Geant4 implementation of interference effects in X-ray coherent scattering

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Interference effects in coherent X-ray scattering

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^{-1}]

$$x = \frac{q}{2h} = \frac{1}{\lambda}\sin(\theta/2) \qquad \tilde{q} = \frac{q}{m_e c} \text{ (used in Geant4)}$$

Common MC approach for molecules: IAM

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

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

Interference effects in coherent X-ray scattering

Molecular Form Factor of water

The FF peaks are characteristic of the material
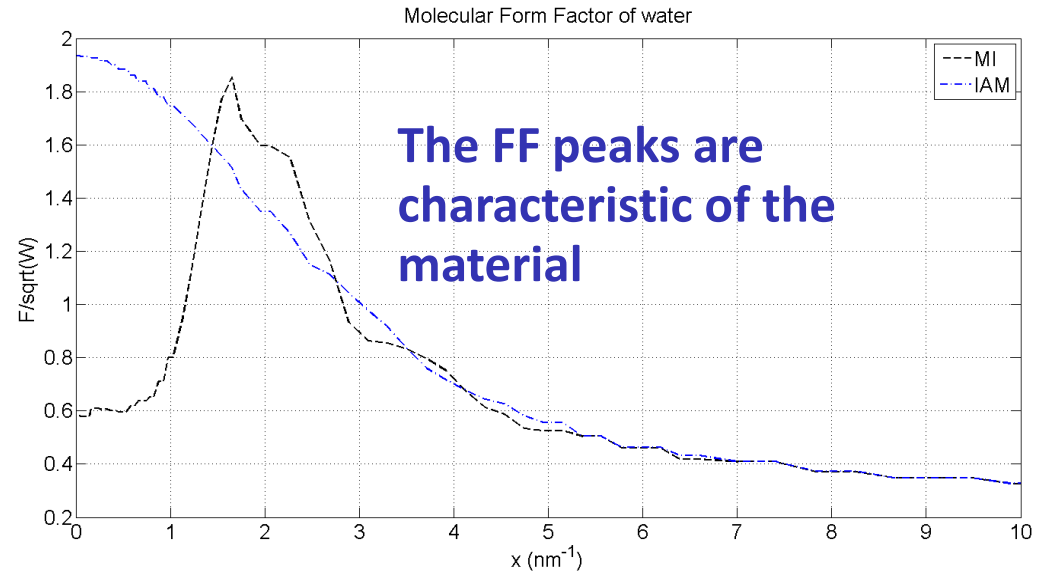
Effect of Molecular Interference (MI)

Coherent scattering **dominates** Compton scattering at low angles and it is **distinguishable** from primary beam.

With MI

8°

12°

Without MI
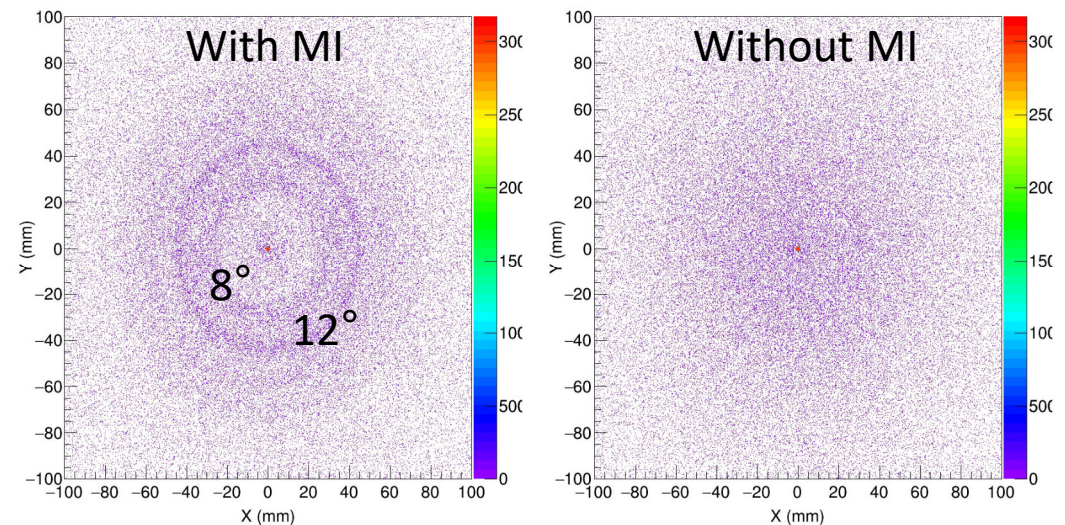
Scattering of a **20 keV photon beam** in a **human breast** sample

G4 implementation of interference (MI) effects

- The Penelope model was extended **(G4PenelopeRayleighModelMI)** to **read molecular form factors (FF) with interference effects** *[G. Paterno et al, Physica Medica 51 (2018) 64–70]*.

- **G4PenelopeRayleighModelMI** class coexists with the "standar" **G4PenelopeRayleighModel** class and it can be selected instead of the standard version in the user **PhysicsList** to activate MI.

- A **library of 32 FFs** is made available. The database was **rationalized** avoiding redundance and fully **validated** with respect to previous implementation.

- 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**).

- **The cross-section is re-calculated integrating the DCS**.

- A significant amount of work was done to make the developed code **compliant** with the **Geant4 official guidelines** and **avoid** any possible **bug** and **memory waste**.

G4 implementation of interference (MI) effects

Read the Form Factors with Molecular Interference (MIFF)

A new method of G4PenelopeRayleighModelMI: **ReadMolInterferenceData(const G4String&,const G4String& filename="NULL")** is used to read the form factor (FF) with molecular interference (MI) of a **selected variety of materials**, according to a well-defined association "matname" <-> "MIFF" (reported in the documentation page).

```
fKnownMaterials->insert(std::pair<G4String,G4String>("Fat_MI","FF_fat_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("Water_MI","FF_water_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("BoneMatrix_MI","FF_bonematrix_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("Mineral_MI","FF_mineral_Tartari2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("adipose_MI","FF_adipose_Poletti2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("glandular_MI","FF_glandular_Poletti2002.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("breast5050_MI","FF_human_breast_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("carcinoma_MI","FF_carcinoma_Kidane1999.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("muscle_MI","FF_pork_muscle_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("kidney_MI","FF_pork_kidney_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("liver_MI","FF_pork_liver_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("heart_MI","FF_pork_heart_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("blood_MI","FF_beef_blood_Peplow1998.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("grayMatter_MI","FF_gbrain_DeFelici2008.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("whiteMatter_MI","FF_wbrain_DeFelici2008.dat"));
fKnownMaterials->insert(std::pair<G4String,G4String>("bone_MI","FF_bone_King2011.dat"));
```

MIFF then are stored in a dedicated map (matname is the key):
std::map<G4String,G4PhysicsFreeVector*> ***MolInterferenceData**;
This map is recalled in **BuildFormFactorTable(const G4Material*)** method. **MT compliant**, *Tables are computed by master thread and passed to the secondary threads*.

For materials with MIFF, the cross-section is calculated by integrating the DCS (overriding of **ComputeCrossSectionPerVolume(const G4Material*)** of G4VEmModel). If a coherent scattering event occurs, the scattering angle is sampled according to RITA algorithm, which was not modified.

Decomposition of tissues in basis components

Beef Adipose tissue (Peplow-Verghese, 1998) = 76% fat + 24% water
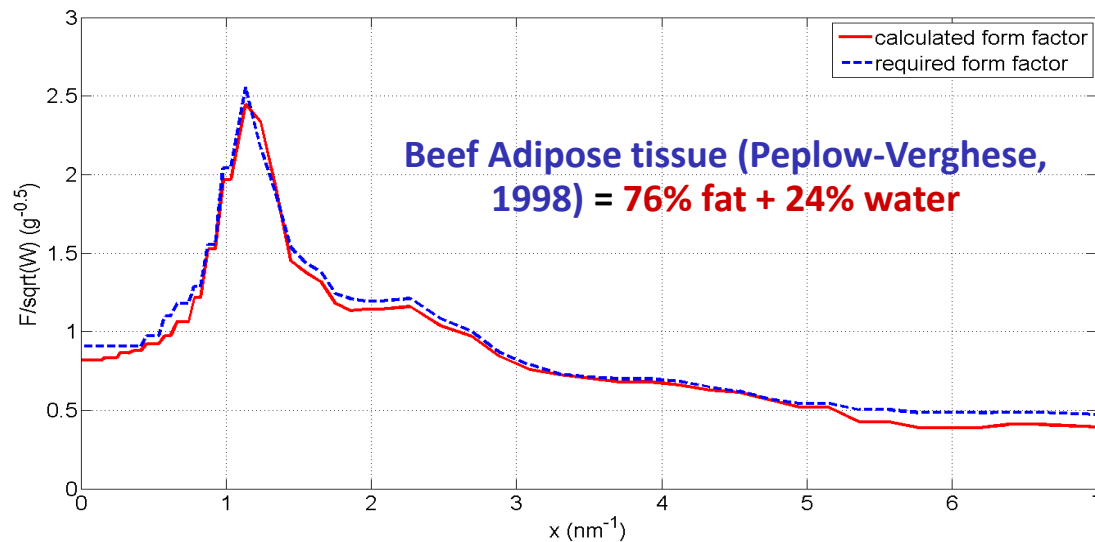
$$\frac{F^2}{W} = \sum_{i=1}^{4} a_i \frac{F_i^2}{W_i}$$

i=fat, water, collagen, hydroxyapatite

Avoid to use unclassified tissues

No extension needed, simply define a material and label it as "**MedMat_a1_a2_a3_a4**", where **ai are the weight fractions of the 4 basis materials** (example: "MedMat_0.80_0.20_0.00_0.00").

In the **BuildFormFactorTable(const G4Material*)** method, the basis FFs are mixed accordingly.

Form factor defined by the user

NH4NO3
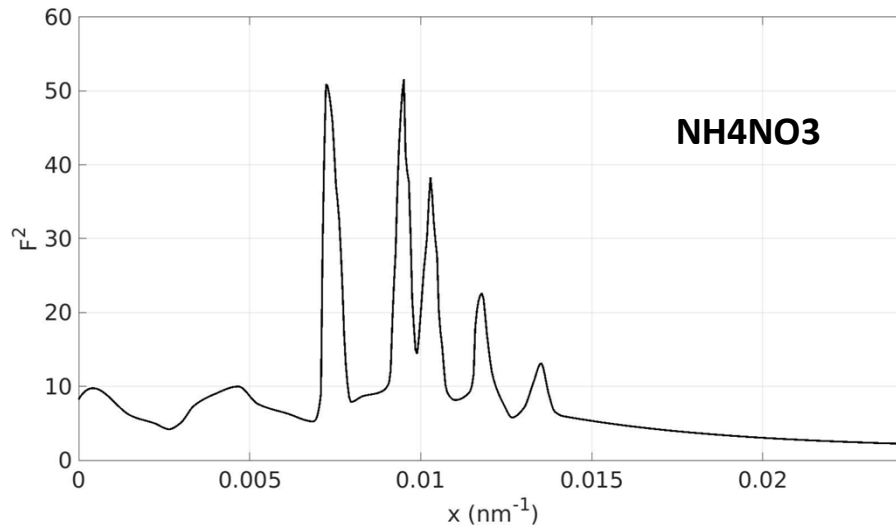
Useful for materials with partial crystalline behavior

In the **DetectorConstrucion.cc**, use the new **G4MIdata** extension to provide the path of the FF file of the material (through **setFilenameFF(G4String)** method).

```
d = CustomMatDensity*g/cm3;
matname = "CustomMat";
CustomMat = new G4ExtendedMaterial(matname, d, nel);
if (CustomMatHmassfract) CustomMat->AddElement(elH, CustomMatHmassfract);
if (CustomMatCmassfract) CustomMat->AddElement(elC, CustomMatCmassfract);
if (CustomMatNmassfract) CustomMat->AddElement(elN, CustomMatNmassfract);
if (CustomMatOmassfract) CustomMat->AddElement(elO, CustomMatOmassfract);
if (CustomMatNamassfract) CustomMat->AddElement(elNa, CustomMatNamassfract);
if (CustomMatPmassfract) CustomMat->AddElement(elP, CustomMatPmassfract);
if (CustomMatSmassfract) CustomMat->AddElement(elS, CustomMatSmassfract);
if (CustomMatClmassfract) CustomMat->AddElement(elCl, CustomMatClmassfract);
if (CustomMatKmassfract) CustomMat->AddElement(elK, CustomMatKmassfract);
if (CustomMatCamassfract) CustomMat->AddElement(elCa, CustomMatCamassfract);
//Extend the material
CustomMat->RegisterExtension(std::unique_ptr<MIdata>(new MIdata("MI")));
MIdata* dataMICustomMat = (MIdata*)CustomMat->RetrieveExtension("MI");
dataMICustomMat->SetFilenameFF(fCustomMatFF);
```

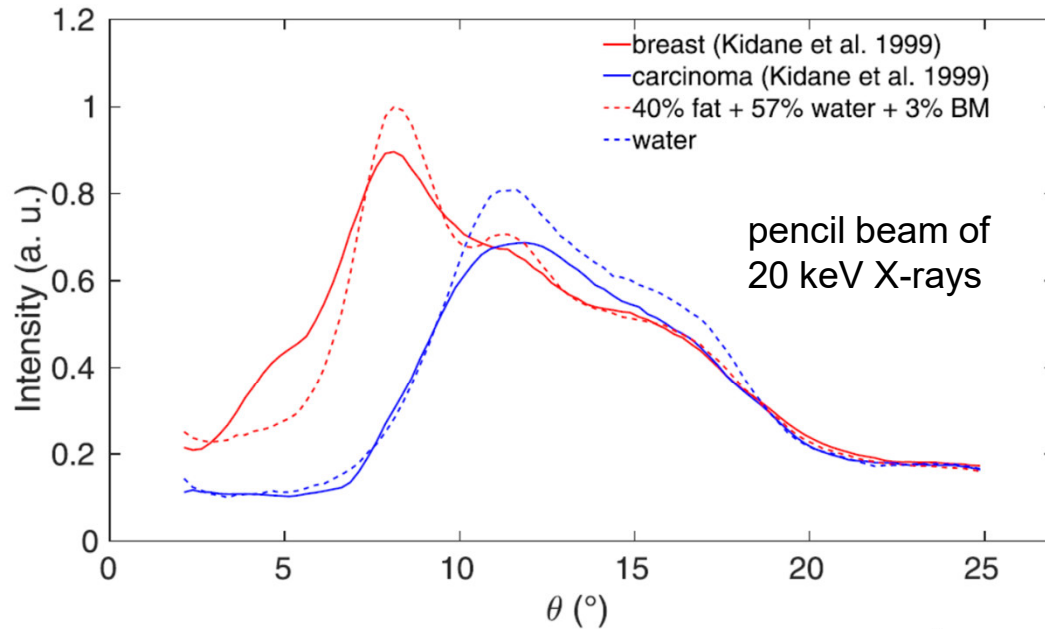It will be used in the **BuildFormFactorTable**(const G4Material*) method.

Validation
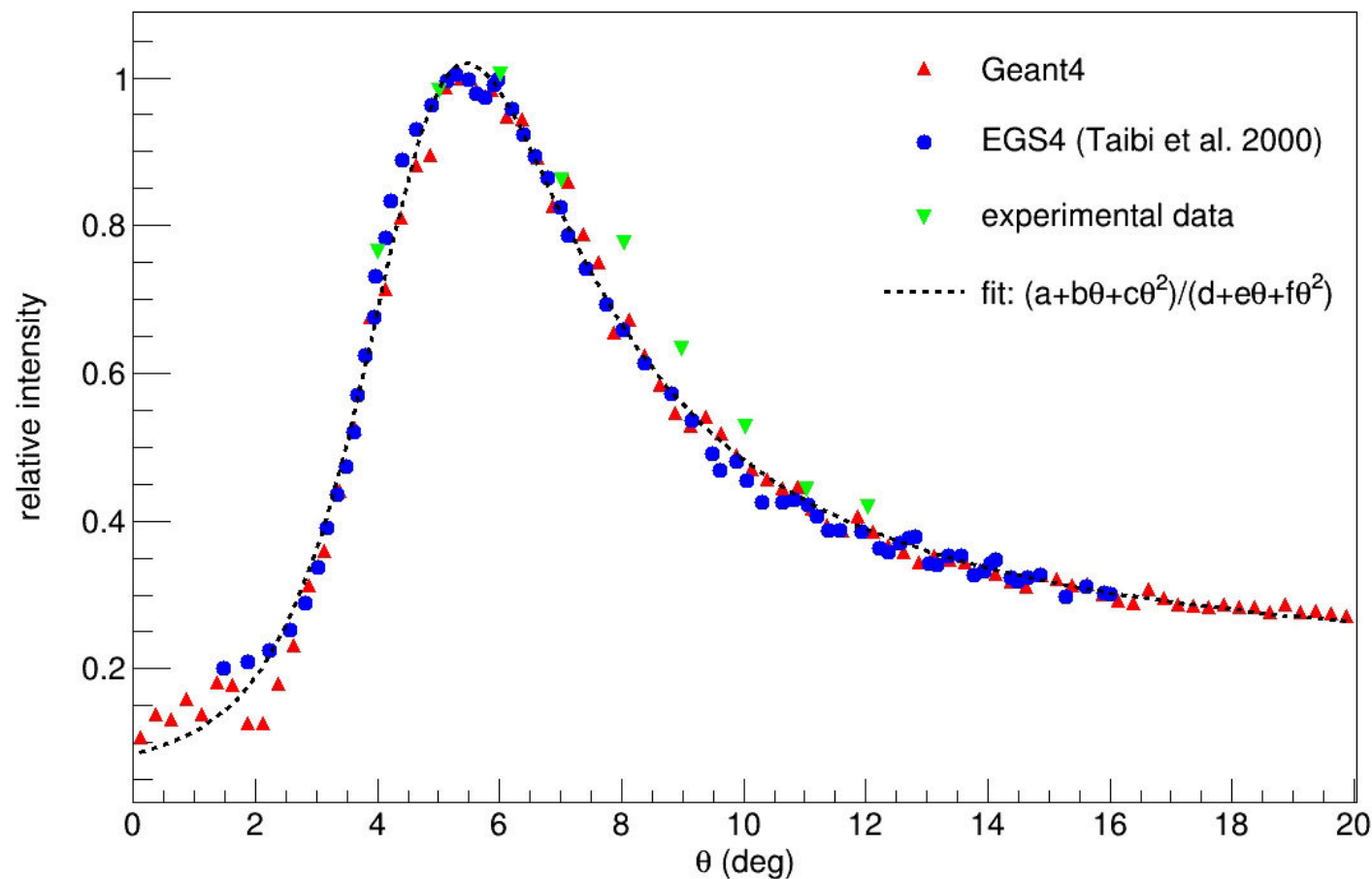
Simulation of the experiment by Evans et al., 1991: Scattering of **polychromatic X-rays** (60 kVp and filtration of 0.5 mm Cu) **from a 5 mm-thick carcinoma sample.**

Simulations agree with the experiment.
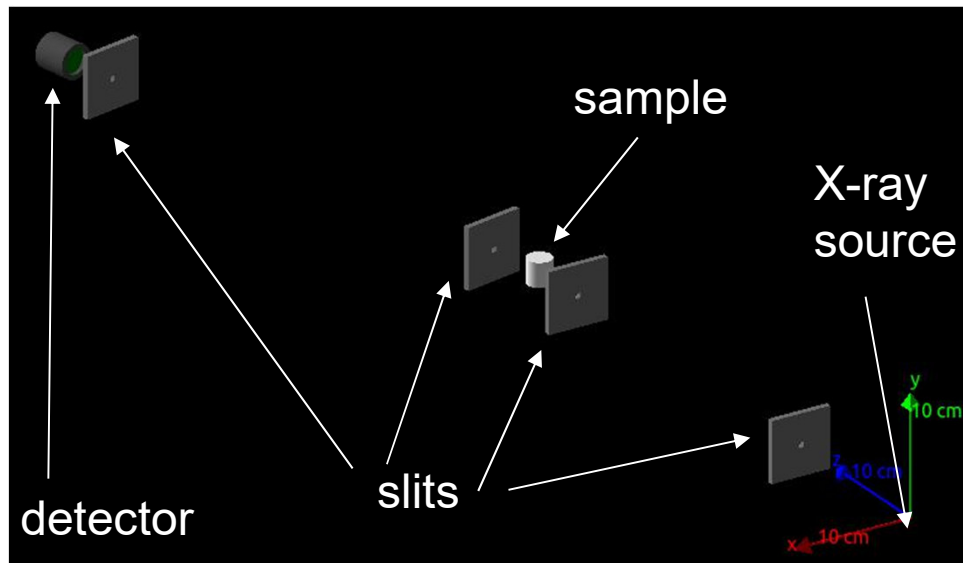
G. Paternò et al., Physica Medica 51 (2018) 64 -70

Validation and possible use: classification of tissues

pencil beam of 20 keV X-rays

Polychromatic X-ray beam

G. Paterno et al, Physics in Medicine and Biology Vol. 65(2020), 245002
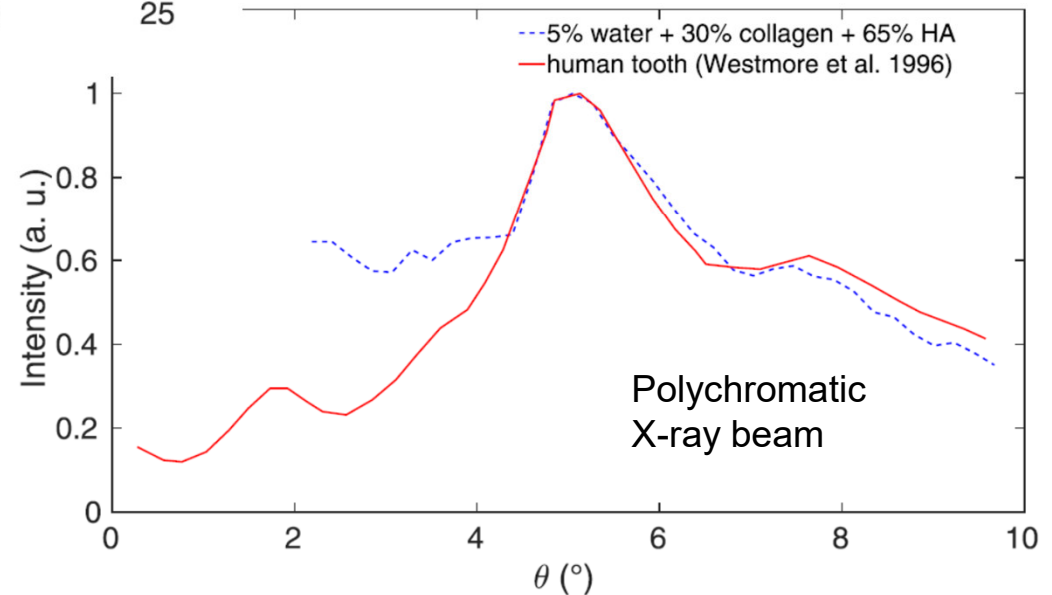
saxs example (see dedicated slides)

A **dedicated (extended) example** was developed to show how to enable and exploit molecular interference implementation.

• **Geometry, materials and X-ray source** can be set through **custom commands** (to be used in a macro file)

• **Material management** (the "**basis approach**" is foreseen and can be activated by codifying the material composition in its name, e. g., "*MedMat_0.25_0.36_0.13_0.36*")

• **Scoring** through *SteppingAction* and *SensitiveDetector* (simple scoring screen or Ge detector) -> **root scripts** are provided for data analysis

Documentation

considered material. To take into account the molecular interference effect (MI), form factors extracted from the measured scattering (diffraction) patterns can be used. A database of form factors including MI effect for a variety of materials, mainly biological tissue and plastics, is available. In order to use the files of the database, the user has to label the defined materials according to the following table:

material	label
fat	Fat_MI
water	Water_MI
collagen	BoneMatrix_MI
hydroxyapatite	Mineral_MI
PMMA	PMMA_MI
adipose	adipose_MI
glandular	glandular_MI
breast (50%fat + 50%water)	breast5050_MI
liver	liver_MI
kidney	kidney_MI
muscle	muscle_MI
heart	heart_MI
blood	blood_MI
bone	bone_MI
carcinoma	carcinoma_MI

Sidebar

⌂ Geant4 Homepage

Geant4 Documentation

10.7 (doc Rev5.0)

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Installation Guide

Book For Application Developers

Physics Reference Manual

General Information

Particle Decay

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Electromagnetic Physics in GEANT4

Gamma incident

Introduction to Gamma

Documentation

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Physics Reference Manual

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CIRS30-70	CIRS30-70_MI
CIRS50-50	CIRS50-50_MI
CIRS70-30	CIRS70-30_MI
RMI454	RMI454_MI

Due to the tissue variability, the measured diffraction patterns of two samples of the same tissue type may differ significantly. To overcome this problem, a generic tissue can be decomposed in simpler basis materials with well-defined elemental composition. In particular, each tissue is considered as a composition of four components, namely fat, water, collagen or bone matrix, and hydroxyapatite (see [PaternoCC+18], [PaternoCGT20]). The form factor of a generic tissue can be then expressed through the mixture rule using tissues (molecules or supramolecules) instead of atoms as:

$$\frac{F^2(q)}{W} = \sum_{i=1}^{4} \frac{a_i F_i^2(q)}{W_i}, \qquad (3)$$

where a_i is the mass fraction of i-th basis component.

In order to enable this functionality, the user has to create the mixture of basis materials (whose composition and density are defined in [PaternoCGT20] and label the material as *MedMat_a1_a2_a3_a4*, where *ai* are three digit numbers representing the mass fraction of the basis components. Then, the form factor of the material is automatically calculated according to Eq.(3).

In order to gain generality, the user has the faculty of providing the form factor of the materials he wants to consider. This is obtained by defining a material as *G4ExtendedMaterial* and registering *G4MIData* extension. The *SetFilenameFF()* method of this class allows to specify the path of the file with the form factor of the material. This functionality is particularly suited for modeling materials with partial crystalline beahviour, such as powder and polycrystals, which are characterize by a large number of sharp diffraction peaks.

Conclusions

- The development of **interference effects in coherent X-ray scattering model** is completed and it was introduced in the official Geant4 release (from 10.7). A dedicated example was also implemented and made available to users as an official extended example. All the documentation describing the developed code was also produced.

- **The code developed allows** the user to:

  - remove scatter from images,

  - simulate WAXS/SAXS experiments,

  - classify unknown tissues.

Back-up slides

Sampling the scattering angle: RITA algorithm

First, the occurrence of a coh. scatt. event is determined from σ_{Ra}, then the angular deflection is sampled

$$P_{Ra}(\cos\theta) = \frac{1+\cos^2\theta}{2} F^2(q) \qquad 0 \le q \le q_{max} = 2E/c = 2m_e c\kappa$$

$$P_{Ra}(\cos\theta) = g(\cos\theta)\, \pi(q^2) \qquad g(\cos\theta) = \frac{1+\cos^2\theta}{2} \qquad \pi(q^2) = F^2(q)$$

rejection method

1. Using the **RITA algorithm**, sample a random value of q^2 from the distribution $\pi(q^2)$, restricted to the interval $[0, q_{max}^2]$.

2. Set $\cos\theta = 1 - 1/2 * q^2/k^2$ ($k = E/m_e c^2$).   *(it comes from the definition of $q = 2E/c[\sin(\vartheta/2)] = (E/c[2(1-\cos\vartheta)]^{1/2}$)*

3. Generate a new random number ξ (uniformly distributed in the interval $[0,1]$).

4. If $\xi > g(\cos\theta)$, go to step 3.   *(note that **g is a valid rejection function** since $0 < g \le 1$)*

5. Deliver $\cos\theta$.

Sampling efficiency higher than 66%