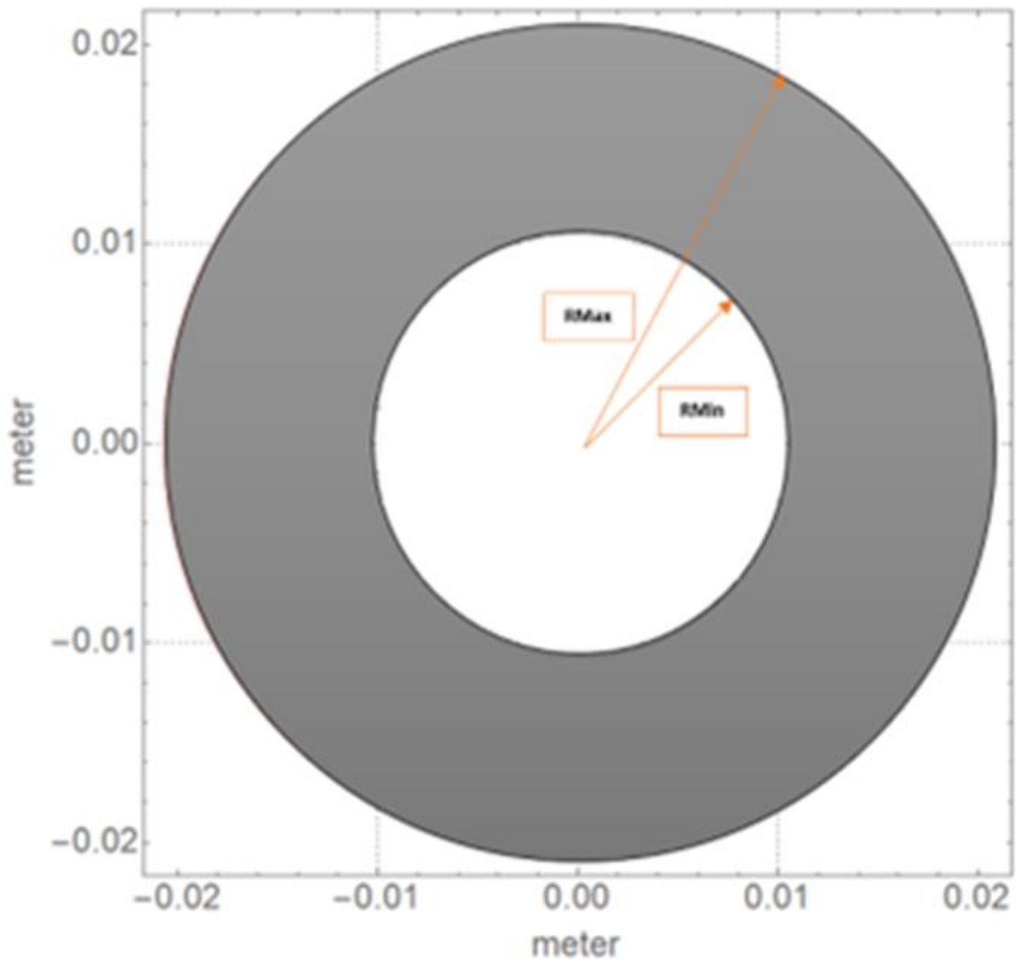


- The spaces between the Laue lens rings, namely the white spaces, are where there are no crystals.
- Still, the photons here are transmitted or absorbed at these spaces.
- Thus, shielding for the lens frame is needed. However, to keep the complexity of this example to a reasonable level, this is not considered in the developed process.

SIMPLIFICATIONS AND ASSUMPTIONS

- In the algorithm, the behaviour of the Laue lens consisting of seven rings was simplified by dealing with a tube with inner and outer diameters.

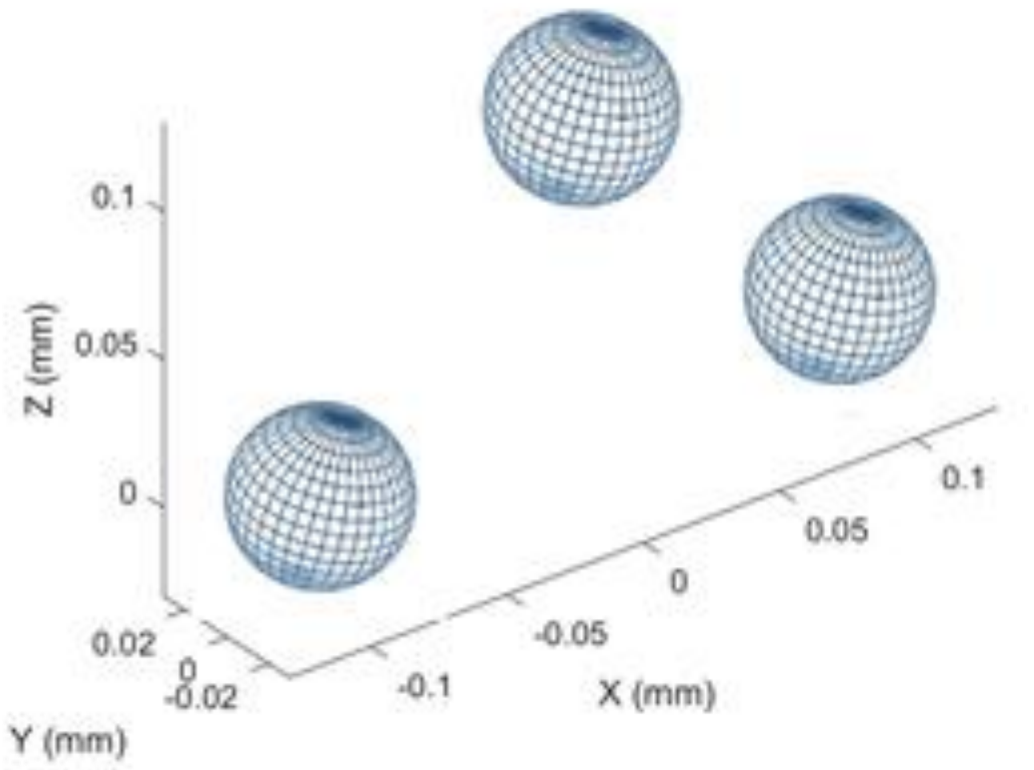
- There are no empty spaces between the minimum and maximum Laue lens radii.



INITIAL CODE VALIDATION

- This example can reproduce the main features of most of the relevant observables as measured in the real Laue lens behaviour.

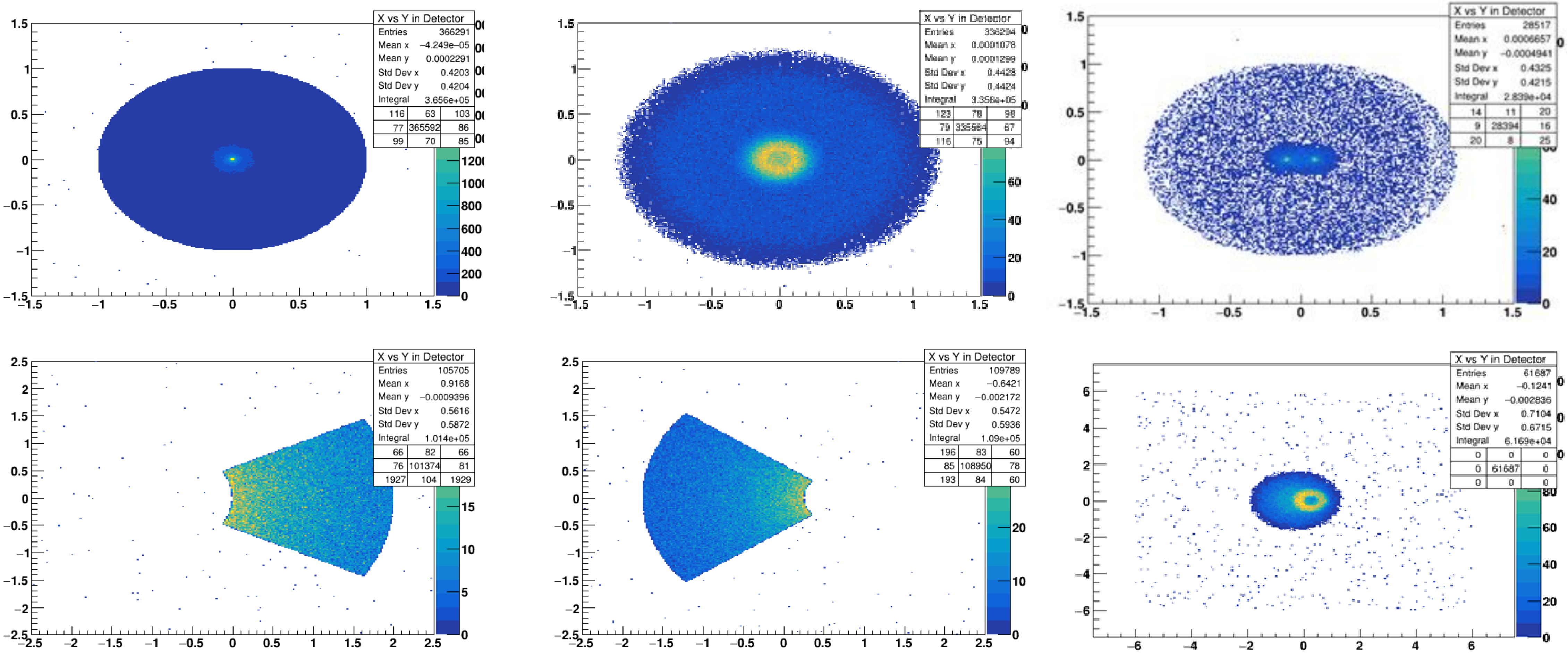
- Simplified simulation of a Laue lens with one, and two-point sources along with all possible interactions with a detector placed at the lens focus were recorded for the purpose of code validation.



INITIAL CODE VALIDATION

- This is initially used to validate Geant4 Laue lens code against real data taken in Laue lens experiments for medical imaging.
- Moreover, it also reproduces the results of the original developed Mathematica that was developed by Dr. Riccardo Camattari.
- We benchmark these first results based on the developed initially code in Mathematica using the Laue genetic tool and the particle tracking Carlo code we developed in MATLAB.

SHIFT VALIDATION



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CODE FLEXIBILITY

SCALING FACTOR

- The $ScaleFactor$, is set as an input parameter so the user can change the Laue lens design and apply the diffraction for different system designs and configurations.

- The default value for this parameter is set to 1. Changing the scaling factor would consequently modify the parameters inner and outer radius of the lens

- Moreover, the set focal length (where the detector should be placed) Ld, as well as the optimal distance from source to Laue volume Ls will be automatically modified depending on the modified scale factor parameter.

CODE FLEXIBILITY

SCALING FACTOR

The Laue lens volume is represented as a tube of dimensions (mm):

$$RMin = Default\ set\ Value \times ScaleFactor.$$

$$RMax = Default\ set\ Value \times ScaleFactor.$$

The focal length of the lens is also multiplied by the ScaleFactor as in below:

$$Focal\ Length = Default\ set\ Value \times ScaleFactor$$

$$Source\ Location = Ls = Focal\ Length$$

$$Detector\ Location = Ld = Focal\ Length$$

CODE FLEXIBILITY

Detector Position

- Important Note: The source location (Ls) and the detector location (Ld) can be placed at any distance from the Laue lens Centre.

- However, the optimal case is achieved by placing the source at a distance equal to the lens’s focal length, namely Ls=Ld = Focal Length.

- The user can change the detector position along the lens axis, and as a result, the efficiency would be smaller.

DIFFRACTED AND TRANSMITTED

SCALE FACTOR – Diffracted And Transmitted

- Appending the final locations of the diffracted gamma-rays will be dependent on the focal length which by itself affected by scale Factor.

```
AppendTo[diffracted[$KernelID],
 {xinter, yinter, beamOut[focalLenght][[1]], beamOut[focalLenght][[2]]}];

,
AppendTo[transmitted[$KernelID],
   {xinter, yinter, beamIn[focalLenght][[1]], beamIn[focalLenght][[2]]}];
(*the photon goes stright*)
```

CODE FLEXIBILITY

Point Source And Extended Source

- The code works for both point and extended source.

- In the extended source code, there is the parameter "rSphereMax", which is the radius of the spherical source.

- The code will automatically work for both cases once the source is selected.

EVENT: THE PRIMARY GENERATOR

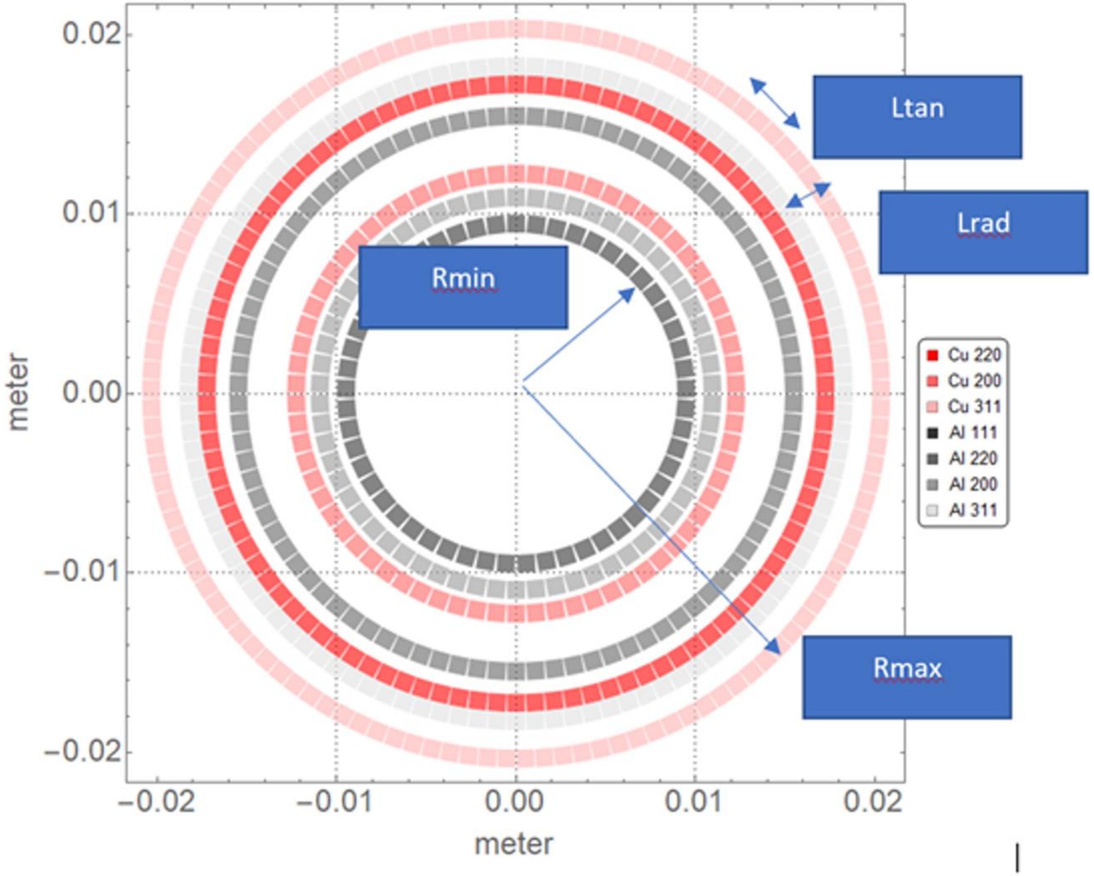
- The particle, its energy, position, and direction, are set in the PrimaryGeneratorAction class.
- The primary kinematics consists by default of a single 150 keV gamma placed at position (0,0,0).
- It is directed to interact with the lens (i.e. lens LensRmin and LensRmax define the gamma theta limits).

GEOMETRY DEFINITION

- The Laue lens volume is represented as a tube of dimensions (mm) with RMax and RMin.
- The initial parameters are set as shown in the below table:

Parameter	Default Set Values (mm)
Inner Radius ($RMin$).	8.97
Outer Radius ($RMax$).	20.83
Focal Length	500
Scale Factor ($ScaleFactor$).	1
Detector position	(0,0,1000)
Lens position	(0,0,500)
Source Position	(0,0,0)

Geometry Definition



The following properties are defined by the command /exLaueLens/LaueConstProperty(with their default values):

- LensLRad: length of the crystals along the radial direction with respect to the lens, on the lens plane.
- LensLTan: length of the crystals along the tangential direction with respect to the lens, perpendicular to LensRad, on the lens plane.

The GEANT4 Developed Process

First, position of the diffracted and transmitted xD,yD are determined based on the Monte Carlo simulation and the lens diffraction. And then use this position to pass it to the Geant4 track:

```
G4double localFocusZ = fabs((prePos.z()+postPos.z())/2.-vtxPos.z());
   G4ThreeVector localFocus(xyD.x(),xyD.y(),localFocusZ);
   const G4VTouchable* lensTouch = preStepPoint->GetTouchable();
   localFocus += G4ThreeVector(0.,0.,fFocalLength);
   //    G4cout << " localFocus TRANSL " << localFocus << " " << lensTouch->GetTranslation() << G4endl; //GDEB
   localFocus *= *(lensTouch->GetRotation());
   //  G4cout << " localFocus ROT " << localFocus << " " << *(lensTouch->GetRotation()) << G4endl; //GDEB
   G4ThreeVector globalFocus = localFocus;
```

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The GEANT4 Developed Process

- This work presents the first attempt to model X-ray and gamma ray focusing based on Laue diffraction in the GEANT4 toolkit.

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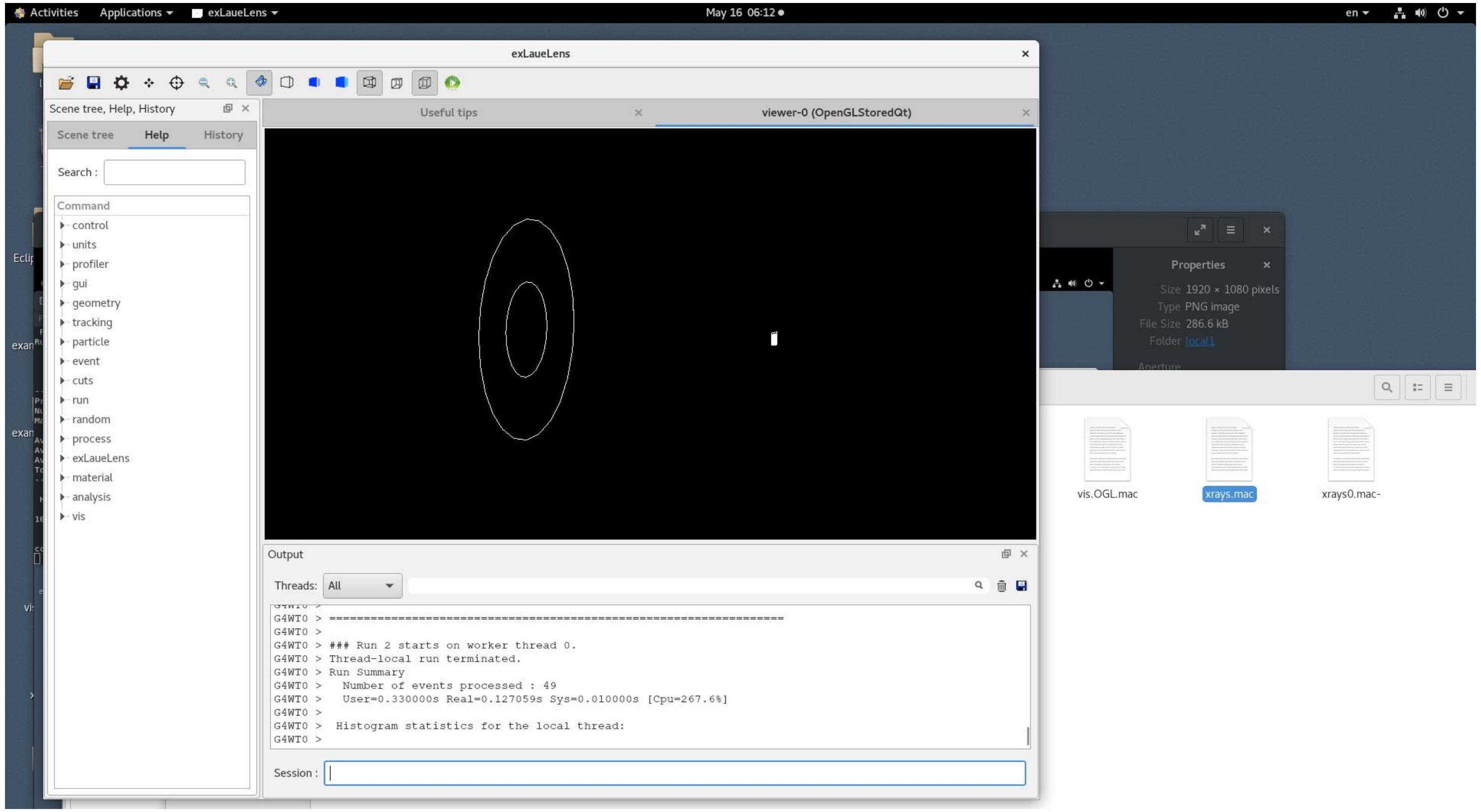

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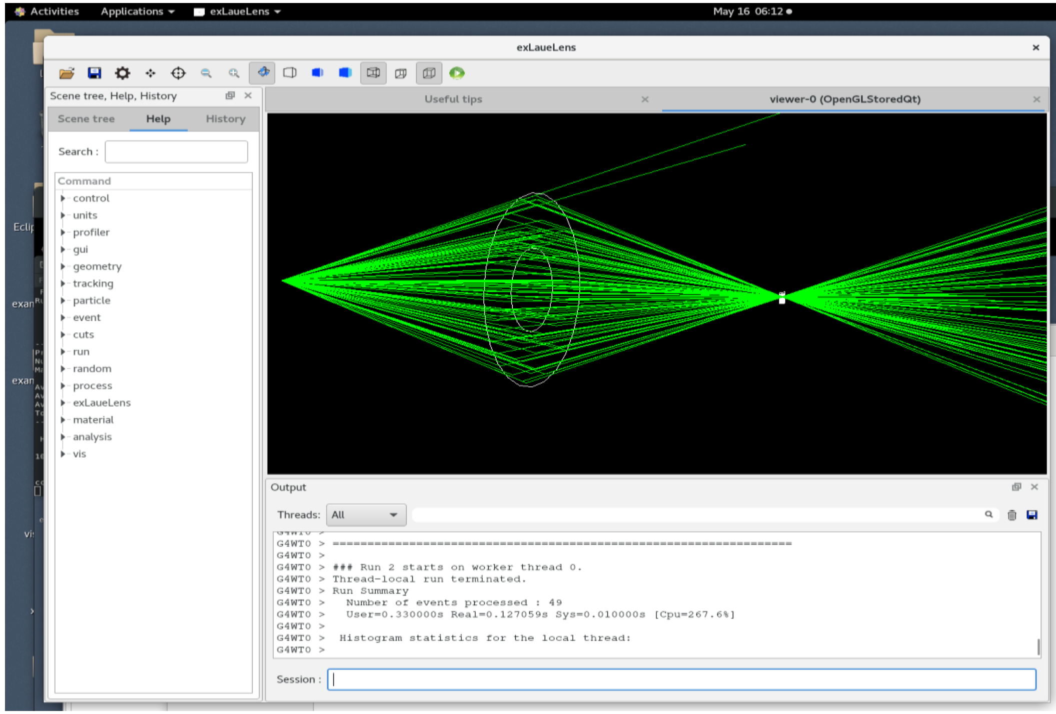
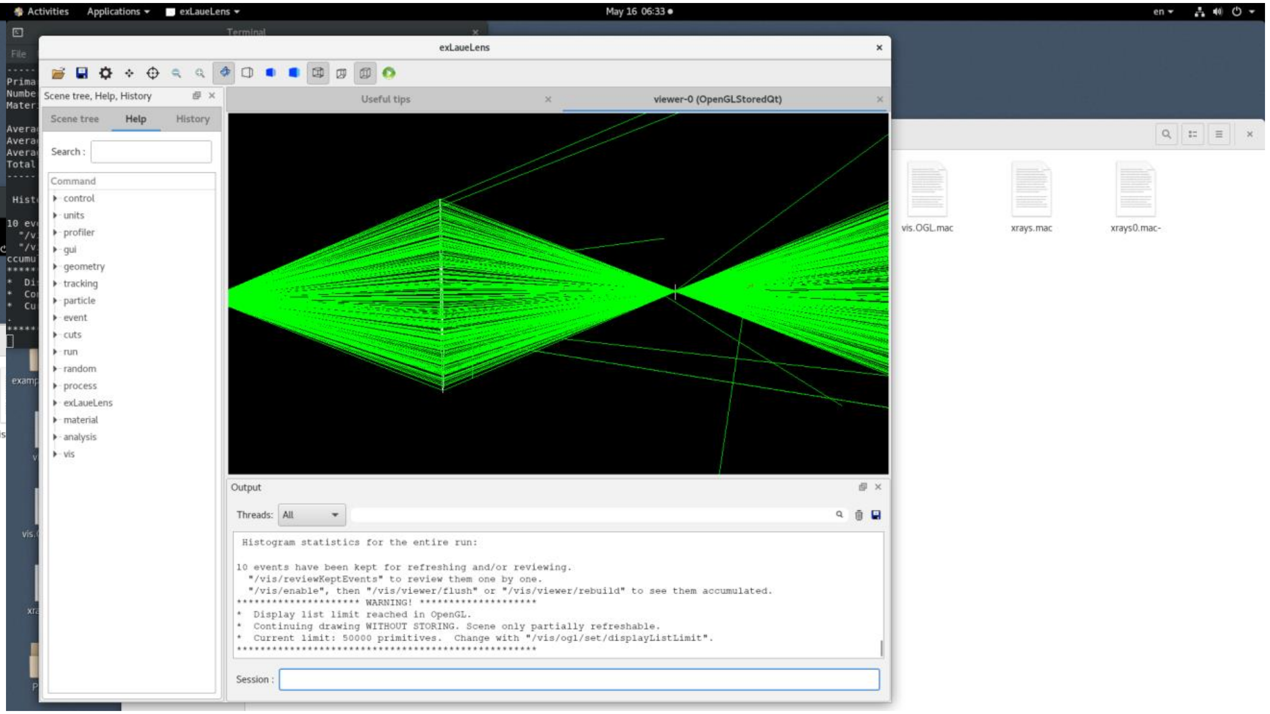
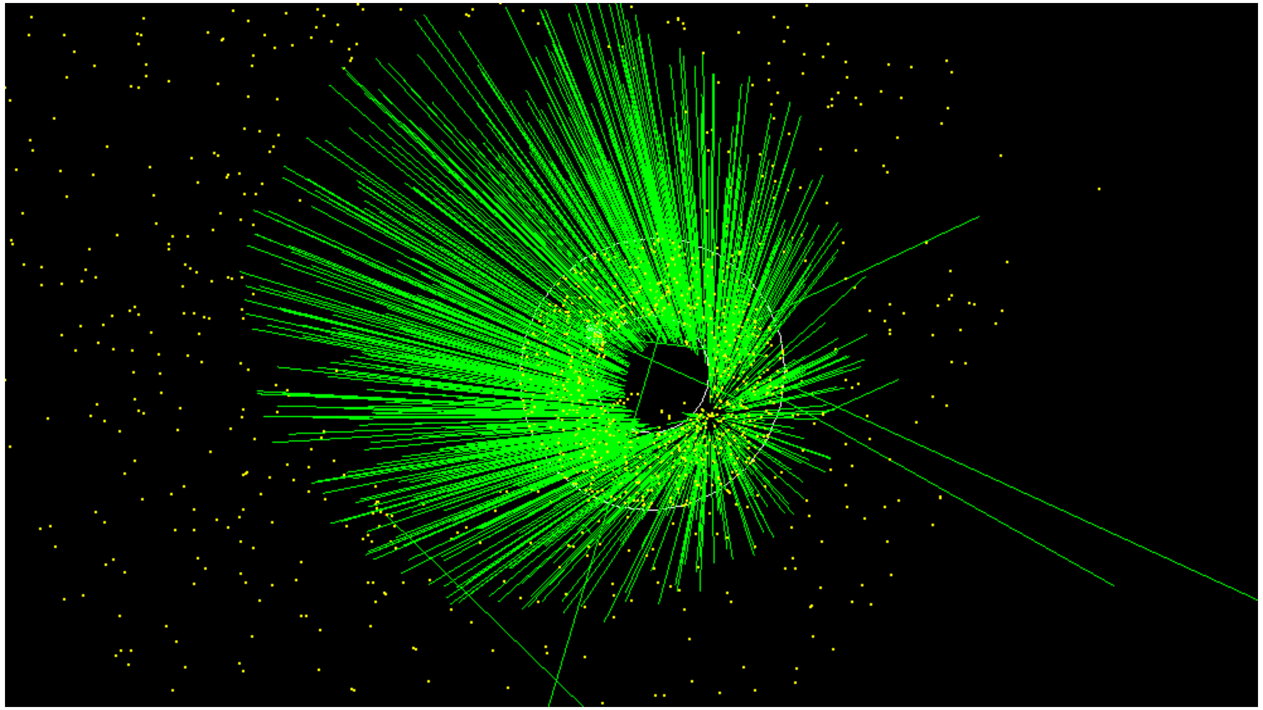
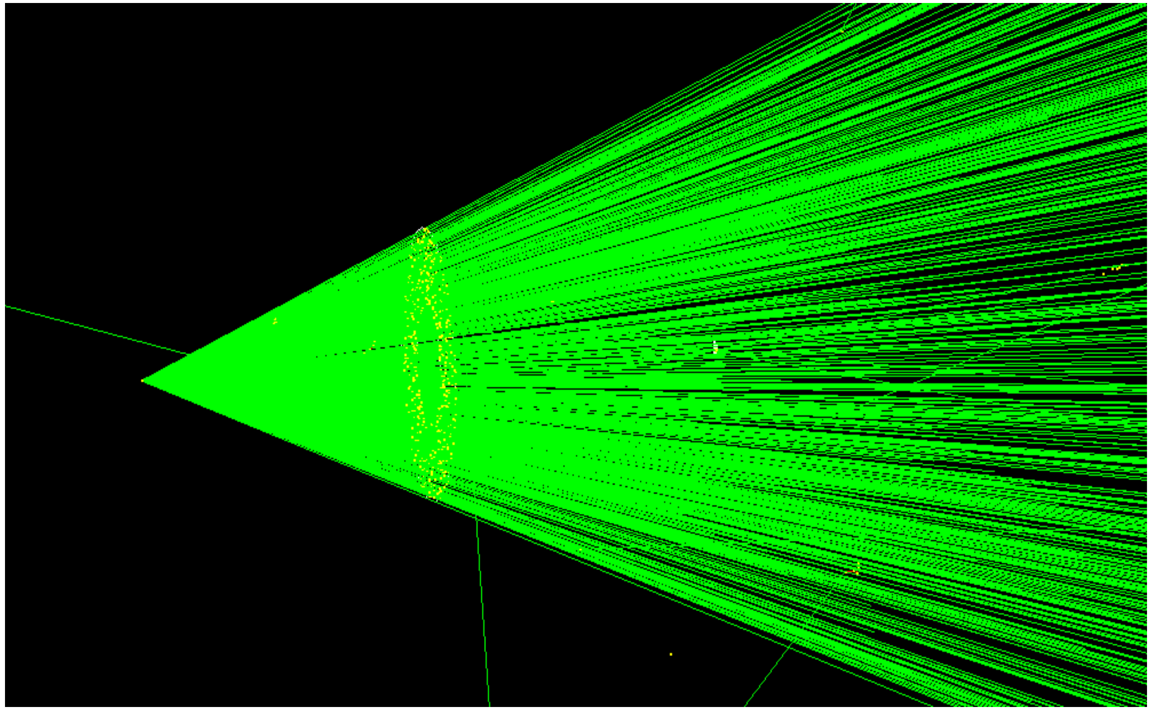
The GEANT4 Developed Process





The GEANT4 Developed Process





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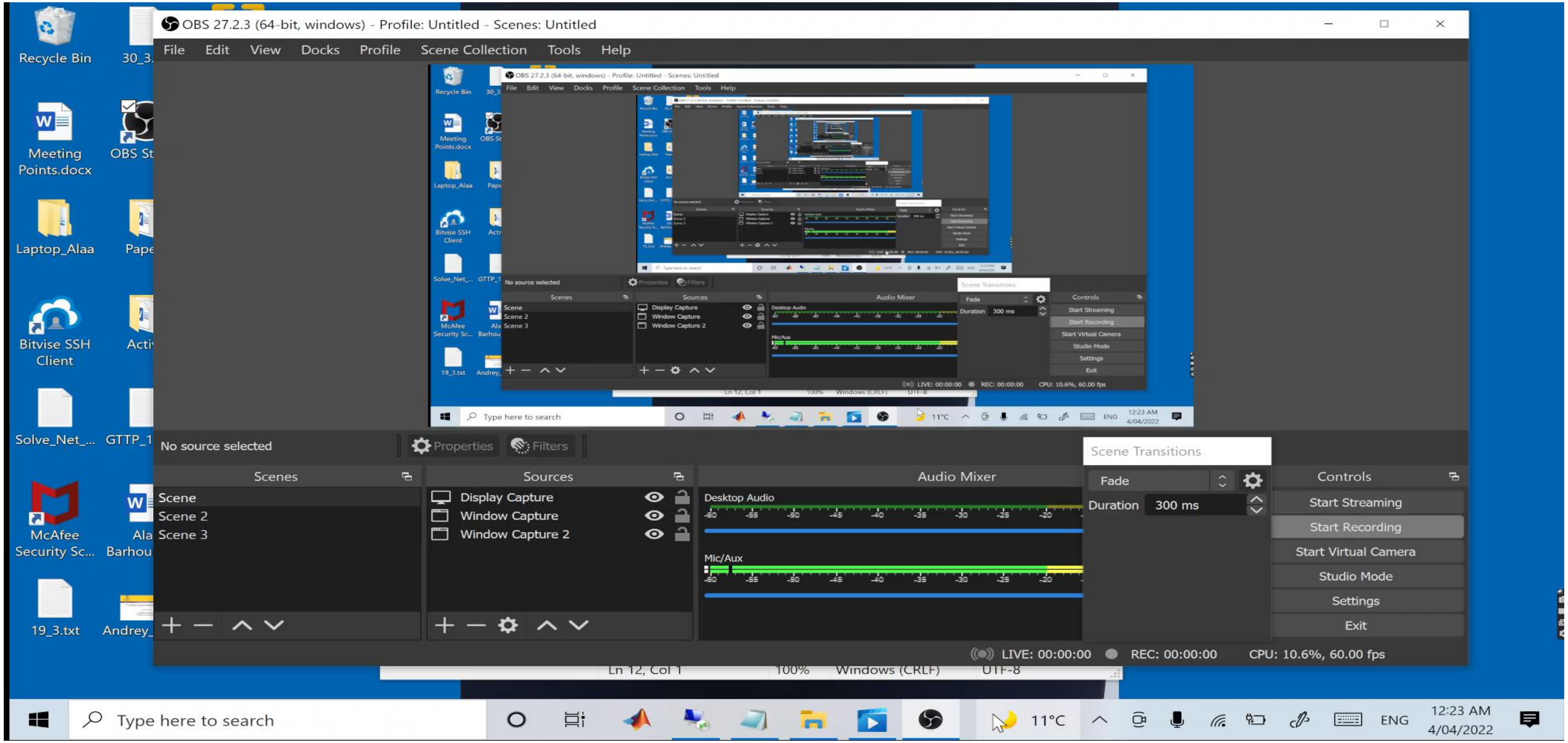
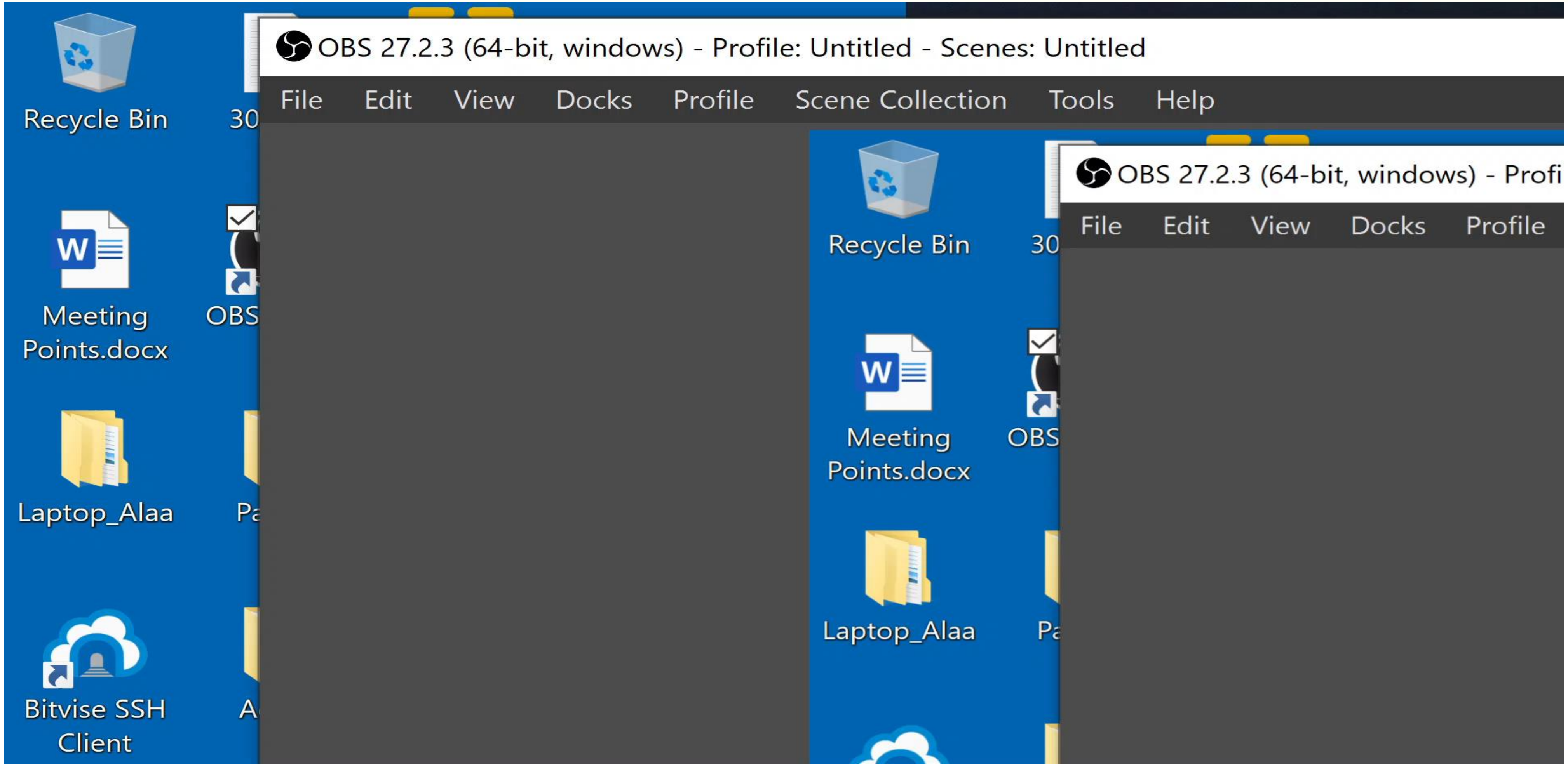
The GEANT4 Developed Process



The GEANT4 Developed Process



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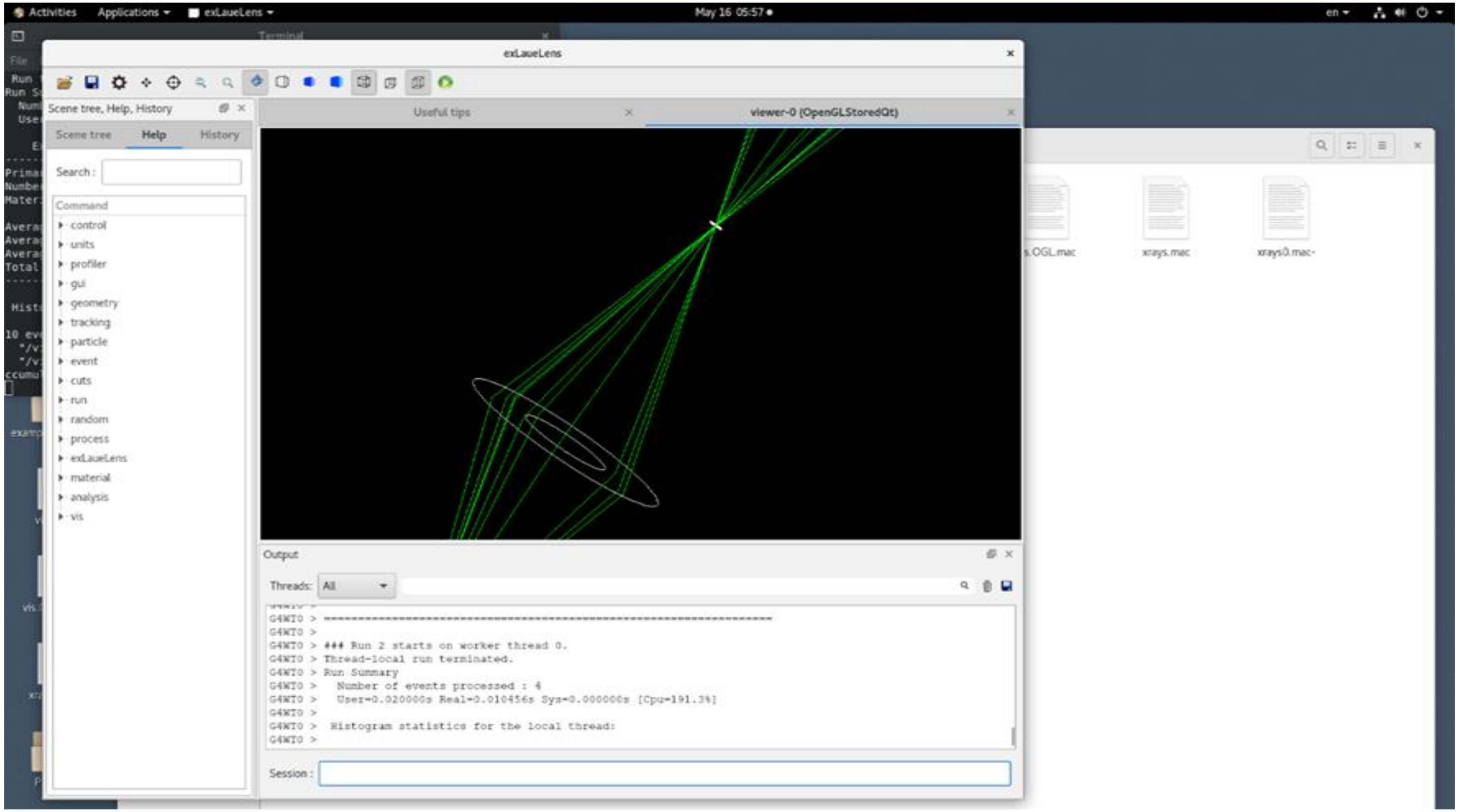
The GEANT4 Developed Process



CONTRIBUTION TO KNOWLEDGE

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- Facilitating the Laue lens simulations in a stable environment for high energy physics would help address specific needs in measuring extreme astrophysical sources that probe some of the most pressing questions in fundamental physics for the next decade.

- The diffraction mechanism hasn't been implemented in the existing Monte Carlo. Thus, the wave nature effect can't be imitated. This is one of the significant limitations scientists encounter when attempting to model Laue lens gamma focusing in a realistic particle tracking environment.

- The upcoming advancements in SPECT and the need for high-resolution systems have motivated the development of a particle transport code for the Gamma rays focusing by a particular type of lens named Laue lens with the focus on its application SPECT oncology.

CONCLUSION

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- The developed example models the wave-based properties of gamma rays and predicts the diffracted, transmitted, and absorbed gamma ray and Z locations on the detector plane based on a Monte Carlo simulation.

- The mode provides flexibility to control several input parameters for various Laue lens designs.

- The Laue diffraction code is a particle transport code developed to simulate the propagation of energetic particles through any volume of interest. It is established by defining this volume as the Laue lens by default.

CONCLUSION

- The Geant4 Laue diffraction project proposed in the hope produce an open-source simulation software fully integrated into the Geant4 Monte-Carlo simulation toolkit to simulate the diffraction of the gamma rays based on the Laue lens focusing effect.

- Its functionality and capabilities carry on expanding at the same time as its performance is being improved.