A novel extended example for the generation and tracking of inverse Compton scattering photons
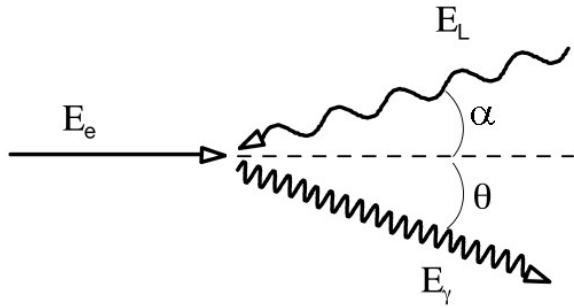
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Outline

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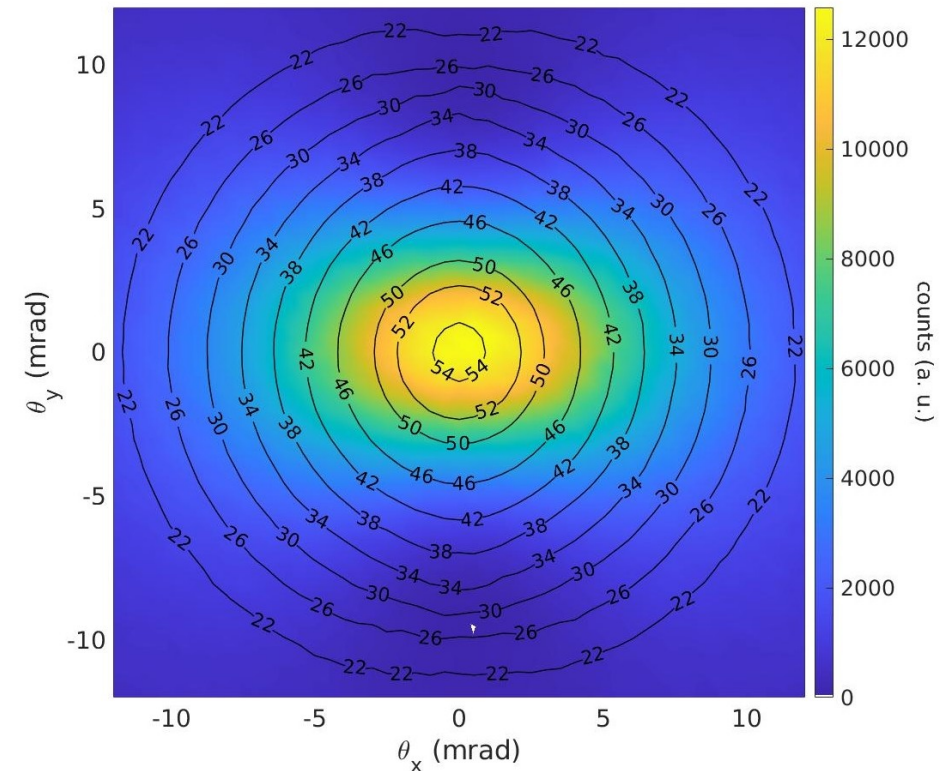
Short introduction to Inverse Compton Scattering

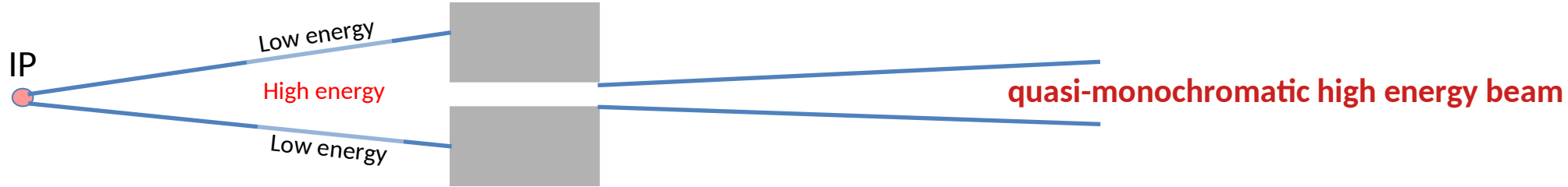$$E_\gamma \approx \frac{2\gamma^2(1+\cos\alpha)}{1+(\gamma\theta)^2+\dfrac{4\gamma E_L}{m_e c^2}} E_L$$

- Laser photons interacts 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_γ and polar scattering angle θ exists (E_γ does not depend on ϕ).

- 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_ψ, is:

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

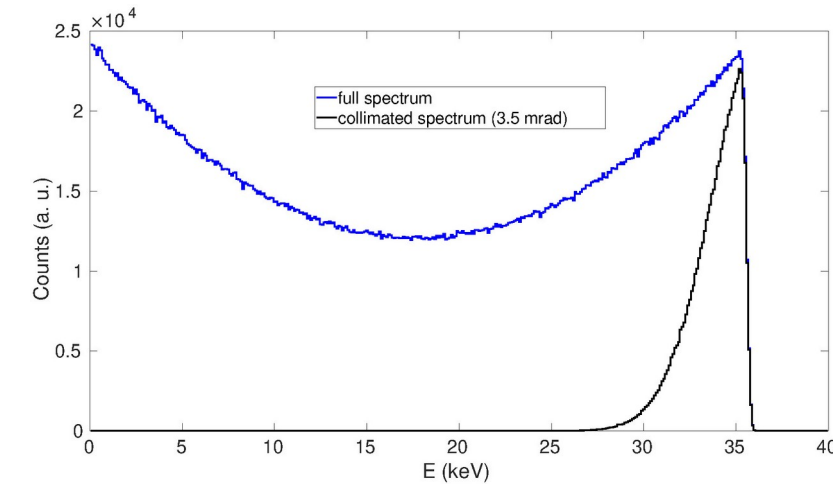**BriXS**: L. Serafini et al., NIM A 930 (2019) 167–172

Short introduction to Inverse Compton Scattering

IP

Low energy

High energy

Low energy

quasi-monochromatic high energy beam

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

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

- **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 θ there is a **local energy distribution**.

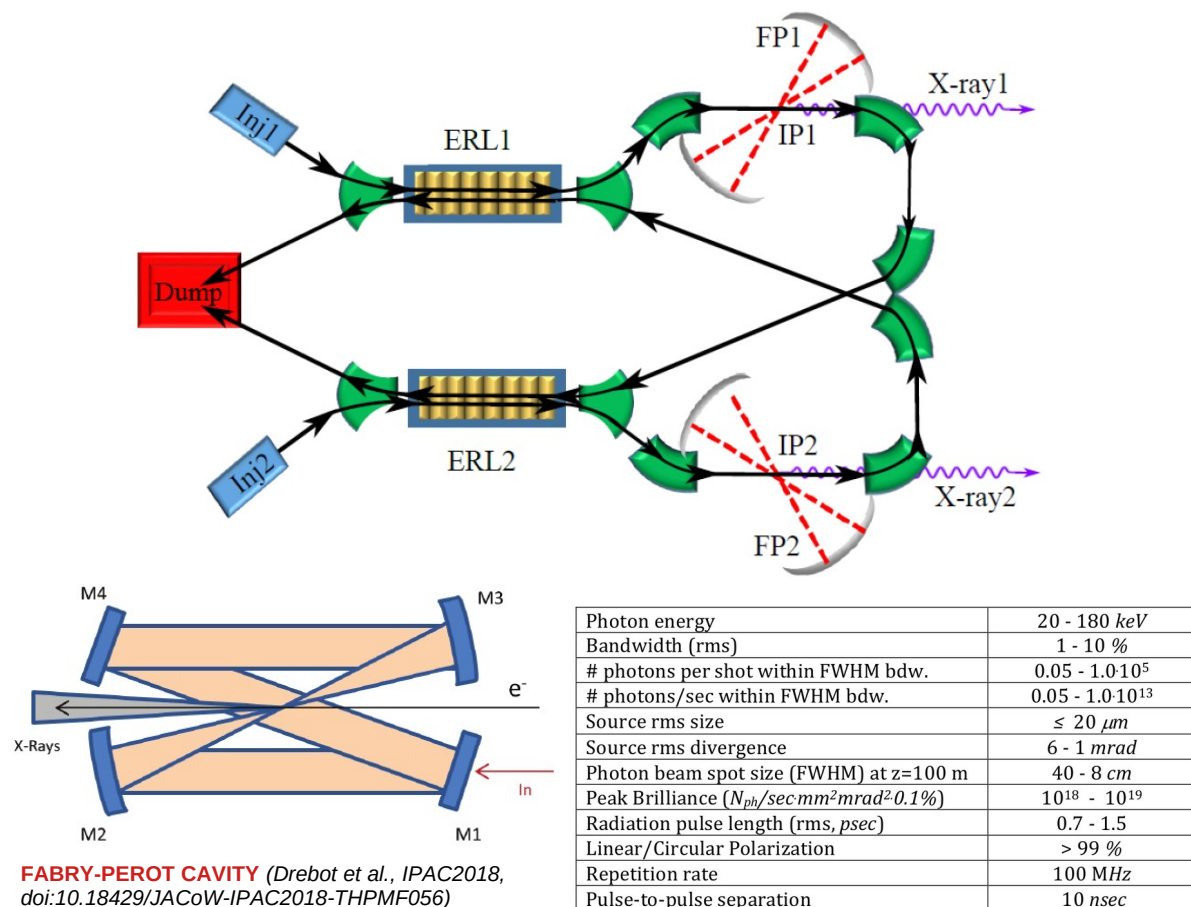**Collimator design**: G. Paternò et al., NIM B 402 (2017), 349-353

FP1

X-ray1

IP1

ERL1

Inj1

Dump

ERL2

Inj2

IP2

X-ray2

FP2

M4 M3

e⁻

X-Rays

In

M2 M1

FABRY-PEROT CAVITY *(Drebot et al., IPAC2018, doi:10.18429/JACoW-IPAC2018-THPMF056)*

Photon energy	20 - 180 keV
Bandwidth (rms)	1 - 10 %
# photons per shot within FWHM bdw.	$0.05 - 1.0 \cdot 10^5$
# photons/sec within FWHM bdw.	$0.05 - 1.0 \cdot 10^{13}$
Source rms size	$\leq 20~\mu m$
Source rms divergence	6 - 1 $mrad$
Photon beam spot size (FWHM) at z=100 m	40 - 8 cm
Peak Brilliance ($N_{ph}/sec \cdot mm^2 mrad^2 0.1\%$)	$10^{18} - 10^{19}$
Radiation pulse length (rms, $psec$)	0.7 - 1.5
Linear/Circular Polarization	> 99 %
Repetition rate	100 MHz
Pulse-to-pulse separation	10 $nsec$

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

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^2 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 μm) → good transverse coherence

- 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, μCT, PCI, SAXS, DE and KES, ...

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

Simulation of ICS

- 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 source**, 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

- **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**.

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

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

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.

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

$$\frac{d\sigma}{dE'_g} = \pi r_e^2 \frac{mc^2}{E_p'^2} \left(2 + \frac{2E'_p}{mc^2}\right) f(E'_g)$$

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

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

- Generate a uniform random number r within 0 and 1 and check if r $\leqslant$ 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 θ'** as: $\dfrac{1}{E'_g} = \dfrac{1}{E'_p} + \dfrac{1}{mc^2}(1 - \cos\theta')$

- calculate the **azimuthal scattering angle in the electron rest frame φ'** according according to the double differential cross section d^{2}σ/dE'$_g$dφ' through the rejection method.

Example of input macro

- The **features** of the **colliding beams at IP** have to be defined.

- **A collimation angle** θ_{max} can be set and only photons within this polar angle will be accepted (the smaller this angle, the longer the simulation)
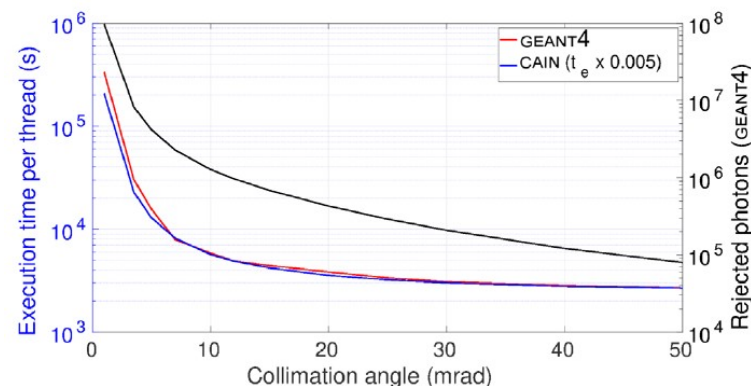

```
/lcsgs/ebeam/energy 43.3e6      #mean energy (eV)
/lcsgs/ebeam/espread 2.e-3      #relative spread (sigma)
/lcsgs/ebeam/emitx 1.5e-6       #x norm. emitt. (m*rad)
/lcsgs/ebeam/emity 1.5e-6       #y norm. emitt. (m*rad)
/lcsgs/ebeam/alphax 0.0015      #Twiss parameters
/lcsgs/ebeam/alphay 0.0021
/lcsgs/ebeam/betax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

/run/printProgress 100000
/run/beamOn 1000000
```
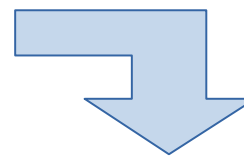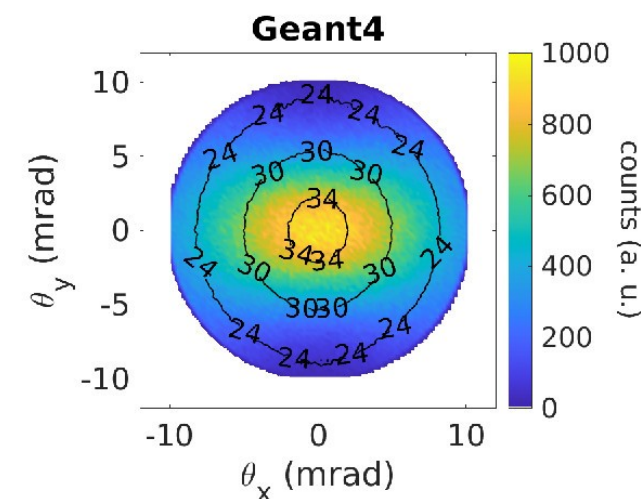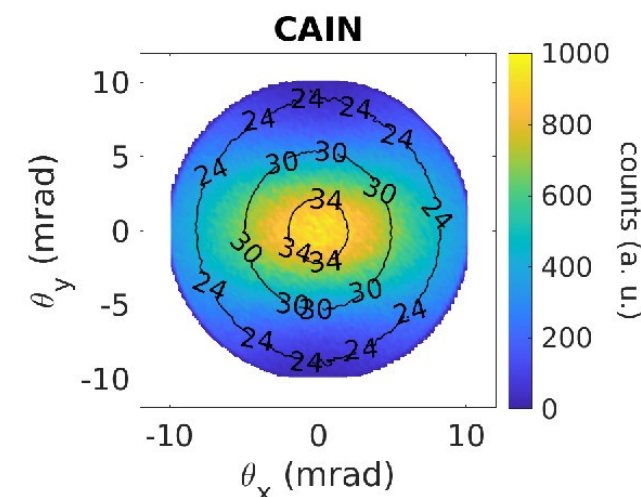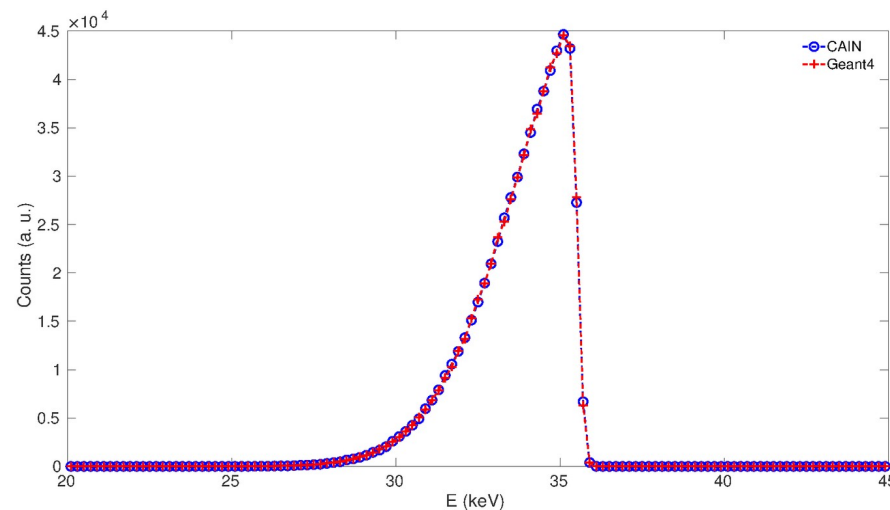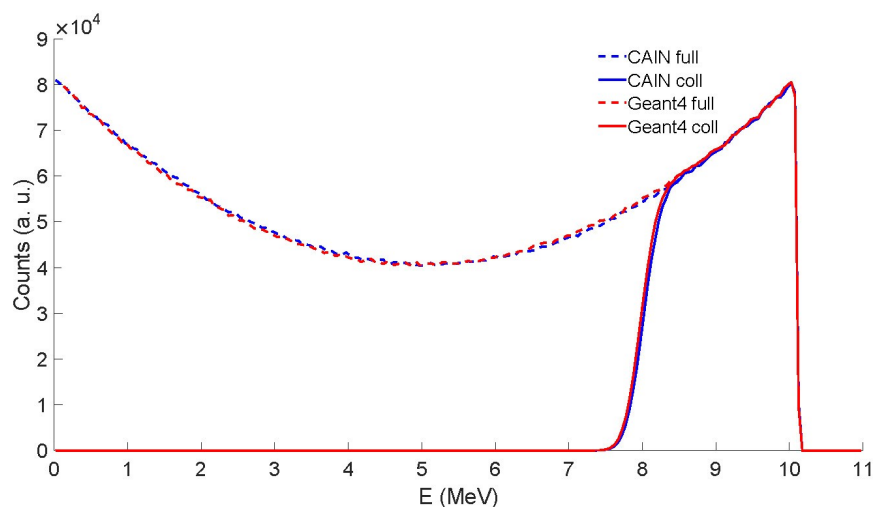
LCS emitted flux estimation

Number of emitted ph/s = 2.30e+13

Nphs_psi = 2.74e+12

Simulation of ICS

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
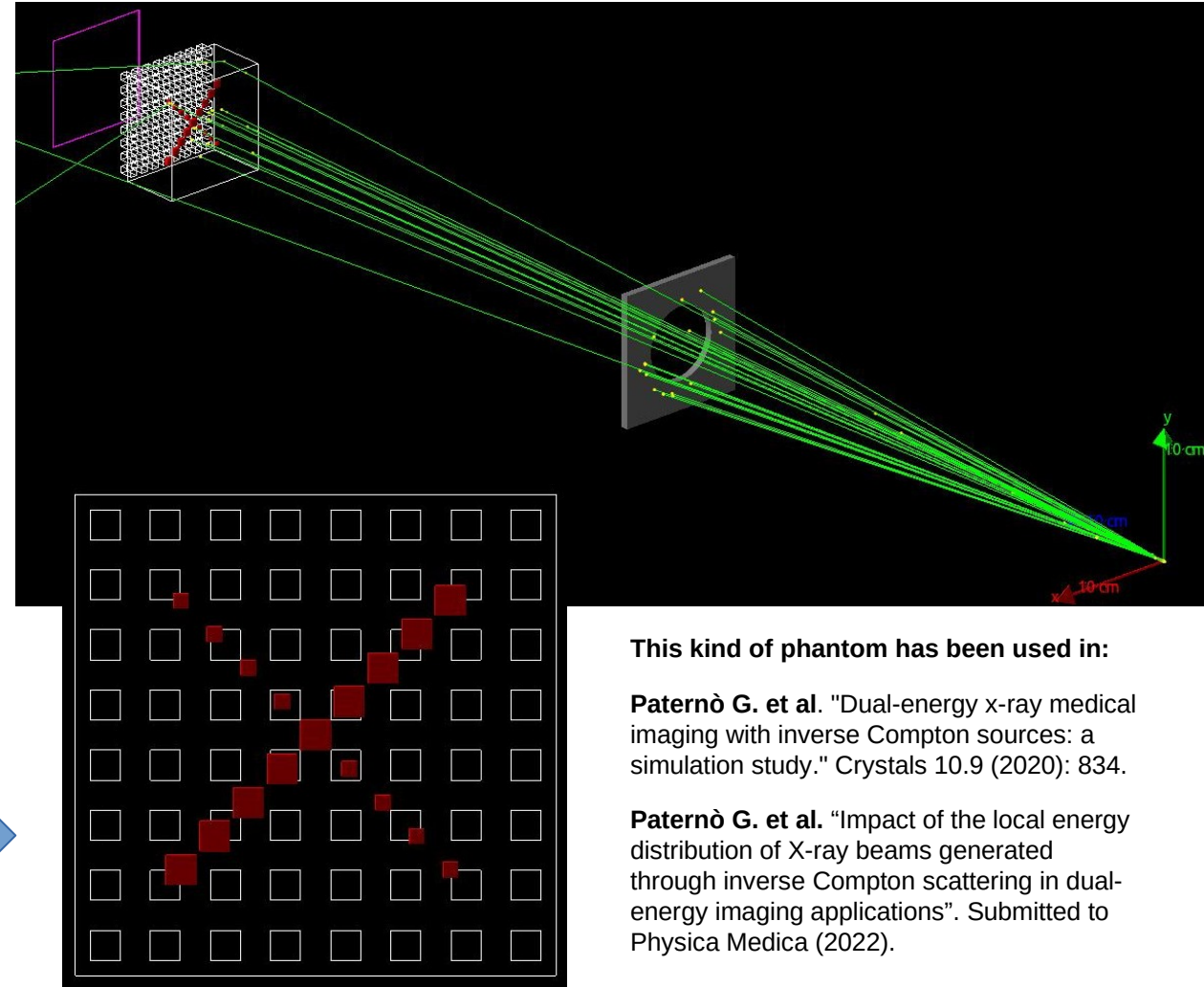
We propose the novel "ics" extended example

- 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 saved)

- It is thus possible to track, generate and track or generate only the primary (ICS) photons.

- The **phantom** is conceived for studies of medical imaging (in particular, KES imaging) with ICS sources.

- **Geometry and Source** can be set through **macro**.

This kind of phantom has been used in:

Paternò G. et al. "Dual-energy x-ray medical imaging with inverse Compton sources: a simulation study." Crystals 10.9 (2020): 834.

Paternò G. et al. "Impact of the local energy distribution of X-ray beams generated through inverse Compton scattering in dual-energy imaging applications". Submitted to Physica Medica (2022).

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).

The example **can be downloaded** from: *https://www.fe.infn.it/medical_physics/Geant4/*

Tracking of ICS radiation

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 θ from a liner distribution from 0 to θ_{max}.

4) Calculating the nominal photon energy E_{nom} through the analytical relationship with the polar angle.

5) Sampling the photon energy form an approximated asymmetrical spectrum with $E_{peak} = E_{nom}$ and spread calculated according to the **local energy BW** (properly parametrized as a function of θ -> 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

Example of input macro to be used in "mode 3": ICS parametrization

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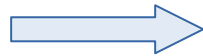
Parameters used to describe the local energy distribution of a ICS source
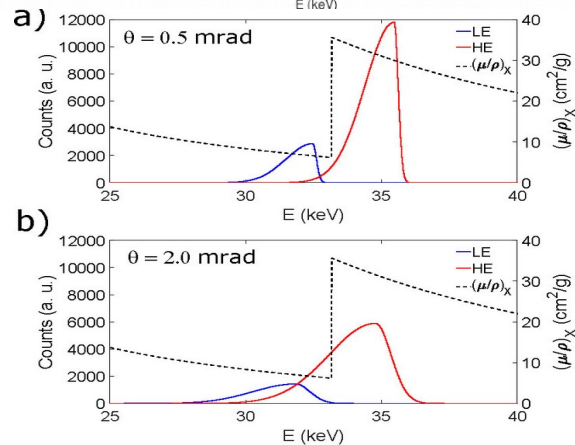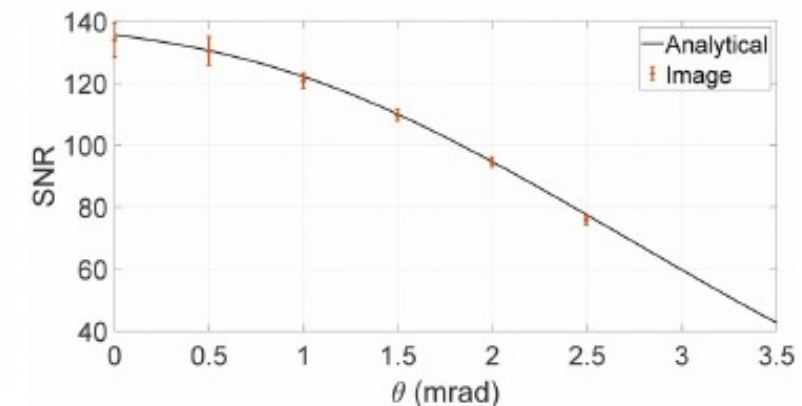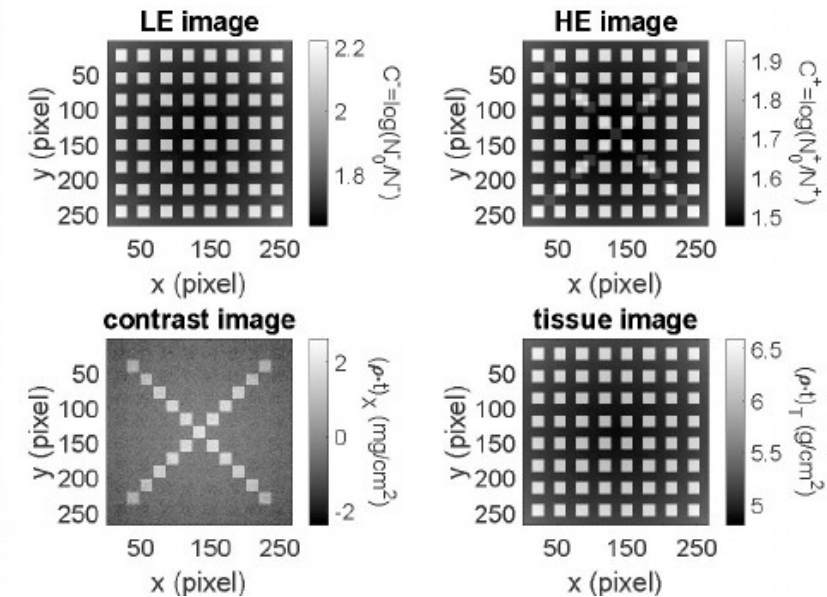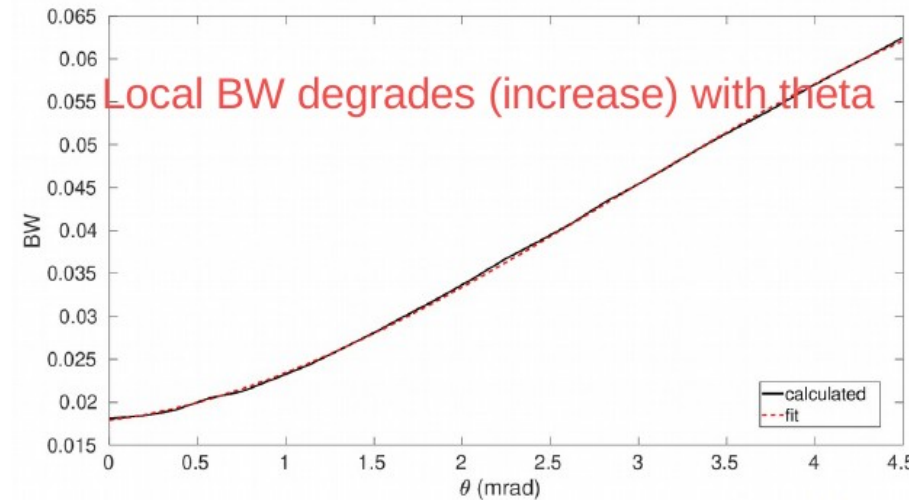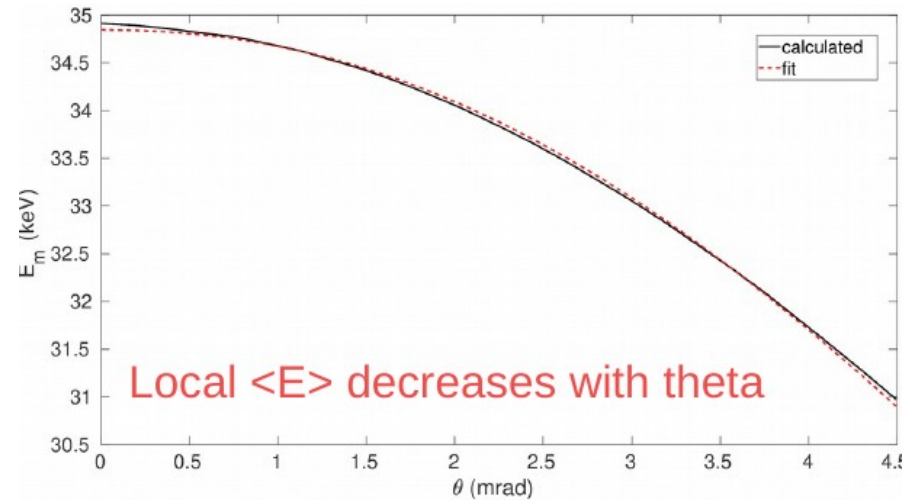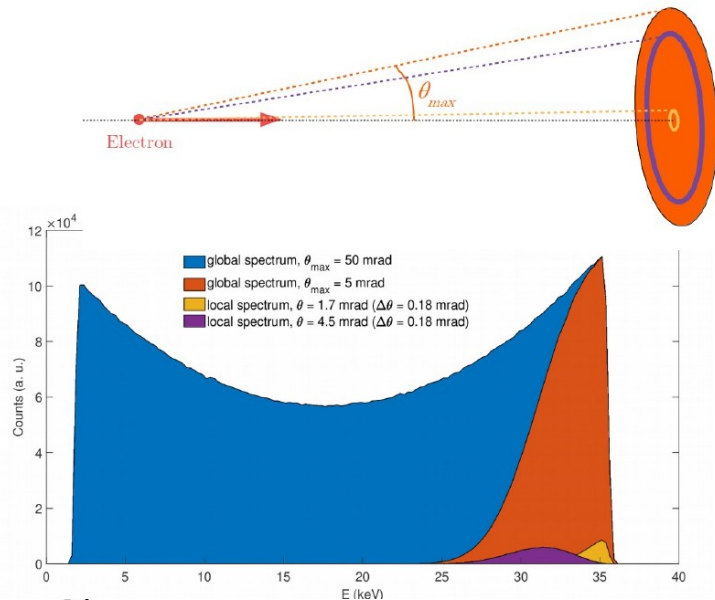
Conclusions

- 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

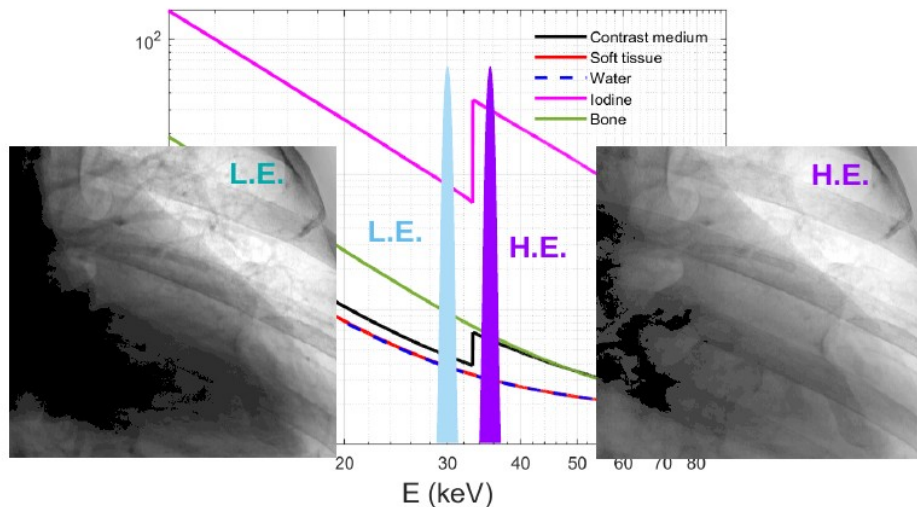**Sampling of the azimuthal scattering angle in the electron rest frame ф'**

$$\frac{d^2\sigma}{dE'_g d\phi'} = \frac{mc^2 r_e^2}{2E'^2_p} \left\{ [1 + P_t \cos(2\tau' - 2\phi')] \right.$$

$$\times \left[\left(\frac{mc^2}{E'_p} - \frac{mc^2}{E'_g} \right)^2 + 2\left(\frac{mc^2}{E'_p} - \frac{mc^2}{E'_g} \right) \right]$$

$$\left. + \frac{E'_p}{E'_g} + \frac{E'_g}{E'_p} \right\},$$

- τ' is the 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).
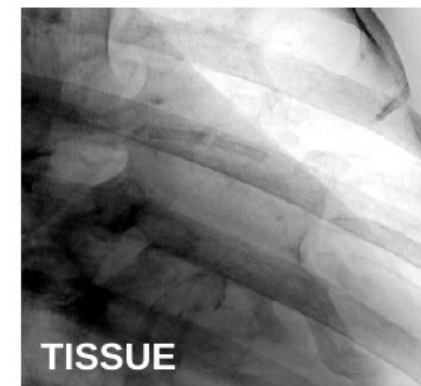
KES imaging

- 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**

All the parameters at play are interconnected and difficult to disentagle
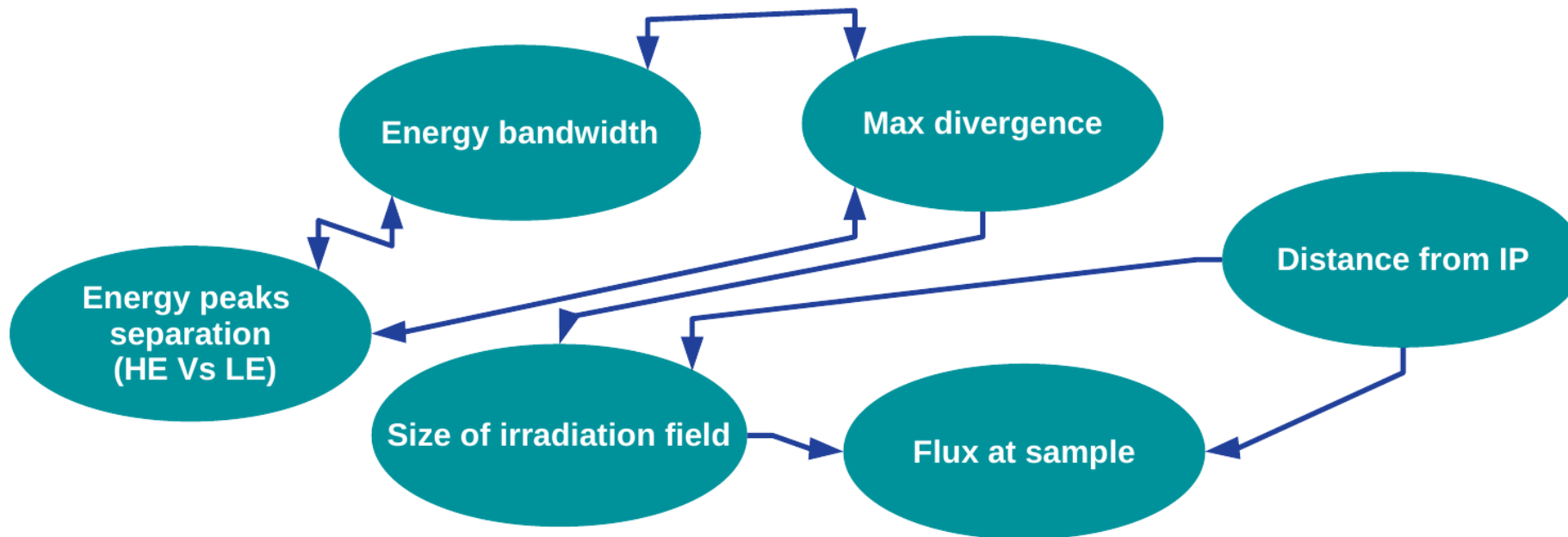
The process is strongly dependent on the foreseen imaging task, there **is not a good-for-all recipe**

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. Submitted to Physica Medica (2022).