

Welcome! 🖐️



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Workshop Materials

<https://www.comet-toolkit.org/user-guide/training/tuwien/>



Today's Agenda



1. **Presentation 1:** *Uncertainties & CoMet Toolkit Introduction (15 min)*
2. **Exercise 1:** *"Punpy Uncertainty Propagation" (15 min)*
3. **Presentation 2:** *"Error Correlation" (15 min)*
4. **Exercise 2:** *"Punpy with Error Correlation" (15 min)*



Break (10 min)

5. **Exercise 3:** *"Spectrometer example" (20 min)*
6. **Exercise 4:** *"Uncertainties in time series" (20 min)*
7. **Wrap-up:** *"Applications & Outlook" (10 min)*





The CoMet Toolkit – Uncertainties Made Easy

Rasma Ormane, Pieter De Vis, Sam Hunt

National Physical Laboratory

TU Wien workshop - 18/10/2026



NPL



NPL Bushy House

What is National Physical Laboratory?

- ❑ UK's **National Metrology Institute** (NMI)
- ❑ *“Realises, maintains and develops the UK's primary measurement standards”*
- ❑ Established in 1900



NPL, Teddington





Knowledge Exchange

- **ESA's SIRENE** project established NPL & TU Wien collaboration
 - Vegetation Optical Depth uncertainty propagation
 - Closely working with *Ruxandra, Nicolas, Wouter*
- Visiting scientist placement
 - 19th – 23rd October, 2026
 - Funded by the **UK ITSS**

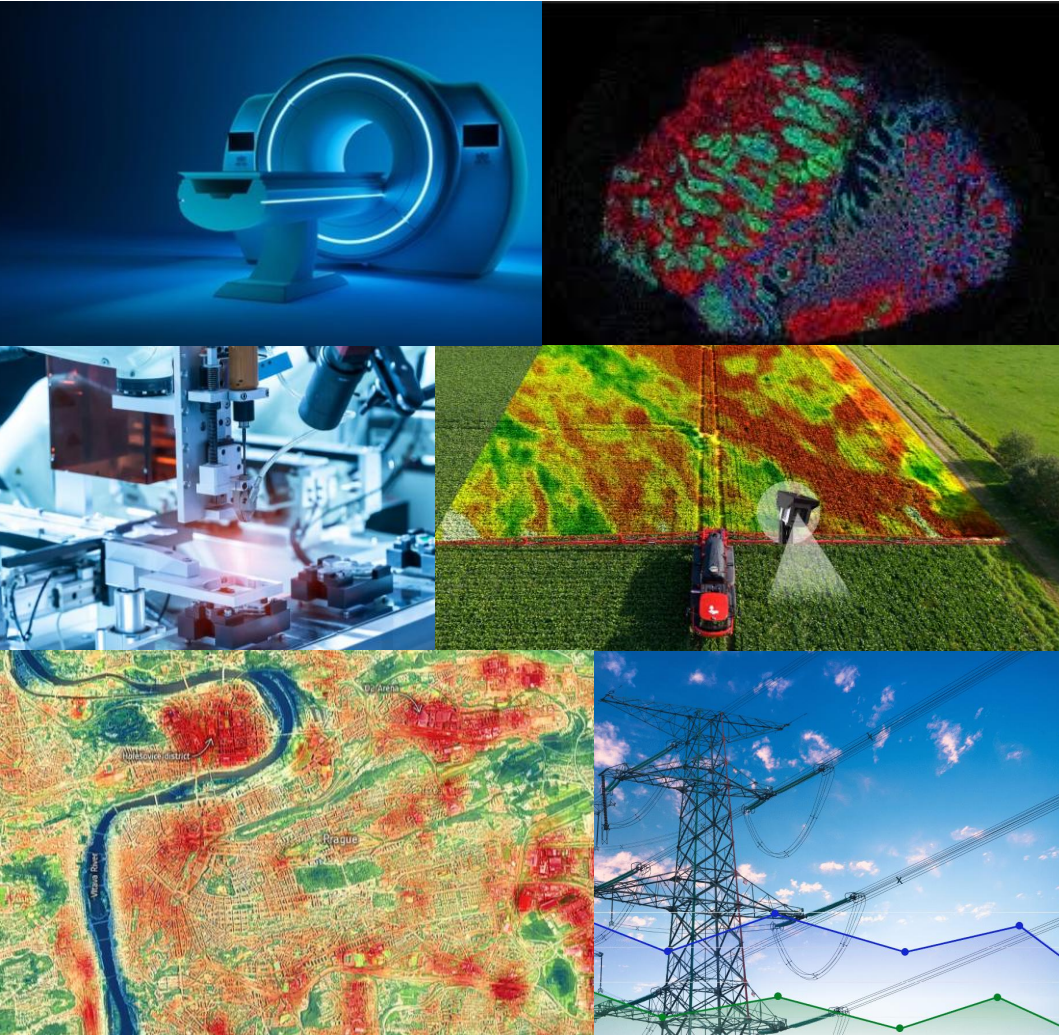
NPL



UK INSTITUTE FOR
TECHNICAL
SKILLS & STRATEGY



Measurements in Society

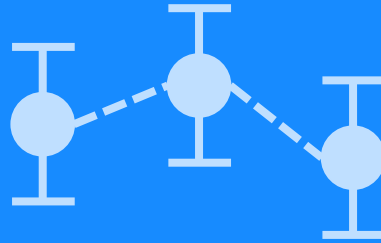


- ❑ Critical for e.g. **health**, **manufacturing**, and **environmental** monitoring.
- ❑ Growing in **size** and **complexity**.
- ❑ Reliable interpretation requires **uncertainty** and **error-covariance** information, often overlooked or non-standardised.
- ❑ **Error correlation** important to get uncertainties right when combining data

CoMet Toolkit



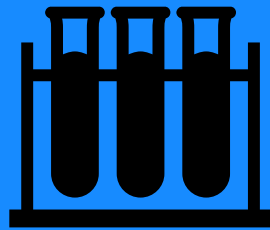
**Python
Tools**



**Uncertainty
Handling**



**Open
Source**



Tested



Applied

IDEAS-QA4EO

CoMet Toolkit



 **punpy**

Propagation UNcertainties in Python

 **obsarray**

Handling uncertainty and error-covariance in datasets

 **comet_maths**

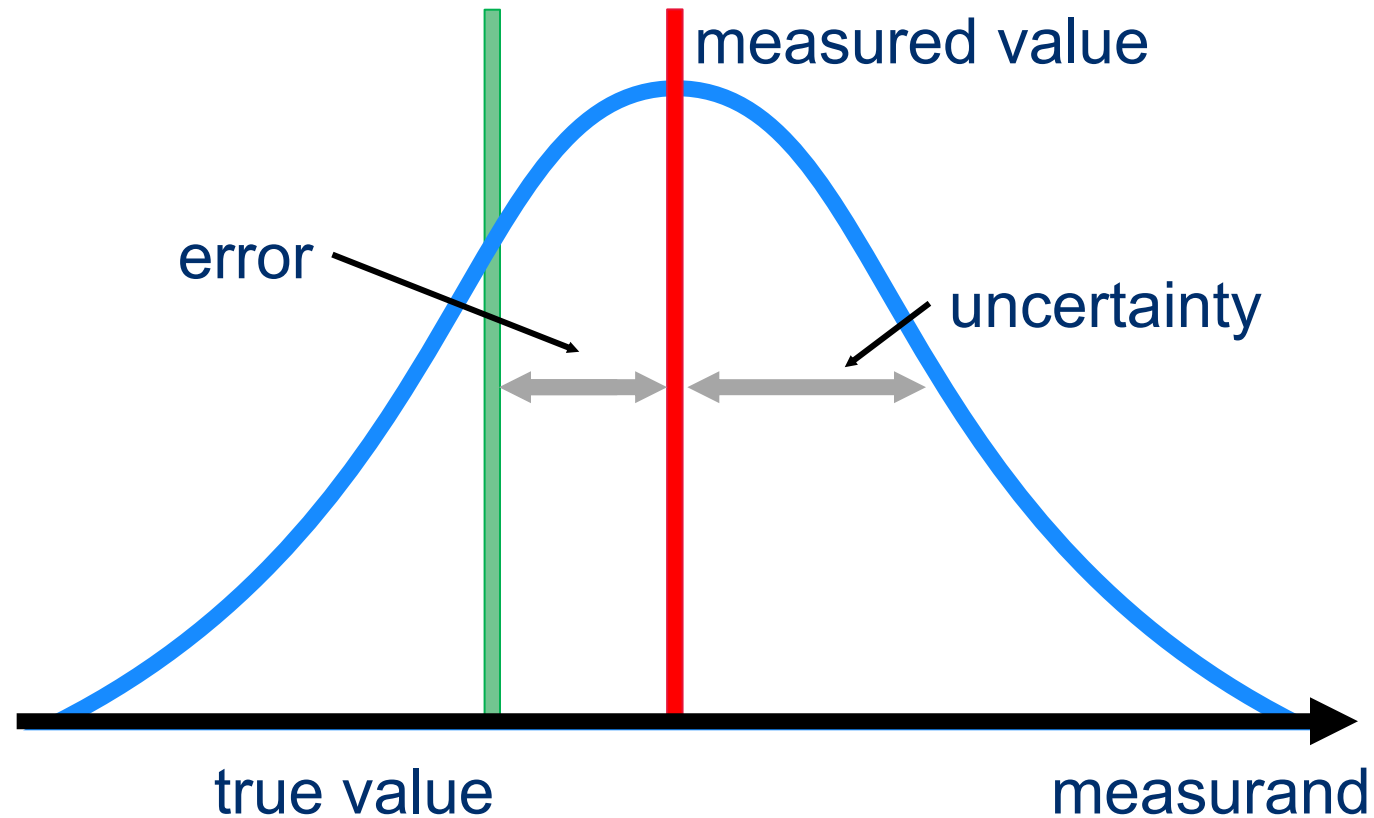
CoMet mathematical algorithms and interpolation tools

 **UNC Specification**

Uncertainty metadata naming conventions



Uncertainties 101

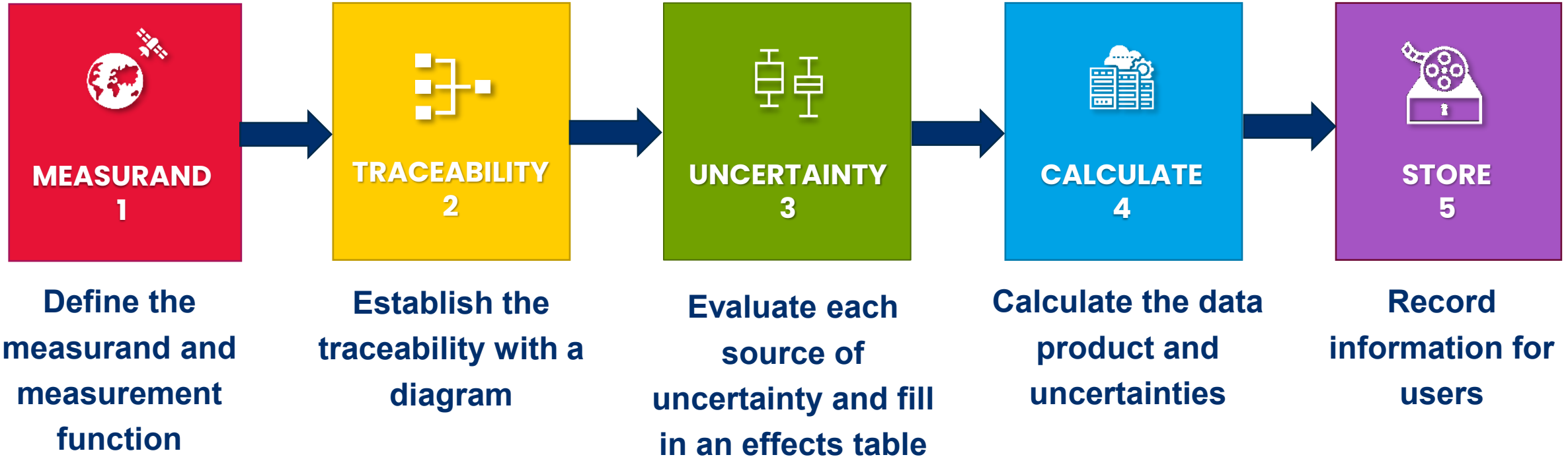




A Metrological Approach

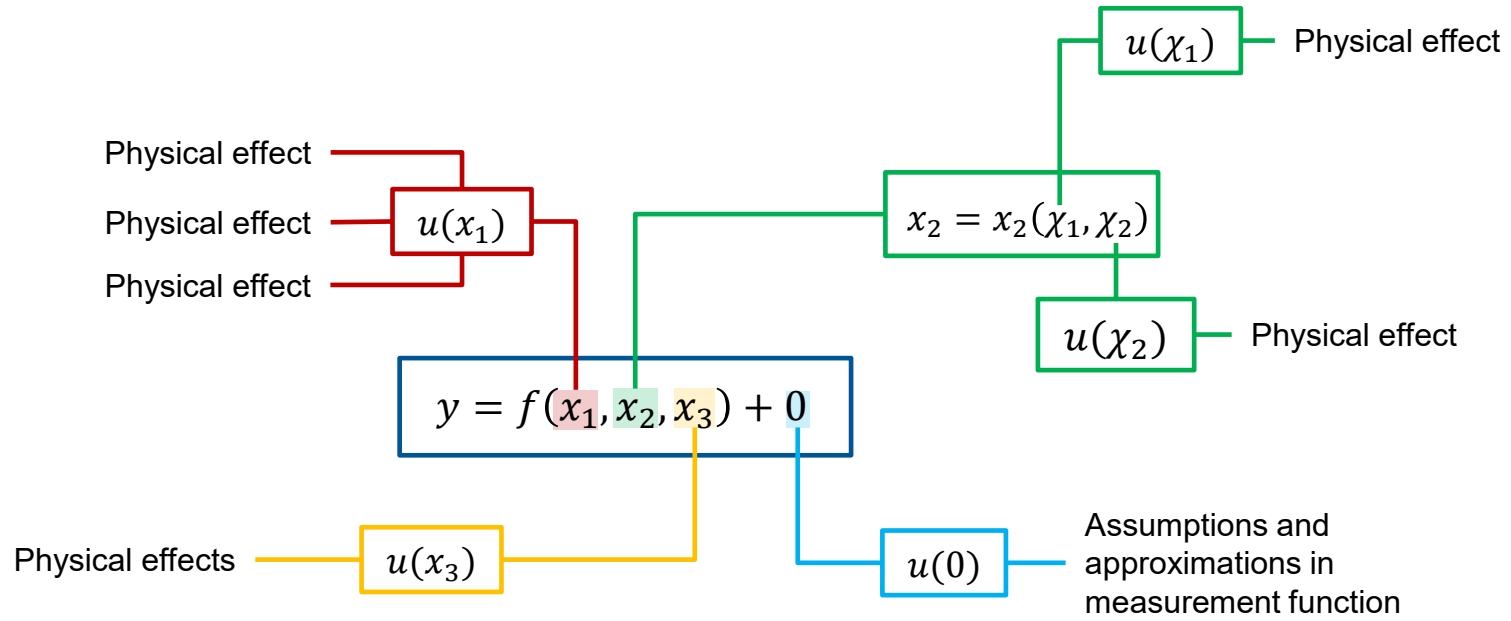
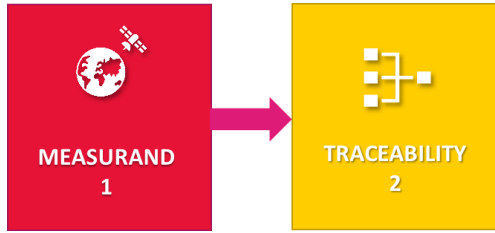


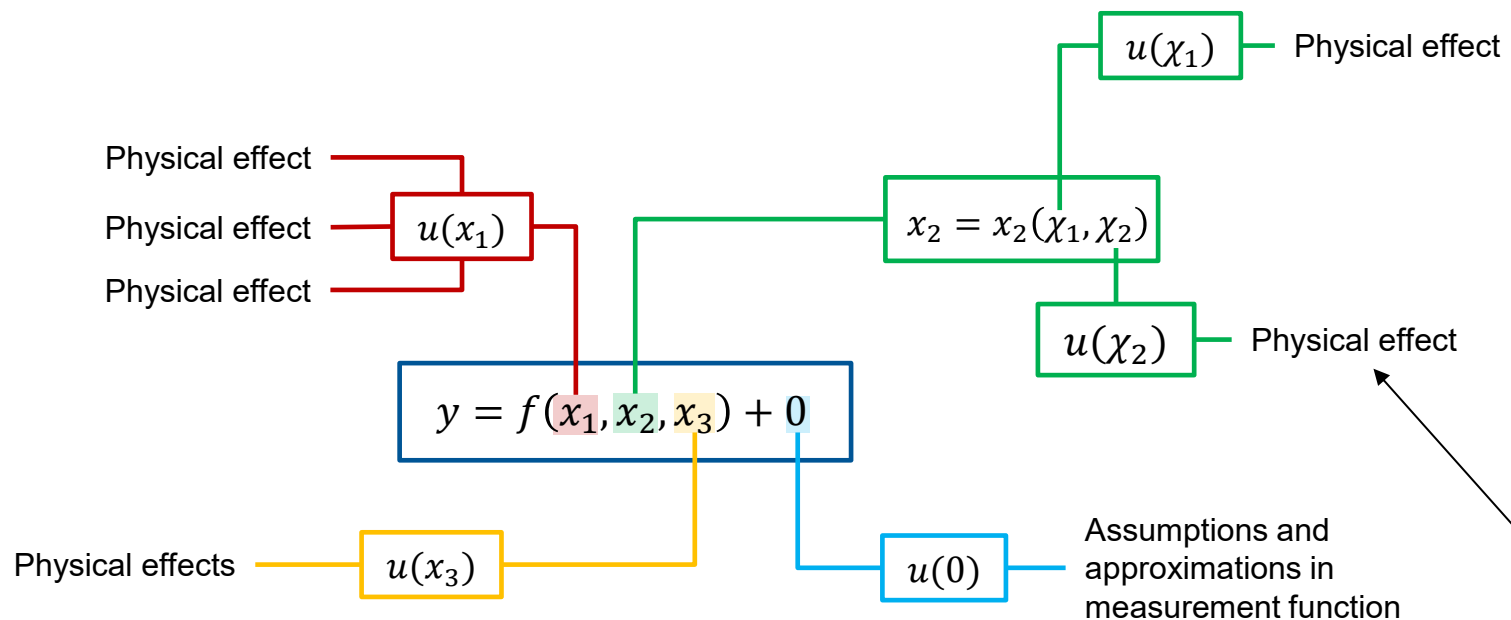
Uncertainties are evaluated and expressed following [QA4EO Five Steps](#), a framework which employs the principles of metrology.



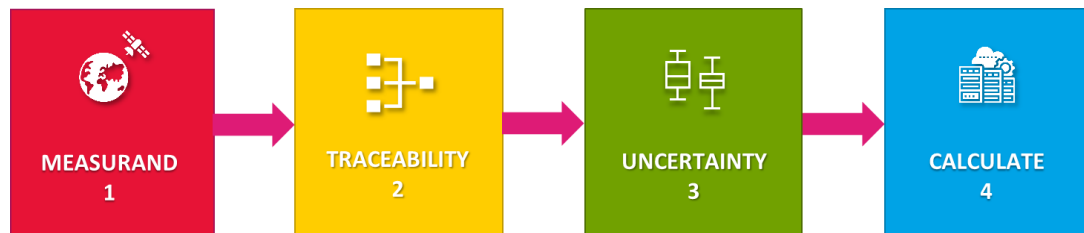


$$y = f(x_1, x_2, x_3) + 0$$

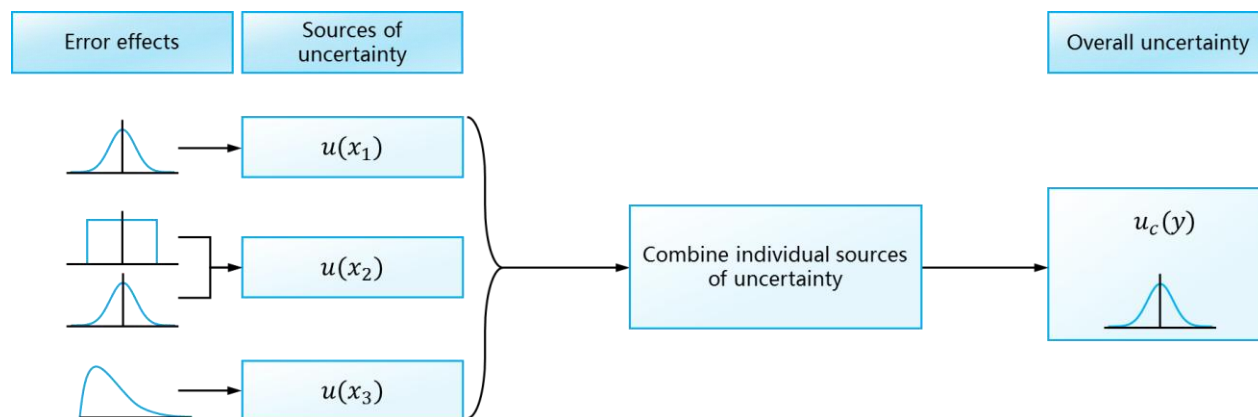




		Comments
Name of effect		A unique name
Affected term in measurement function		Name and standard symbol
Instruments in the series affected		List names
Correlation type and form	Pixel-to-pixel [pixels]	From a set of defined correlation forms
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Correlation scale	Pixel-to-pixel [pixels]	As needed to define type
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Channels/bands	List of channels / bands affected	Channel names
	Error correlation coefficient matrix	A matrix
Uncertainty	PDF shape	Functional form
	units magnitude	Units
Sensitivity coefficient		Value, equation or parameterisation of sensitivity of measurand to term



 **punpy**



- Monte Carlo (MC)
 - ❑ Draw random input samples
 - ❑ Correlate samples
 - ❑ Run samples through measurement function
 - ❑ Calculate statistics

- Law of Propagation of Uncertainty (LPU)

$$\square u^2(y) = \sum_{i=1}^N c_i^2 u^2(x_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N c_i c_j u(x_i, x_j).$$

$$\square S_y = J^T S_x J$$



obsarray

		Comments
Name of effect		A unique name
Affected term in measurement function		Name and standard symbol
Instruments in the series affected		List names
Correlation type and form	Pixel-to-pixel [pixels]	From a set of defined correlation forms
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Correlation scale	Pixel-to-pixel [pixels]	As needed to define type
	from scanline to scanline [scanlines]	
	between images [images]	
	Between orbits [orbit]	
	Over time [time]	
Channels/bands	List of channels / bands affected	Channel names
	Error correlation coefficient matrix	A matrix
Uncertainty	PDF shape	Functional form
	units magnitude	Units
Sensitivity coefficient		Value, equation or parameterisation of sensitivity of measurand to term



```

double u_str_temperature(x=2, y=2, time=3);
:_FillValue = 9.969209968386869E36; // double
:err_corr_1_dim = "x";
:err_corr_1_form = "custom";
:err_corr_1_units = ; // double
:err_corr_1_params = "err_corr_str_temperature_x";
:err_corr_2_dim = "y";
:err_corr_2_form = "systematic";
:err_corr_2_units = ; // double
:err_corr_2_params = ; // double
:err_corr_3_dim = "time";
:err_corr_3_form = "systematic";
:err_corr_3_units = ; // double
:err_corr_3_params = ; // double
:pdf_shape = "gaussian";
  
```

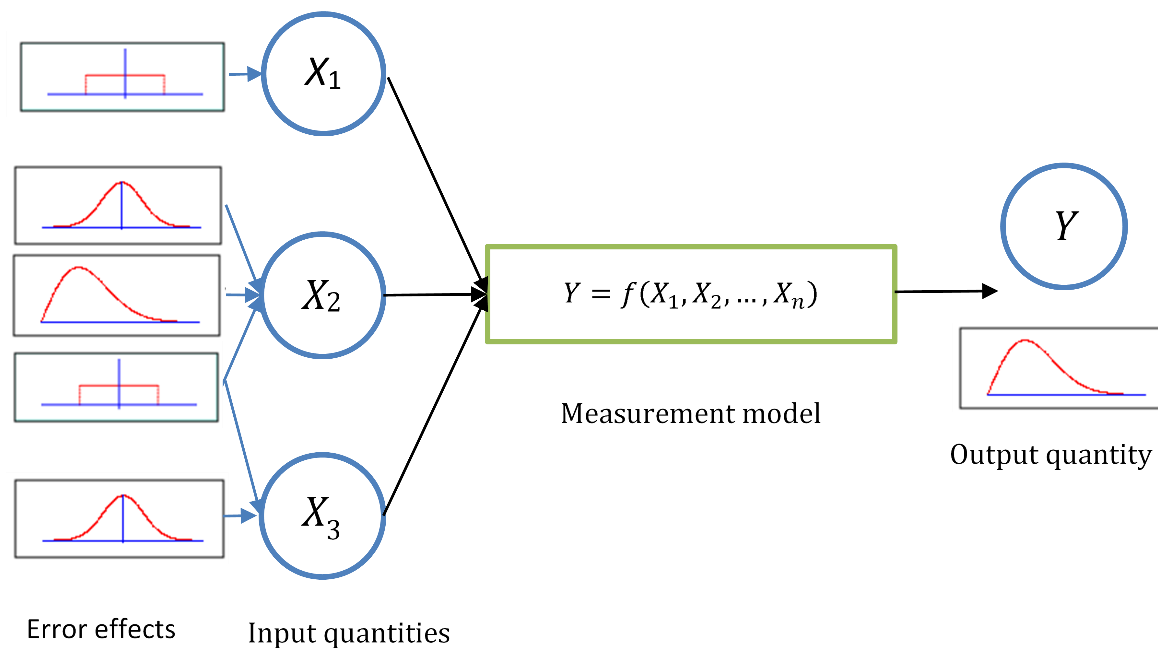
CoMet Packages:



 punpy

Propagating Uncertainties with

- ❑ Python module for propagating **random**, **systematic** and **structured uncertainties** through any Python measurement function
- ❑ Flexible in terms of the **specified correlations** along given dimensions or between input quantities
- ❑ **Monte Carlo** and **Law of Propagation of uncertainties** methods available



Punpy as a Standalone Tool



□ Simple user **interface**:

1. Import punpy
2. Define measurement function
3. Create MC or LPU object
4. Propagate uncertainties

```
import punpy
prop=punpy.MCPropagation(10000)
unc_measurand=prop.propagate_random(measurement_func,
                                     [input_qt1,input_qt2],[unc_qt1,unc_qt2])
```

□ **Measurement function** are defined as python functions that take arrays as input quantities and return an array as measurand

□ Many optional **keywords** for flexible functionality

- *return_corr*
- *Corr_between*
- *Repeat_dims*
- *Parallel_cores*
- *Output_vars*
- ...



Exercise 1



Please go to <https://www.comet-toolkit.org/user-guide/training/tuwien/>

Objective: use punpy to apply sensor calibration to digital numbers to obtain radiance with uncertainties



Measurement function → $f(L0, gains)$

L1 uncertainties → *punpy*

Input values →

$L0, gains$

Input uncertainties →

$u(L0), u(gains)$

$L1$

$u(L1)$



The CoMet Toolkit – Error Correlation

Sam Hunt, Pieter De Vis, Rasma Ormane

National Physical Laboratory

TU Wien workshop - 18/10/2026



Error Correlation



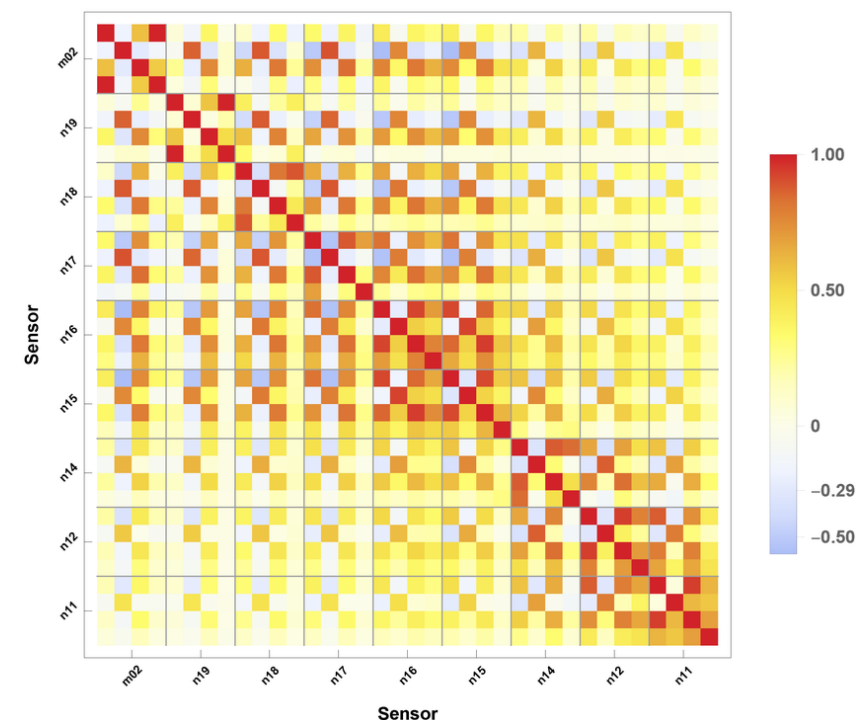
What is Error Correlation?

Errors in a dataset are **not always independent** — e.g., when errors in pixels, bands instruments, or time steps are systematically related.



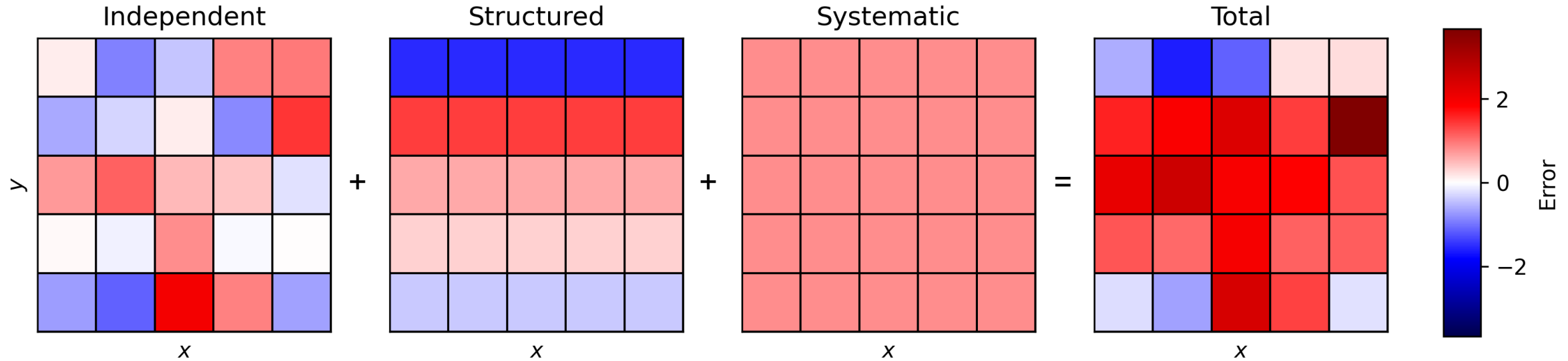
Why does it Matter?

- ☐ Bias uncertainties persist – averaging doesn't help!
- ☐ Band ratios might be off – affecting retrieval uncertainty
- ☐ Misleading confidence in trends

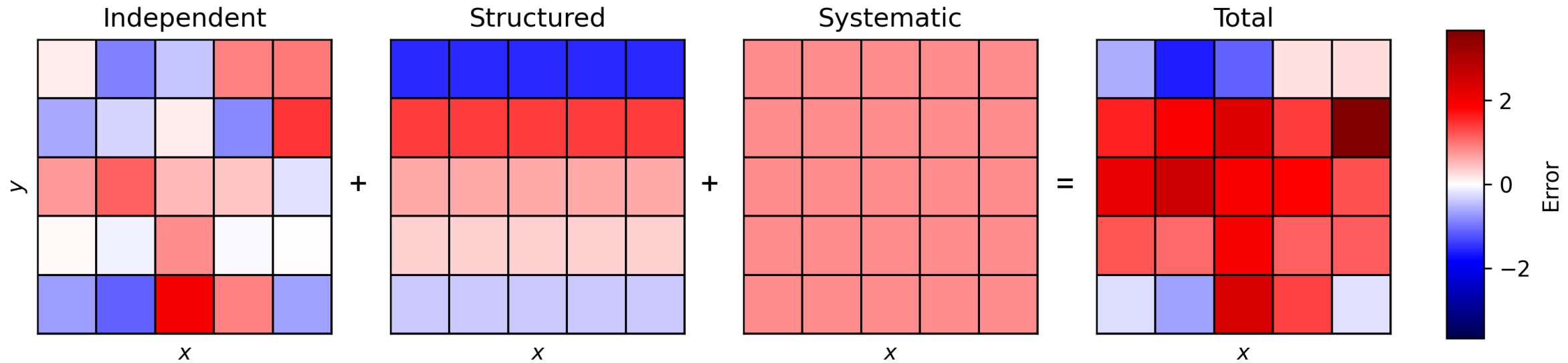


*Error correlation matrix from
Giering et al. 2019*

ND Datasets & Error-Correlation



ND Datasets & Error-Correlation



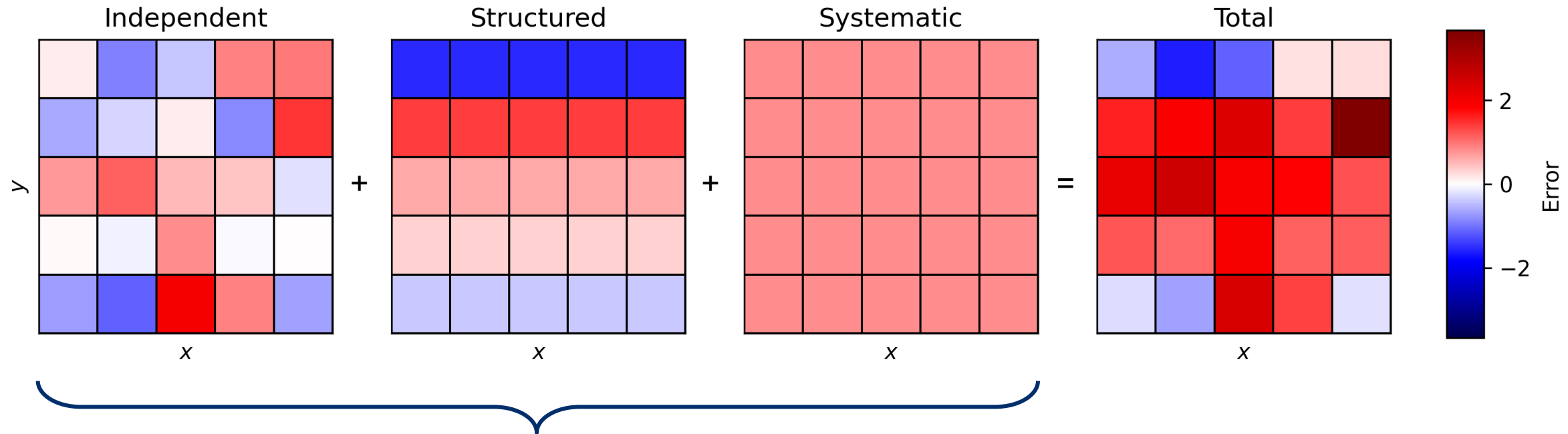
Examples

Noise from
detector

Periodically
updated
correction

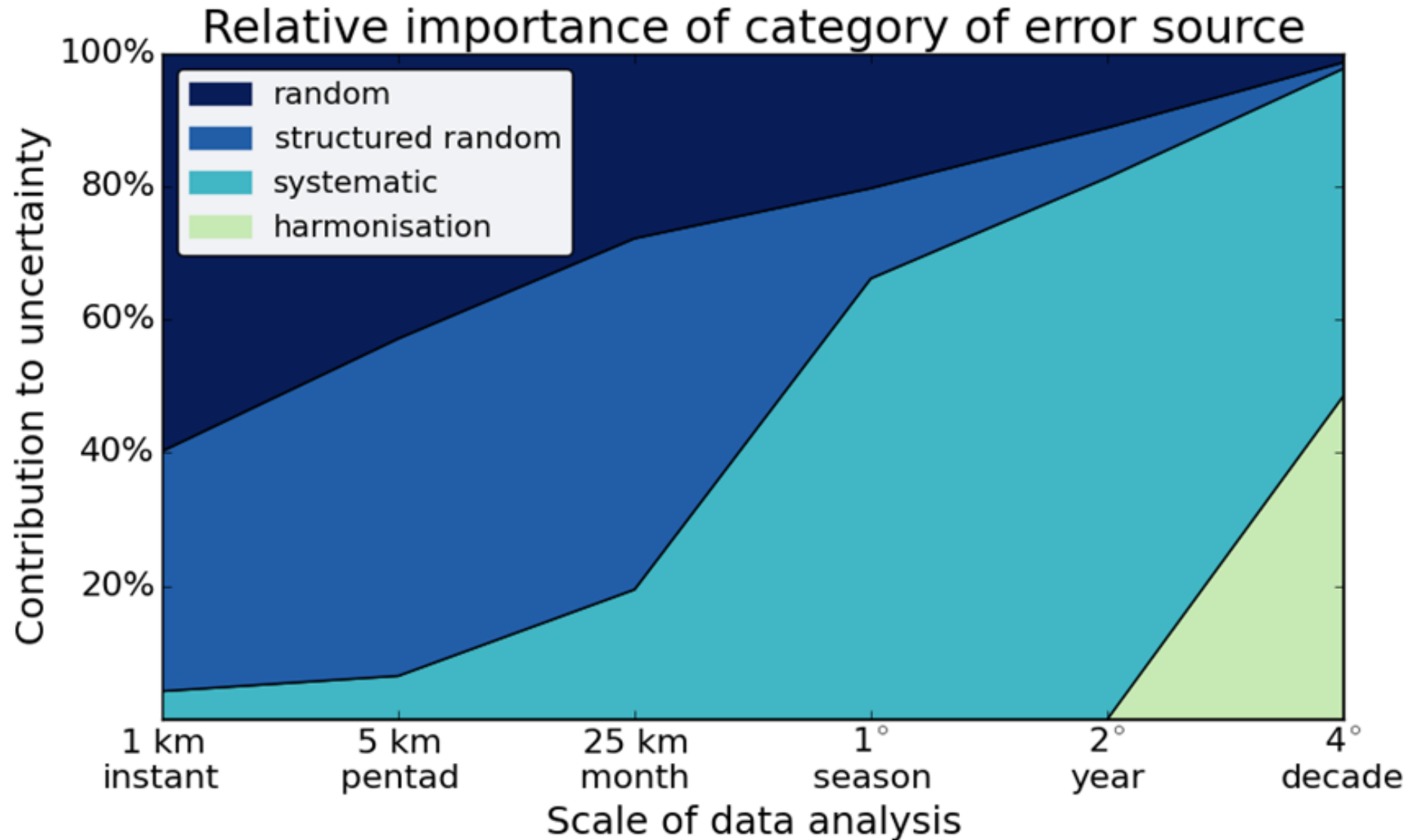
Pre-flight
calibration
error

ND Datasets & Error-Correlation



All three effects have the **same uncertainty** ($u=1$)
BUT a very **different behaviour** in the overall dataset!
This matters!

Why does error-correlation matter?



ND Datasets & Error-Correlation



For an image, define this with an **error-correlation matrix**

Defining the **cross-pixel error-correlation**, $r_{i,j}$, for all pixels – label as:

1	2	3	4	5
6	7	8	9	10
11	12	13	14	15
16	17	18	19	20
21	22	23	24	25

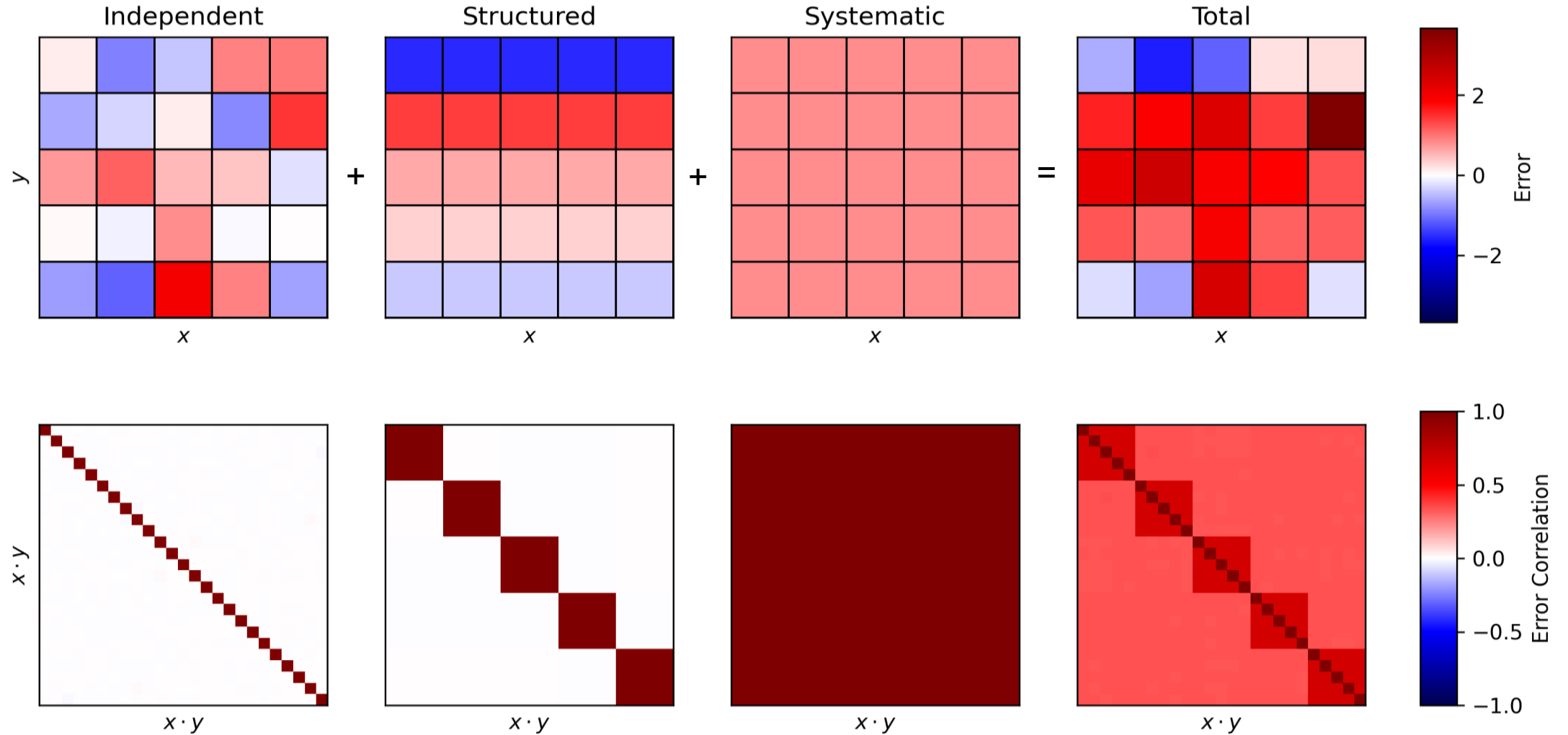
Pixels



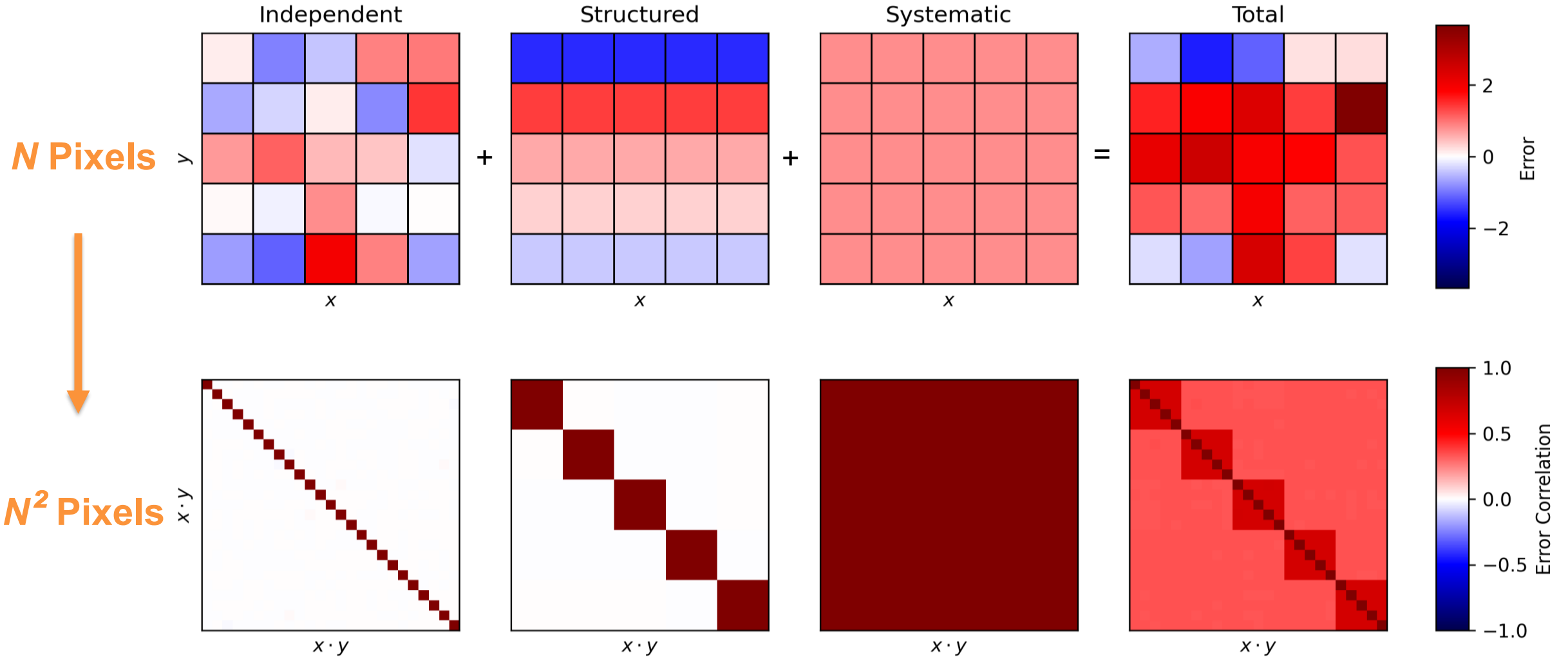
$r_{1,1}$	$r_{2,1}$	$r_{3,1}$	$r_{4,1}$	$r_{5,1}$	$r_{6,1}$	...
$r_{1,2}$	$r_{2,2}$	$r_{3,2}$				
$r_{1,3}$	$r_{2,3}$	$r_{3,3}$				
$r_{1,4}$			$\ddots$			
$r_{1,5}$						
$r_{1,6}$						
$r_{1,7}$						
$r_{1,8}$						
$\vdots$						

Cross-pixel error-correlation

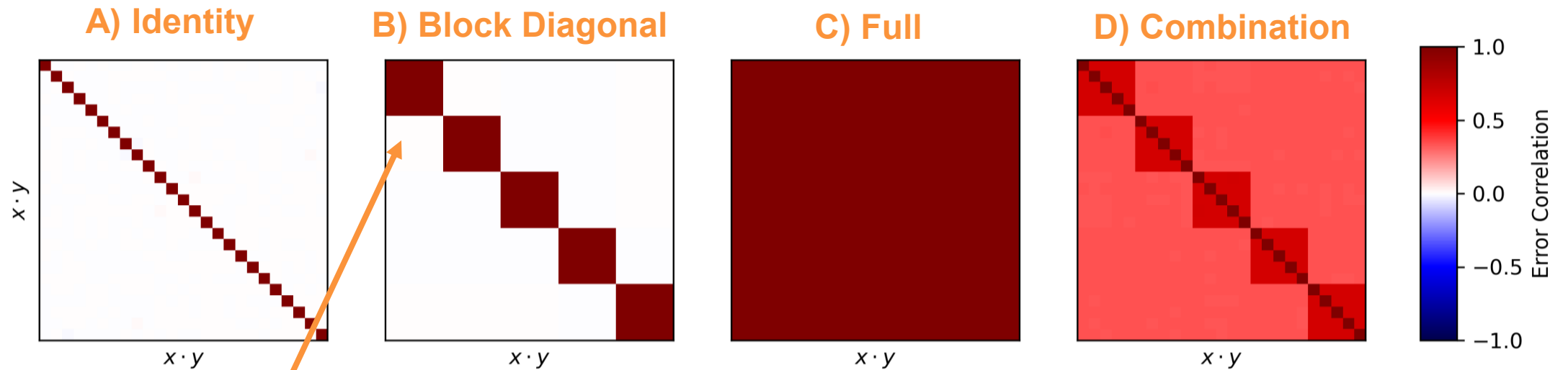
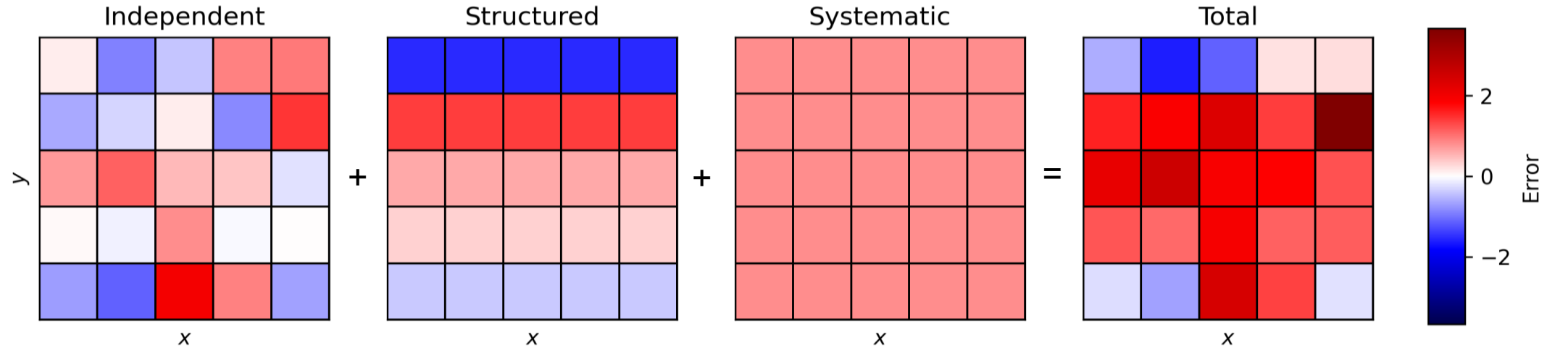
ND Datasets & Error-Correlation



ND Datasets & Error-Correlation

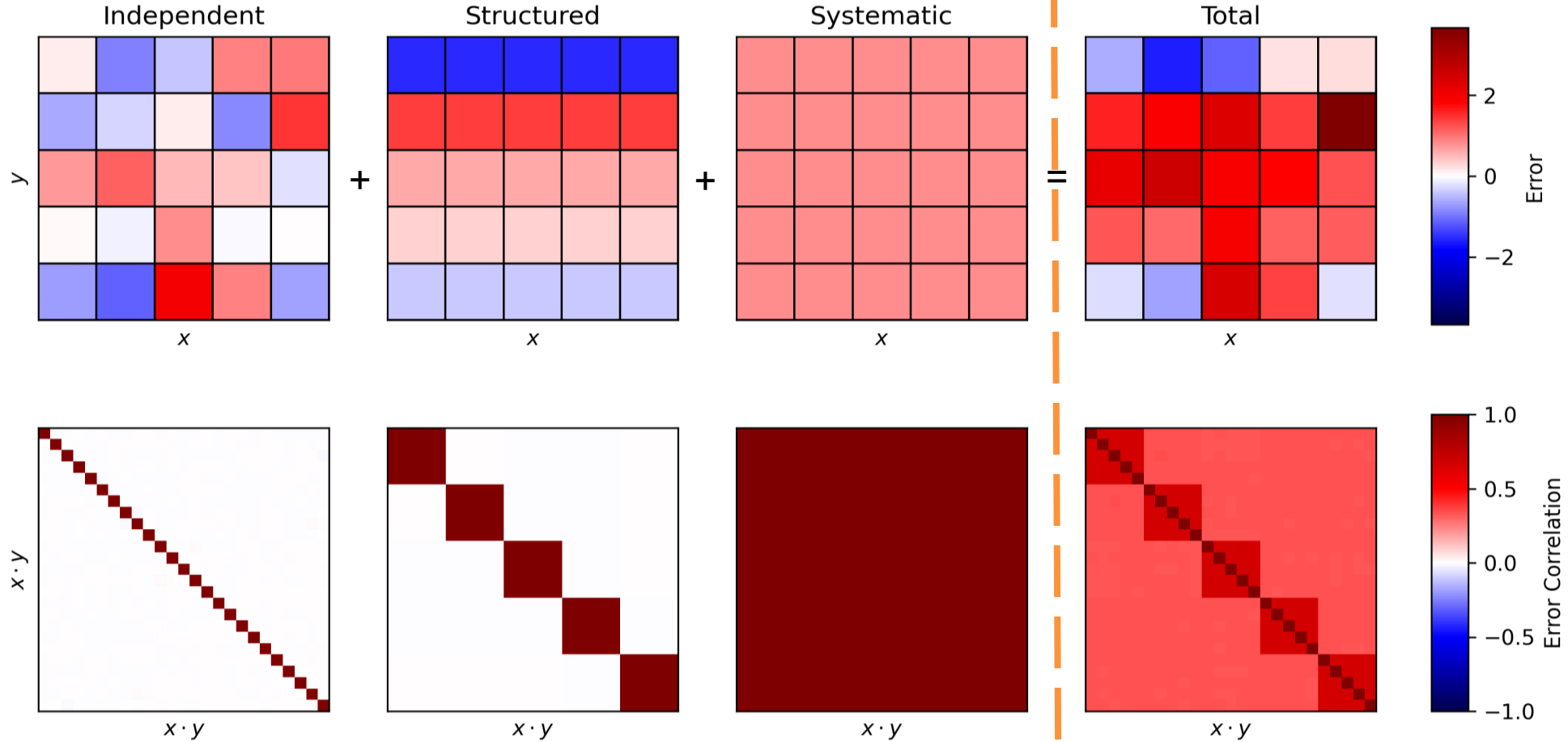


ND Datasets & Error-Correlation



Sub-matrices for systematic
error-correlation within row

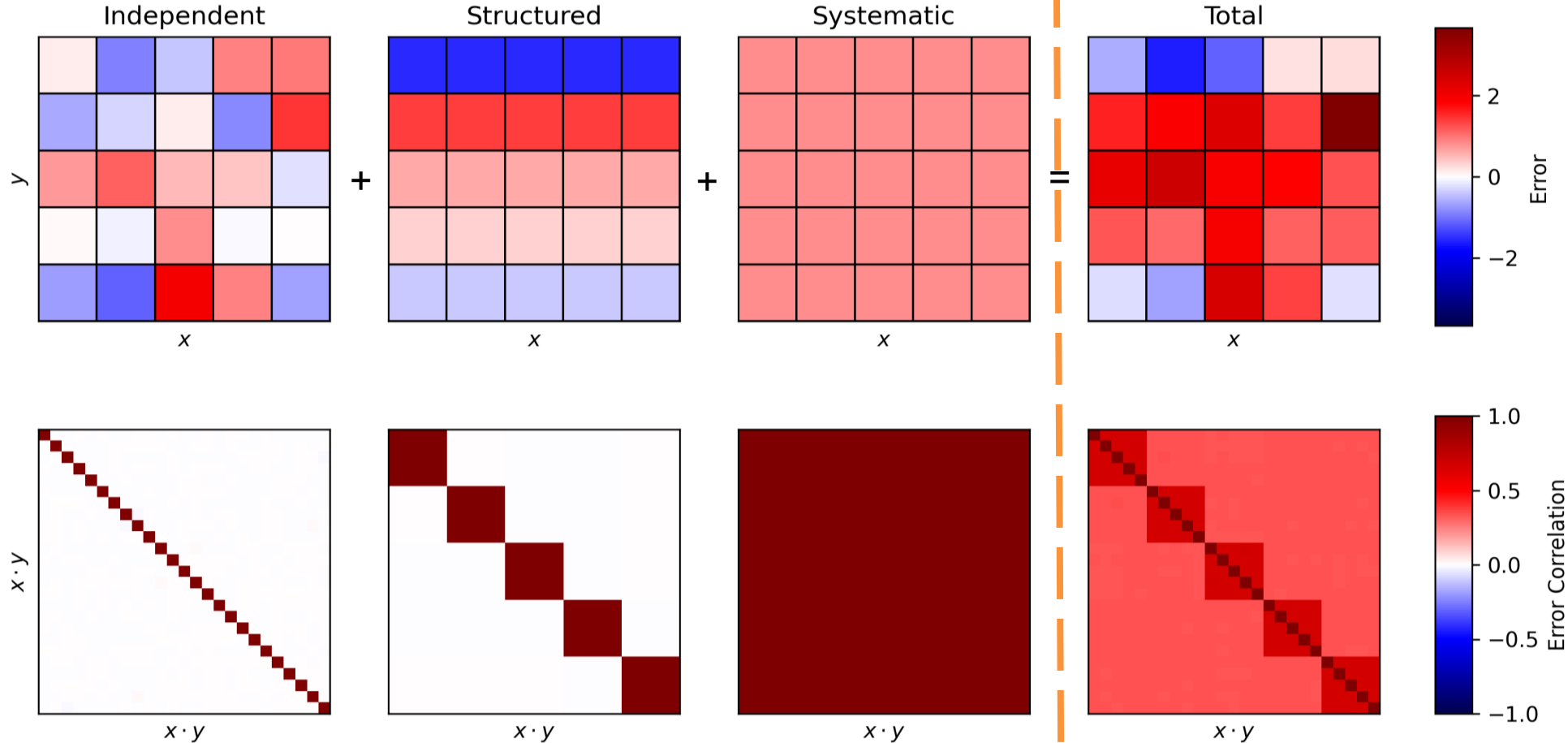
ND Datasets & Error-Correlation



✓ *Simply parameterizable*

✓ *Parameterisable via other terms*

ND Datasets & Error-Correlation



- ✓ *Simply parameterizable*
- ✓ *One term might dominate at different scales*

- ✓ *Parameterisable via other terms*
- ✓ *Same complexity at all scales*



Error Correlation



What is Error Covariance?

Combines error correlation and uncertainty

$$S = U R U^T$$



Random, systematic and structured uncertainty

- ❑ It is the errors that are correlated, not the uncertainty values
- ❑ **Random** means completely uncorrelated, i.e. error correlation is identity matrix
- ❑ **Systematic** means fully correlated, i.e. error correlation filled with 1's



Exercise 2



Please go to <https://www.comet-toolkit.org/user-guide/training/tuwien/>

Objective: repeat analysis of Exercise 1, this time accounting for error correlation



Measurement function → $f(L0, gains)$ *L1 uncertainties* → *punpy*

<i>Input values</i> →	$L0, gains$	$L1$	$corr$
<i>Random uncertainties</i> →	$u_r(L0), u_r(gains)$	$u_r(L1)$	cov
<i>Systematic uncertainties</i> →	$u_s(L0), u_s(gains)$	$u_s(L1)$	
		$u_t(L1)$	



The CoMet Toolkit – UNC & obsarray

Pieter De Vis, Sam Hunt, Rasma Ormane

National Physical Laboratory

TU Wien workshop - 18/10/2026



UNC



What is UNC?

- ☐ *Uncertainty metadata Naming Convention (UNC)*
- ☐ Provide a **standardised metadata format** for uncertainty/error-covariance information
- ☐ Contribute to & build upon an **existing ecosystem of standards** and best practices:
 - **JCGM GUM**: Guide to the expression of uncertainty in measurement
 - **JGCM VIM**: International Vocabulary for Metrology
 - **The NetCDF** data model
 - **The Climate and Forecast (CF)**: metadata for weather and climate data.

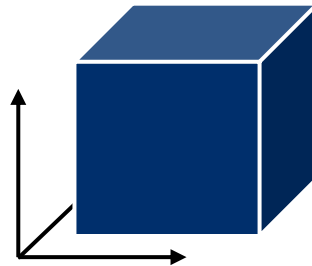


UNC Specification



Uncertainty Variable Metadata

Observation Variables

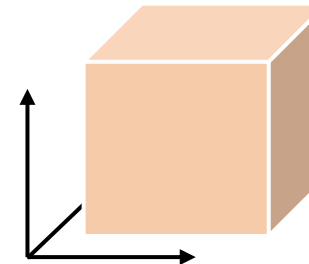
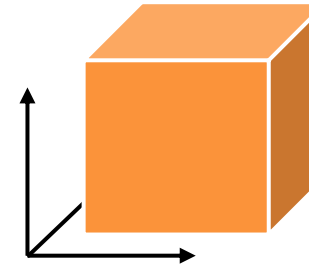


Metadata:

- Uncertainty Components

associated with

Uncertainty Variables



...

Metadata:

- **PDF Shape** (gaussian, ...)
- **Units** (abs. or rel.)
- **Error-Correlation...**

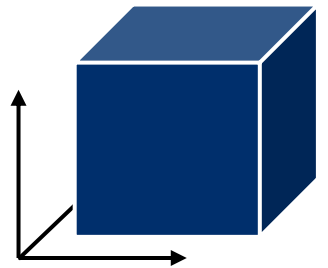


UNC Specification



Example – Temperature Dataset

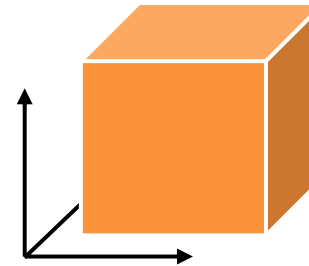
Observation Variables



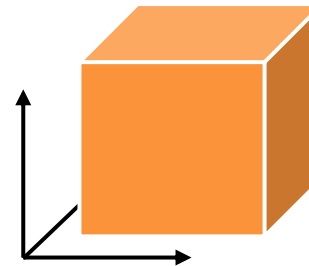
temperature

associated with

Uncertainty Variables



u_noise



u_calibration

Metadata:

- PDF Shape – “gaussian”
- Units – %
- Error-Correlation:
 - All dims - Random

Metadata:

- PDF Shape – “rectangular”
- Units – “K”
- Error-Correlation:
 - **x, y** – systematic
 - **time** – defined by matrix



Measurement data handling in Python

- ❑ **obsarray** is an extension to xarray to support defining, storing and interfacing with measurement data – using the UNC specification.
- ❑ Also has functionality for defining flags following **CF Conventions**.
- ❑ It is designed to work well with netCDF files and for the **Earth Observation** community.

Plugs straight into punpy for propagation through measurement functions!

Punpy with digital effects tables



- ❑ **punpy** interfaces with **obsarray** to make uncertainty propagation as efficient and easy to use as possible
- ❑ **propagate_ds()** function returns an **obsarray** dataset with combined random, systematic and structured uncertainties on measurand

```
from punpy import MeasurementFunction

# Define your measurement function inside a subclass of MeasurementFunction
class IdealGasLaw(MeasurementFunction):
    def meas_function(self, pres, temp, n):
        return (n * temp * 8.134) / pres

# create object of the measurement function class and specify the variable names
gl = IdealGasLaw(["pressure", "temperature", "n_moles"], "volume", yunit="m^3")

# propagate uncertainties on the input quantities in ds to measurand in ds_y
ds_y = gl.propagate_ds(ds)
```



Exercise 3



Please go to <https://www.comet-toolkit.org/user-guide/training/tuwien/>

Objective: propagate uncertainties through a complete measurement workflow, from raw spectrometer data to a vegetation index: NDVI





Exercise 4



Please go to <https://www.comet-toolkit.org/user-guide/training/tuwien/>

Objective: propagate uncertainties on spectrometer measurements separated in time and combine them into time series

- ☐ **Process** individual uncertainties
- ☐ **Store** uncertainty information (magnitudes, correlation)
- ☐ **Combine** uncertainties (random and systematic treated separately)
- ☐ **Analyse** depending on application (temporal correlation)



The CoMet Toolkit – Wrap-up

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CoMet Toolkit in Action

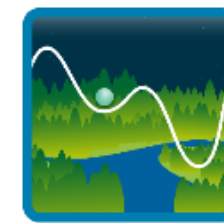


- ❑ Validated against **NIST** uncertainty engine:

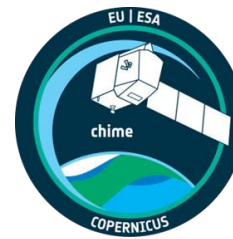
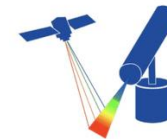
https://colab.research.google.com/github/comet-toolkit/comet_training/blob/main/NIST_example.ipynb

- ❑ *CoMet Toolkit* applications:

- ❑ Satellite **calibration** and **validation**
- ❑ Remote sensing **product** processing
- ❑ Climate and atmospheric **observations**
- ❑ Digital twins and RT **modelling**



HYPERNETS





Outlook



- ❑ Looking to continue to expand the use cases the developed tools
 - Aiming to enable uncertainty propagation through **any python measurement function**
 -  Please get in touch if you are interested!
- ❑ Recently released **MetEOR Toolkit!**
 - *Metrology for Earth Observation and Radiometry*
 - Open source Python toolkit for the comparison of satellite and reference measurements.
 - <https://www.comet-toolkit.org/meteor/>

