Caveats concerning the G4-DF simulation

Julio Ureña, Justo Martín-Albo, Anselmo Cervera

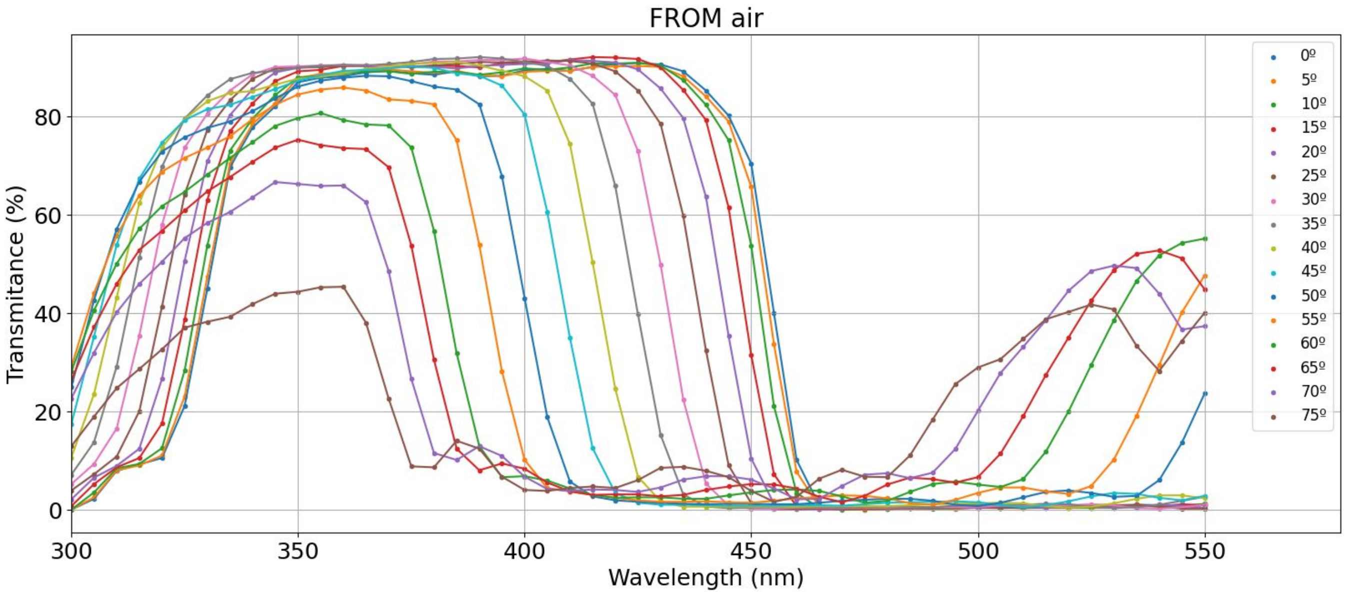
Photon Collectors WG - 7 February 2023

DEEP UNDERGROUND NEUTRINO EXPERIMENT

INSTITUT DE FÍSICA CORPUSCULAR

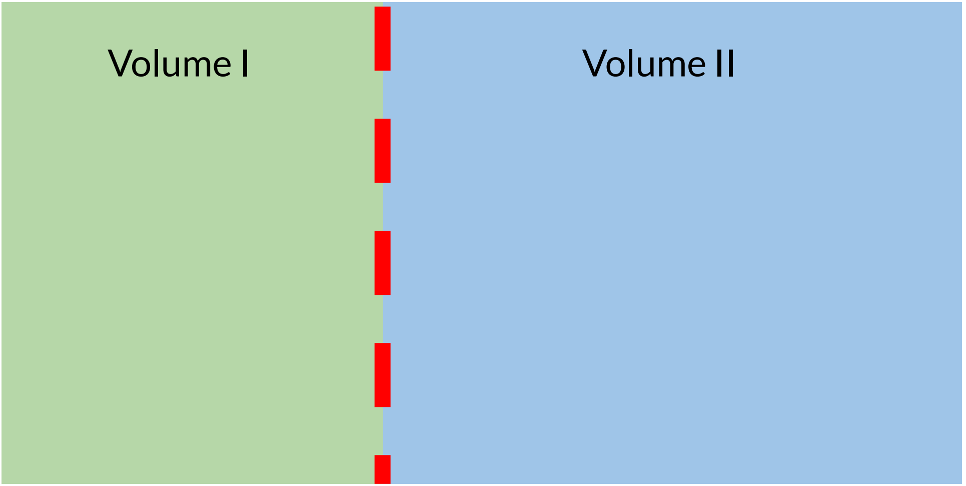
G4 tool for simulating DF

- **G4 receives a set of wavelength-dependent transmitance curves**
- **Each curve is defined for a certain angle of incidence (AOI)**
- We endow a surface with the provided transmitance data
- When a photon reaches such surface, G4 performs a 2D-interpolation (wavelength and AOI) and comes up with a transmitance value for such event
- The photon is transmitted or specularly-reflected up to the interpolated transmitance



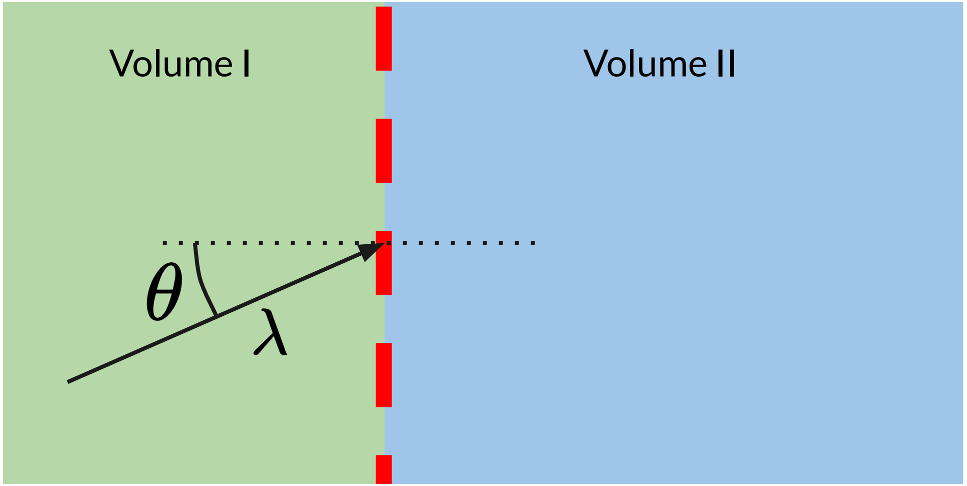
G4 tool for simulating DF

- G4 receives a set of wavelength-dependent transmitance curves
- Each curve is defined for a certain angle of incidence (AOI)
- **We endow a surface with the provided transmitance data**
- When a photon reaches such surface, G4 performs a 2D-interpolation (wavelength and AOI) and comes up with a transmitance value for such event
- The photon is transmitted or specularly-reflected up to the interpolated transmitance



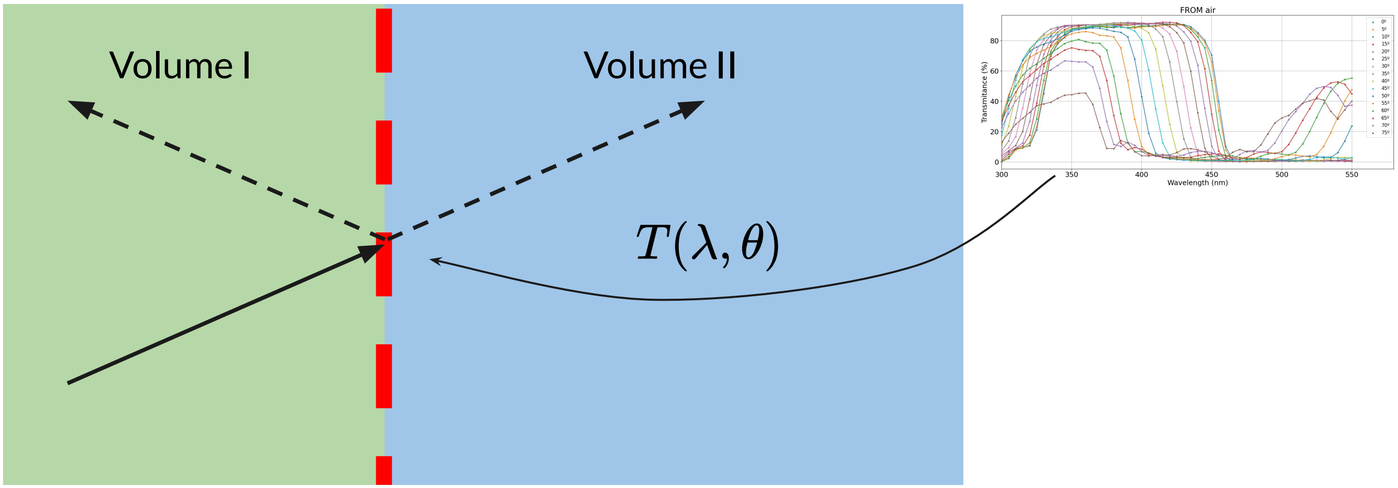
G4 tool for simulating DF

- G4 receives a set of wavelength-dependent transmitance curves
- Each curve is defined for a certain angle of incidence (AOI)
- We endow a surface with the provided transmitance data
- **When a photon reaches such surface, G4 performs a 2D-interpolation (wavelength and AOI) and comes up with a transmitance value for such event**
- The photon is transmitted or specularly-reflected up to the interpolated transmitance

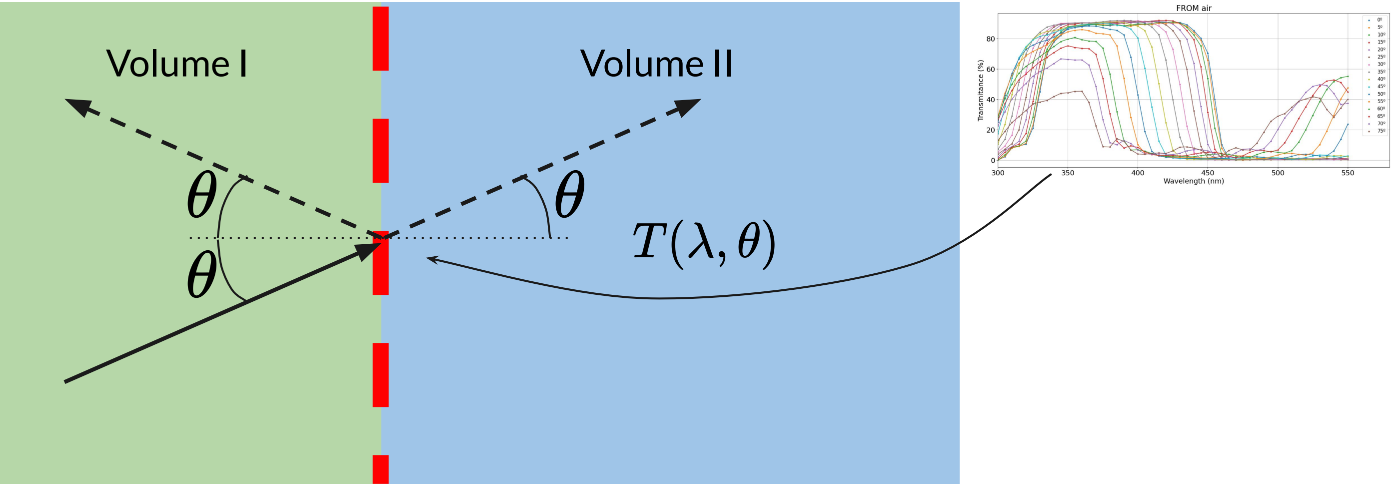


G4 tool for simulating DF

- G4 receives a set of wavelength-dependent transmitance curves
- Each curve is defined for a certain angle of incidence (AOI)
- We endow a surface with the provided transmitance data
- When a photon reaches such surface, G4 performs a 2D-interpolation (wavelength and AOI) and comes up with a transmitance value for such event
- **The photon is transmitted or specularly-reflected up to the interpolated transmitance**



If reflection takes place, the photon is specularly reflected
If transmission takes place, **no snell refraction is applied!**

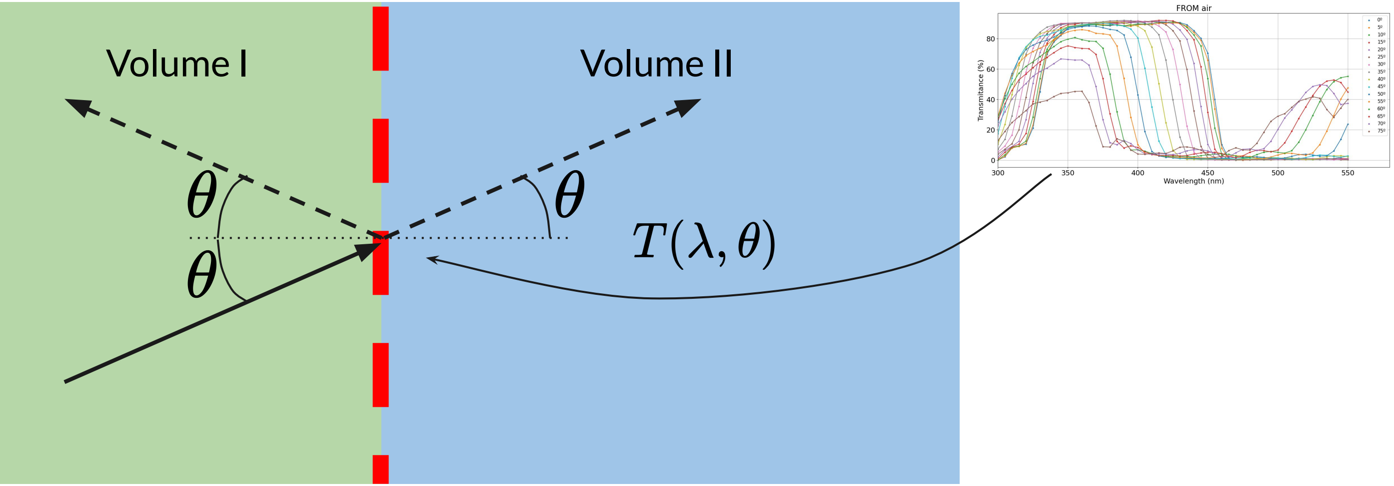


G4 tool for simulating DF

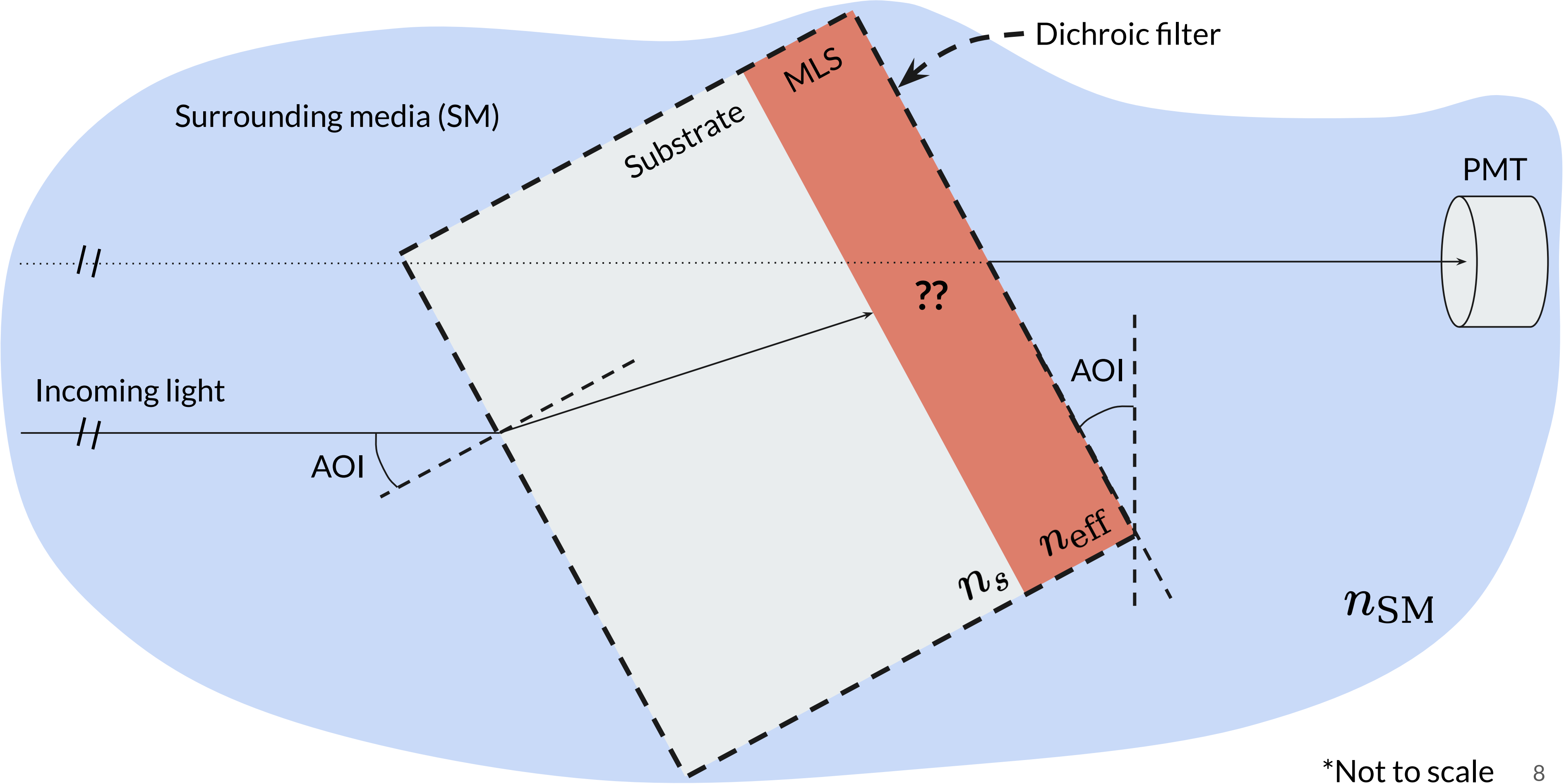
From Geant4 user's guide > Tracking and physics > Physics processes > Optical photon processes > Boundary process:

> "*As expressed in Maxwell's equations,* ***Fresnel reflection and refraction are intertwined through their relative probabilities of occurrence****. Therefore neither of these processes, nor total internal reflection, are viewed as individual processes deserving separate class implementation.*"

Fresnel reflection/refraction are regarded as processes which are ruled-by and inseparable-from their relative probabilities. Thus, setting a custom transmission probability destroys such processes: now just reflection and "raw" transmission are considered.

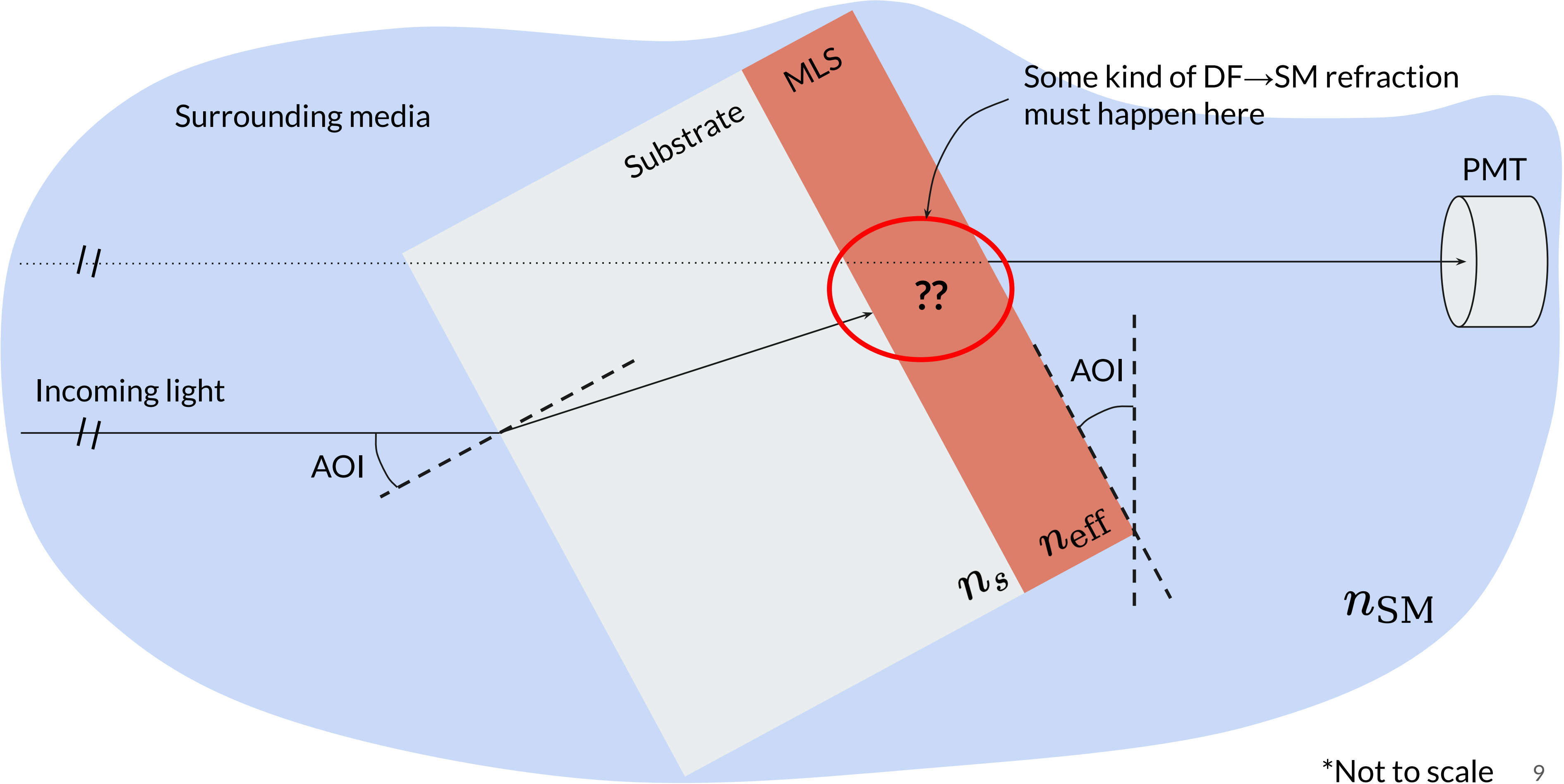


DF previous considerations



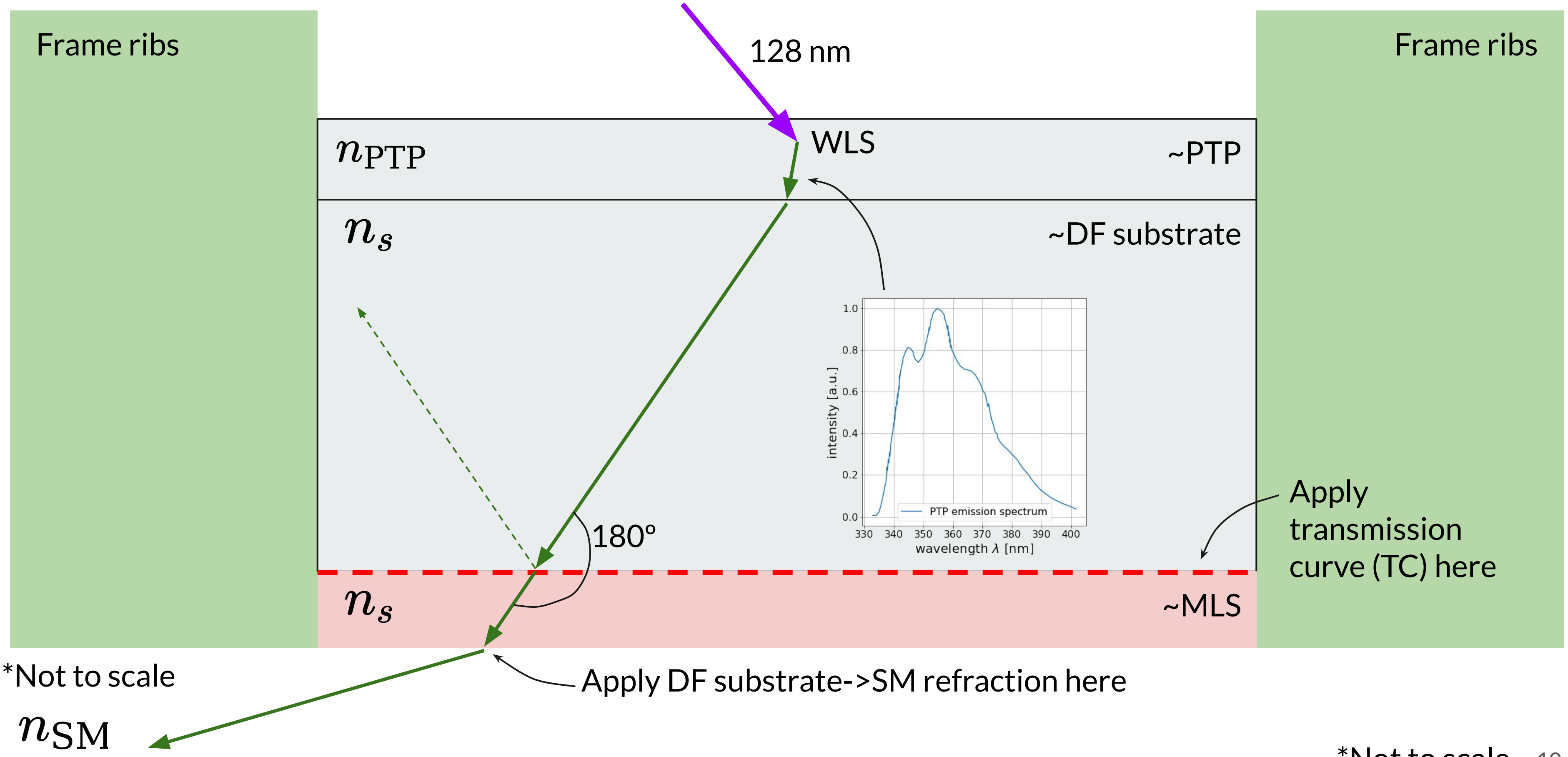
*Not to scale

DF previous considerations



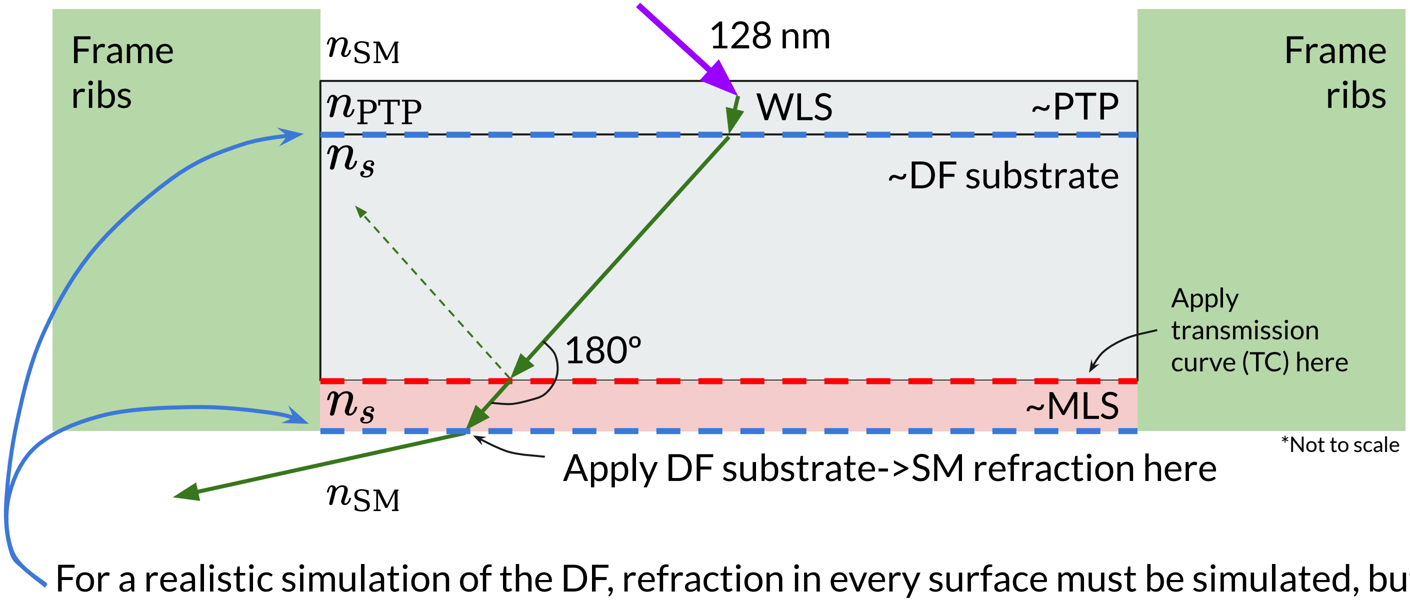
*Not to scale

DF computational model



*Not to scale

First caveat

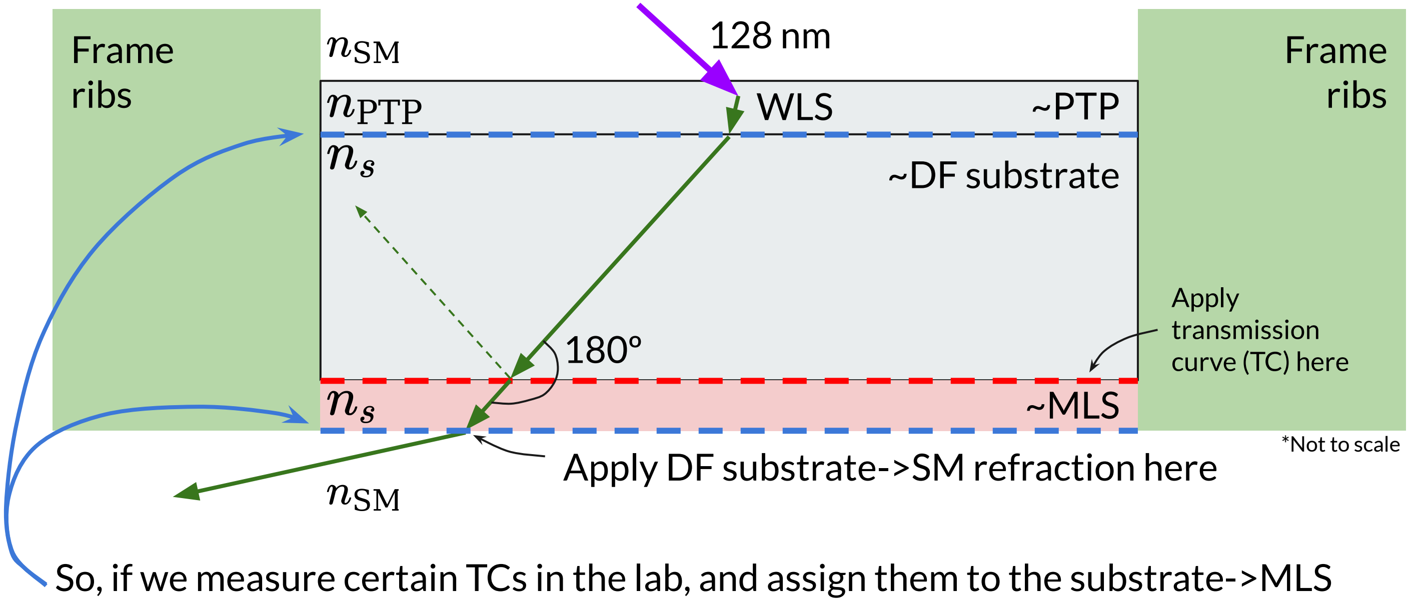


For a realistic simulation of the DF, refraction in every surface must be simulated, but as we have seen, refraction cannot be separated from reflection

From Geant4 user's guide > Tracking and physics > Physics processes > Optical photon processes > Boundary process:

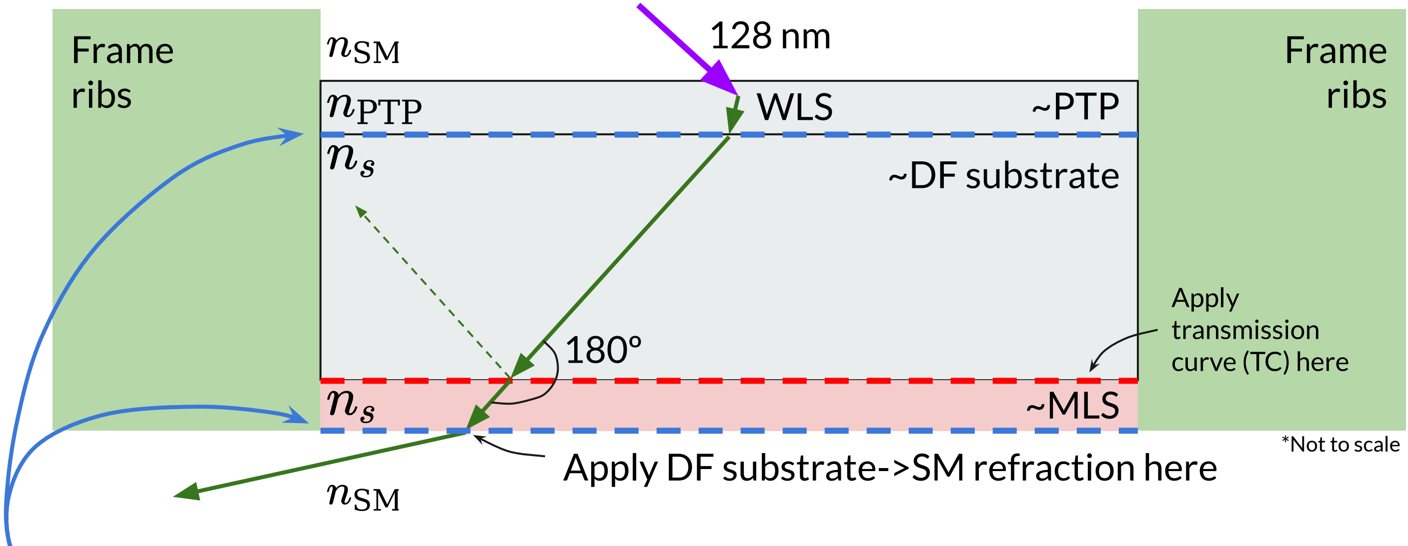
"As expressed in Maxwell's equations, ***Fresnel reflection and refraction are intertwined through their relative probabilities of occurrence****. Therefore neither of these processes, nor total internal reflection, are viewed as individual processes deserving separate class implementation."*

First caveat



So, if we measure certain TCs in the lab, and assign them to the substrate->MLS interface, these interfaces will contribute with an extra reflection probability.

First caveat

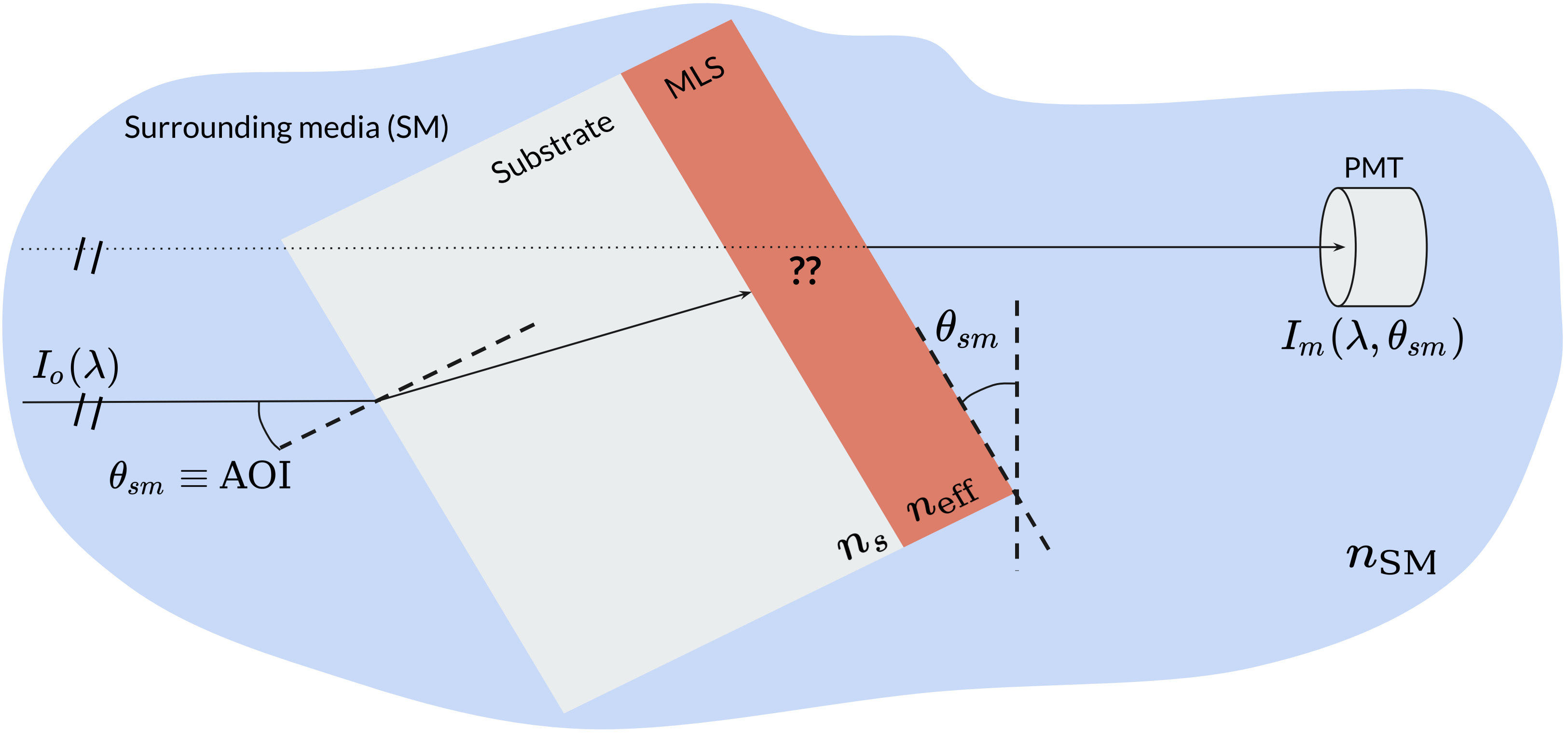


This extra reflection is given by Geant4 which automatically simulates reflection/refraction probability using Fresnel equations

'Fresnel Transmission'

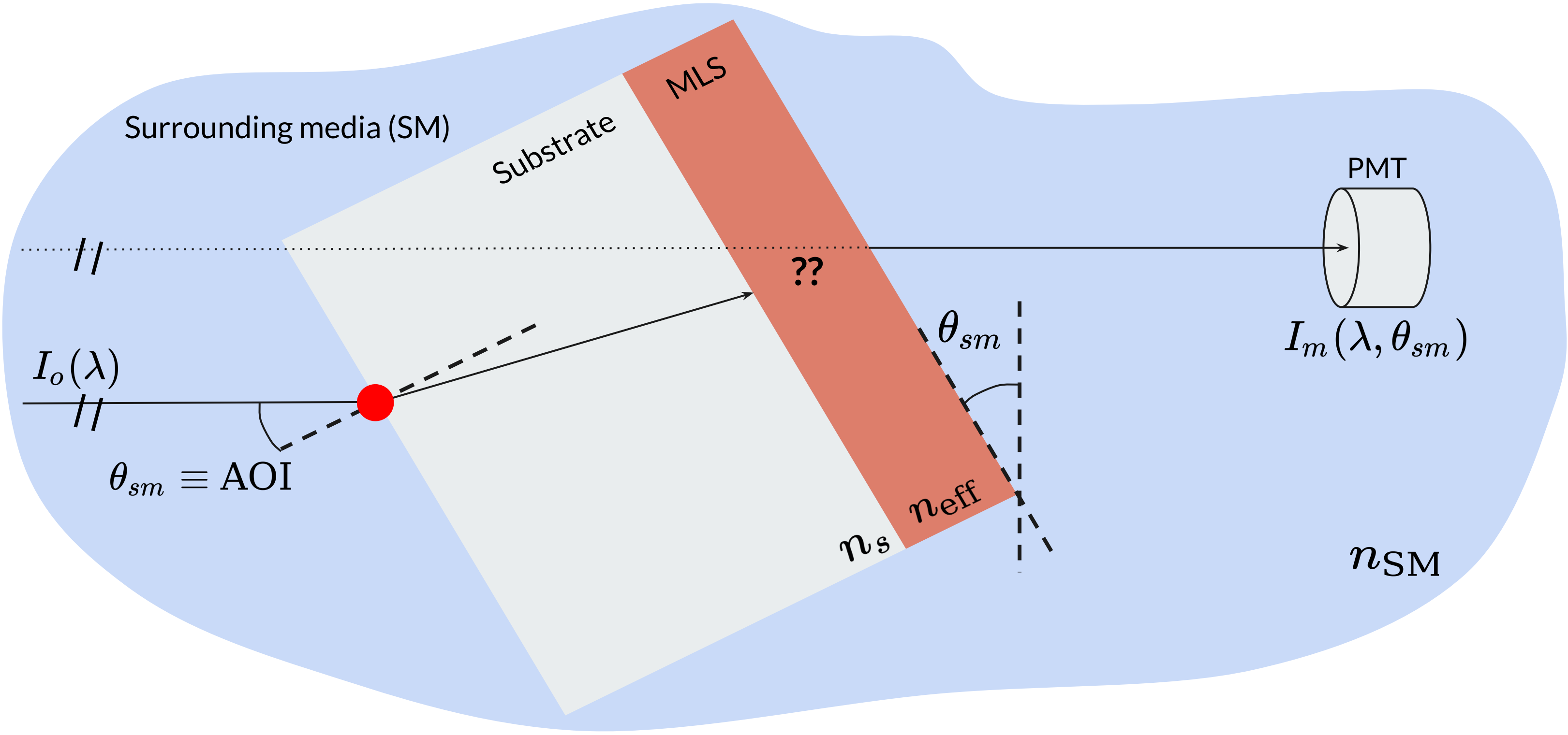
$$R_S = \left(\frac{n_1 \cos\theta_i - n_2 \cos\theta_t}{n_1 \cos\theta_i + n_2 \cos\theta_t} \right)^2 \qquad R = \frac{R_S + R_P}{2} \qquad FT \equiv T = 1 - R$$

First caveat



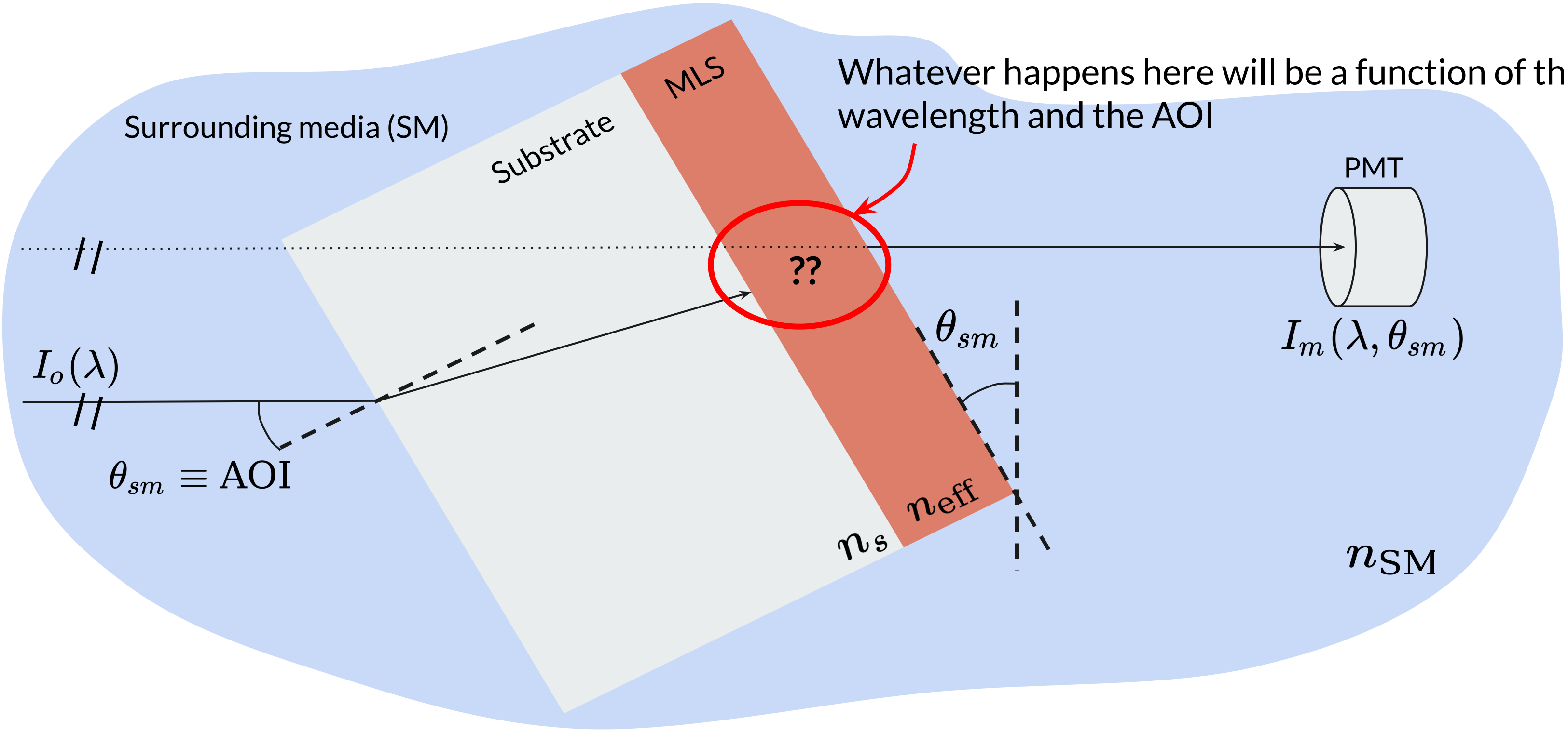
$$I_m(\lambda, \theta_{sm}) = I_o(\lambda) \cdot \ldots$$

First caveat



$$I_m(\lambda, \theta_{sm}) = I_o(\lambda) \cdot FT_{n_{su}}^{n_{sm}}(\theta_{sm}) \cdot \ldots$$

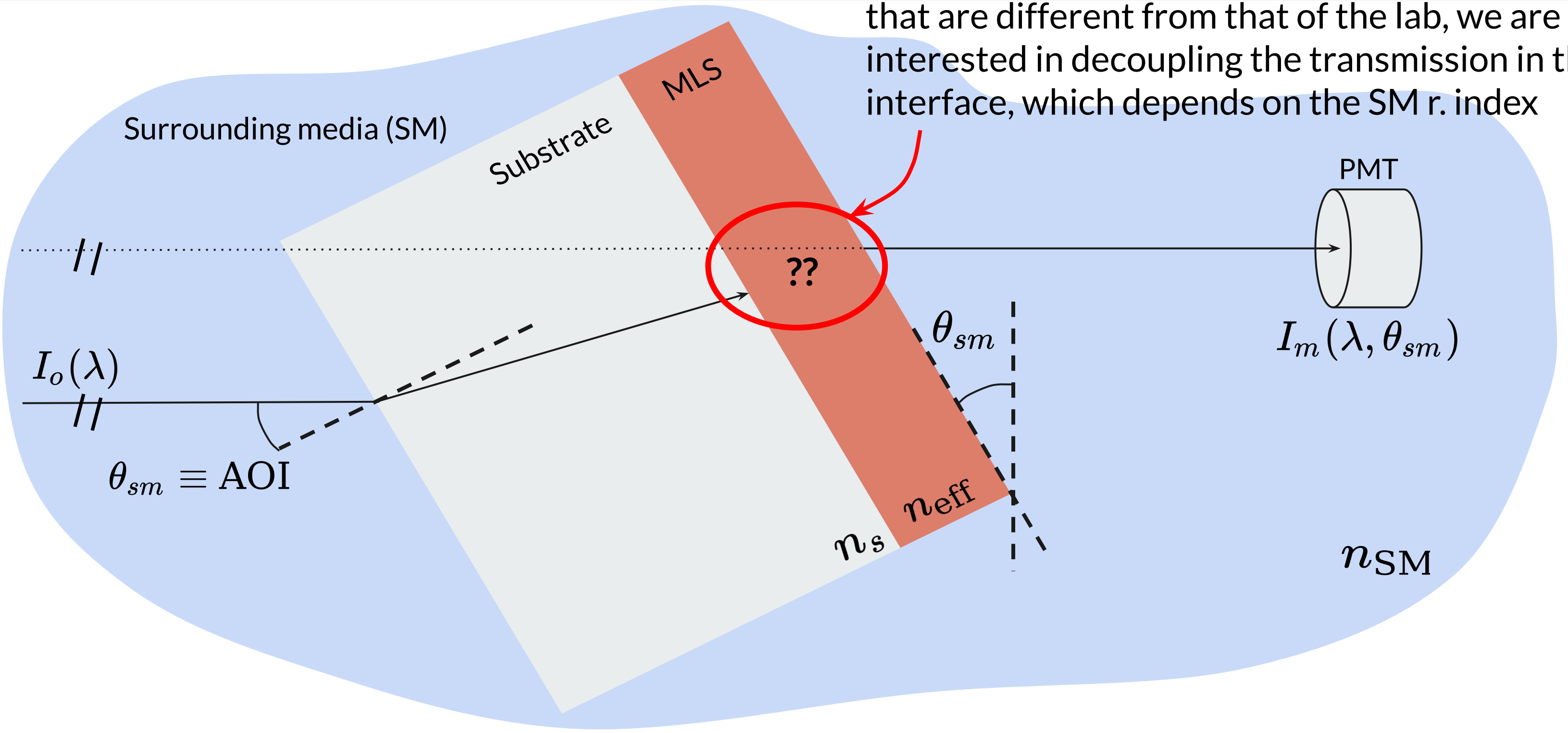
First caveat



$$I_m(\lambda, \theta_{sm}) = I_o(\lambda) \cdot FT_{n_{su}}^{n_{sm}}(\theta_{sm}) \cdot X(\lambda, \theta_{sm})$$

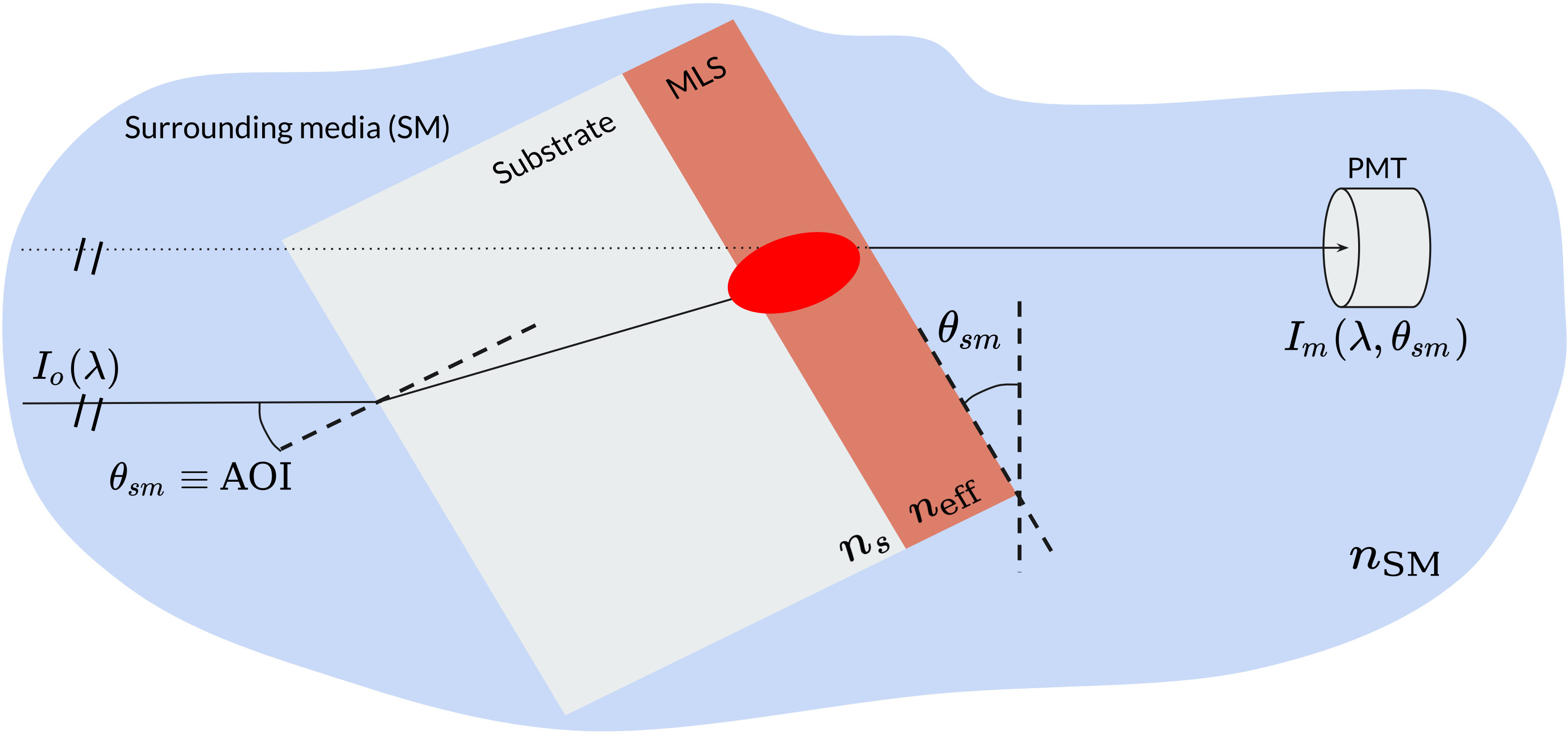
First caveat

But, since we want to simulate the DF in medias that are different from that of the lab, we are interested in decoupling the transmission in the last interface, which depends on the SM r. index



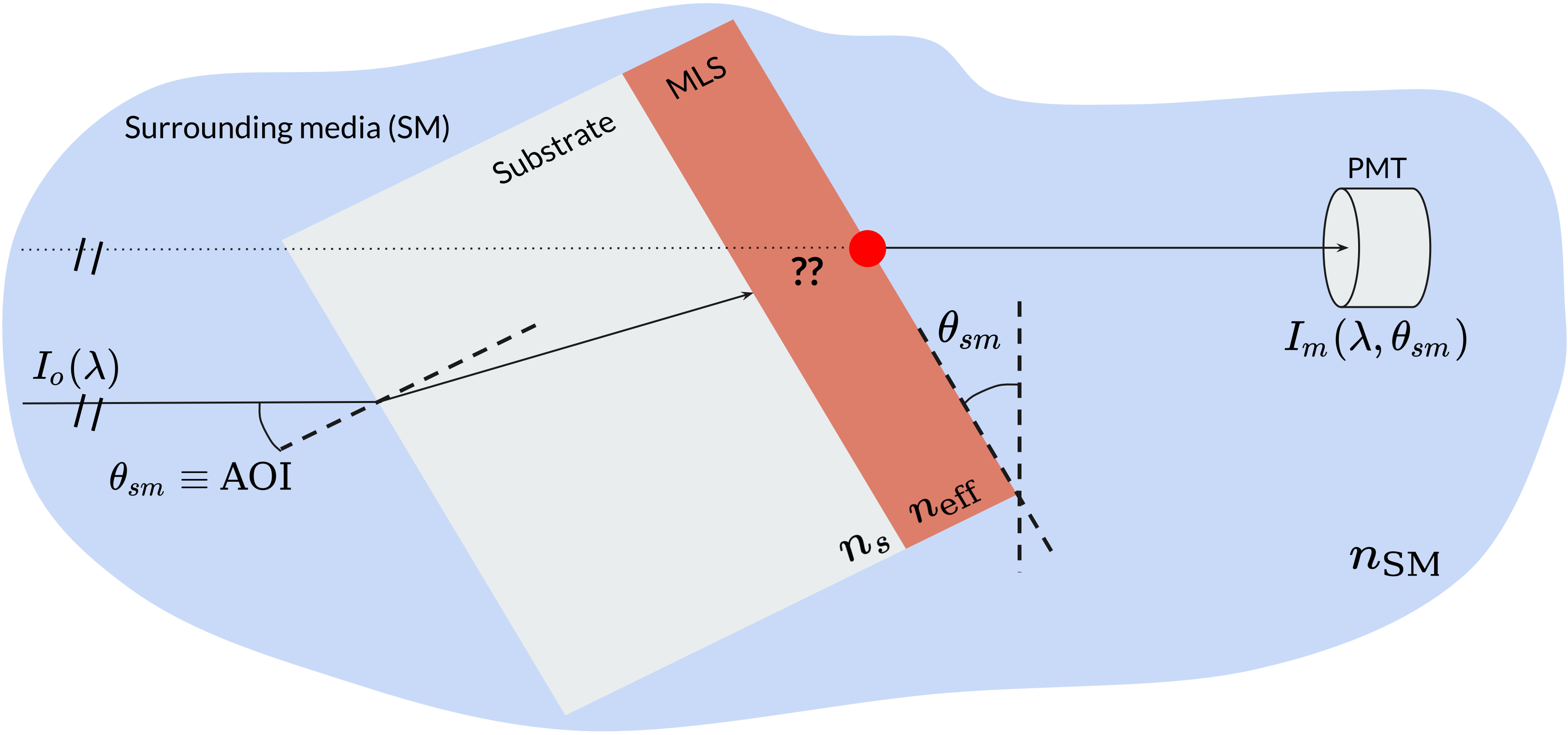
$$I_m(\lambda, \theta_{sm}) = I_o(\lambda) \cdot FT_{n_{su}}^{n_{sm}}(\theta_{sm}) \cdot X(\lambda, \theta_{sm})$$

First caveat



$$I_m(\lambda, \theta_{sm}) = I_o(\lambda) \cdot FT_{n_{su}}^{n_{sm}}(\theta_{sm}) \cdot ITC(\lambda, \theta_{sm}) \cdot \ldots$$

First caveat



$$I_m(\lambda, \theta_{sm}) = I_o(\lambda) \cdot FT_{n_{su}}^{n_{sm}}(\theta_{sm}) \cdot ITC(\lambda, \theta_{sm}) \cdot FT_{n_{sm}}^{n_{DF}}(\alpha(\theta_{sm}))$$

First caveat

$$ITC(\lambda, \theta_{sm}) = \frac{T_m(\lambda,\theta_{sm})}{FT_{n_{su}}^{n_{sm}}(\theta_{sm}) \cdot FT_{n_{sm}}^{n_{DF}}(\alpha(\theta_{sm}))}$$

If we knew everything here, we could compute the ‘intrinsic’ transmitance curve of the dichroic filter as shown above

$$I_m(\lambda, \theta_{sm}) = I_o(\lambda) \cdot FT_{n_{su}}^{n_{sm}}(\theta_{sm}) \cdot ITC(\lambda, \theta_{sm}) \cdot FT_{n_{sm}}^{n_{DF}}(\alpha(\theta_{sm}))$$

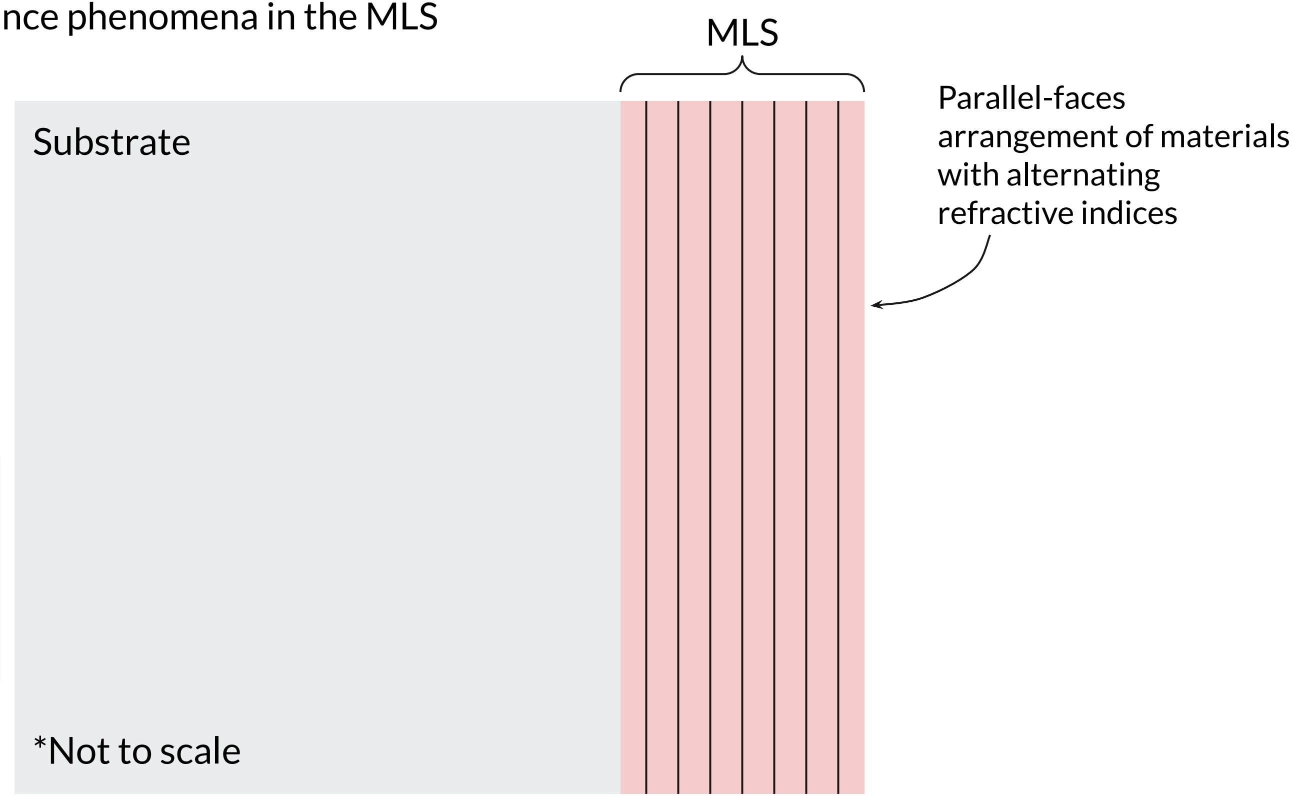
First caveat

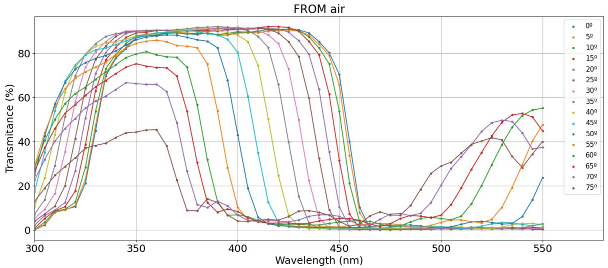
$$ITC(\lambda, \theta_{sm}) = \frac{T_m(\lambda,\theta_{sm})}{FT_{nsu}^{nsm}(\theta_{sm}) \cdot FT_{nsm}^{nDF}(\alpha(\theta_{sm}))}$$

The truth is we know everything except for **this**, but we can overcome this if we assume the following conceptual model:

DF conceptual model

The TC emerges from the interference phenomena in the MLS

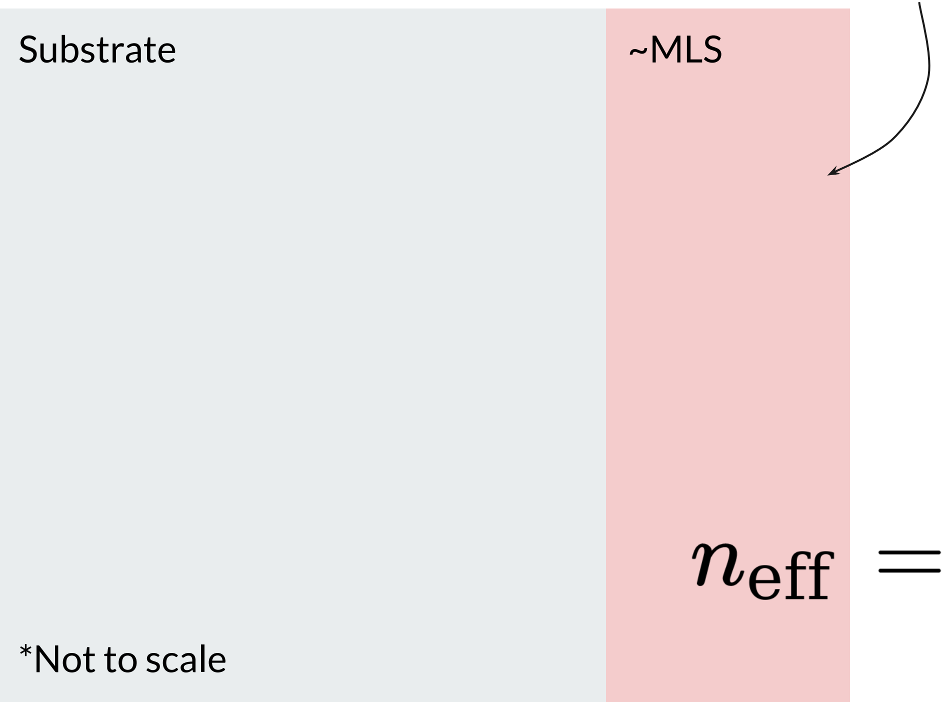




Different AOI's result in different TCs (we already knew this), but different SM also result in different TCs

DF conceptual model

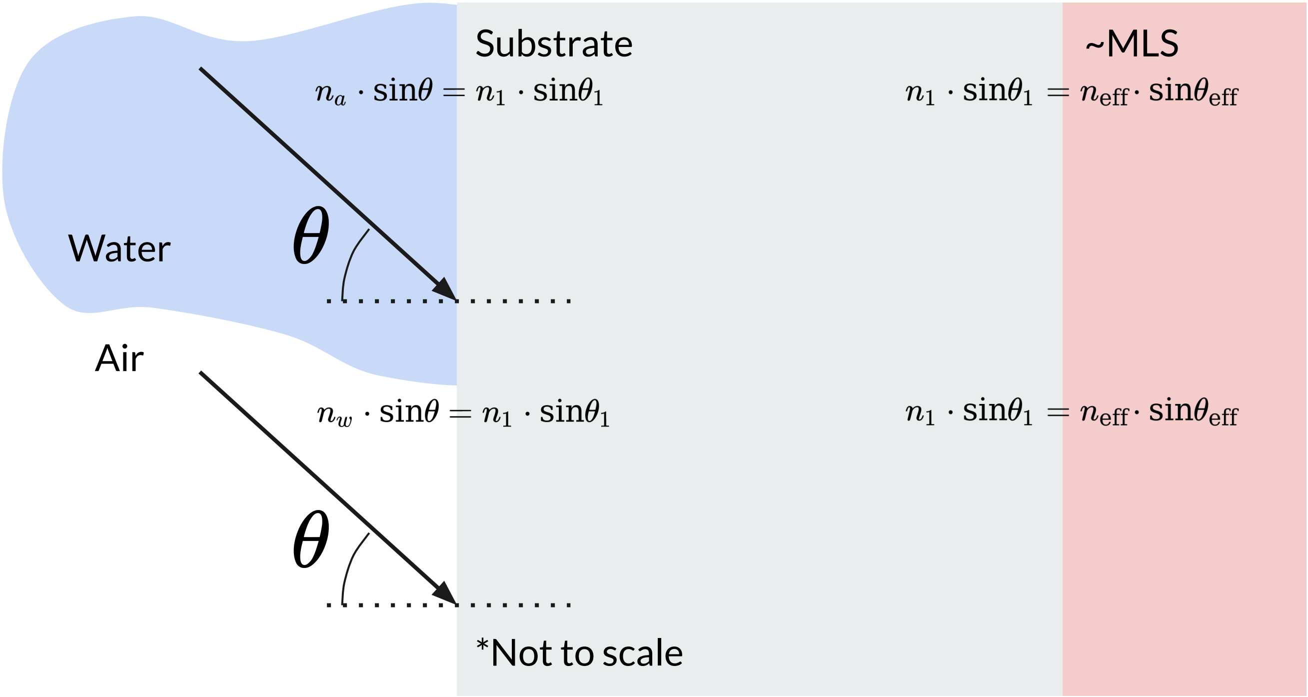
→ Substitute the MLS by an homogeneous volume with an effective refractive index



$$n_{\text{eff}} = \frac{\sum_i d_i}{\sum_i \frac{d_i}{n_i}}$$

Within this model, to explain the dependence of TCs with the surrounding media, our current hypothesis is that **what determines the TC is the angle of refraction (AOR) within the ~MLS.**

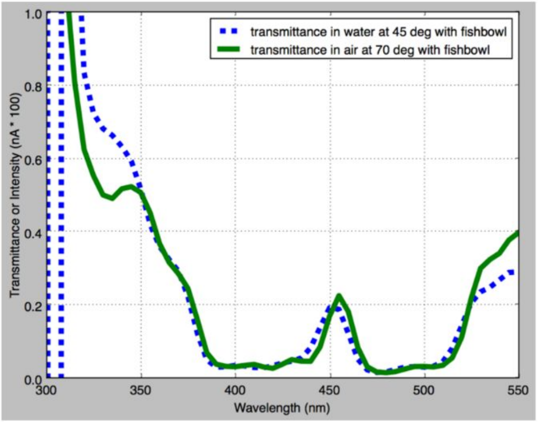
DF conceptual model



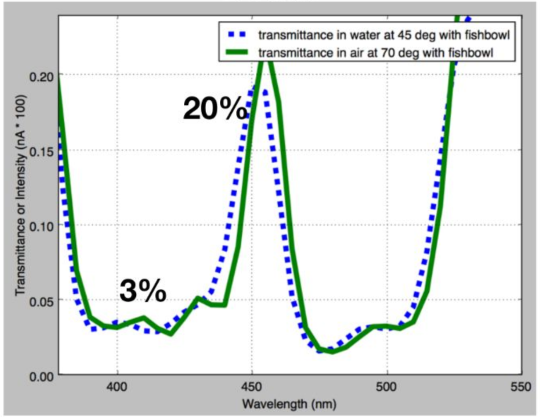
Within this model, to explain the dependence of TCs with the surrounding media, our current hypothesis is that **what determines the TC is the angle of refraction (AOR) within the ~MLS.**

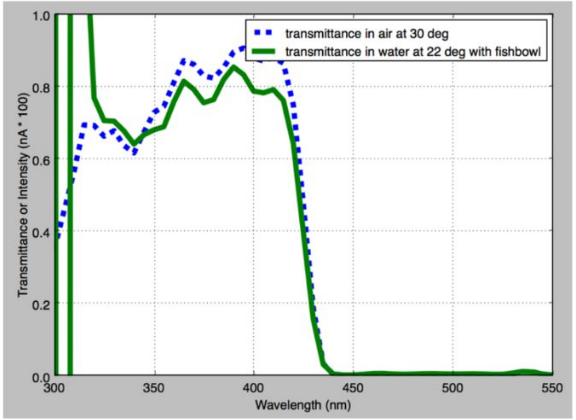
Model backups

There are **experimental** measurements and Transfer-matrix-method simulations backing up this hypothesis:

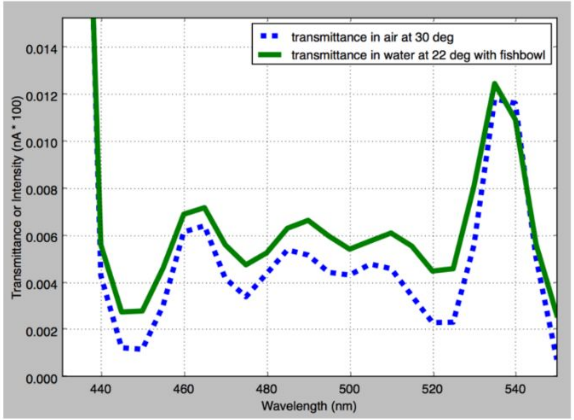


ZOOM



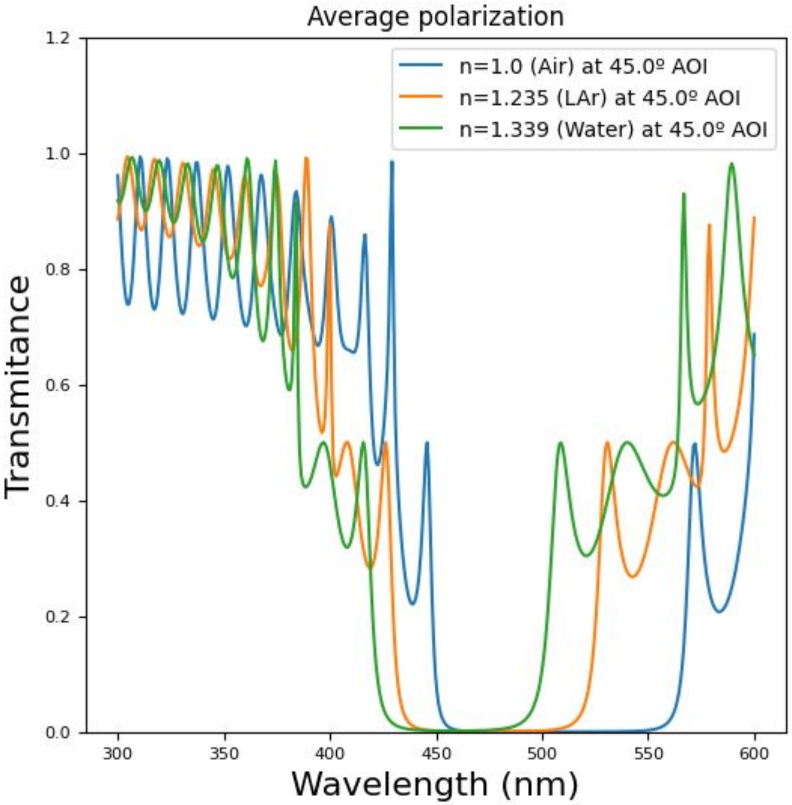


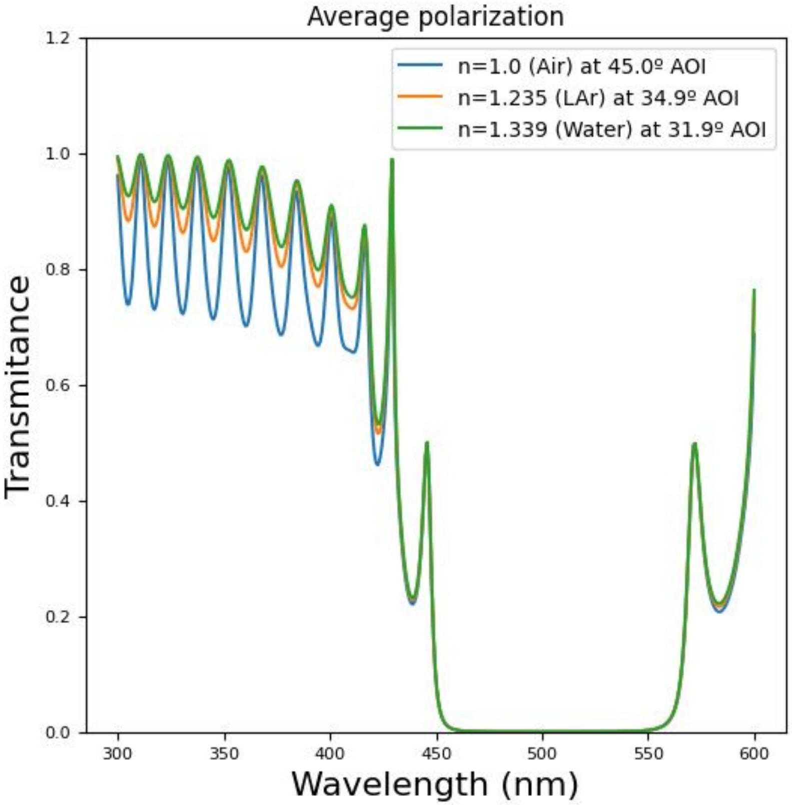
ZOOM



Model backups

There are experimental measurements and Transfer-matrix-method **simulations** backing up this hypothesis:





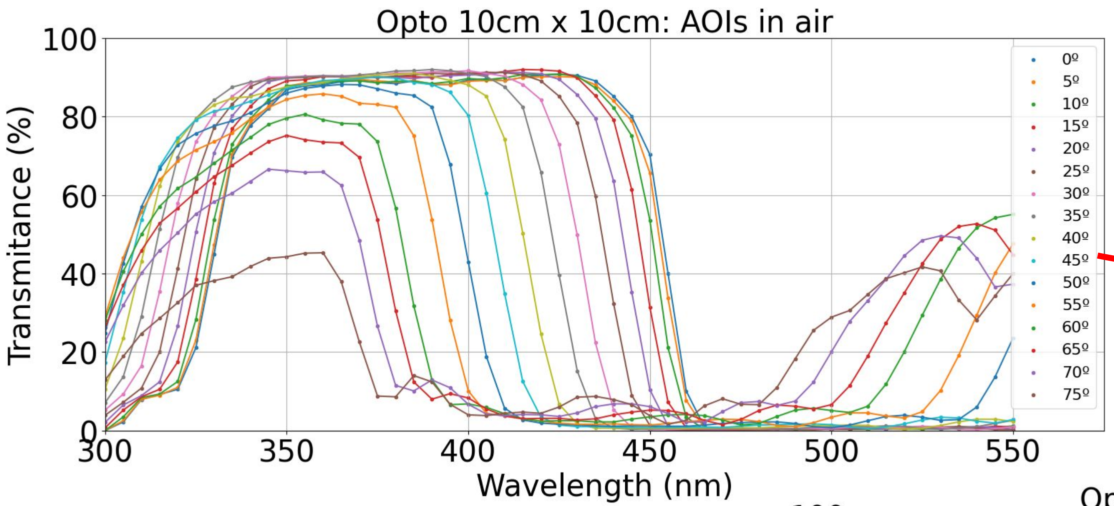
First caveat

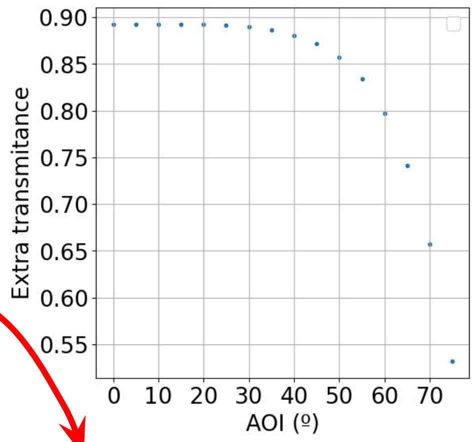
$$ITC(\lambda, \theta_{sm}) = \frac{T_m(\lambda, \theta_{sm})}{FT_{nsu}^{nsm}(\theta_{sm}) \cdot FT_{nsm}^{nDF}(\alpha(\theta_{sm}))}$$

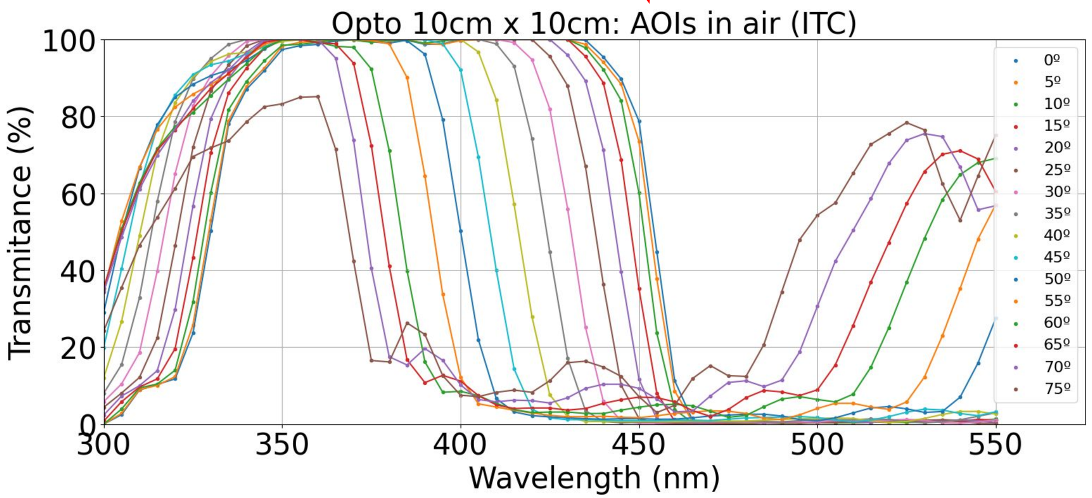
Within this approximation, we know what the refractive index of the dichroic filter is (the effective r. index of the MLS) and we can compute the angle of the light that propagates within the ~MLS using Snell's law

$$ITC(\lambda, \theta_{sm}) = \frac{T_m(\lambda, \theta_{sm})}{FT_{nsu}^{nsm}(\theta_{sm}) \cdot FT_{nsm}^{n_{\text{eff}}}(S(\theta_{sm}))}$$

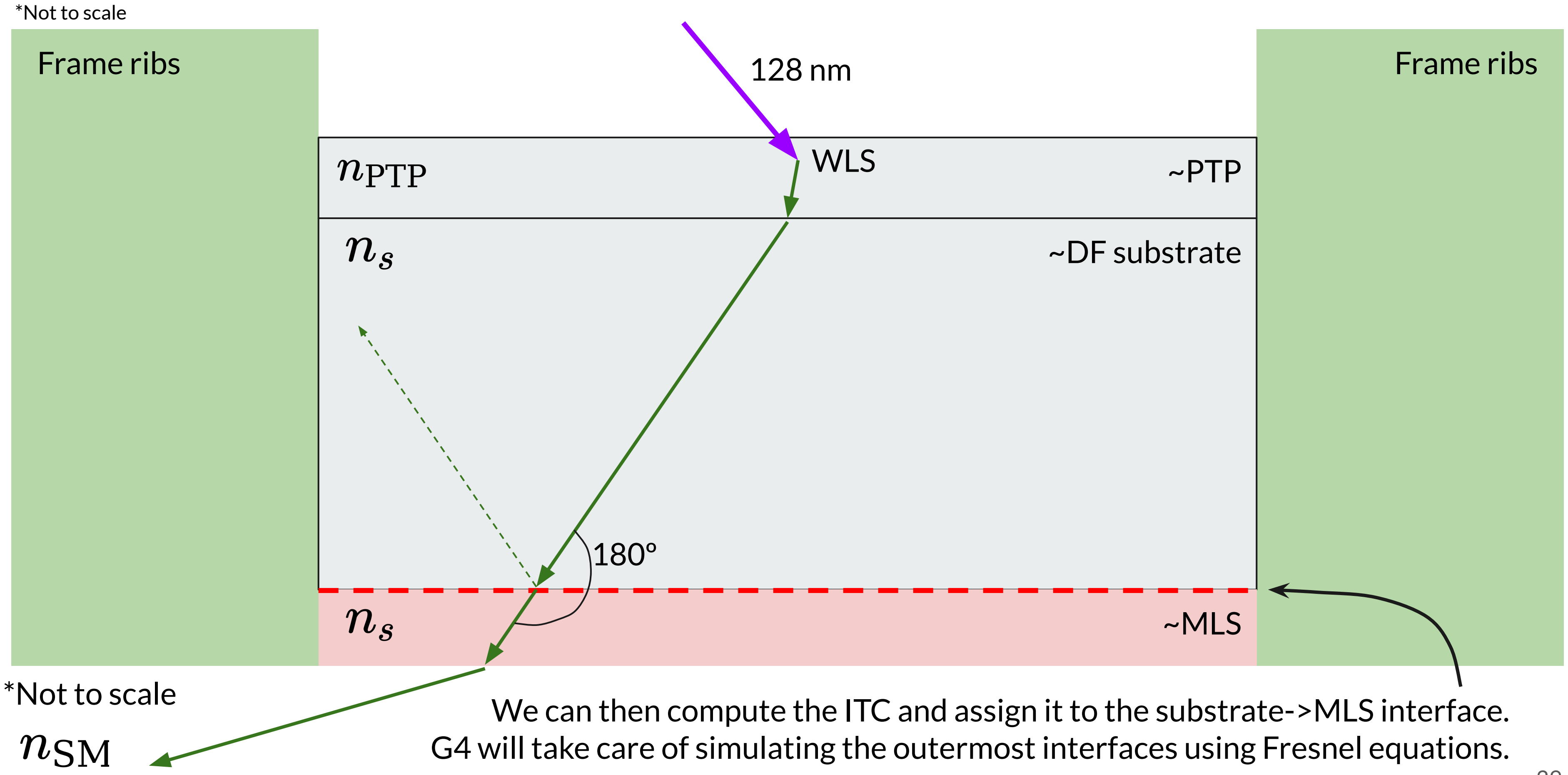
First caveat





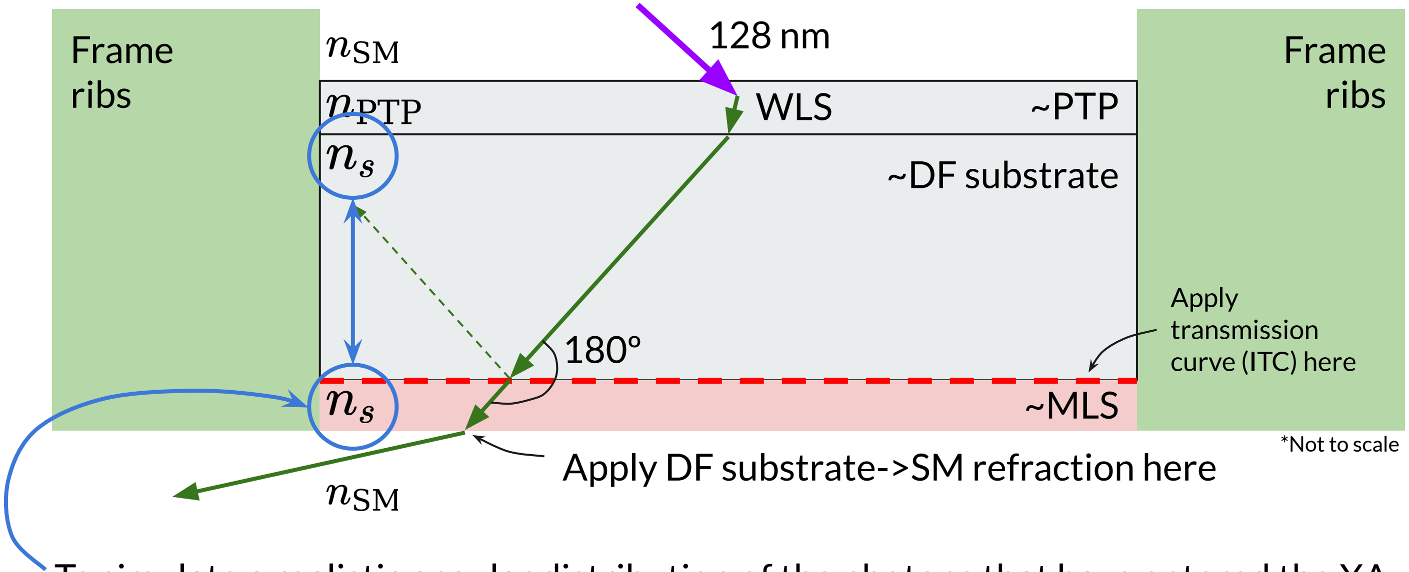


DF computational model



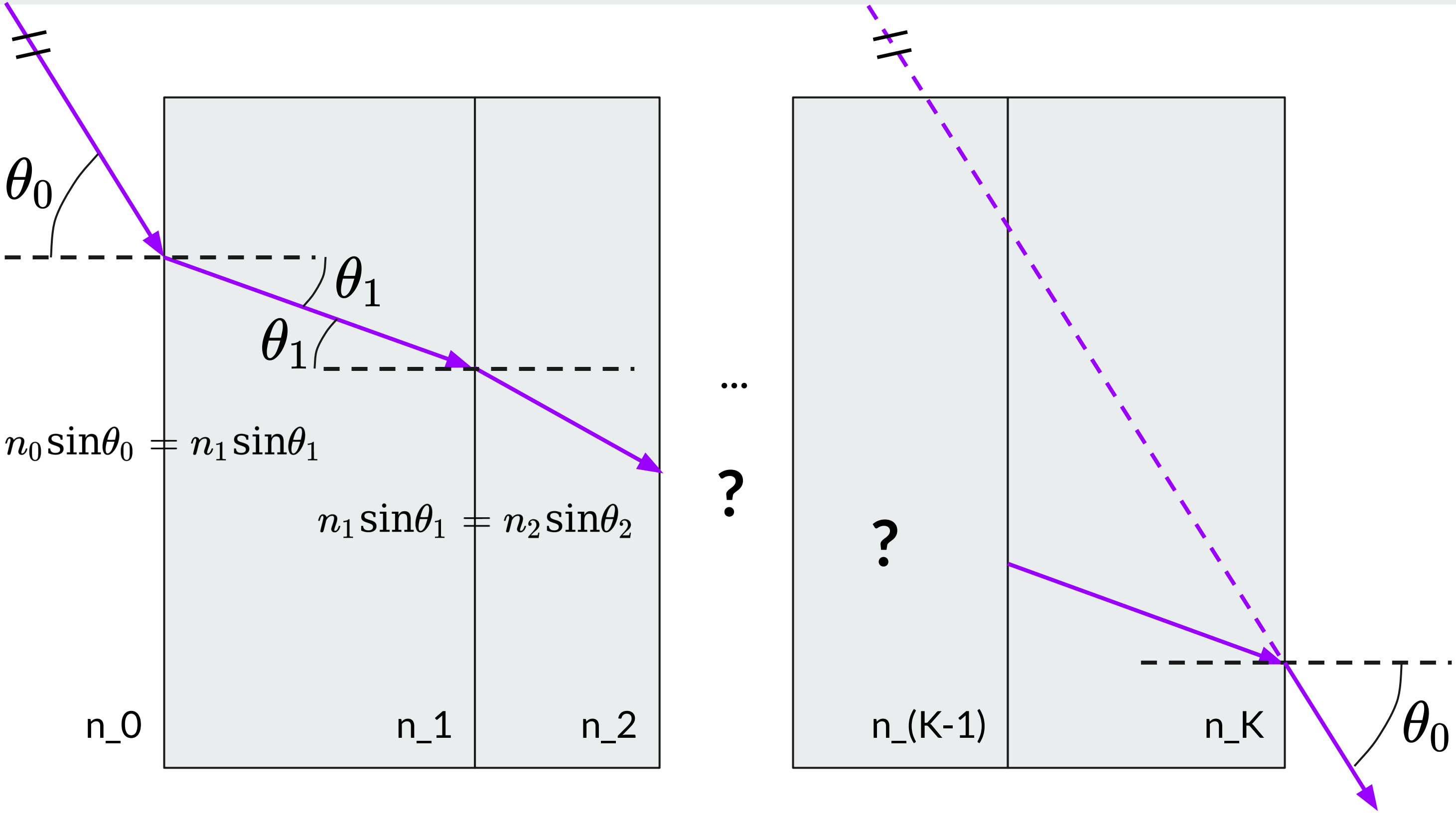
We can then compute the ITC and assign it to the substrate->MLS interface.
G4 will take care of simulating the outermost interfaces using Fresnel equations.

Second caveat

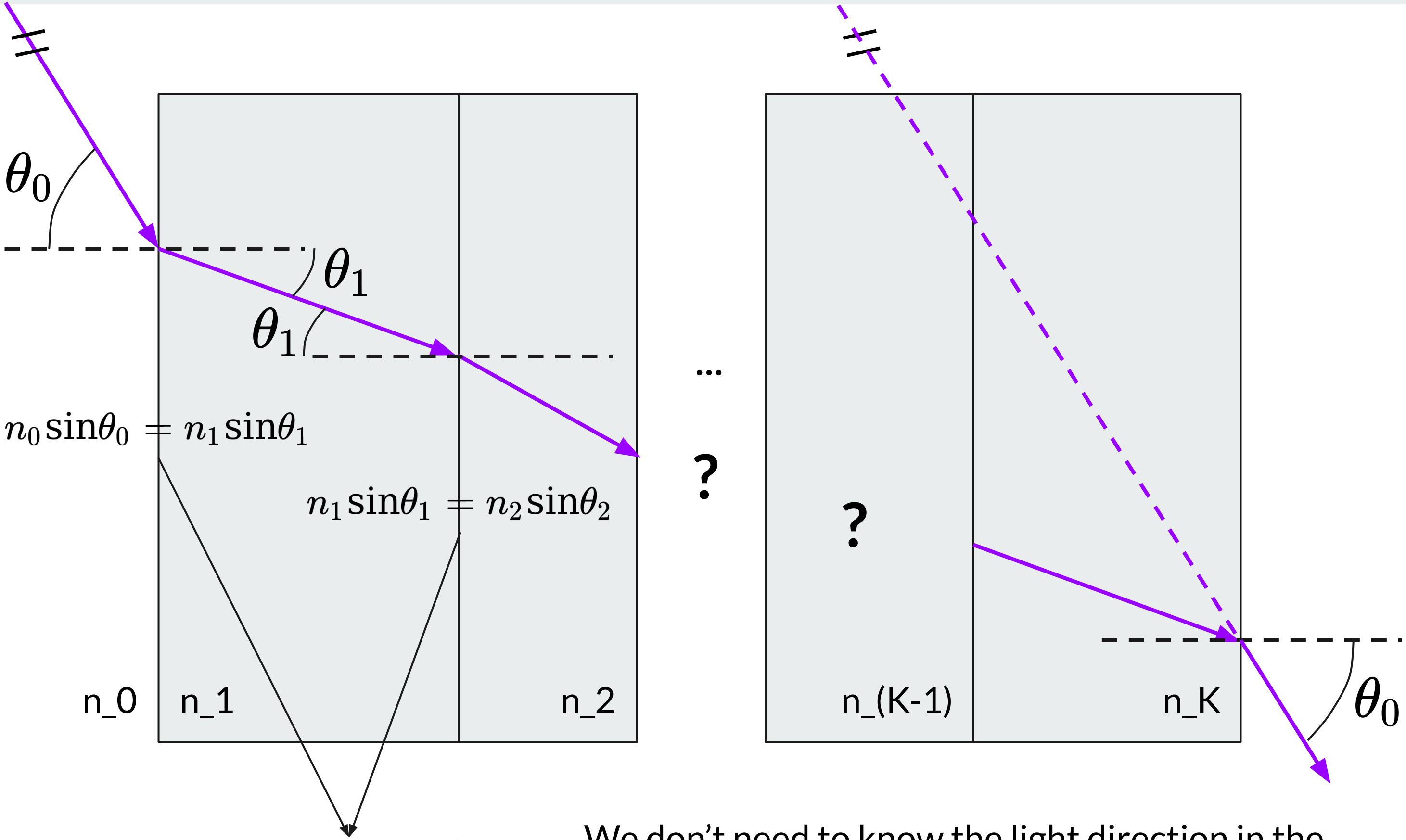


To simulate a realistic angular distribution of the photons that have entered the XA, we need to set the ~MLS volume refractive index to that of the substrate

Previous considerations on parallel-faces stackings



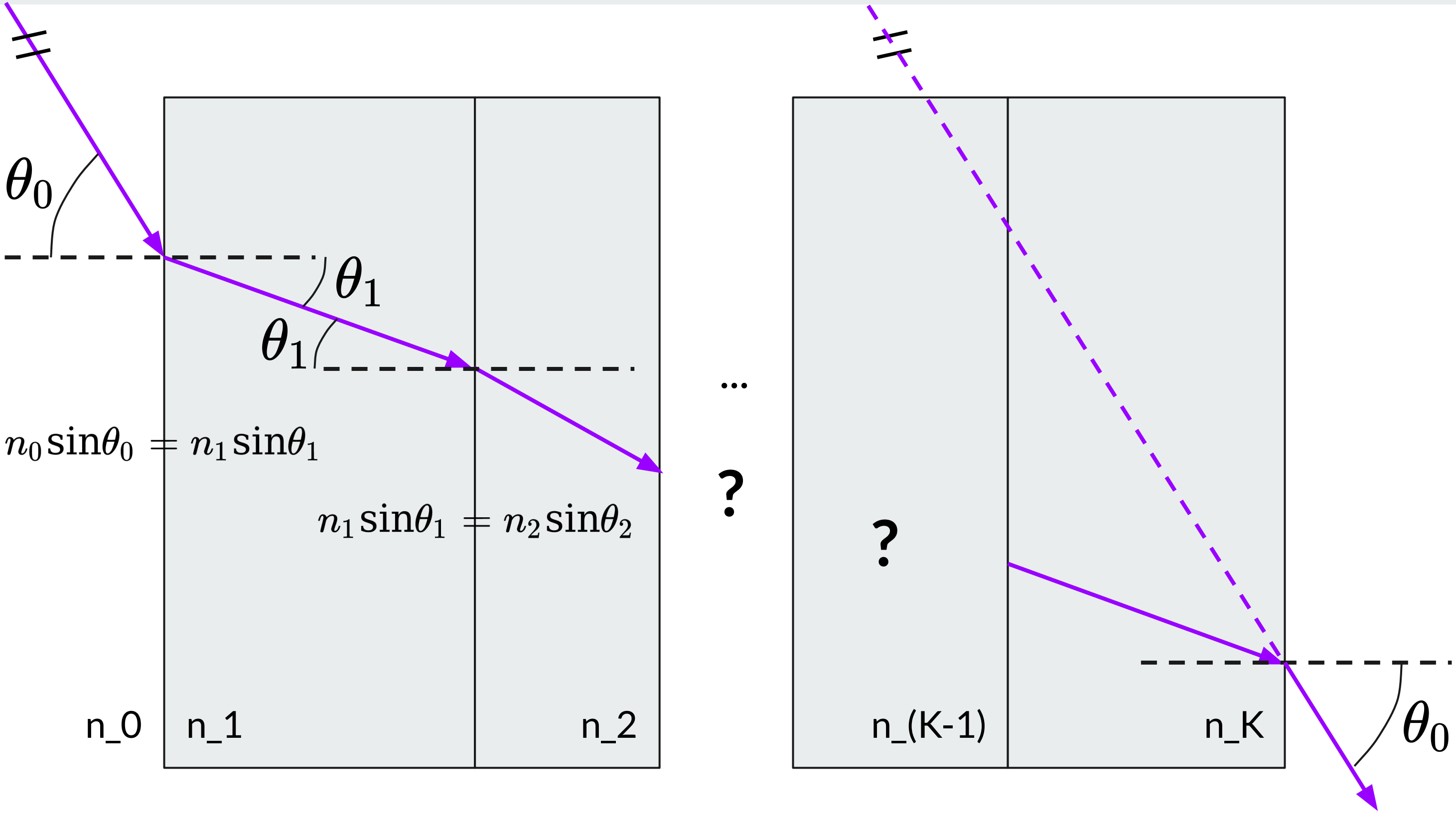
Previous considerations on parallel-faces stackings



$$n_0 \sin\theta_0 = n_2 \sin\theta_2$$

We don't need to know the light direction in the first layer to compute it for the second layer

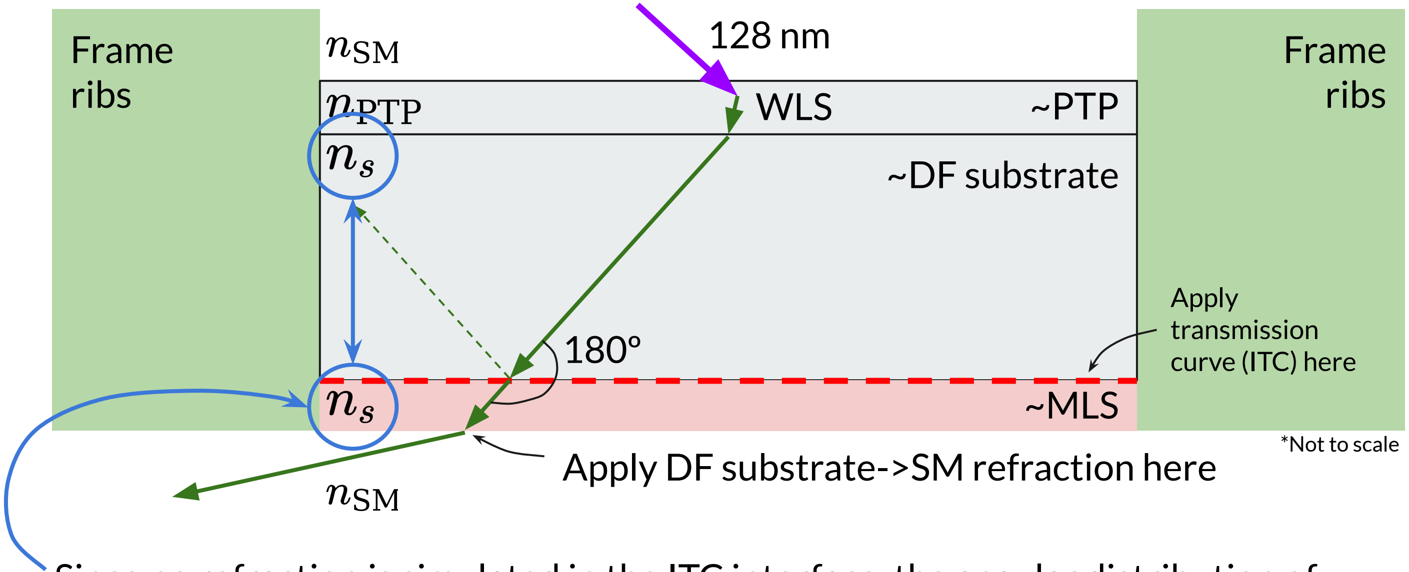
Previous considerations on parallel-faces stackings



$$n_i \sin\theta_i = \text{cte} \ \forall i$$

Indeed, **we only need to know the pair (theta_i, n_i) for some layer**, to know the light propagation direction in any other layer

Second caveat



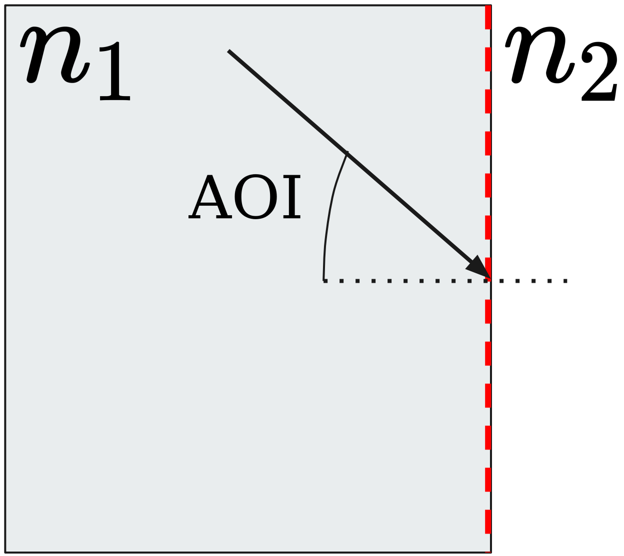
Since no refraction is simulated in the ITC interface, the angular distribution of photons within the ~MLS volume is that of the photons in the substrate volume (this is a simulation artifact). To prevent this artifact from spoiling a realistic simulation of the angular distribution of photons in LAr, the refraction in the ~MLS->LAr interface must account for the substrate refractive index.

Third caveat

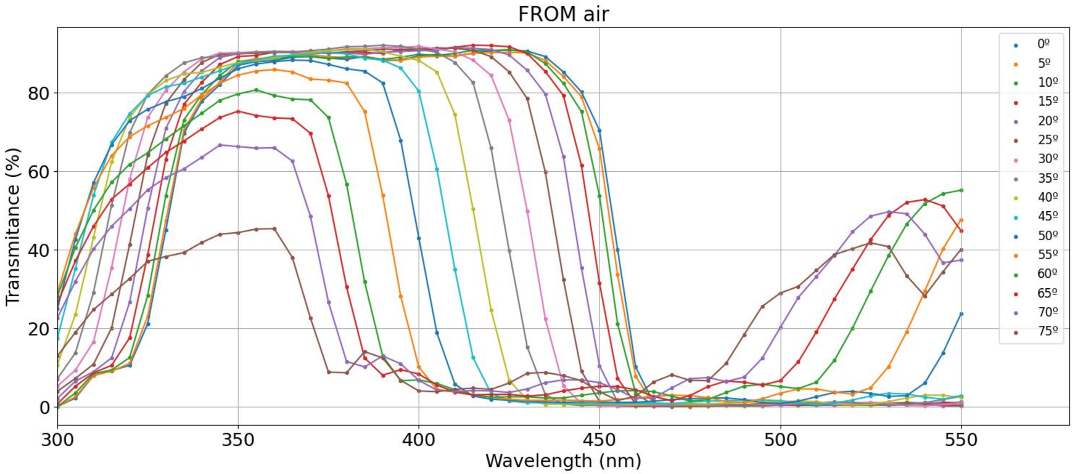
In G4, the TC is applied at some boundary, so there's actually no volume where an AOR is defined. I.e. when a photon reaches the dichroic boundary, G4 won't have access to any AOR information:

<u>The only information that G4 counts on to decide which TC to apply is the AOI</u>

Assuming the AOR model, a way to proceed is the following one:



0) Assume we have measured certain TCs **in air** for a DF which **we want to simulate within another media** using a dichroic boundary

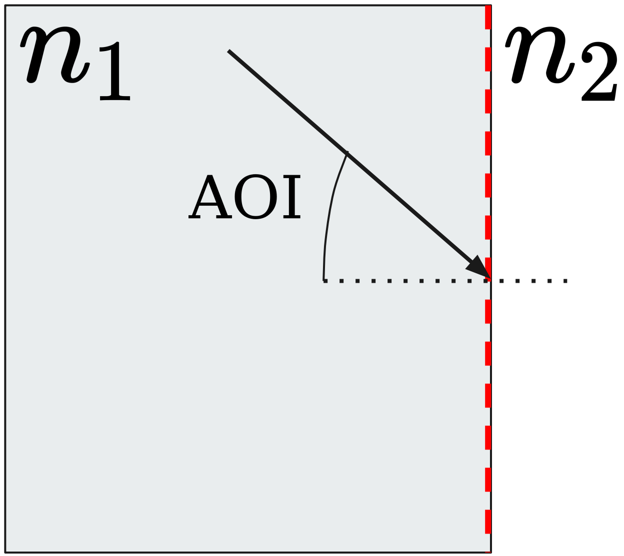


Third caveat

In G4, the TC is applied at some boundary, so there's actually no volume where an AOR is defined. I.e. when a photon reaches the dichroic boundary, G4 won't have access to any AOR information:

<u>**The only information that G4 counts on to decide which TC to apply is the AOI**</u>

Assuming the AOR model, a way to proceed is the following one:

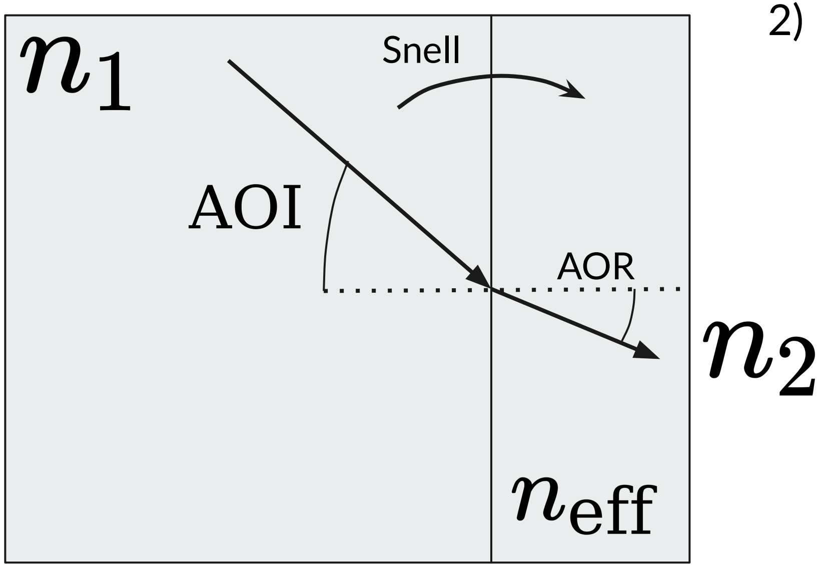


1) A photon impinges on the dichroic boundary with a certain AOI theta, from a media with refractive index n_1

Third caveat

In G4, the TC is applied at some boundary, so there's actually no volume where an AOR is defined. I.e. when a photon reaches the dichroic boundary, G4 won't have access to any AOR information:
<u>**The only information that G4 counts on to decide which TC to apply is the AOI**</u>

Assuming the AOR model, a way to proceed is the following one:



2) Ask yourself, what would the AOR be if there was actually a volume with a refractive index equal to the MLS effective refractive index?

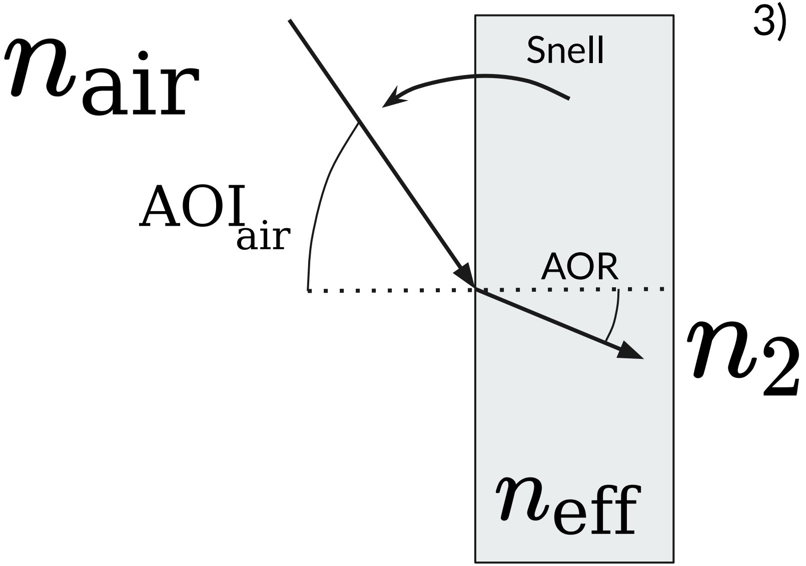
   I.e. compute "forward" snell's law

Third caveat

In G4, the TC is applied at some boundary, so there's actually no volume where an AOR is defined. I.e. when a photon reaches the dichroic boundary, G4 won't have access to any AOR information:

<u>**The only information that G4 counts on to decide which TC to apply is the AOI**</u>

Assuming the AOR model, a way to proceed is the following one:



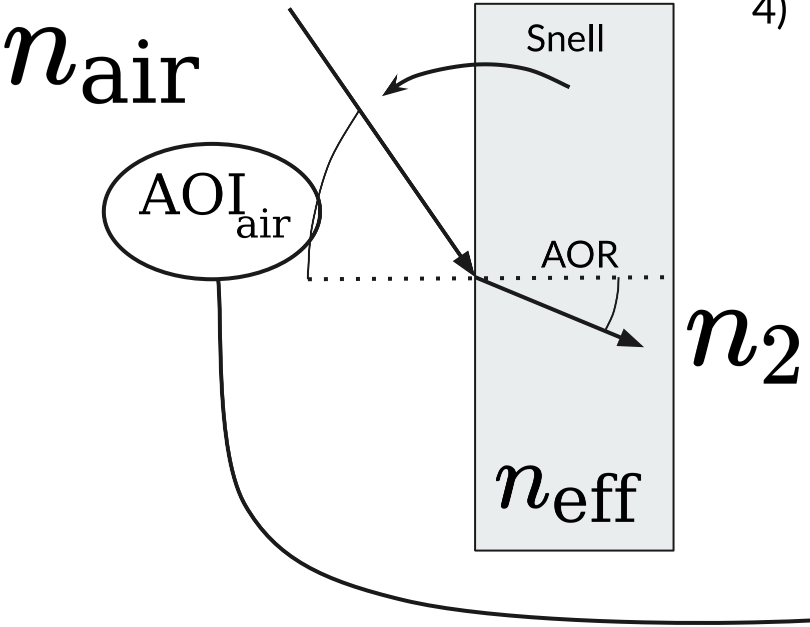
3) Ask yourself, what AOI in air would give rise to such AOR?

   I.e. compute "backward" snell's law

Third caveat

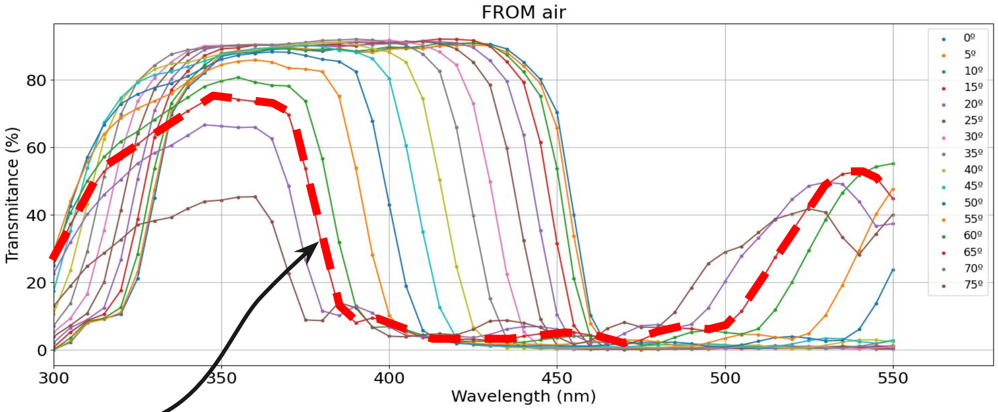
In G4, the TC is applied at some boundary, so there's actually no volume where an AOR is defined. I.e. when a photon reaches the dichroic boundary, G4 won't have access to any AOR information:
<u>The only information that G4 counts on to decide which TC to apply is the AOI</u>

Assuming the AOR model, a way to proceed is the following one:



4) Identify the TC that matches such AOI in air

I.e. compute "backward" snell's law



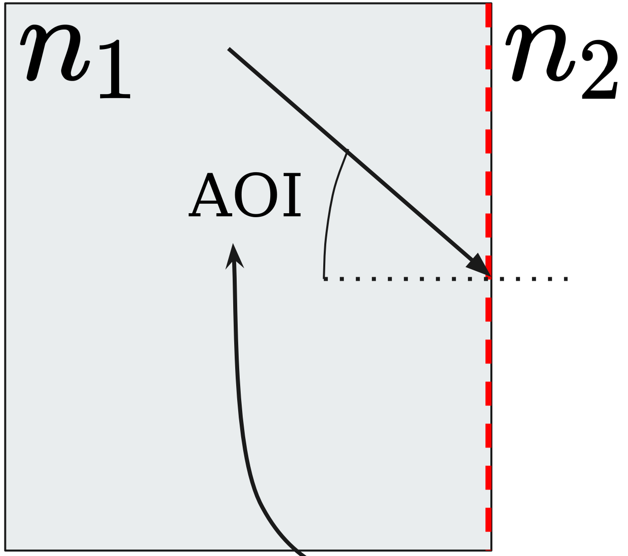
Third caveat

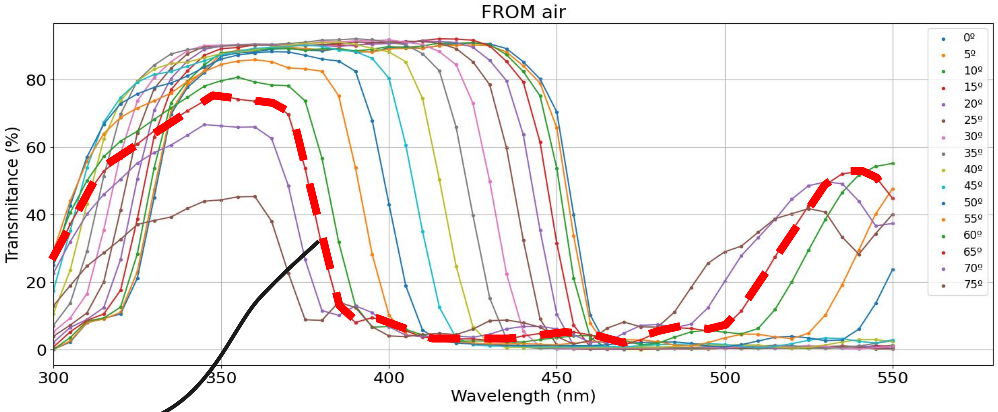
In G4, the TC is applied at some boundary, so there's actually no volume where an AOR is defined. I.e. when a photon reaches the dichroic boundary, G4 won't have access to any AOR information:

<u>The only information that G4 counts on to decide which TC to apply is the AOI</u>

Assuming the AOR model, a way to proceed is the following one:

5) Assign such TC to the actual AOI in the n_1 media



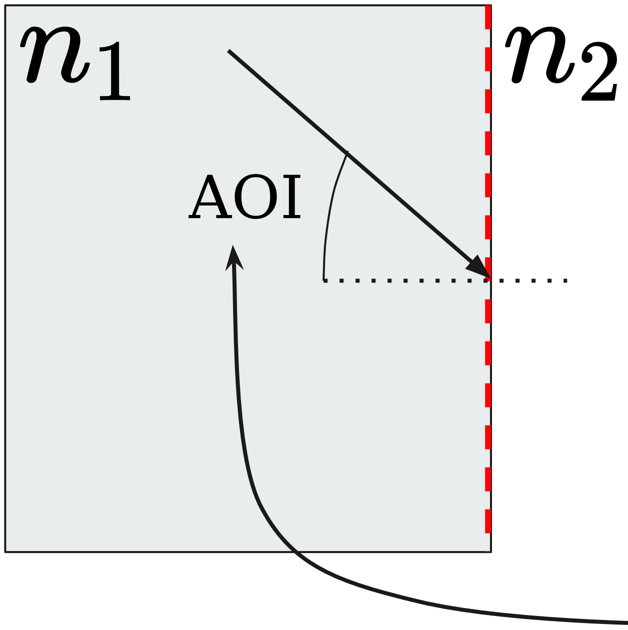


Third caveat

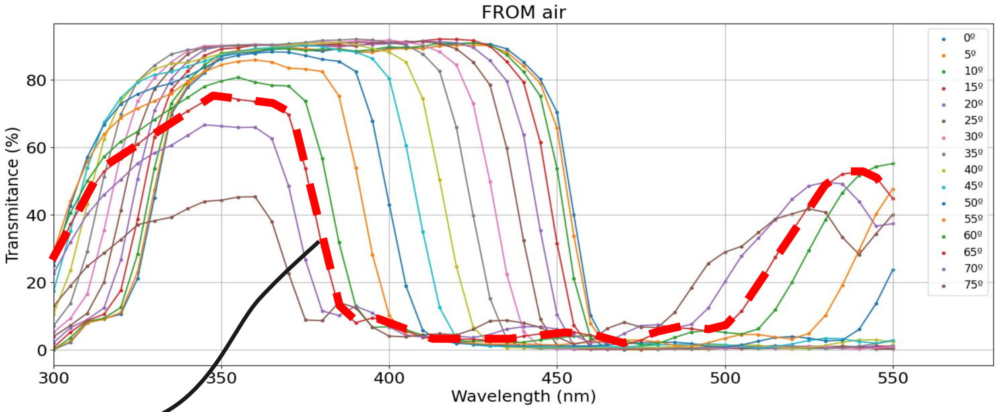
In G4, the TC is applied at some boundary, so there's actually no volume where an AOR is defined. I.e. when a photon reaches the dichroic boundary, G4 won't have access to any AOR information:

<u>The only information that G4 counts on to decide which TC to apply is the AOI</u>

Assuming the AOR model, a way to proceed is the following one:

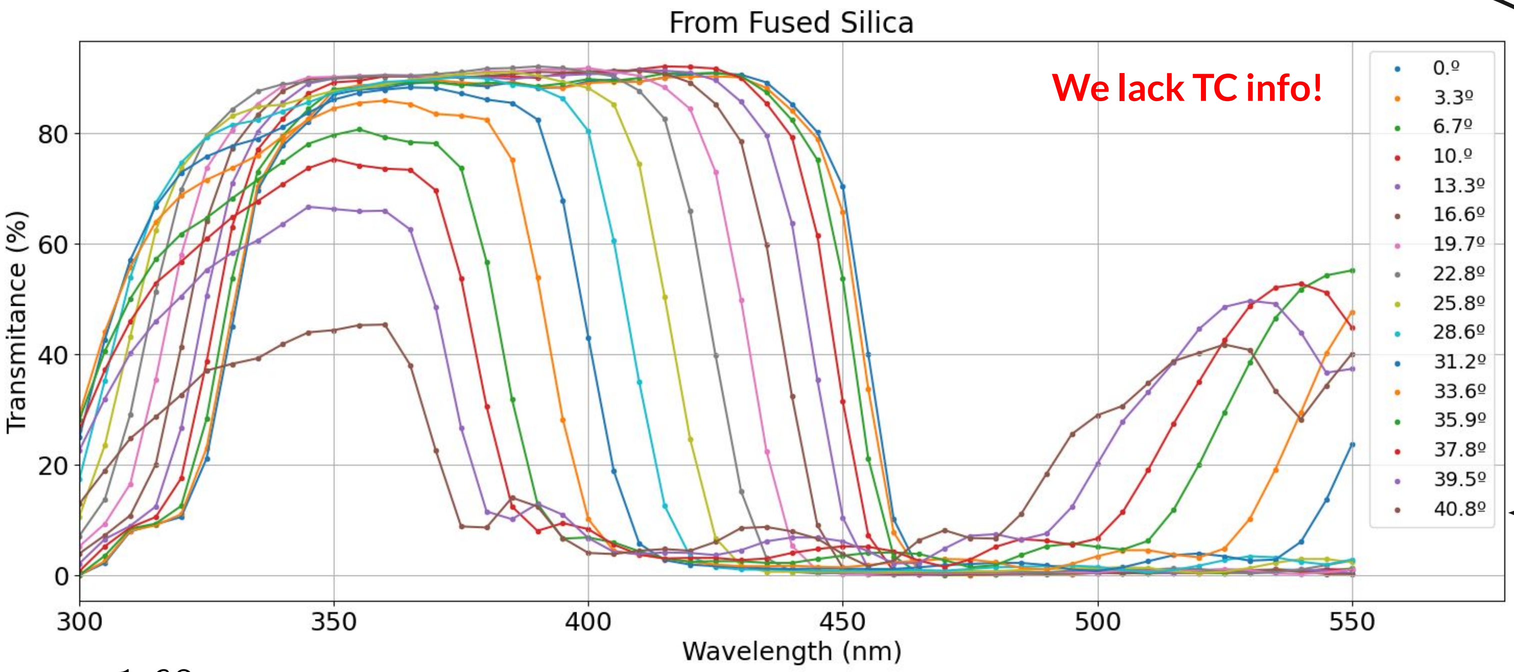


As a result, we redefine the angles of the TCs we measured in air to overcome the fact that no MLS refraction happens in the simulation



Derived issue: Lack of TC info

Assume we have measured a DF in air from 0º to 75º AOI, and assume we are modelling the DF using the first approach, where photons impinge over the dichroic boundary from a fused silica (FS) media (n≈1.47). Then, this method assigns the 0º TC curve in air to the 0º TC curve in FS, and **the 75º TC curve in air to the 41º TC curve in FS**

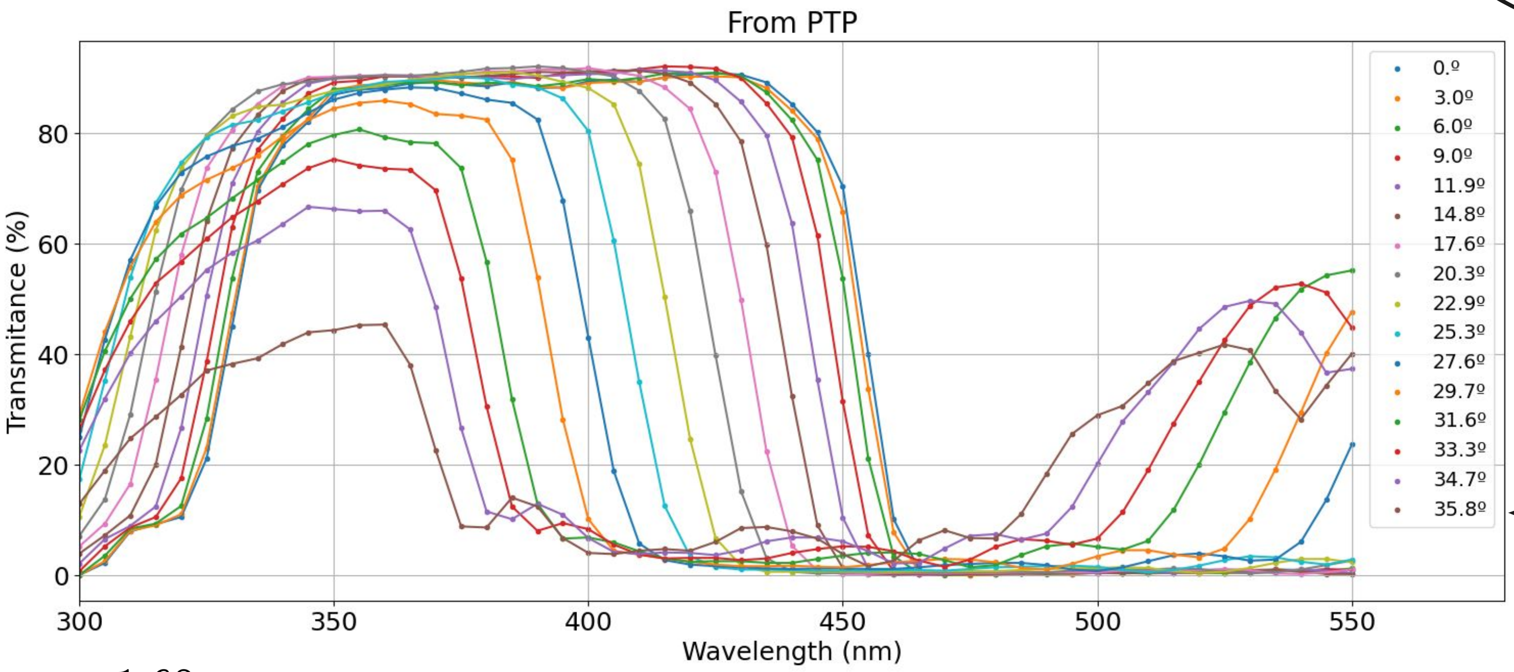


Assuming $n_{\mathrm{eff}} \simeq 1.68$

Derived issue: Lack of TC info

*The information loss is actually the same in both cases, if we assume that for both cases, the incoming light was emitted by PTP with a fixed AD

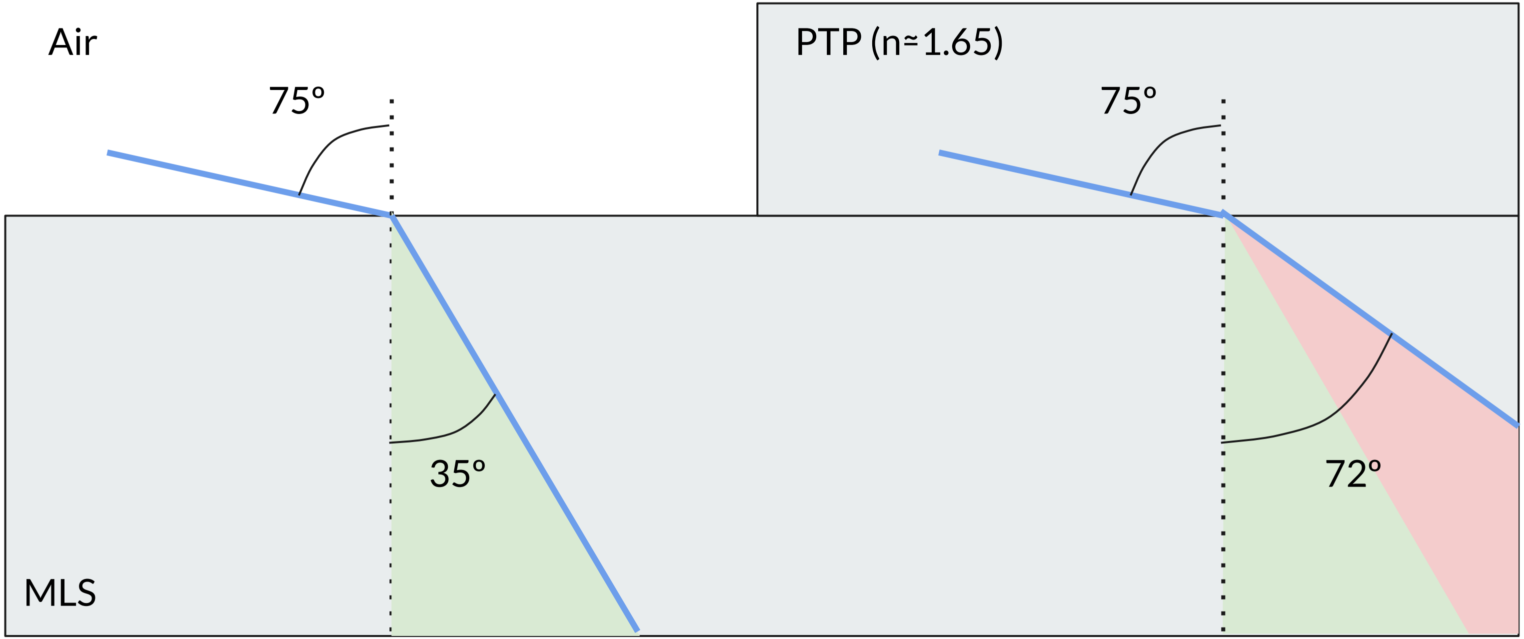
If we want to simulate a PTP (n≃1.65) layer right above the dichroic boundary, the information loss is even worse*



Assuming $n_{\rm eff} \simeq 1.68$

Derived issue: Lack of TC info

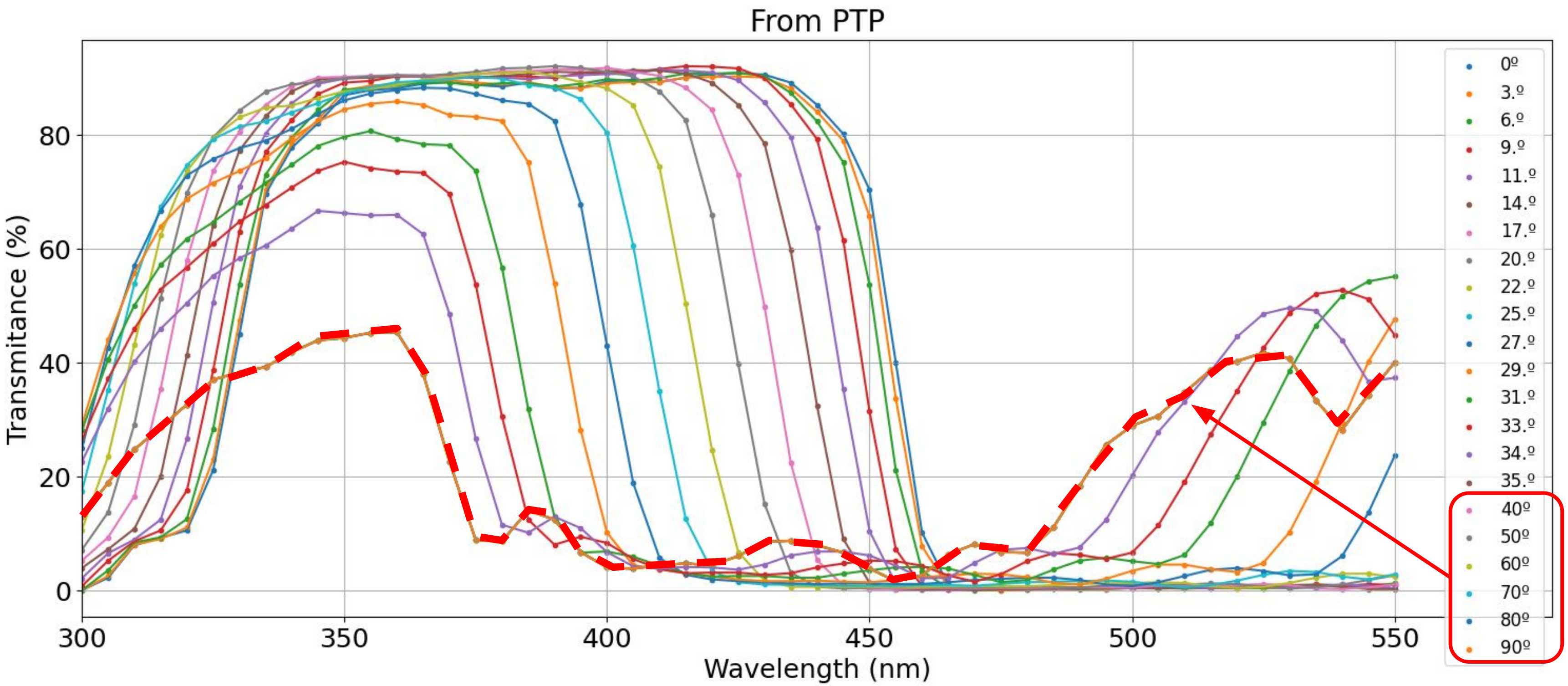
The underlying cause is that sweeping 0-75º AOI in air does not let us explore the full range of AOR that refraction from PTP gives:



Assuming $n_{\text{eff}} \simeq 1.68$

Derived issue: Lack of TC info

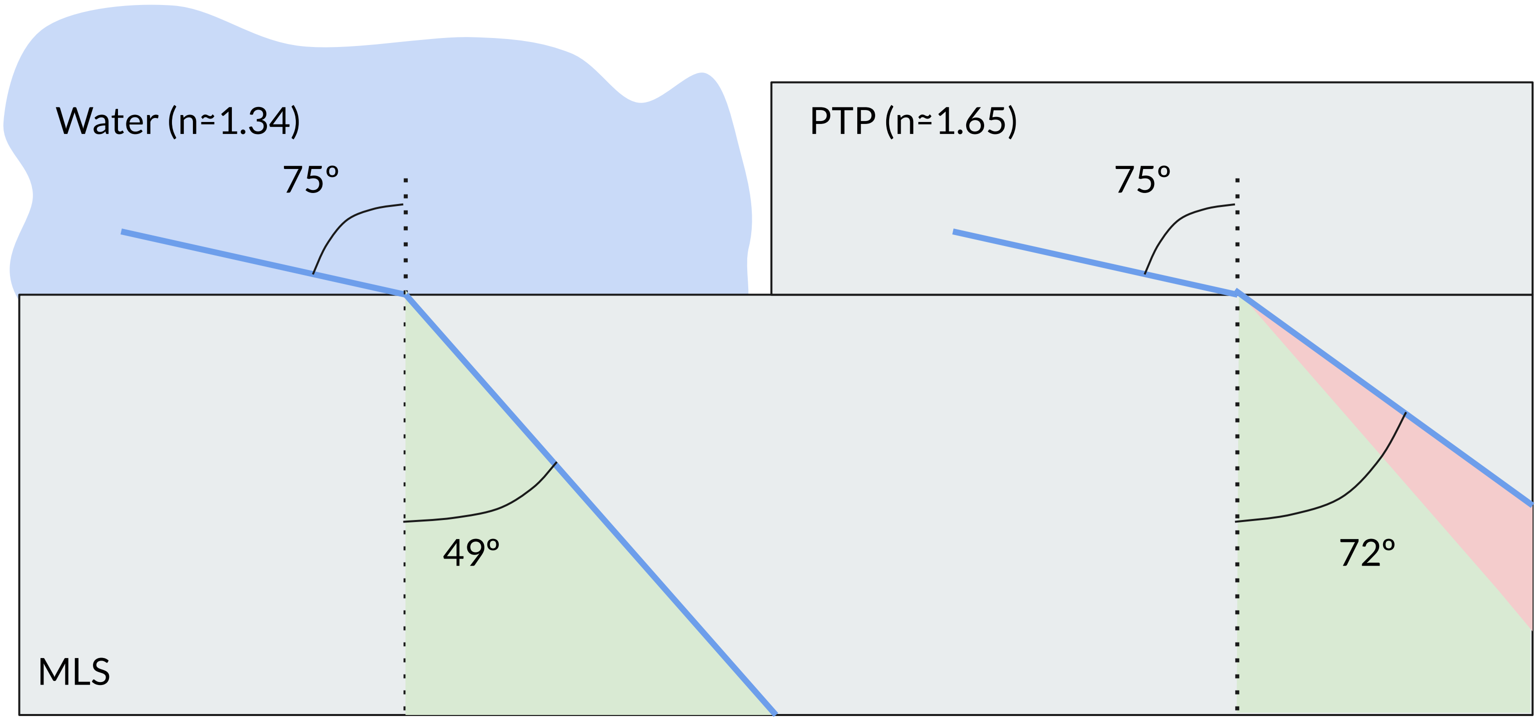
The most immediate ‘solution’ is to extrapolate the nearest (angle–wise) TC to every unknown value:



Since the bigger the AOI, the worse DF performance, extrapolating the biggest-AOI available TC to bigger angles sets an upper bound to the DF performance for AOIs whose TC we have not measured yet.

Derived issue: Lack of TC info

Measuring the TCs within water would widen our AOR scope



Assuming $n_{\mathrm{eff}} \simeq 1.68$