Copernicus FICE 2024

Training on In situ Ocean Colour Above-Water Radiometry towards Satellite Validation

GUM general metrological framework

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6-17 May 2024 Venice, Italy



Outline



- Methodology and resources
- Basic uncertainty concepts
- Absolute calibration measurement equation
- Above water radiometry measurement equation
- Uncertainty propagation in HyperCP

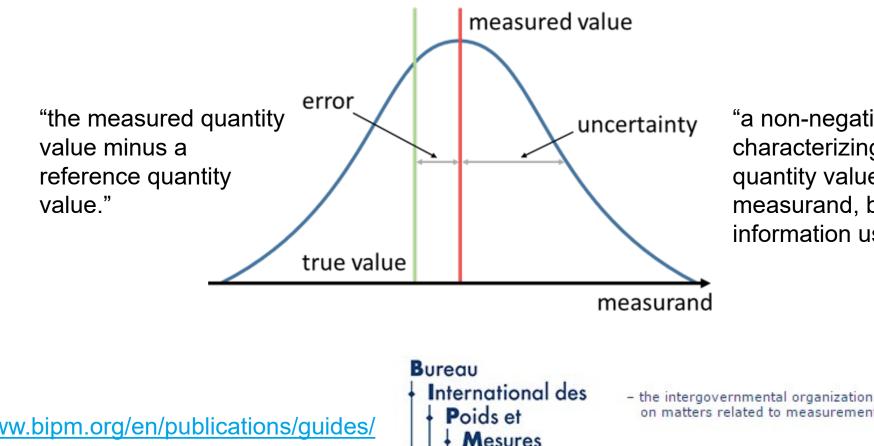


Methodology and resources

Methodology and resources



The International Vocabulary of Metrology (VIM)



"a non-negative parameter characterizing the dispersion of the quantity values being attributed to a measurand, based on the information used."

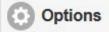
http://www.bipm.org/en/publications/guides/

- the intergovernmental organization through which Member States act together on matters related to measurement science and measurement standards.





[VIM3] 2.26 measurement uncertainty uncertainty of measurement, uncertainty



non-negative parameter characterizing the dispersion of the <u>quantity values</u> being attributed to a <u>measurand</u>, based on the information used



NOTE 1 Measurement uncertainty includes components arising from systematic effects, such as components associated with <u>corrections</u> and the assigned quantity values of <u>measurement standards</u>, as well as the <u>definitional uncertainty</u>. Sometimes estimated systematic effects are not corrected for but, instead, associated measurement uncertainty components are incorporated.

NOTE 2 The parameter may be, for example, a standard deviation called <u>standard measurement uncertainty</u> (or a specified multiple of it), or the half-width of an interval, having a stated <u>coverage probability</u>.

NOTE 3 Measurement uncertainty comprises, in general, many components. Some of these may be evaluated by <u>Type A evaluation of measurement</u> <u>uncertainty</u> from the statistical distribution of the quantity values from series of <u>measurements</u> and can be characterized by standard deviations. The other components, which may be evaluated by <u>Type B evaluation of measurement uncertainty</u>, can also be characterized by standard deviations, evaluated from probability density functions based on experience or other information.

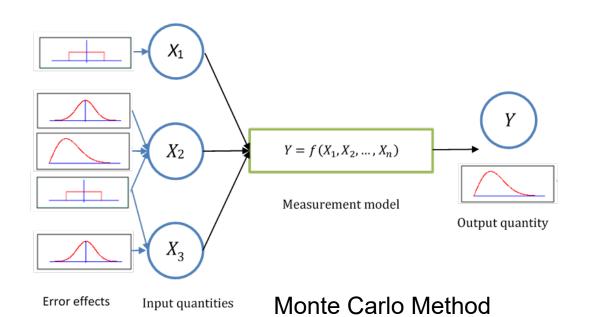
NOTE 4 In general, for a given set of information, it is understood that the measurement uncertainty is associated with a stated quantity value attributed to the measurand. A modification of this value results in a modification of the associated uncertainty.

https://jcgm.bipm.org/vim/en/2.26.html

Methodology and resources



 the Guide to the expression of Uncertainty in Measurement (GUM) and its supplements



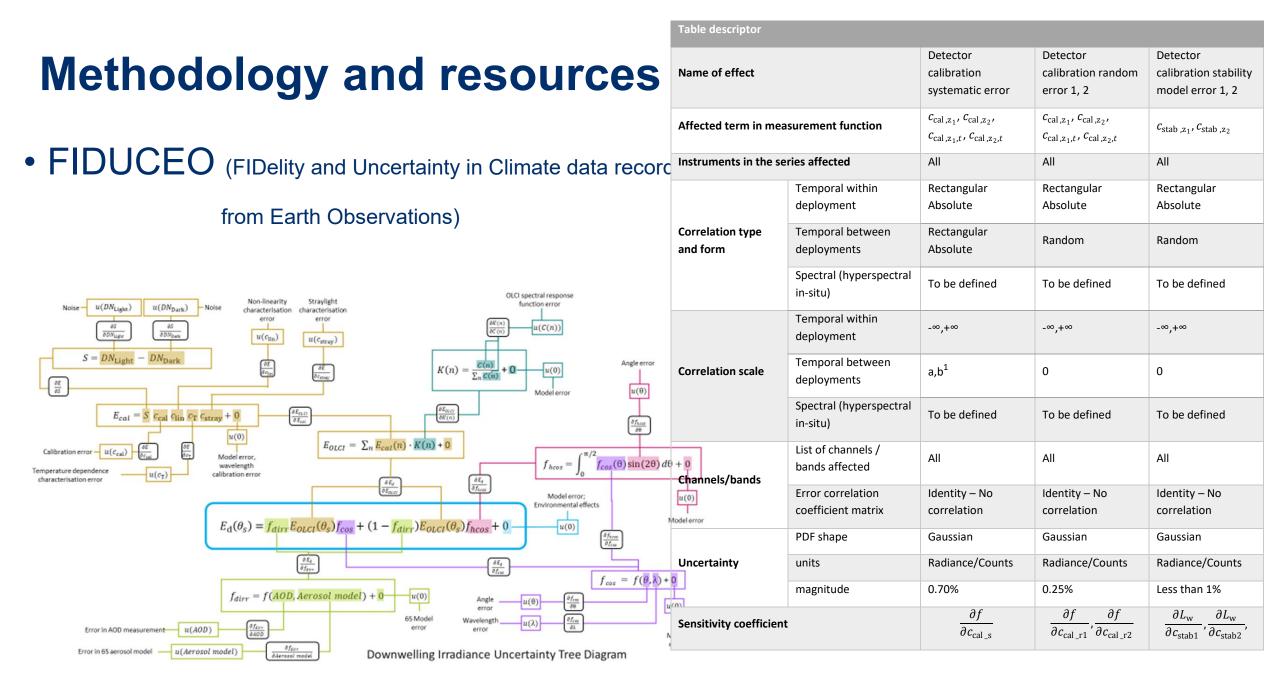
$$u^{2}(y) = \sum_{i=1}^{N} c_{i}^{2} u^{2}(x_{i}) + 2 \sum_{i=1}^{N-1} \sum_{j=i}^{N} c_{i} c_{j} u(x_{i}, x_{j}),$$

The Law of Propagation of Uncertainties

http://www.bipm.org/en/publications/guides/

Bureau International des Poids et Mesures

 the intergovernmental organization through which Member States act together on matters related to measurement science and measurement standards.





Q

News People

CoMet Toolkit

The **CoMet Toolkit** (Community Metrology Toolkit) is an open-source software project to develop Python tools for the handling of errorcovariance information in the analysis of measurement data.

```
import xarray as xr
import obsarray
from punpy import MeasurementFunction, MCPropagation
```

```
# read digital effects table
ds = xr.open_dataset("digital_effects_table_gaslaw_example.nc")
```

About

Tools -

Define your measurement function inside a subclass of MeasurementFunction
class IdealGasLaw(MeasurementFunction):

Examples

```
def meas_function(self, pres, temp, n):
    return (n *temp * 8.134)/pres
```

propagate the uncertainties on the input quantites in ds to the measurand # uncertainties in ds_y (propagate_ds returns random, systematic and structured) ds_y = gl.propagate_ds(ds, store_unc_percent=True)



Basic uncertainty concepts

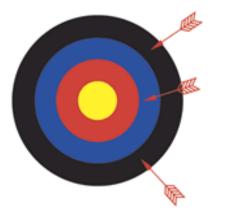
What is not a measurement uncertainty?



- Mistakes made by operators are not measurement uncertainties. They should not be counted as contributing to uncertainty. They should be avoided by working carefully and by checking work.
- Accuracy (or rather inaccuracy) is not the same as uncertainty. Unfortunately, usage of these words is often confused. Correctly speaking, 'accuracy' is a qualitative term (e.g. you could say that a measurement was 'accurate' or 'not accurate'). Uncertainty is quantitative. When a 'plus or minus' figure is quoted, it may be called an uncertainty, but not an accuracy.
- Errors are not the same as uncertainties (even though it has been common in the past to use the words interchangeably in phrases like 'error analysis').
- Statistical analysis is not the same as uncertainty analysis. Statistics can be used to draw all kinds of conclusions which do not by themselves tell us anything about uncertainty. Uncertainty analysis is only one of the uses of statistics.

Measurement Uncertainty: Accuracy and Precision





Poor precision, poor accuracy

Accuracy \Rightarrow qualitative term relating the mean of the measurements to the true value

 $\begin{array}{l} \mbox{Precision} \Rightarrow \mbox{represents the spread of the} \\ \mbox{measurements} \end{array}$





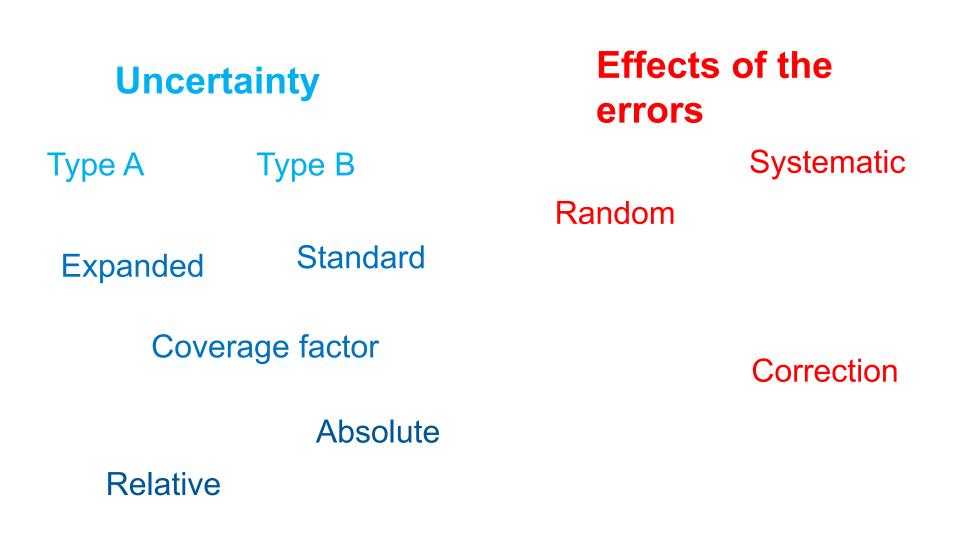
Good precision, poor accuracy



Good precision, good accuracy







Uncertainty types



There are two methods for estimating uncertainties:

Type-A:

uncertainty estimates using statistics i.e. by taking multiple readings and using that information

Type-B:

uncertainty estimates from any other information, e.g. past experience, calibration certificates, etc.

Confidence intervals



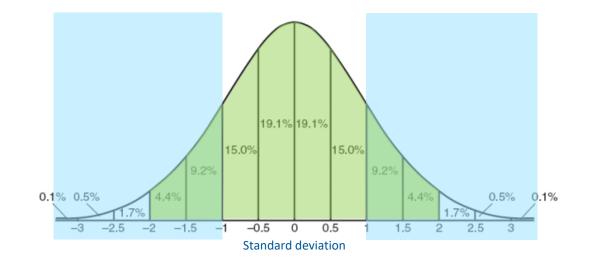
Uncertainty is given with respect to a given confidence interval:

 $u(y) = \pm 3 \text{ cm}$

at the 68.2% coverage probability $(1\sigma \text{ or } k = 1)$ at the 95.4% confidence level

 $u(y) = \pm 6 \text{ cm}$

at the 95.4% coverage probability (2σ or k = 2)



Uncertainty expression



Relative uncertainty: $5 \text{ mW m}^{-2} \text{ nm}^{-1} \pm 0.2 \%$ i.e. uncertainty expressed as a percentage

Absolute uncertainty: $5 \text{ mW m}^{-2} \text{ nm}^{-1} \pm 0.01 \text{ mW m}^{-2} \text{ nm}^{-1} \text{ i.e.}$ uncertainty expressed in the native measurement units

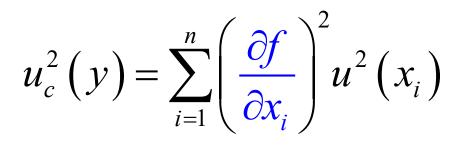


First order Taylor series approximation uncorrelated input quantities version

$$u_{c}^{2}(y) = \sum_{i=1}^{n} \left(\frac{\partial f}{\partial x_{i}}\right)^{2} u^{2}(x_{i})$$

THE LAW OF PROPAGATION OF UNCERTAINTIES





Sensitivity Coefficients

Sensitivity coefficients cheatsheets



Summation in quadrature for addition and subtraction

e=*a*+*b*-*c*,

Combined uncertainty = $\sqrt{a^2 + b^2 + c^2 + ...etc}$.

Summation in quadrature for multiplication or division $A=L\cdot W$,

$$\frac{u(A)}{A} = \sqrt{\left(\frac{u(L)}{L}\right)^2 + \left(\frac{u(W)}{W}\right)^2} \ .$$

Sensitivity coefficients cheatsheets



Squared value

 Z^{2} ,

 $\frac{2u(Z)}{Z}$

Summation in quadrature for more complicated function

$$P=\frac{V^2}{R},$$

$$\frac{u(P)}{P} = \sqrt{\left(\frac{2u(V)}{V}\right)^2 + \left(\frac{u(R)}{R}\right)^2} \ .$$

Steps to an uncertainty budget



1. Traceability Chain

- 2. Calculation Equation
- 3. Sources of Uncertainty
- 4. Measurement Equation
- 5. Sensitivity Coefficients
- 6. Assigning Uncertainties
- 7. Combining your uncertainties
- 8. Expanding your uncertainties

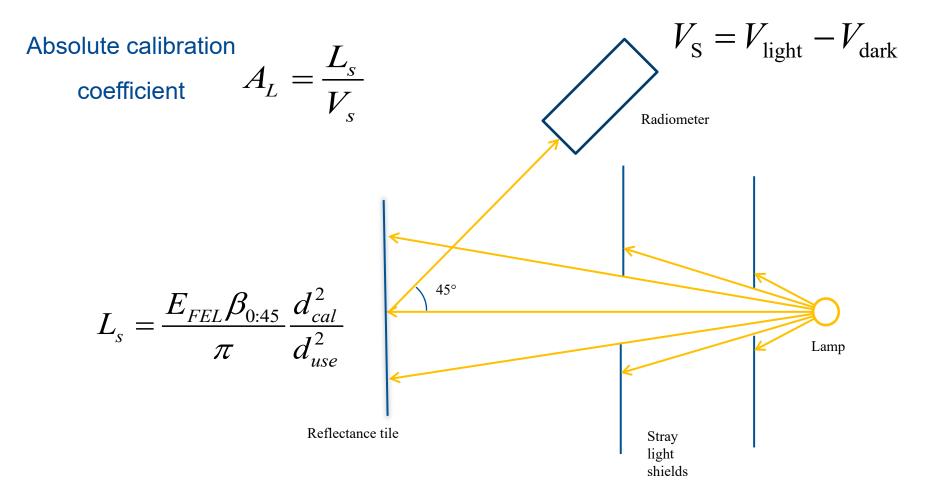
Symbol	Uncertainty component	Size of effect	Correction applied?	Residual uncertainty	Divisor	Sensitivity coefficient	Uncertainty associated with final value due to effect	
Combined standard uncertainty								
Expanded uncertainty								



Absolute calibration measurement equation

Calculation equation





Sources of uncertainty





Calibration certificate Lamp additional effects

- Ageing
- Alignment
- Current stability



Calibration certificate

Diffuser additional effects

- Ageing
- Uniformity



Distance accuracy



Random noise

Instrument additional effects

- Stability (drift)
- Room stray light

Measurement equations



$$L_{\rm s} = \frac{E_{\rm FEL}\beta_{0:45}}{\pi} \frac{d_{\rm cal}^2}{d_{\rm use}^2}$$

$$L_{\rm s} = \frac{E_{\rm FEL}\beta_{0:45}}{\pi} \frac{d_{\rm cal}^2}{d_{\rm use}^2} K_{\rm lamp_stab} K_{\rm align} K_{\rm current} K_{\rm diff_stab} K_{\rm unif}$$

$$V_{\rm S} = V_{\rm light} - V_{\rm dark}$$

$$V_{\rm S} = V_{\rm light} K_{\rm light_stab} + K_{\rm stray} - V_{\rm dark} K_{\rm dark_stab}$$





Remember calibration certificates almost always quote uncertainties at *k* = 2 !

Rectangular uncertainty distributions

 $-2 \cdot u(d_{use})/d_{use}$

1

1

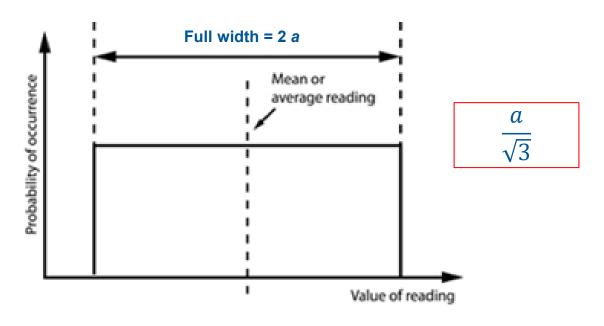


Resolution of distance measuring instrument = 0.1 mm

Measurement distance = 500.0 mm

Uncertainty associated with distance measurement = $(0.05 / 500) / \sqrt{3} = 0.006 \%$

Uncertainty in irradiance from distance measurement = 2×0.006 % = 0.012 %



Uncertainty budget



Symbol	Uncertainty component	Size of effect	Correction applied?	Residual uncertainty	Divisor	Sensitivity coefficient	Uncertainty associated with final value due to effect		
$u(E_{\rm FEL})$	Ref. lamp irradiance	1.5 %	N	1.5 %	2	1	0.75 %		
$u(\beta_{0:45})$	Tile radiance factor	2.0 %	N	2.0 %	2	1	1.00 %		
$u(d_{use})$	Lamp distance (500 mm)	0.05 mm	N	0.01 %	√3	2	0.012 %		
$u(K_{align})$	Lamp alignment	0.15 %	N	0.15 %	1	1	0.15 %		
$u(K_{l_{stab}})$	Light reading stability	negligible	N	negligible			negligible		
$u(K_{d_{stab}})$	Dark reading stability	negligible	N	negligible			negligible		
$u(K_{\text{lamp_stab}})$	Lamp stability	0.083 %	N	0.083 %	√3	1	0.048 %		
$u(K_{\text{diff_stab}})$	Diffuser stability	0.125 %	N	0.125 %	√3	1	0.072 %		
$u(K_{\text{stray}})$	Stray light in lab	negligible	N	negligible			negligible		
u(K _{current})	Lamp current (8.000 A)	0.004 A	Ν	0.25 % in <i>I</i> , or 0.99 % in <i>E</i> _{FEL} at 600 nm	√3	1	0.572 % (at 600 nm)		
$u(K_{\text{unif}})$	Radiance uniformity	1.50 %	N	1.50 %	√3	1	0.866 %		
Combined standard uncertainty									
Expanded uncertainty (k=2)									

Uncertainty budget

1. Traceability Chain

Uncertainty evaluation type ?

Type B – information form calibration certificates !

Symbol	Uncertainty component	Size of effect	Correction applied?	Residual uncertainty	Divisor	Sensitivity coefficient	Uncertainty associated with final value due to effect
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$u(\beta_{0:45})$	Tile radiance factor	2.0 %	N	2.0 %	2	1	1.00 %

Coverage factor ? Probability distribution?

k = 2, Gaussian







Uncertainty evaluation type?

Type B – information form calibration certificates Type A – repeated measurements

Symbol	Uncertainty component	Size of effect	Correction applied?	Residual uncertainty	Divisor	Sensitivity coefficient	Uncertainty associated with final value due to effect
$u(E_{FEL})$	Ref. lamp irradiance	1.5 %	N	1.5 %	2	1	0.75 %
$u(\beta_{0:45})$	Tile radiance factor	2.0 %	N	2.0 %	2	1	1.00 %
$u(d_{use})$	Lamp distance (500 mm)	0.05 mm	N	0.01 %	√3	2	0.012 %

Absolute uncertainty

Relative uncertainty

Uncertainty budget



- 3. Sources of uncertainty
- 4. Measurement equation (all components with assigned size of effect)
- 5. Sensitivity coefficient

Symbol	Uncertainty component	Size of effect	Correction applied?	Residual uncertainty	Divisor	Sensitivity coefficient	Uncertainty associated with final value due to effect	
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Combined standard uncertainty								
Expanded uncertainty (k=2)								

Uncertainty budget



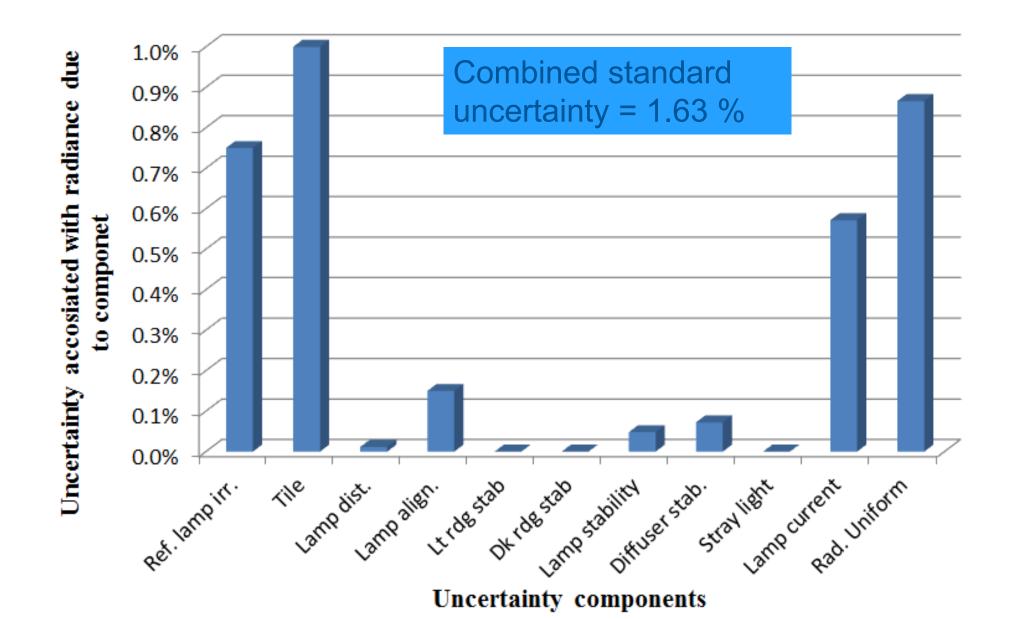
6. Assigning Uncertainties

7. Combining your uncertainties

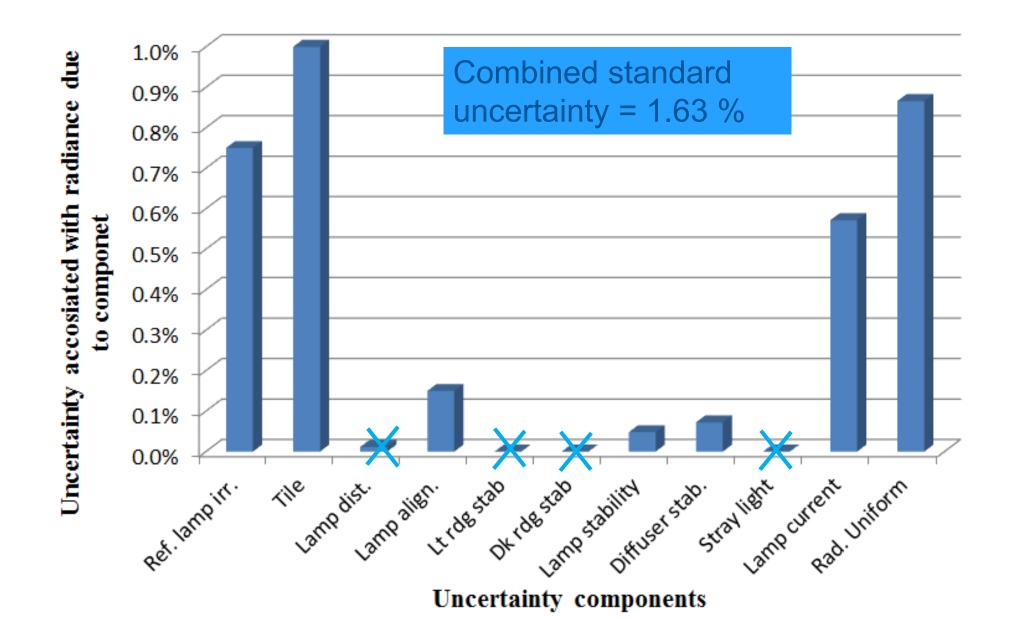
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8. Expanding your uncertainties

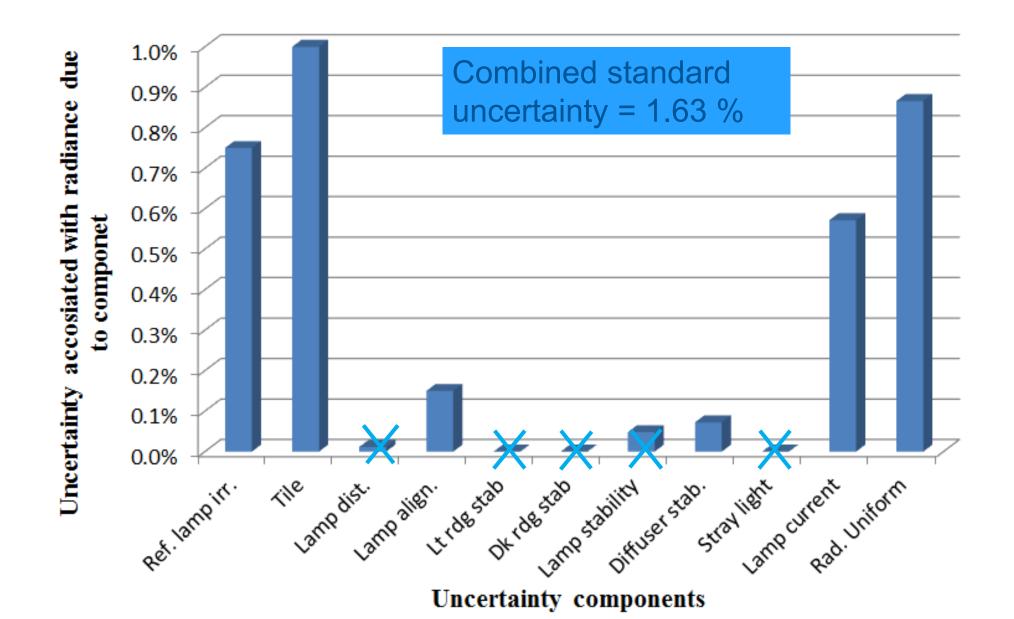




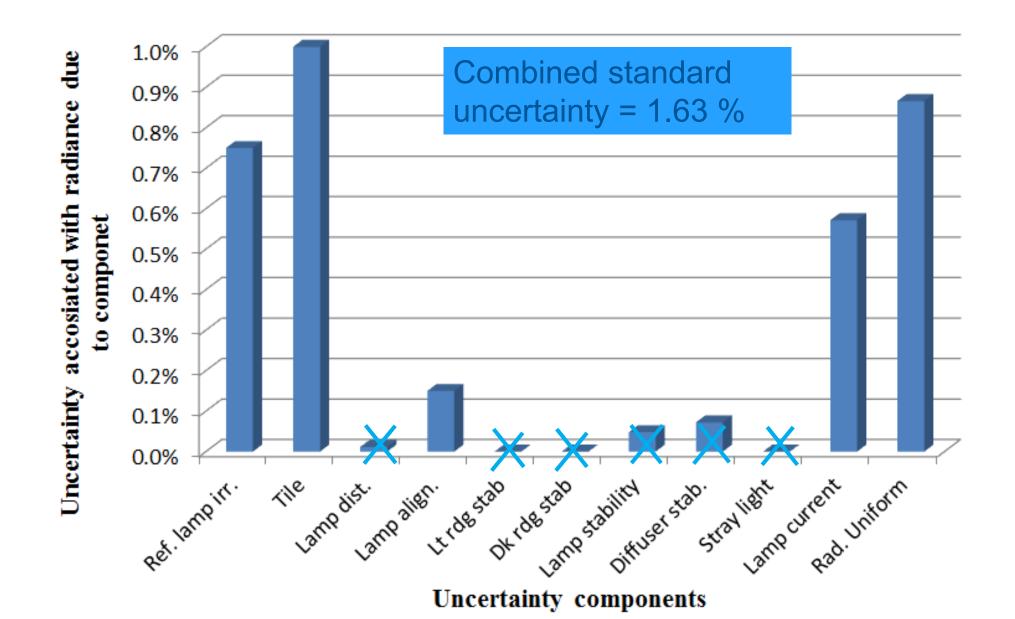




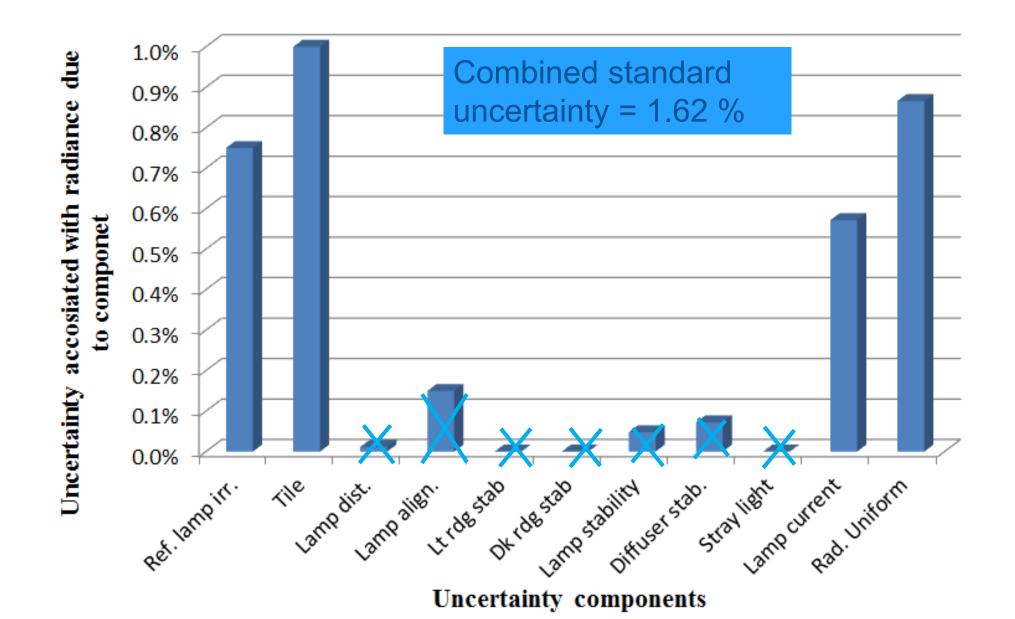














Above water radiometry measurement equation

Remote sensing reflectance cheatsheet



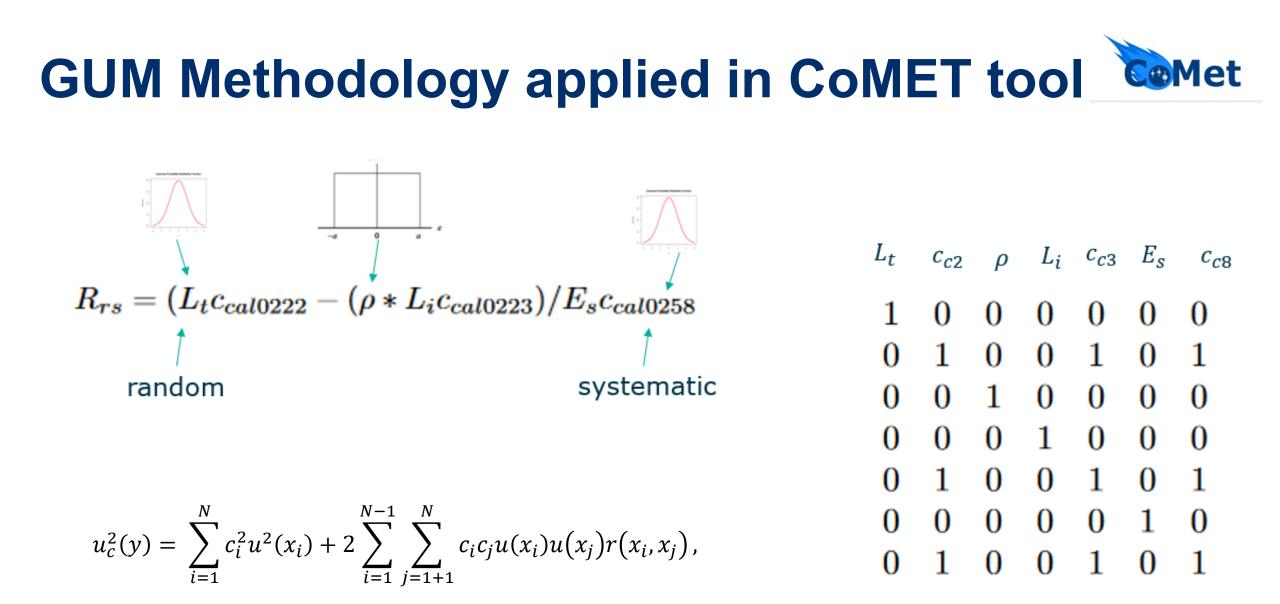
$$R_{rs} = \frac{L_t - \rho L_i}{E_s}$$

$$u_{rel}(L_r) = \sqrt{u_{rel}(\rho)^2 + u_{rel}(L_i)^2}$$

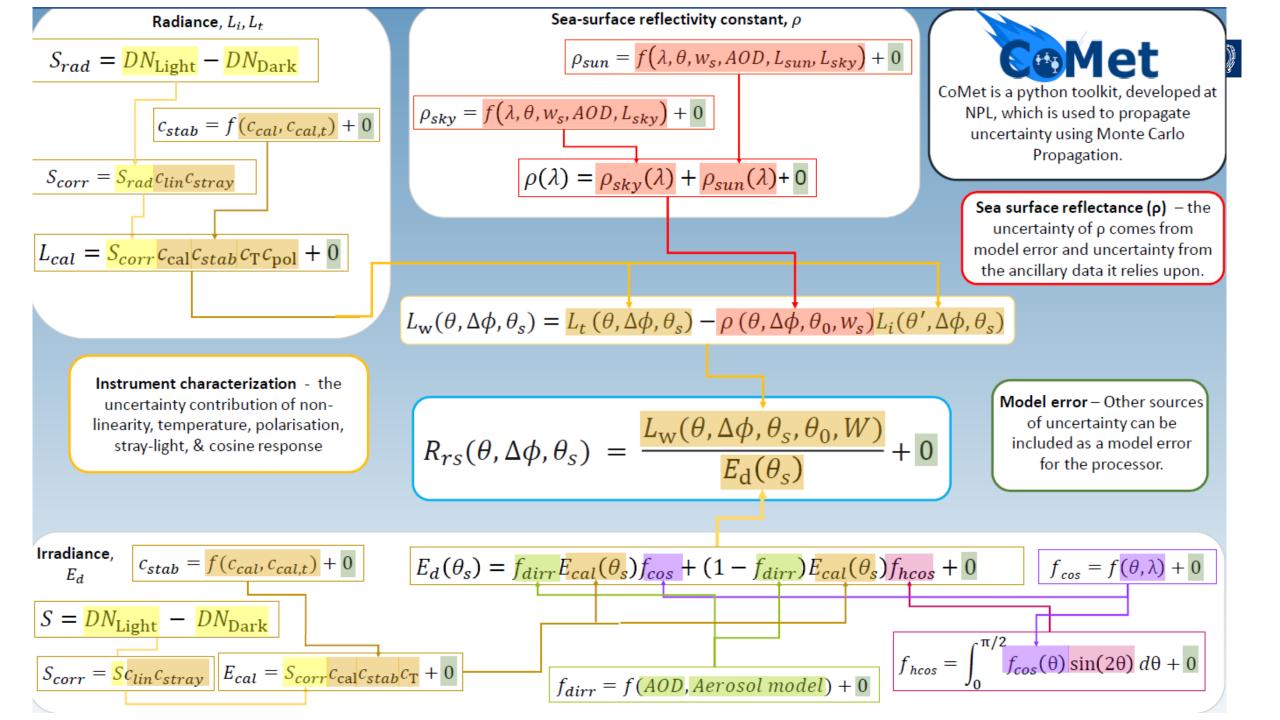
$$u_{asbl}(L_w) = \sqrt{u_{abs}(L_t)^2 + u_{abs}(L_r)^2}$$

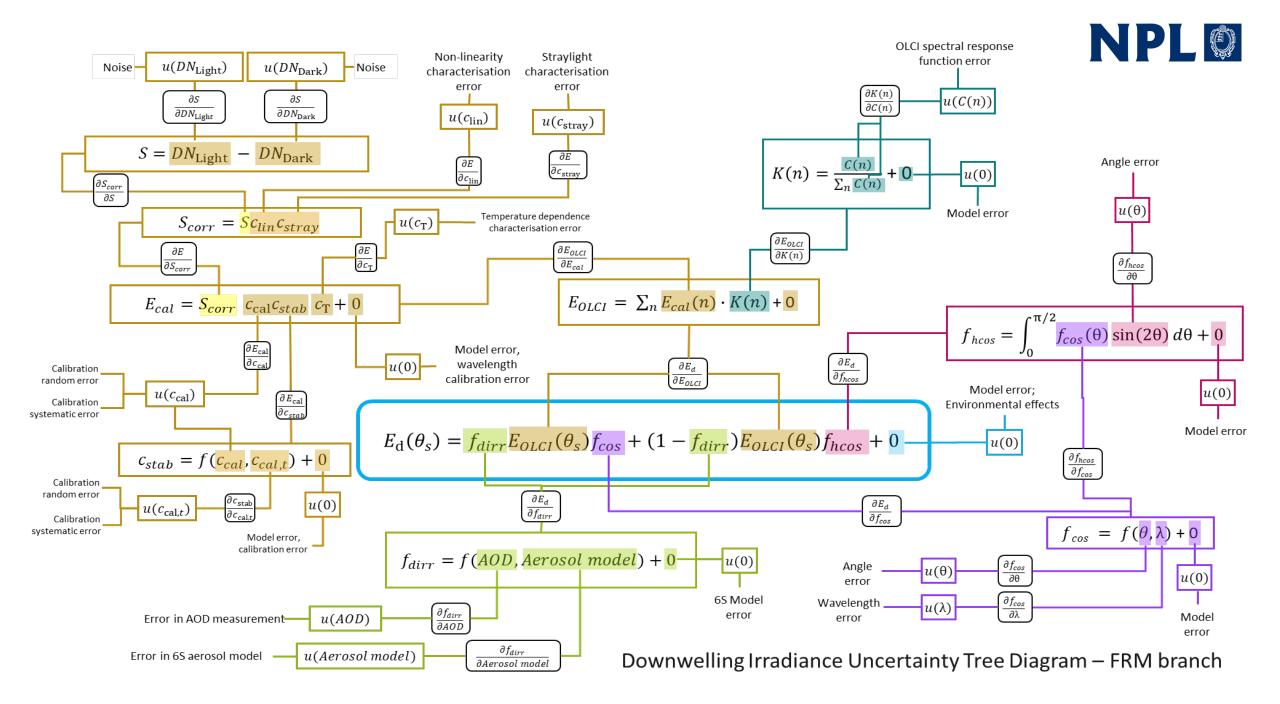
$$u_{rel}(L_w) = \sqrt{\frac{u_{abs}(L_t)^2 + u_{abs}(L_r)^2}{L_w^2}}$$

$$u_{rel}(R_{rs}) = \sqrt{u_{rel}(L_w)^2 + u_{rel}(E_s)^2}$$



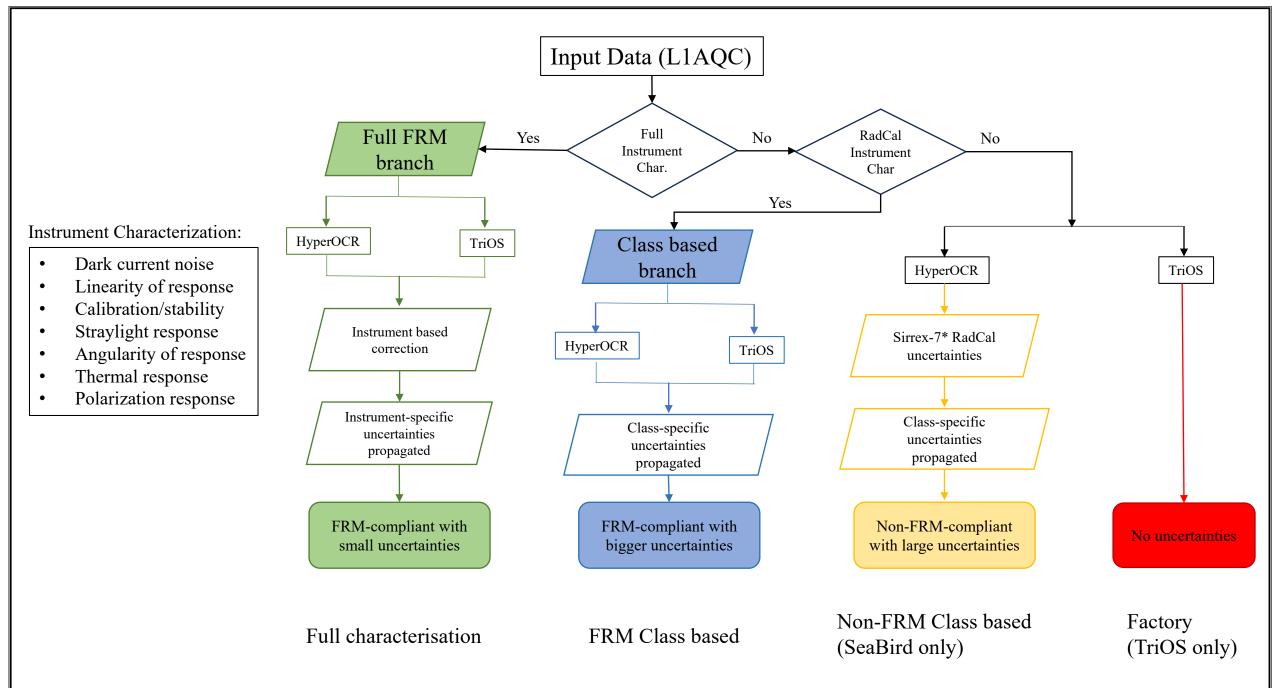
JCGM100:2008. Evaluation of measurement data - Guide to the expression of uncertainty in measurement JCGM101:2008. Evaluation of measurement data - Supplement 1 to the Guide to the expression of uncertainty in measurement - Propagation of distributions using a Monte Carlo method.







Uncertainty propagation in HyperCP



* The Seventh SeaWiFS Intercalibration Round-Robin Experiment (SIRREX-7), March 1999.

Default branch measurements equations **NPL**

• Irradiance

 $E_{d}(\lambda) = \overline{E_{d}(\lambda)} \cdot c_{cal}(\lambda) c_{stab}(\lambda) c_{lin}(\lambda) c_{stray}(\lambda) c_{T}(\lambda) f_{cos}$



Approach



Table 3. Summary information about each uncertainty component values for class-based approach (blue branch, Fig. 5)

Variable crmbel	Variable name/description	Exemplary uncertainty magnitude for class-based characterisation		PDF shape	Correlation	Correlation between 'corr_between'
Variable symbol		TRIOS	HyperOCR			
$ \begin{pmatrix} DN_{\text{light},L_X} - DN_{dark,L_X} \end{pmatrix} \\ \begin{pmatrix} DN_{\text{light},E_S} - DN_{dark,E_S} \end{pmatrix} $	Mean value of DNs measured by a single instrument at a "station"	Standard deviation calculated per measurement from data statistics		Normal	Random	N/A
C _{cal}	Absolute radiometric calibration	Uncertainty values from calibration certificate divided by 2 to convert them back into standard uncertainty, <i>k</i> =1		Normal	Systematic	Between all three instruments
C _{stab}	Absolute calibration stability	1%		Rectangular	Systematic	N/A
$c_{\rm lin}$	Detector non-linearity	2%		Normal	Systematic	Between all three instruments
C _{stray}	Spectral stray light	Vary spectrally and per instrument due to difference in spectral shape of the signal, should come from the class-based stray light file		Normal	Systematic	Between all three instruments
c_T	Temperature sensitivity	Vary spectrally come from the class-based temperature sensitivity file		Normal	Systematic	Between all three instruments
C _{pol}	Polarisation sensitivity (Radiance only)	Vary spectrally and per instrument to use published data from (Talone and Zibordi, 2016)	Vary spectrally and per instrument triple values for TRIOS, as shown in [AD-1]	Normal	Systematic	Between two radiance instruments
C _{cos}	Cosine response (Irradiance only)	Directional 3.5%	Directional 2%	Normal	Systematic	N/A



Approach

Table 4 – Summary information about each uncertainty component for sea surface reflectance factor (ρ) estimation using Mobley method

Variable symbol	Variable name/description	Exemplary uncertainty magnitude	PDF shape	Correlation	Correlation between 'corr_between'	
ρ	Sea surface reflectance	Calculated for each cast depends on all input components, especially wind speed	Normal	Random	N/A	
Ws	Wind speed	1ms ⁻¹	Normal	Random	N/A	
$\Delta \phi$	Relative azimuth	3°	Normal	Random ²	N/A	
θ_s	Solar zenith angle	0.5°	Normal	Random	N/A	
+0	Model error	Difference between Mobley and Zhang method	Rectangular	Systematic	N/A	

Default Branch CP Implementation Example

Source of Uncertainty	Input Uncertainty
DN _{light}	Std (k=1)
DN _{dark}	Std (k=1)
C _{cal}	Tartu file
C _{stab}	1%
C _{lin}	2%
C _{stray}	FRM4SOC- 1
C _{temp}	Tartu file
C _{COS}	2%

179	
180	@staticmethod
181	def Es(DNLight, DNDark, Ccal, Cstab, Clin, Cstray, Ct, Ccos):
182	"""(DNLIGHT-DNDARK).Ccal.Cstab.Clin.Cstray.Ct.Ccos"""
183	<pre>return (DNLight - DNDark) * Ccal * Cstab * Clin * Cstray * Ct * Ccos</pre>
10/	

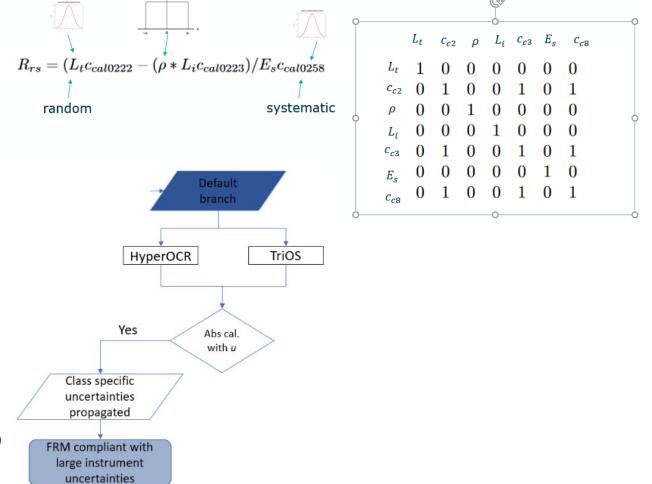
- Occurs at L1B during dark correction, c_{cal} is taken from Tartu file.
- Time average *DN*_{light} & *DN*_{dark}.
- Remaining coefficients are set to 1.
- Measurement function is defined in python.
- Punpy generates samples from inputs and uncertainties.
- Runs M=10000 Monte Carlo uncertainty propagation according to the GUM.
- Output is divided by signal to generate relative uncertainty.
- Saved in the uncertainty budget group.

NPLO

Using Monte Carlo

- First, we need to identify our measurement function, *f*
- We need our inputs to the measurement function with their associated uncertainties
- Then we build samples of *M* draws, based on known input correlation
- We run those samples through f
- $u_c(y)$ can be found from the statistics o the output

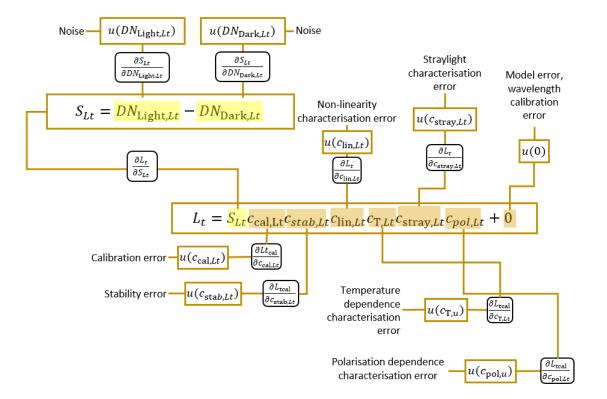






How FRM Uncertainties are Propagated

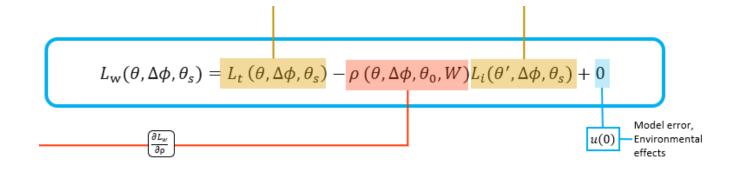
- We combine and process samples directly
- We calculate uncertainty (in theory) alongside the processor
- Correlations are engendered within the samples
- L2 uncertainties (*R_{rs}, Lw, NLw*), are calculated using distributions of Es, Li, Lt, & Rho which contain information of uncertainty and correlation



NPLØ

FRM Uncertainties – an example





404 405		gate.Lw_FRM, MC_x: [ltSample, rhoSample, liSample]) agate.Rrs_FRM, MC_x: [ltSample, rhoSample, liSample, esSample])
	≡ 3 usages ≛ AKamsay17	349 @staticmethod
344	@staticmethod	
345	def Lw_FRM(lt, rho, li):	350 def Rrs_FRM(lt, rho, li, es):
346	*** Lw FRM branch measurment function ***	351 """ Rrs FRM branch measurment function """
347	return lt - (rho * li)	352 🔶 return (lt - (rho * li)) / es
348		353

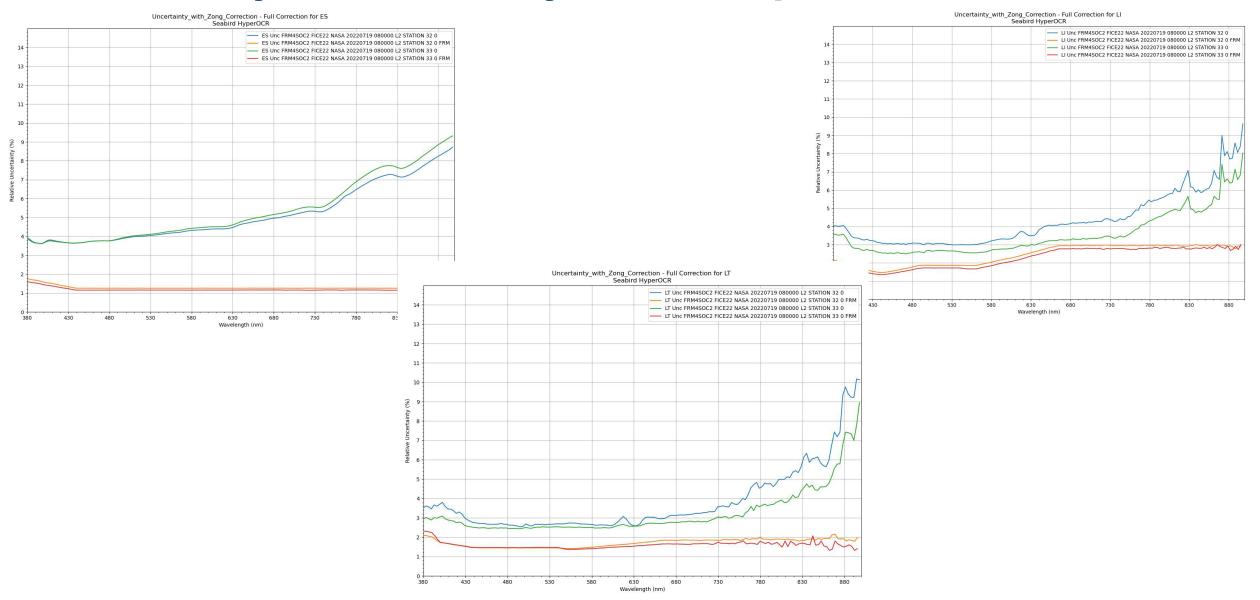
HyperCP



Variable Symbol	Variable Name	Uncertainty Source	Class Based	FRM
			Correction Applied	
$ \begin{pmatrix} DN_{light,L_X} - DN_{dark,L_X} \end{pmatrix} \\ \begin{pmatrix} DN_{light,E_S} - DN_{dark,E_S} \end{pmatrix} $	Mean value of DNs measured by a single instrument at a "station"	Standard deviation calculated from statistics of filtered measurements	NA	NA
^c cal	Absolute Radiometric Calibration	Instrument specific characterisation	NA	NA
^c stab	Absolute Calibration Stability	Instrument specific characterisation	NA	NA
^c lin	Detector Non-Linearity	Instrument specific characterisation	No	Yes
^c stray	Spectral Stray Light	Zong stray light correction method	No	Yes
C _T	Temperature Sensitivity	Instrument specific characterisation	No	Yes
^c pol	Polarisation Sensitivity (Radiance)	Class specific characterisation	No	No
ccos	Cosine Response (Irradiance)	Instrument specific characterisation	No	Yes

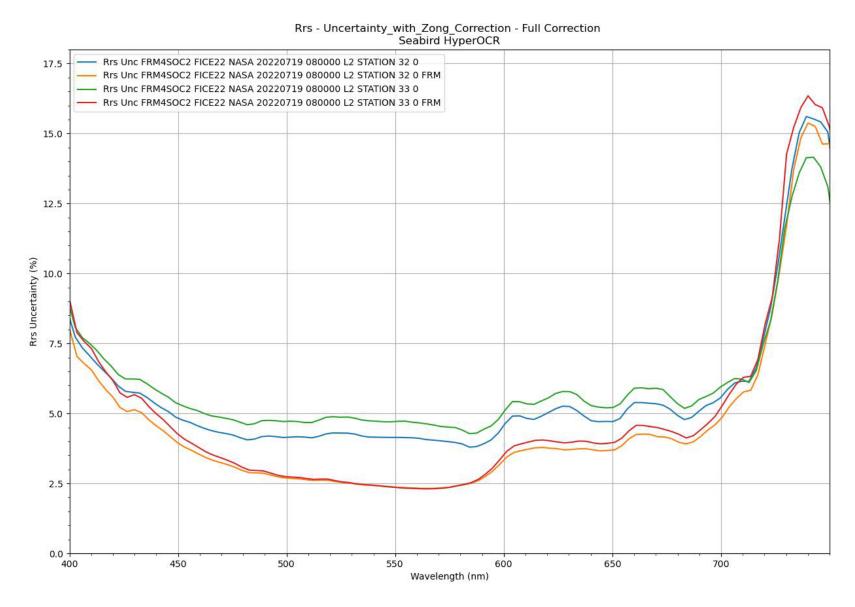


Uncertainty Results – PySAS sample data





Uncertainty Results – PySAS sample data





Congratulation!

I finished and you survived ;-)