

### **Optical photons**

OPT-PROD, OPT-PROP, MAT-PROP, TCQUENCH

Advanced course – ANL, June 2023

# Simulating optical photons

Scintillators (Eljen technology)



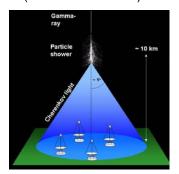
CT scanner (Siemens corporation)





Optical/scintillating fibers

Gamma-ray astronomy (Hess collaboration)



Neutrino observatories (Super Kamiokande collaboration)

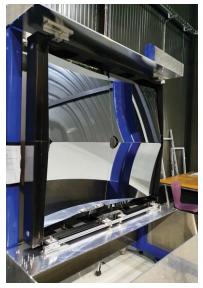


- Applications:
  - Gamma-ray and neutrino observatories
  - Dosimetry and area monitoring
  - Medical imaging
  - Hadron and electromagnetic calorimetry
  - Geophysical probing
- Why simulate optical photons?
  - Detection efficiency
  - Energy and time resolution
  - Material and geometry optimizations
  - Background estimation and event reconstruction

Tile calorimeter (CERN – ATLAS collaboration)



RICH detector (CERN – LHCb collaboration)





# **Optical photons in FLUKA?**

• In FLUKA, photons and optical photons are **NOT** the same particle!

Particle	FLUKA name	FLUKA particle ID	
Photon	PHOTON	7	
Optical photon	OPTIPHOT	-1	

- Difference unrelated with the particle energy.
- Each associated to different physics processes but both:
  - transport and deposit energy,
  - can be used as primary particles,
  - have a defined energy range for transport and production,
  - have scattering and absorption cross-sections and,
  - have a polarization vector (which can be defined as "random").



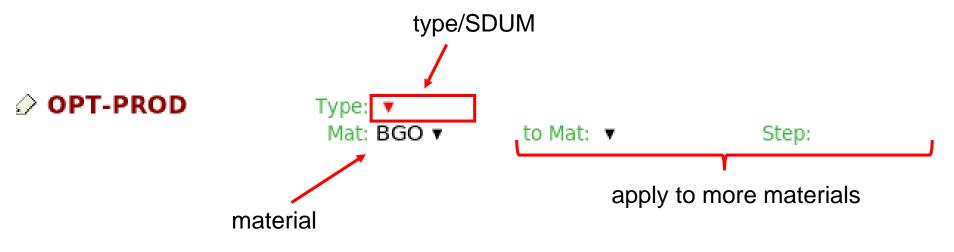
# **Optical photons in FLUKA**

- Optical photon production and transport disabled by default.
- Important mandatory cards:
  - **OPT-PROD**: Activates production (scintillation, Cherenkov)
  - **OPT-PROP**: Activates transport (energy cuts, reflections, boundary crossing, etc)
- Optional card:
  - **TCQUENCH**: Activates quenching (following Birk's law). Applies for scoring only.
- Plethora of user routines available for fine tuning of transport options.



# **Optical photon production (OPT-PROD card)**

- Creation of secondary optical photons handled by the OPT-PROD card.
- Processes:
  - Scintillation
  - Cherenkov
- Production options applied to materials.



• Note: Transition radiation is not supported by FLUKA. Ignore the placeholder options.



### **Scintillation**

- SDUM=SCINTILL:
  - Activate scintillation with defined peak photon energy  $(E_i)$ .
- Other **SDUM**:
  - **SCINT-WV**: Define the peak wavelength  $(\lambda_i)$
  - **SCINT-OM**: Define the peak angular frequency ( $\omega_i = 2\pi f$ )

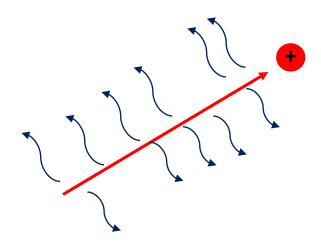


- Time: Scintillation decay time in seconds.
- Fraction: Fraction of deposited energy converted in optical photons with energy E<sub>i</sub>
  - fraction = yield (photons/MeV) ×  $E_i$  (eV) × 10<sup>-6</sup> or yield (photons/MeV) × 1.2398 × 10<sup>-3</sup> /  $\lambda_i$  (nm)
- Scintillation photons are monochromatic.
  - Or up to 3 peaks can be defined combining 3 OPT-PROD cards.



#### **Scintillation**

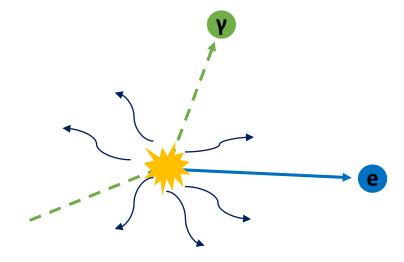
#### **Continuous losses**



- Optical photons generated randomly along tracks of charged particles.
- Photon momentum direction isotropic.
- Average number of photons proportional to the electronic stopping power (dE/dx).
- Exact number of photons Poisson distributed at each step.

#### **Discrete losses**

(electron below production cut-off)



- Optical photons created at the scattering vertex.
- Photon momentum direction isotropic.
- Number of photons proportional to the discrete energy loss.



## **Cherenkov radiation**

- Produced with charged particles travelling faster than the speed of light in the material (i.e.  $\beta > n^{-1}$ ).
- Activated with **SDUM=CERENKOV**. Must define the energy spectrum range for production.
- Other SDUM:
  - CEREN-WV: Define the wavelength range.
  - **CEREN-OM**: Define the angular frequency range ( $\omega = 2\pi f$ ).



- Optical photon produced along track in a characteristic cone with angle θ (cos(θ)=1/(nβ)).
- Uniform energy spectrum.



## **Conservation of energy**

#### WARNING

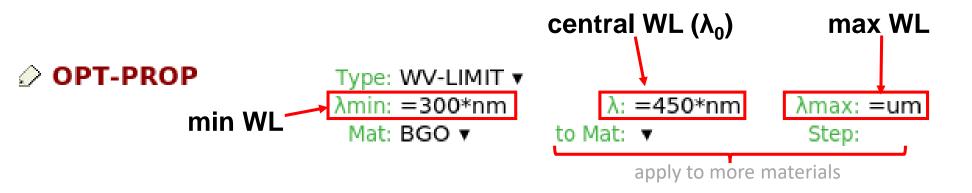
Energy conservation applies for production of optical photons with FLUKA. Therefore, you should expect different results from **ENERGY** or **DOSE** scoring when using the **OPT-PROD** and **OPT-PROP** cards. Other MC codes (e.g. Geant4) may manage energy conservation laws differently.

- Total stopping power of particles, from electronic losses, elastic scattering and inelastic scattering unchanged with optical photons.
- But! Fraction of energy losses **converted** into optical photons.
- Photons transport energy far from the interaction, therefore:
  - Scored local energy deposition or dose is lower!



## **Transport cuts (OPT-PROP card)**

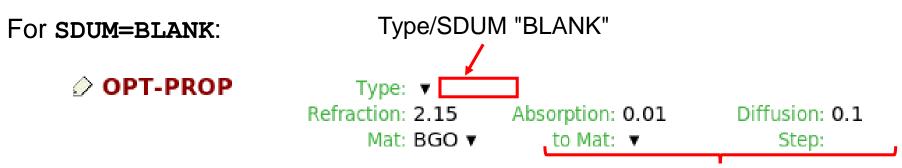
- Transport cuts defined using:
  - **SDUM=WV-LIMIT**: Wavelength cuts
  - **SDUM=OM-LIMIT**: Angular frequency cut



- The card defines the energy range. Central wavelength used for series expansions.
- Note: Transport cuts have no impact on the number of optical photon produced (for example when looking at the numbers found in the output file).
- Warning: The default cuts are 250 nm to 600 nm with central WL of 289 nm. To keep in mind when configuring OPT-PROD cards!
- Tip: More efficient to instead define narrow production cuts.



## **Transport properties – The OPT-PROP card**



Index of refraction (n):

apply to more materials

- Related to Snell's law, total internal reflections and Fresnel reflections.
- Changes the velocity of optical photons in the material (v=c/n).
- Must be defined for production and transport of optical photons in all materials! (exception: vacuum)
- Absorption:
  - Equal to the inverse absorption length (in cm<sup>-1</sup>) (follows the survival curve  $exp(-s/\lambda)$ ).
  - Energy of absorbed photons scored normally like for other particles.
  - Default: no absorption (=0.0)

#### Diffusion:

- Equal to inverse diffusion length (in cm<sup>-1</sup>).
- Random elastic scattering of photon with survival curve  $exp(-s/\lambda)$ .
- Photons scattered isotopically.
- Default: no diffusion (=0.0)



## **Transport properties – Series expansion**

- Series expansion of the index of refraction, the absorption coefficient and the diffusion coefficient can be defined.
- Taylor series around central wavelength  $\lambda_0$  (central angular frequency also available). Example for the index of refraction:

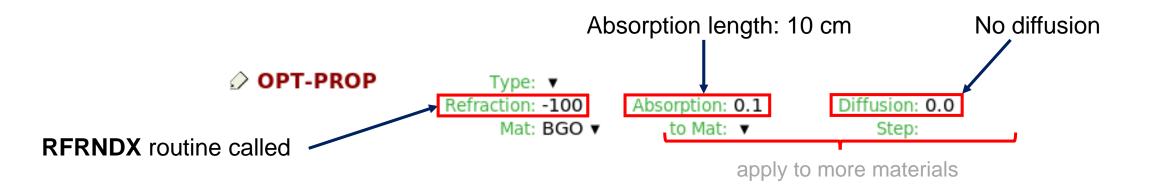
$$n(\lambda) = n(\lambda_0) + \frac{dn}{dx}x + \frac{1}{2}\frac{d^2n}{dx^2}x^2 + \frac{1}{6}\frac{d^3n}{dx^3}x^3 \quad \text{where} \quad x \equiv \frac{\lambda - \lambda_0}{\lambda_0}$$

- 0<sup>th</sup> order of the series defined with **SDUM=BLANK**.
- Derivatives defined with complementary **OPT-PROP** cards:
  - **SDUM=&1**: First derivatives
  - **SDUM=&2**: Second derivatives
  - SDUM=&3: Third derivatives



## **Transport properties – User routines**

- Arbitrary transport properties defined with user routines:
  - **RFRNDX**: Refraction index
  - **ABSCFF**: Absorption coefficient
  - **DFFCFF**: Diffusion coefficient
- Routine inputs:
  - Wavelength
  - Angular frequency
  - Material
- User routine called only if the property value is less than -99.





## **Reflections (OPT-PROP card)**

• With **SDUM=METAL**, the material behaves like a reflector.



- Reflectivity (r) can be defined. In practice, the user sets the value of "3rd 1-r".
- Other card options (1st, 2nd) are not used.
- User routine RFLCTV for arbitrary reflectivities.
  - Inputs: wavelength, angular frequency, material
  - Return value: the material reflectivity



# Sensitivity (OPT-PROP card)

• With **SDUM=SENSITIV**, the quantum efficiency of an optical sensor can be simulated.

🖉 OPT-PROP	Type: SENSITIV 🔻	0th: 0.5	1st: 0.0
	2nd: -5.0	3rd: 0.0	Max sensitivity: 0.5

- For efficiency reasons, the option is applied at the production stage, not during scoring. The option is not material or region dependent.
- The n<sup>th</sup> derivatives of the sensitivity curve at the central wavelength  $\lambda_0$  (or angular frequency  $\omega_0$ ) are specified on the card. Similar series expansion as for transport properties:

$$\epsilon(\lambda) = \epsilon(\lambda_0) + \frac{d\epsilon}{dx}x + \frac{1}{2}\frac{d^2\epsilon}{dx^2}x^2 + \frac{1}{6}\frac{d^3\epsilon}{dx^3}x^3$$
 where  $x \equiv \frac{\lambda - \lambda_0}{\lambda_0}$ 

 Central wavelength (angular frequency) defined using SDUM=WV-SENSI (SDUM=OM-SENSI) along with the sensitivity curve domain.

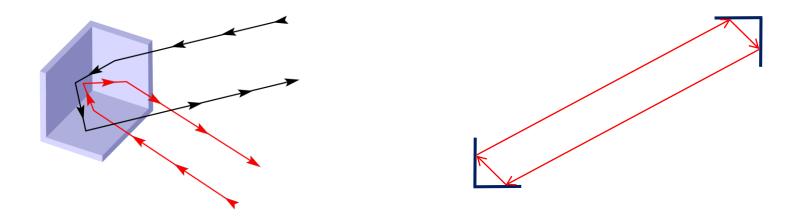
OPT-PROP Type: WV-SENSI ▼
λmin: =300\*nm λ: =500\*nm λmax: =1059\*nm

• User routine **QUEFFC** for defining arbitrary sensitivities.



### Photons trapped in locked modes

- Optical photons produced in a box can be trapped in "locked modes", meaning they undergo an infinite number of reflections. Simulation appears stuck.
- Reason: Light rays incoming on a mirror corner made up of 3 perpendicular surfaces are reflected in the same but opposite direction. A region which contains 2 of such corners can trap photons indefinitely.



• **Solution:** Open paths for optical photons to exits the locked modes. Recommend setting a small absorption or a reflectivity which is not exactly 100%.



# **Boundary crossing routine (OPHBDX)**

- Special boundary crossing treatment with the OPHBDX routine to override the treatment defined using the OPT-PROP card.
- Routine called each time an optical photon crosses boundaries predefined using the OPT-PROP card (SDUM=SPEC-BDX). Can define up to 40 boundaries using multiple OPT-PROP cards.

🖉 OPT-PROP	Type: SPEC-BDX <b>v</b>			
	Activate: On 🔻	Reg: R1 🔻	to Reg: R2 🔻	
	Activate: 🔻	Reg: 🔻	to Reg: 🔻	

#### • Input variables of **OPHBDX**:

- Wavelength / angular frequency
- Current region and new region

#### • Output variables of **OPHBDX**:

- Index of refraction, absorption coefficient and diffusion coefficient for the new region.
- Group velocity in the new region.
- Option to kill the photon.
- See the dedicated lecture on user routines for details on applying OPHBDX to all particle types.



# Wavelength shifting

- Option implemented as a user routine: **WVLNSH**
- Routine called every time an optical photon is absorbed.
  - Must set an absorption coefficient larger than 0 with the **OPT-PROP** card.
- Input variables:
  - Absorbed photon energy (wavelength)
  - Current material and region
- Output variables:
  - Number of secondary photons
  - Lists of energies (wavelengths) and production delays

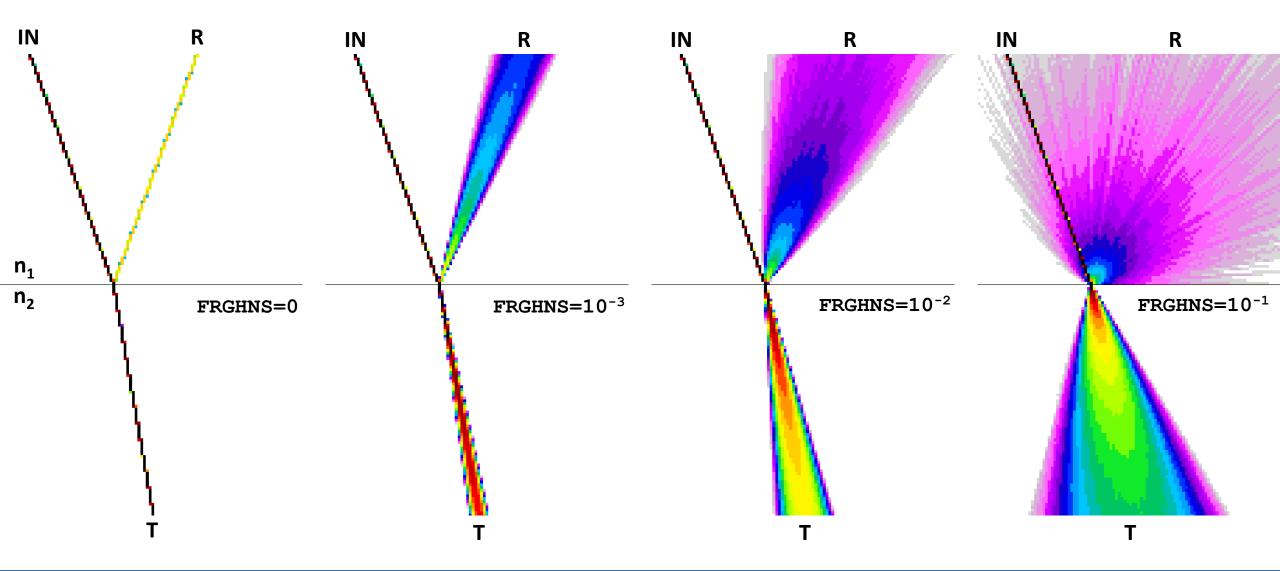


## **Boundary roughness (FRGHNS routine)**

- The roughness of a boundary can be simulated using the FRGHNS routine.
  - Routine called every time an optical photon is reflected or crosses between two regions.
  - Returns a roughness parameter, used to smear the direction of the outgoing photon.
  - New angle normally distributed. Gaussian width related to the roughness parameter.
- Input variables of **FRGHNS**:
  - Particle direction cosines (TXX, TYY, TZZ)
  - Particle direction normal to surface (UXSRFC, UYSRFC, UZSRFC)
  - Current material/region (MMAT, MREG) and new material/region (MMATNW, NEWREG)



# **Boundary roughness (FRGHNS routine)**





# Arbitrary transport properties: the USRMED routine

- USRMED routine can be used to take full control of the optical photon track in a material and at boundaries.
- Activated setting **SDUM=USERDIRE** in the **MAT-PROP** card.
  - Called for ANY particle travelling in the specified materials (not just for optical photons).



- Input/Output variables:
  - New region
  - Particle weight
  - Particle position at boundary
  - Momentum and polarization unit vectors
- Useful to define arbitrary interface physics for optical photons when a more complex model than generic
  options is required.
  - For reflection and transmission: Override the track direction.
  - For absorption: Override the particle weight (set w=0 to simply kill the particle).



### **Polarization**

- All particles in FLUKA have a dynamic polarization state.
- The polarization vector is accessible for **ALL** simulated particles regardless if it makes sense or not. Only used for some physics processes in FLUKA, for example:
  - Fresnel transmission and reflection of optical photons.
  - Compton scattering of photons.
- **Note:** The **POLARIZAti** card sets the polarization of primary photons. This card does not work with optical photons.
  - To change the polarization of primary optical photons, you must use a source routine.



## **Quenching effects (Birk's saturation)**

Birk's law relates the stopping power in the material to the scintillation light production.
 Quenching or saturation of the light production occurs for high stopping powers.

$$\frac{dL}{dx} = S \frac{\frac{dE}{dx}}{1 + B \frac{dE}{dx} + C \left(\frac{dE}{dx}\right)^2}$$

- FLUKA does not apply Birk's law directly to the production of scintillation photons.
- However, the TCQUENCH card can be applied to an energy detector to reduce the scored energy or dose deposition according to Birk's quenching law.

