

# New extended example exoticphysics/saxs

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# README file of saxs example

```
=====
Geant4 - an Object-Oriented Toolkit for Simulation in HEP
=====
```

```
Extended Example saxs
-----
```

The example saxs implements the typical setup of a Small Angle X-ray Scattering (SAXS) experiment. It is meant to illustrate the usage of molecular interference (MI) of Rayleigh (coherent) scattering of photons inside the matter, which is implemented in the G4PenelopeRayleighModelMI model.

## 1- GEOMETRY

The setup consists of a phantom/sample under investigation, slits to collimate the photon beam and a shielded detector to collect the photons scattered by the phantom (see SAXSDetectorConstruction).

The geometry is scalable through the interactive commands defined in the SAXSDetectorConstructionMessenger class. All the significant quantities, such as the setup (scattering) rotation angle, the position and size of all the volumes, as well as the phantom material can be set via macro commands.

Two macro files come with this example: saxs.in and saxs\_slits.in.

In the saxs.in macro, the phantom is a cylinder with a diameter and a height of 10 mm made of a mixture of 80% fat and 20% water. In general, if the argument of /det/setPhantomMaterial command is 2, as in this case, the material is a biological tissue ("MedMat") defined as a mixture of fat, water, collagen and hydroxyapatite. The weight fraction of the mixture components can be set through commands /det/setComp0, /det/setComp1, /det/setComp2, /det/setComp3, respectively. The tissue form factor (including MI) is automatically calculated as a weighed sum of the form factors of the basis components. In this case, no slits are foreseen and the sensitive detector positioned 400 mm downstream of the phantom collects all the photons transmitted and scattered by the phantom which is illuminated

# Introduction of interference effects in coherent X-ray scattering model

In **Rayleigh (Coherent) Scattering**, photons are scattered by **bound atomic electrons** without excitation of the target atom, i. e., the energy of incident and scattered photons is the same.

**Differential cross-section**  $\frac{d\sigma_{Ra}}{d\Omega} = r_e^2 \frac{1 + \cos^2 \theta}{2} |F(q, Z)|^2$

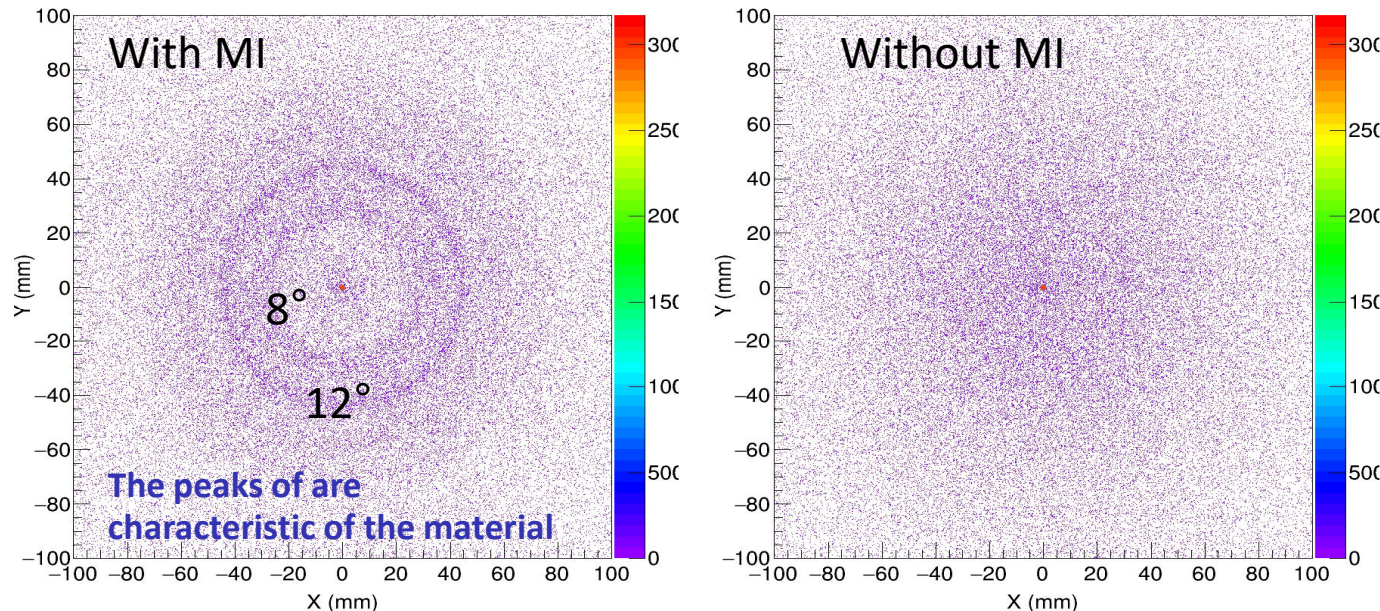
**Momentum transfer [nm<sup>-1</sup>]**  $x = \frac{q}{2h} = \frac{1}{\lambda} \sin(\theta/2)$   $\tilde{q} = \frac{q}{m_e c}$  (used in Geant4)

**Common MC approach for molecules: IAM**

$$F_{mol, IAM}^2(q) = W \sum_i \frac{w_i}{A_i} F^2(q, Z_i) \rightarrow \text{No interference effects}$$

**For each material, a proper Form Factor including interference effects is required**

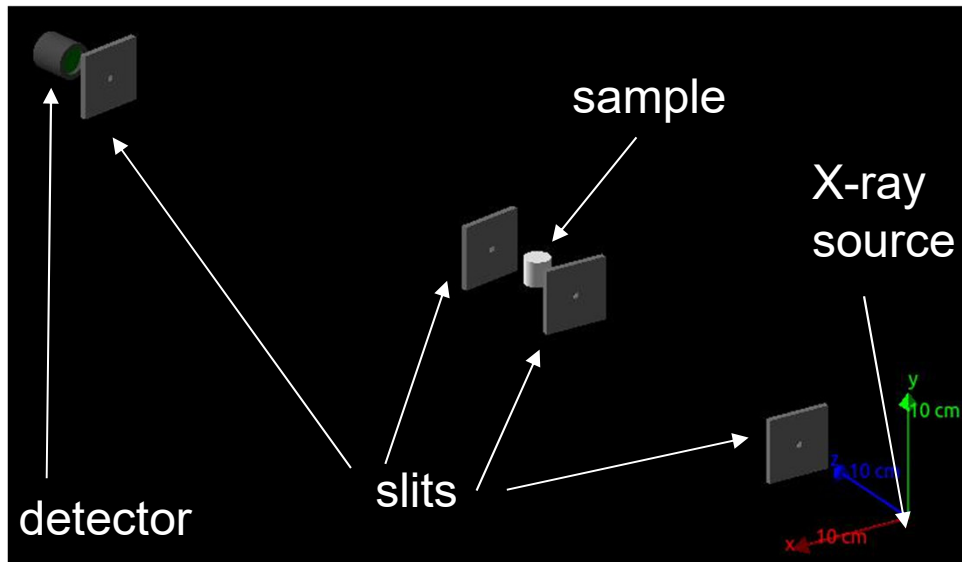
# Introduction of interference effects in coherent X-ray scattering model



Scattering of a 20 keV photon beam in a human breast sample

- The **Penelope model** was modified to read **molecular form factors (FF)** with **interference effects** [G. Paterno et al, *Physica Medica* 51 (2018) 64–70].
- A **library of 32 FFs** is made available.
- Every **biological tissue** can be **segmented in 4 basis components** [G. Paterno et al, *Physics in Medicine and Biology* Vol. 65(2020), 245002].
- The user can introduce **custom form factors** with interference (using the support of **G4ExtendedMaterial**)

# saxs example



The **setup** reproduces that of a **typical SAXS experiment**.

- **Geometry, materials and X-ray source** can be set through **custom user commands**.
- **Sample material management:** the “**basis approach**” is foreseen and it can be activated by codifying the material composition in its name, e. g., “*MedMat\_0.25\_0.36\_0.13\_0.36*” or by dedicated commands. Also, the user can **define a new material** and its FF via macro.

## #Medical material (MedMat) definition

```
/det/setPhantomMaterial 2
/det/setComp0 0.80    #Comp0->Fat
/det/setComp1 0.20    #Comp1->Water
/det/setComp2 0.00    #Comp2->Collagen (BM)
/det/setComp3 0.00    #Comp3->Mineral (HA)
```

## #Custom Material (CustomMat) definition

```
#Z={H,C,N,O,Na,P,S,Cl,K,Ca};
/det/setPhantomMaterial 30
/det/setCustomMatDensity 1.72    #[g/mol]
/det/setCustomMatHmassfract 0.0504
/det/setCustomMatNmassfract 0.3500
/det/setCustomMatOmassfract 0.5996
/det/SetCustomMatFF myFF.dat    #NH4NO3
```

## #materials for the Phantom:

#1->Water, **2->MedMat**, 3->PMMA, 4->Adipose, 5->Glandular, 6->Breast5050, ... , 19->Nylon, #20->Polyethylene, 21->Polystyrene, ... , 27->CIRS7030, 28->RMI454, 29->Air, **30->CustomMat**



# saxs example

From the point of view of the implementation, saxs is a quite standard application.

- MI effects can be activated by instantiating, in the *PhysicsList*, the custom *constructor* **G4emPenelopePhysicsMI**, which builds Penelope EM models and sets **G4PenelopeRayleighModelMI** for coherent scattering. By default, the standard constructor is used, and the MI effects can be set through the user command:  
**/phys/SelectPhysicsList penelopeMI**
- *PrimaryGenerator* is a **GPS** with no default setting -> X-ray source defined via macro. Two macros are provided, one for ADXRD (no slits) and EDXRD (slits used).
- **Scoring** is performed through a *SteppingAction* class and a *SensitiveDetector*. The *SteppingAction* class is used to score the processes that primary photons undergo inside the sample/phantom. Also, the kinetic energy of the photons before the interaction and the deviation angle of the particle are stored. Instead, the *SensitiveDetector* is used to score all the information of the particles impinging on its surface.
- Two **root scripts** are provided to perform **data analysis**: **scattAnalysis.C** can be used to analyze the ntuple scored through the *SteppingAction* class, while **ADXRD.C** can be used for ntuple provided by the *SensitiveDetector*.

# Example of input macro

```
/det/setComp0 0.80
```

```
/det/setComp1 0.20
```

```
/det/setComp2 0.00
```

```
/det/setComp3 0.00
```

```
/det/setPhantomMaterial 2
```

```
/det/setPhantomDiameter 10. mm
```

```
/det/setPhantomHeight 10. mm
```

```
/det/setPhantomZ 500. mm
```

```
/det/setThetaSetup 0.
```

```
/det/setSlits true
```

```
/det/setSlitThickness 20. mm
```

```
/det/setSlit1SampleDistance 200. mm
```

```
/det/setSlit2SampleDistance 100. mm
```

```
/det/setSlit3SampleDistance 100. mm
```

```
/det/setSlit4SampleDistance 200. mm
```

```
/det/setSlit1Aperture 5. mm
```

```
/det/setSlit2Aperture 5. mm
```

```
/det/setSlit3Aperture 5. mm
```

```
/det/setSlit4Aperture 5. mm
```

```
det/setDetectorSize 200. mm
```

```
/det/setDetectorThickness 20. mm
```

```
/det/setDetectorSampleDistance 400. mm
```

```
/phys/SelectPhysicsList penelopeMI
```

```
/phys/setCuts 0.1 mm
```

```
/run/initialize
```

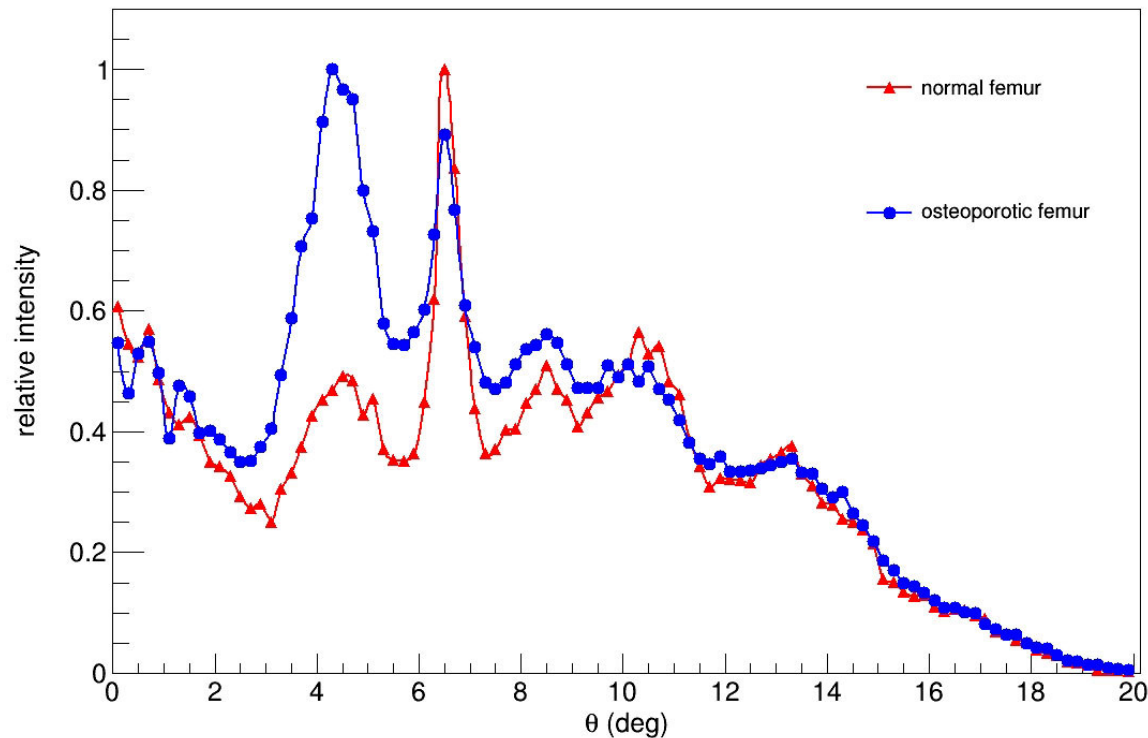
```
/run/setfilenamesave output
```

```
/control/execute beam.mac
```

```
/run/printProgress 100000
```

```
/run/beamOn 1000000
```

# Example of output



**Normal** 36% fat + 15% water +  
13% collagen + 36% HA

**Osteoporotic** = 55% fat + 25%  
water + 05% collagen + 15% HA

Scattering of a 38 keV pencil photon beam incident  
on two samples (5 cm diam) of human femoral  
bone (trabecular tissue)



# Conclusions

- **saxs example allows the user to:**
  - understand how to enable MI effects in X-ray coherent scattering model,
  - define new materials and their FF via user commands,
  - simulate WAXS/SAXS experiments.