

# Generation and tracking of inverse Compton scattering photons in Geant4

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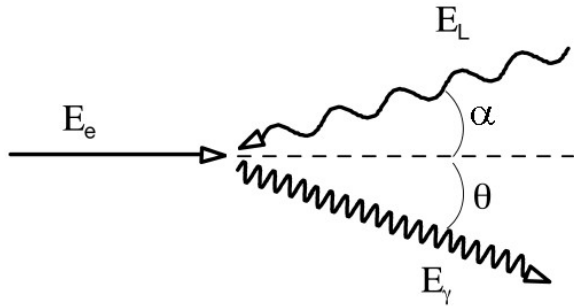
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# Outline

- Short introduction to Inverse Compton Scattering (ICS)
- Implementation of ICS process in Geant4
- An example for the generation and tracking of ICS photons in a medical setup

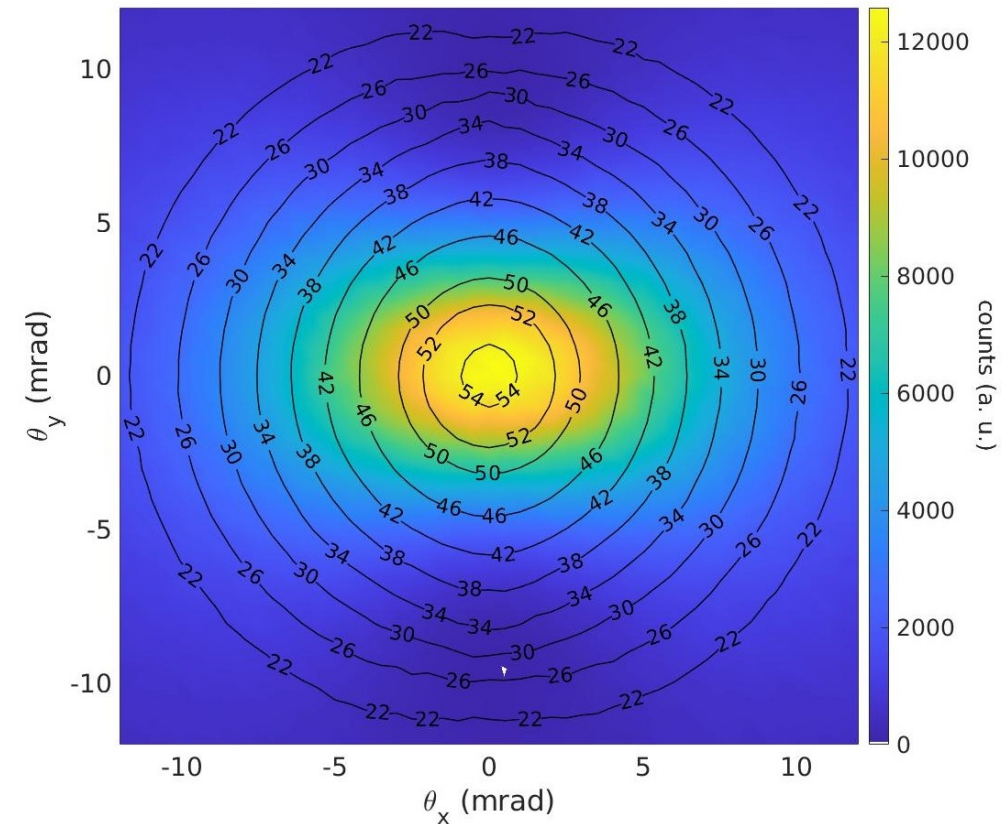
# Short introduction to Inverse Compton Scattering



$$E_\gamma \approx \frac{2\gamma^2(1+\cos\alpha)}{1+(\gamma\theta)^2 + \frac{4\gamma E_L}{m_e c^2}} E_L$$

- Laser photons interact with an accelerated electron beam and gain energy **(from infrared light (eV photons) → to keV or MeV radiation)**.
- A Correlation between the scattered photon energy  $E_\gamma$  and polar scattering angle  $\theta$  exists ( $E_\gamma$  does not depend on  $\phi$ ).
- The intensity distribution depends, in general, on both polar and azimuthal angles.
- The number of scattered photons within a solid angle defined by  $\psi = \gamma\theta_{\max}$ ,  $N_\psi$ , is:

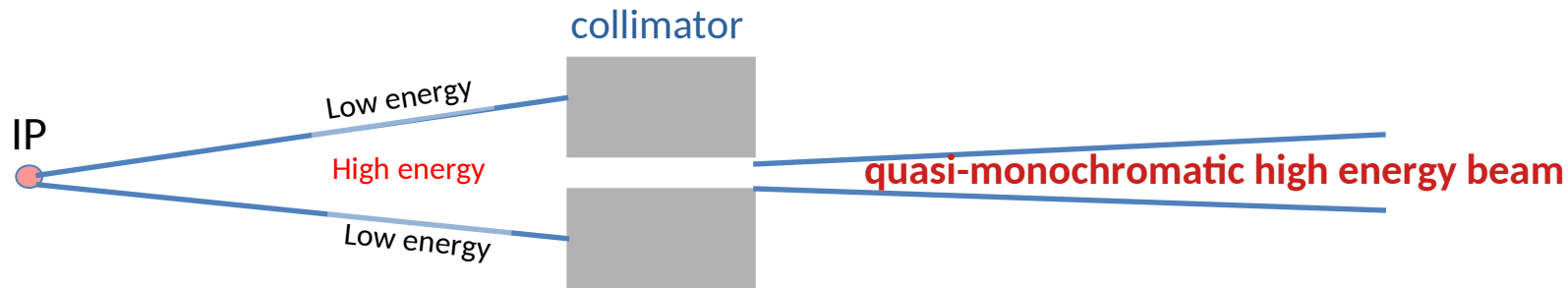
$$N_\psi = L\sigma_\psi = \frac{rN_eN_L \int_0^\psi d\psi' \frac{d\sigma}{d\psi'}}{2\pi \sqrt{\sigma_{y,e}^2 + \sigma_{y,L}^2} \sqrt{\sigma_{x,e}^2 + \sigma_{x,L}^2 + (\sigma_{z,e}^2 + \sigma_{z,L}^2) \tan^2(\alpha/2)}}$$



# Short introduction to Inverse Compton Scattering

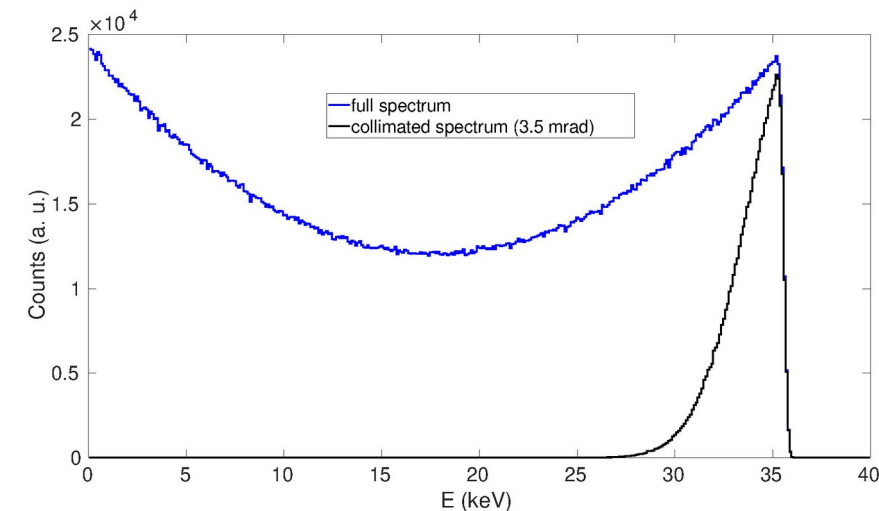
**Inverse Compton radiation is not intrinsically monochromatic**, the energy is related to the polar emission angle.

The required **energy bandwidth** can be obtained by properly **collimating the gamma beam**.



There is a **lower limit** bandwidth achievable (due to energy spread and emittance).

Also, at a given angle  $\theta$  there is a **local energy distribution**.



**example of Collimator design:**

G. Paternò et al., NIM B 402  
(2017), 349-353

$$\frac{\Delta E_{\text{ph}}}{E_{\text{ph}}} \simeq \sqrt{\left[ \frac{\Psi^2/\sqrt{12}}{1+\Psi^2} + \frac{\bar{P}^2}{1+\sqrt{12}\bar{P}^2} \right]^2 + \left[ \left( \frac{2+X}{1+X} \right) \frac{\Delta\gamma}{\gamma} \right]^2 + \left( \frac{1}{1+X} \frac{\Delta E_L}{E_L} \right)^2 + \left( \frac{M^2\lambda_0}{2\pi w_0} \right)^4 + \left( \frac{a_0^2/3}{1+a_0^2/2} \right)^2}$$

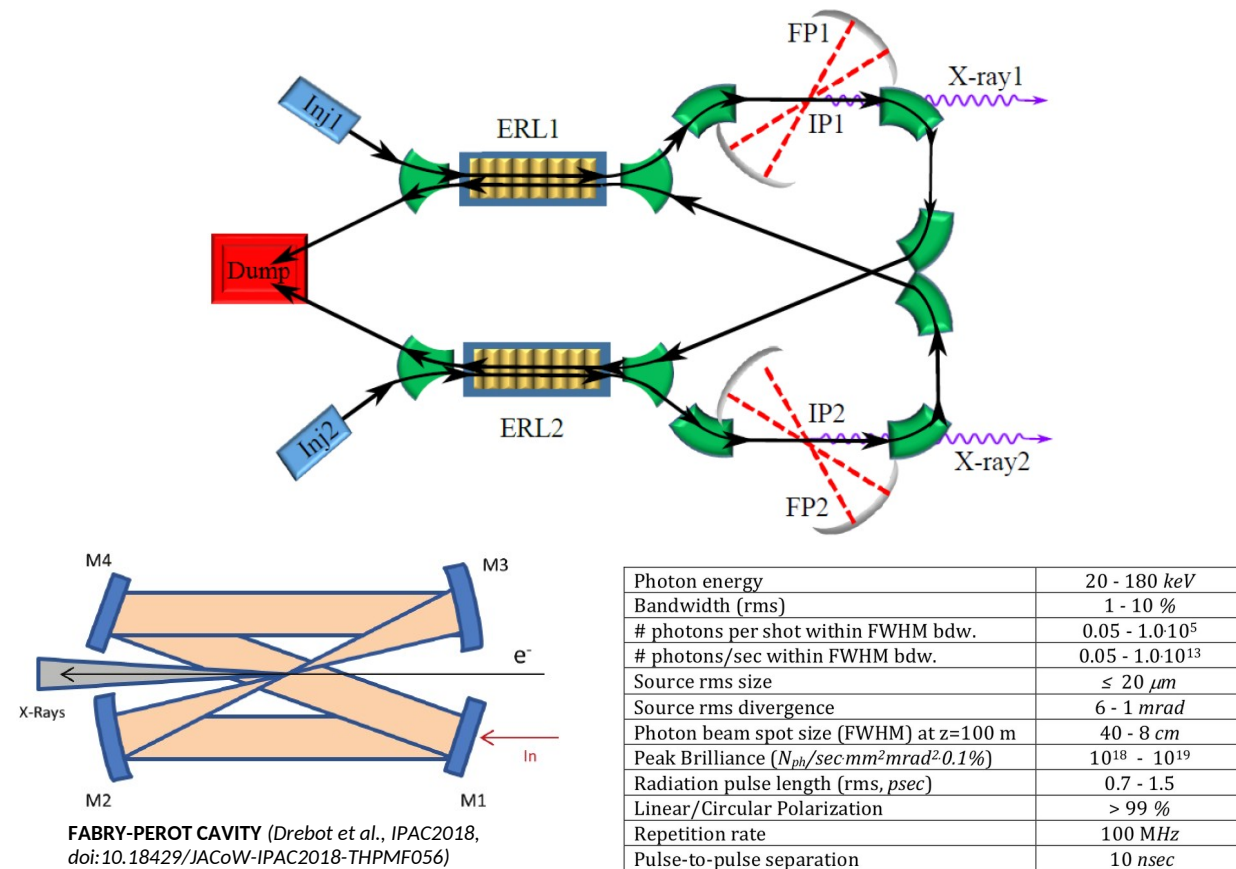
$$\bar{P} = \gamma_{\text{CM}} \frac{\sqrt{2}\epsilon_x}{\sigma_x} = \frac{\sqrt{2}\epsilon_n}{\sigma_x \sqrt{1+X}} \quad X = \frac{4E_e E_L}{M_e^2} \quad a_0 = 6.8 \frac{\lambda_0}{w_0} \sqrt{\frac{U_L(J)}{\sigma_t(ps)}}$$

# Short introduction to Inverse Compton Scattering

## Main features of ICS radiation

- **Energy-angle correlation**
  - Adjustable energy **bandwidth (1-10%)** through simple spatial **collimation**
  - **Moderate divergence** (few mrad) → rather wide (5 - 15 cm diameter) and intense ( $10^6 - 10^8$  ph/(mm<sup>2</sup> s)) irradiation field at distances from the IP of the order few tens of m (**bandwidth/flux vs divergence/field size trade off**)
- **Very small spot size** (few tens of  $\mu\text{m}$ ) → good transverse coherence
- **Intense very short pulses** ( $\sim$  ps)
- Capability of **intense high-energy beams** w.r.t. synchrotrons
- **Negligible harmonic contamination** w.r.t. synchrotrons
- Capability of **multi-color beams** (varying electron beam energy or **collision angle**)

→ **Medical applications:** RX,  $\mu\text{CT}$ , PCI, SAXS, DE and KES, ...



**BriXS:** I. Drebot et al., Instruments 2019, 3, 49

P. Cardarelli et al., Physica Medica 77 (2020) 127-137

# Simulation of ICS radiation

- A reliable tool for the simulation and prediction of the emission characteristics is fundamental for the **design and development of this kind of x-ray sources**, as well as for the operation diagnostics and **optimization of the foreseen applications**.
- Usually, custom codes, both semi-analytical and Monte Carlo, are used and only a few of them are publicly available (e.g. CAIN, RF-Track).
- The purpose is to have a tool, easy to use, through which **simulate the emission of ICS source and track the generated beam in a given experimental setup**.

# Simulation of ICS radiation: “LCS” classes

- **A code to model ICS** (in linear Thomson/Compton regime) **has been developed in Geant4**.
  - It is composed of **3 classes**: *LCSGammaSource*, *LCSGammaSourceData*, *LCSGammaSourceMessenger*, which allow the user to **define an ICS as a primary particle source similarly to the built-in method of Geant4**.
  - The user has to create an instance of ***LCSGammaSource*** in the *PrimaryGeneratorAction* and call the *LCSGammaSource::GeneratePrimaryVertex* method inside *PrimaryGeneratorAction::GeneratePrimaries*.
  - ***LCSGammaSourceData*** (created as singleton when *LCSGammaSource* is instantiated) contains most of data and methods required for the photon sampling.
  - ***LCSGammaSourceMessenger*** allows the user to set the parameters of the interacting beams from a command line or a macro file.
- The developed code allows the user to consider **a wide range of interaction conditions** (non-head-on interactions, laser with elliptical profile at waist, ...)
- **MT fully supported**.
- A complete (external) version of **CLHEP library is required**.

Paternò G. et al. "Generation of primary photons through inverse Compton scattering using a Monte Carlo simulation code." *Physical Review Accelerators and Beams* 25.8 (2022): 084601.

# Simulation of ICS radiation

## Assumptions of the model

- The incident beams have Gaussian distribution in their six-dimensional phase space of motion, but no correlation between the energy and the longitudinal coordinate.
- The laser is monochromatic.
- The laser is unpolarized or linearly polarized.
- The laser intensity is small and non-linear Compton scattering never occurs.
- The incident beams collide so that the center of pulses overlap at the design interaction point (IP) without any position or timing jitters.

# Simulation of ICS radiation

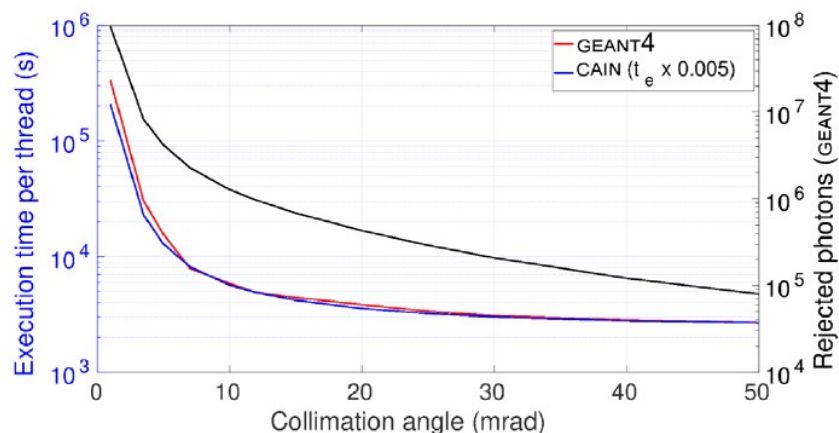
## Steps of LCS algorithm

- 1) A point P is randomly sampled along the electron beam axis as the real interaction point. Point P is located within a range that includes the design collision point and is determined by the duration of the pulses and the envelopes of the colliding beams.
- 2) An electron is sampled from the six-dimensional electron beam phase space and transported to point P.
- 3) The product of the electron and laser photon density at point P is calculated.
- 4) A random sampling through the acceptance-rejection method according to the calculated density product, normalized by its maximum value, is carried out.
- 5) If the sampling is accepted, go to next step. Otherwise return to the first step.
- 6) The laser photon momentum is sampled
- 7) The sampled laser photon momentum is transformed so that it and the polarization vector are in the x-z plane of the laboratory frame with the electron moving along z direction.
- 8) The laser photon momentum is transformed into the electron rest frame.
- 9) **A scattered photon is generated at the electron rest frame, from the sampled electron and laser photon, according to the differential cross-section of Compton scattering.**
- 10) The scattered photon is transformed into the laboratory frame.
- 11) The scattered photon is accepted provided that its momentum is within the **collimator acceptance**.
- 12) The polarization of the scattered photon is evaluated.

# Simulation of ICS radiation

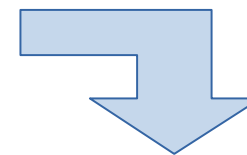
## Example of input macro

- The **features** of the **colliding beams at IP** have to be defined.
- A **collimation angle**  $\theta_{\max}$  can be set and only photons within this polar angle will be accepted (the smaller this angle, the longer the simulation)



```
/lcsge/ebeam/energy 43.3e6 #mean energy (eV)
/lcsge/ebeam/espread 2.e-3 #relative spread (sigma)
/lcsge/ebeam/emittx 1.5e-6 #x norm. emitt. (m*rad)
/lcsge/ebeam/emity 1.5e-6 #y norm. emitt. (m*rad)
/lcsge/ebeam/alphax 0.0015 #Twiss parameters
/lcsge/ebeam/alphay 0.0021
/lcsge/ebeam/betax 0.00814 #(m)
/lcsge/ebeam/betay 0.00814 #(m)
/lcsge/ebeam/sigmaz 4.e-4 m #bunch length
/lcsge/laser/wavelength 1.03e-6 #m
/lcsge/laser/Zrx 0.01098 #x Rayleigh length (m)
/lcsge/laser/Zry 0.01098 #y Rayleigh length (m)
/lcsge/laser/sigmaz 6.e-4 m #pulse length
/lcsge/laser/polphi 0.5 #in units of PI (0->x, 0.5->y)
/lcsge/laser/poldeg 1 #polarization degree
/lcsge/collAngle 7 #collision angle (deg)
/lcsge/collRate 1. #collision rate (Hz)
/lcsge/eBunchCharge 400.e-12 #(C)
/lcsge/laserPulseE 0.01 #(J)
/lcsge/solidangle 50.e-3 #thetamax (rad)
/lcsge/position 0 0 0 cm
/lcsge/zlim1 -0.01 m
/lcsge/zlim2 0.01 m
/lcsge/zcut 0.01
/lcsge/list

/run/printProgress 100000
/run/beamOn 1000000
```



## LCS emitted flux estimation

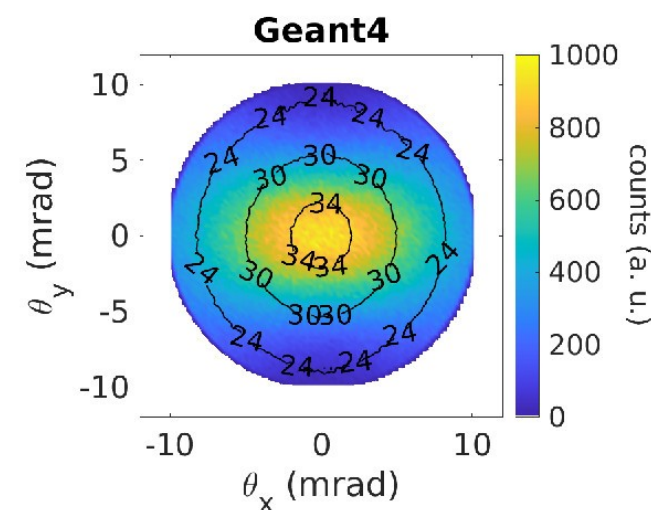
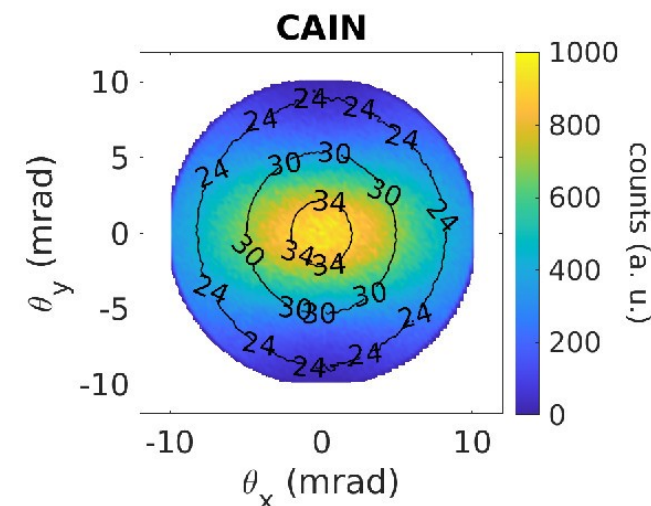
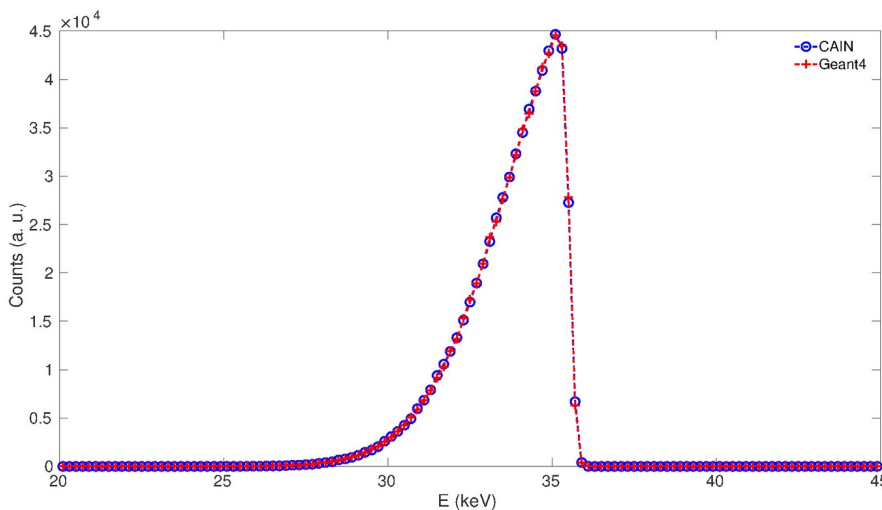
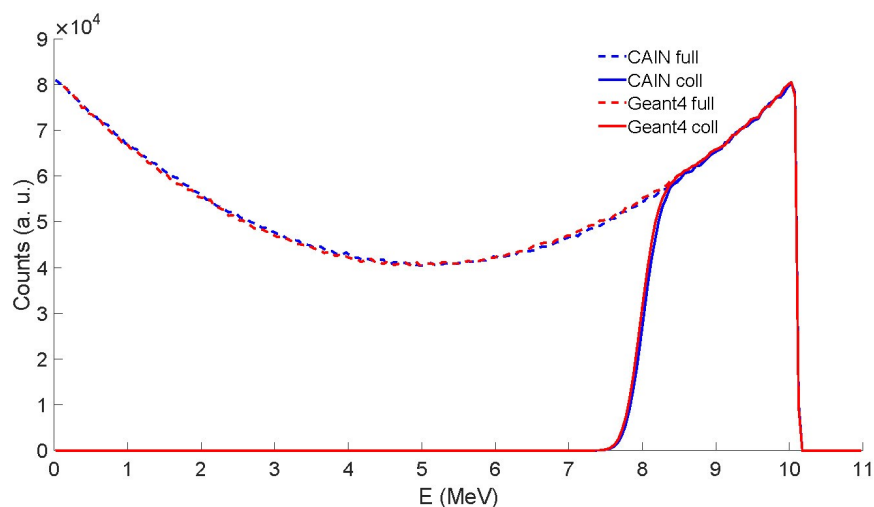
Number of emitted ph/s =  $2.30e+13$

$N_{\text{phs\_psi}} = 2.74e+12$

# Simulation of ICS radiation

## Validation of the developed code: comparison with CAIN

- 3 different cases considered (**BriXS**, NewSUBARU, ELI-NP-GBS)
- excellent agreement in general, slight differences only for high energy collimated beams and in the spatial distribution at IP (larger spots in CAIN)
- LCS turned out about 200 time faster than CAIN

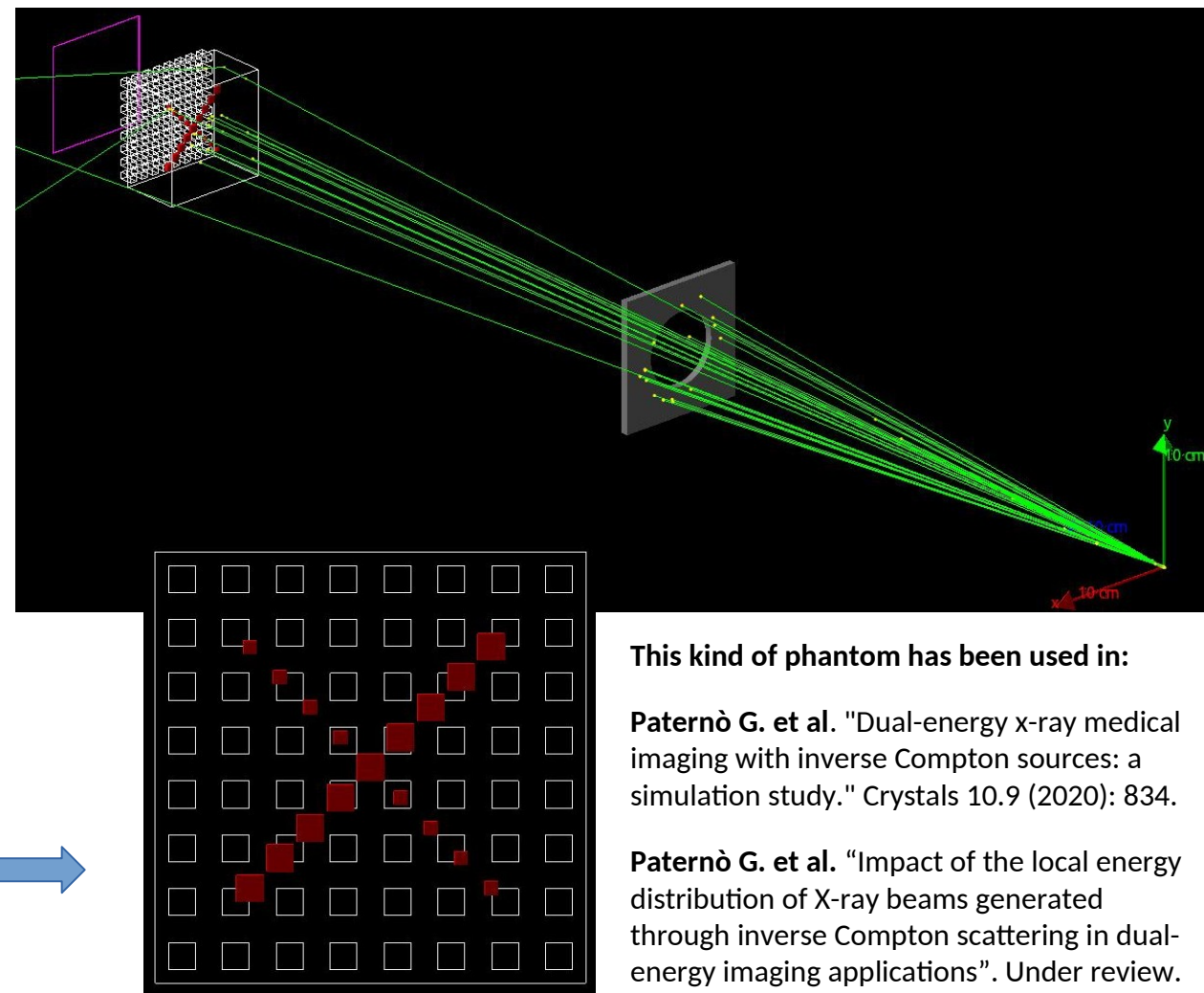


# Tracking of ICS radiation

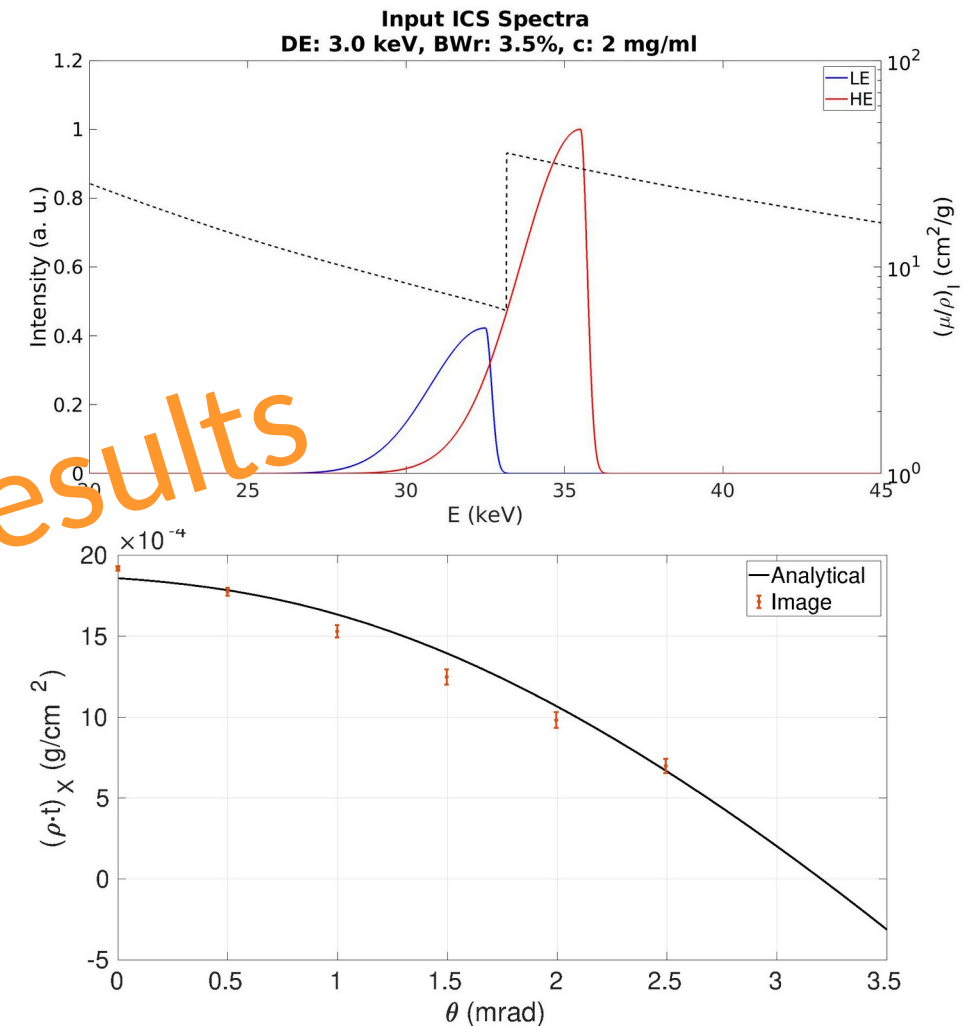
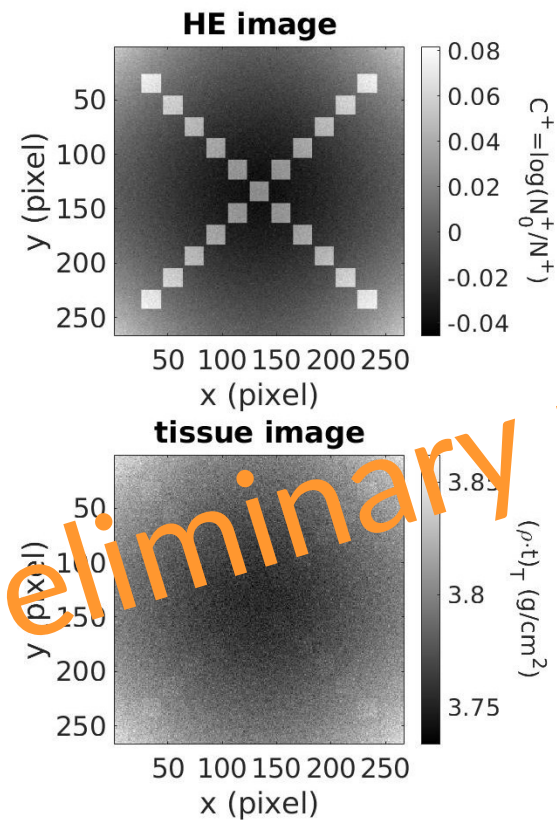
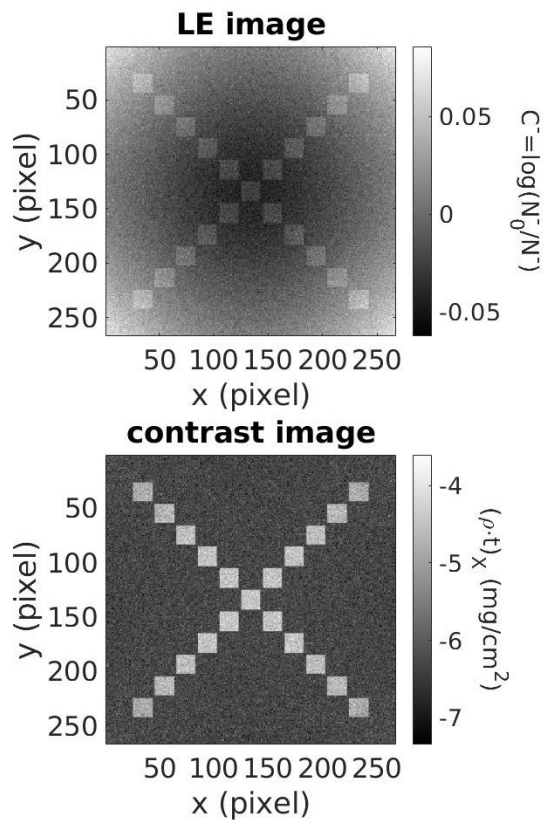
We developed an example called “ics”

- The user can track ICS photons in a simple setup with **slits**, **phantom** and **detector**.
- The particle generator can be chosen between 5 different options:
  - 1) read the phase-space from a text file
  - 2) read the phase-space from a root file
  - 3) **sampling from an ICS parametrization**
  - 4) GPS
  - 5) **exact LCS generation** (phase-space scored)
- It is thus possible to **track**, **generate and track** or **generate only** the **primary (ICS) photons**.
- **Geometry and Source** can be set through **macro**.
- The **phantom** is conceived for **studies of medical imaging** (in particular, **KES imaging**) with ICS sources.

Available at: <https://medical-physics.unife.it/downloads/geant4>



# KES imaging with ICS sources



Preliminary results

# Conclusions

- ICS sources are **“compact” alternative to synchrotrons**. A **reliable tool for the simulation and tracking of their emission** is crucial for assessing their potential in **many fields**.
- **A code has been developed in Geant4** for generating and/or tracking ICS radiation in a simple setup inspired to medical applications.

# Back-up slides

# Simulation of ICS radiation

## Sampling of scattered photons at electron rest frame (step 9)

$$\frac{d\sigma}{dE'_g} = \pi r_e^2 \frac{mc^2}{E'_p{}^2} \left( 2 + \frac{2E'_p}{mc^2} \right) f(E'_g) \quad f(E'_g) = \frac{1}{2 + 2E'_p/mc^2} \left[ \left( \frac{mc^2}{E'_p} - \frac{mc^2}{E'_g} \right)^2 + 2 \left( \frac{mc^2}{E'_p} - \frac{mc^2}{E'_g} \right) + \frac{E'_p}{E'_g} + \frac{E'_g}{E'_p} \right]$$

- Generate the **scattered photon energy**  $E'_g$  by sampling it uniformly within:  $\frac{E'_p}{1 + 2E'_p/mc^2} \leq E'_g \leq E'_p$

- Generate a uniform random number  $r$  within 0 and 1 and check if  $r \leq f(E'_g)$ , in this case accept  $E'_g$ , otherwise reject it and repeat the sampling procedure.

- calculate the **polar scattering angle in the electron rest frame**  $\theta'$  as:  $\frac{1}{E'_g} = \frac{1}{E'_p} + \frac{1}{mc^2} (1 - \cos \theta')$

- calculate the **azimuthal scattering angle in the electron rest frame**  $\phi'$  according to the double differential cross section  $d^2\sigma/dE'_g d\phi'$  through the rejection method.

# Simulation of ICS radiation

## Sampling of the azimuthal scattering angle in the electron rest frame $\phi'$

$$\begin{aligned} \frac{d^2\sigma}{dE'_g d\phi'} = & \frac{mc^2 r_e^2}{2E_p'^2} \left\{ [1 + P_t \cos(2\tau' - 2\phi')] \right. \\ & \times \left[ \left( \frac{mc^2}{E_p'} - \frac{mc^2}{E_g'} \right)^2 + 2 \left( \frac{mc^2}{E_p'} - \frac{mc^2}{E_g'} \right) \right] \\ & \left. + \frac{E_p'}{E_g'} + \frac{E_g'}{E_p'} \right\}, \end{aligned}$$

-  $\tau'$  is the azimuthal angle of the linear polarization direction of the incident photon defined in the electron rest frame.  
 $P_t$  is the degree of linear polarization of the incident photon beam (Lorentz invariant).

# Tracking of ICS radiation

ics example is composed of 20 classes

- apart from the 3 “**LCS**” classes for the exact generation of ICS photons and the **PrimaryGeneratorAction**, we have a **PrimaryGeneratorActionMessenger** class and two custom classes for reading text (**FileReader**) and root files (**RootReader**).
- **StackingAction** class is used to score primary LCS photons (or kill secondaries).
- **SensitiveDetector** is used to score photons impinging on the detector (also mesh scorer can be used for scoring Edep in the detector volume).
- **SteppingAction** is used to score scattering events of primary photons (so as to be able to remove scatter from the obtained images).

# Tracking of ICS radiation: parametrization

## Custom ICS parametrization for imaging simulation purpose:

- A very high number of primary photons to generate (up to  $10^{12}$ ).
- It is necessary to spare CPU time and data space.
- **approximated method** capable of catching the main features of ICS radiation.



## Each primary photon is generated by:

- 1) Sampling (x,y,z) independently from Gaussian distributions.
- 2) Sampling the azimuthal angle from  $U[0,2\pi]$ .
- 3) Sampling a polar angle  $\theta$  from a liner distribution from 0 to  $\theta_{\max}$ .
- 4) Calculating the nominal photon energy  $E_{\text{nom}}$  through the analytical relationship with the polar angle.
- 5) Sampling the photon energy form an approximated asymmetrical spectrum with  $E_{\text{peak}} = E_{\text{nom}}$  and spread calculated according to the **local energy BW (properly parametrized as a function of  $\theta$  -> the source as to be known very well)**.



The collimated spectrum reproduction is approximated, and some correlations are lost, however, the model allow us to effectively simulate imaging with ICS sources (  $\sim 2 \times 10^7$  ph/(h\*threads) vs  $\sim 5 \times 10^5$  ph/(h\*threads) for exact LCS)

# Tracking of ICS radiation: parametrization

## Example of input macro to be used in “mode 3”

```
/gun/setCollAngle 34.5      #deg  
/gun/setEL 1.2037          #eV  
/gun/seta0 0.008  
/gun/setEe 44.             #MeV  
/gun/setX 15.              #um  
/gun/setY 15.              #um  
/gun/setZ 450.             #um
```

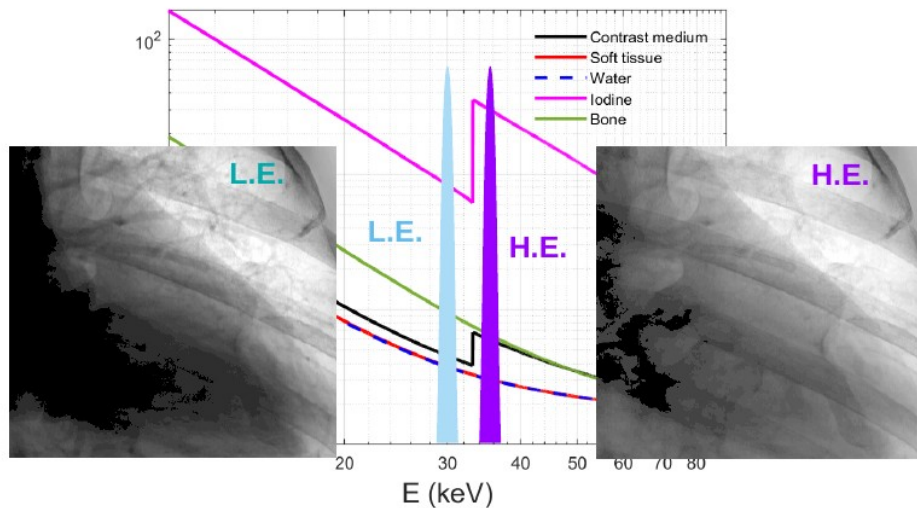
```
/gun/setBW0 0.0145  
/gun/setmBW 10.40  
/gun/SetFitCubic 1  
/gun/setaBW 0.0156  
/gun/setbBW 0.0071  
/gun/setcBW 0.0014  
/gun/setdBW -0.0001  
/gun/setLRr0 9.  
/gun/setTheta1 0.004      #rad  
/gun/setThetamax 0.0035   #rad
```



Parameters used to describe the  
local energy distribution of a ICS  
source

# KES imaging

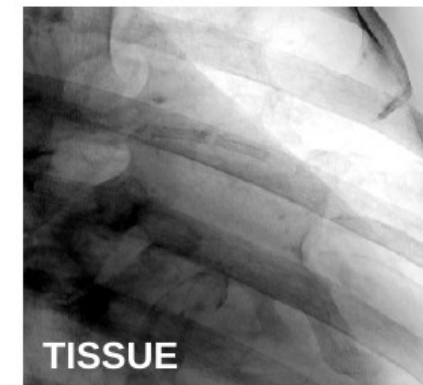
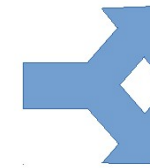
- Details of interest are perfused with a contrast agent having a K-edge (iodine, K-edge @ 33.17 keV).
  - Two images with x-ray beams having energies above and below K-edge are acquired.
  - Two basis materials (X and T) are selected → e. g. contrast agent and water/soft-tissue.
  - By knowing the linear mass attenuation coefficient of 2 basis materials at the LE and HE →
- Obtain two images mapping the distribution of the two basis materials



$$(\rho t)_X = \frac{\left[\frac{\mu^-}{\rho}\right]_T C^+ - \left[\frac{\mu^+}{\rho}\right]_T C^-}{K_0}$$

$$(\rho t)_T = \frac{\left[\frac{\mu^+}{\rho}\right]_X C^- - \left[\frac{\mu^-}{\rho}\right]_X C^+}{K_0}$$

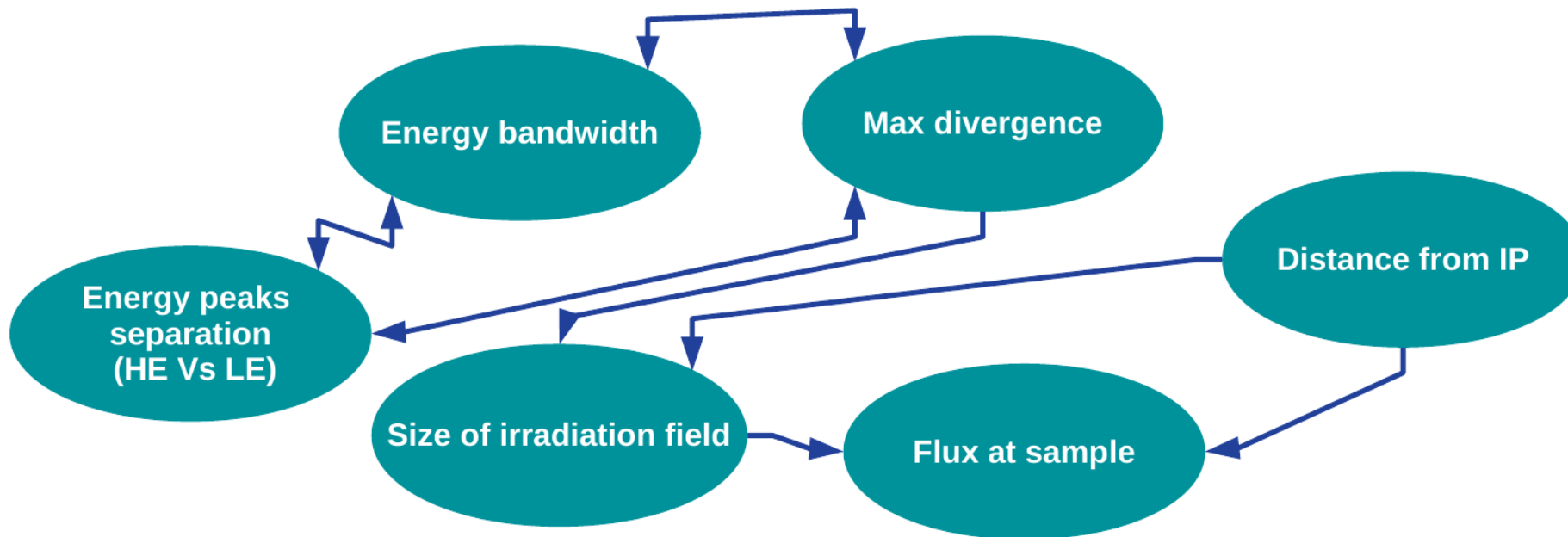
$$K_0 = \left[\frac{\mu^-}{\rho}\right]_T \left[\frac{\mu^+}{\rho}\right]_X - \left[\frac{\mu^+}{\rho}\right]_T \left[\frac{\mu^-}{\rho}\right]_X$$



Several **applications of KES to biomedical imaging** with different contrast agents have been tested and demonstrated **at various synchrotron facilities** (C.A. with I, lung ventilation with Xe, Dynamics of mineralization in growing bones with Ba/Sr,...), **research at ICS sources are ongoing**.

# KES imaging with ICS sources

All the parameters at play are interconnected and difficult to disentangle



The process is strongly dependent on the foreseen imaging task, there **is not a good-for-all recipe**

**Flux requirement for coronary angiography:** Paternò G. et al., Phys. Med. Biol. 64 (2019) 18500.

**Effect of finite energy bandwidth:** Paternò G. et al. Crystals 10.9 (2020): 834.

**Impact of local effects:** Paternò G. et al. Under review.