Welcome! 👋



Maddie Stedman



Sam Hunt

Mentimeter

7302 6971

Workshop Materials

https://www.comet-toolkit.org/user-guide/training/imperial2026/

IDEAS-QA4EO

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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 (15 min)

5. **Exercise 3:** *"Spectrometer example" (30 min)*
6. **Exercise 4:** *"Uncertainties in time series" (30 min)*
7. **Wrap-up:** *"Applications & Outlook" (15 min)*

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The CoMet Toolkit – Uncertainties Made Easy

Maddie Stedman, Sam Hunt, Pieter De Vis, Rasma Ormane

National Physical Laboratory

Imperial workshop - 12/11/2026

NPL





What is National Physical Laboratory?

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

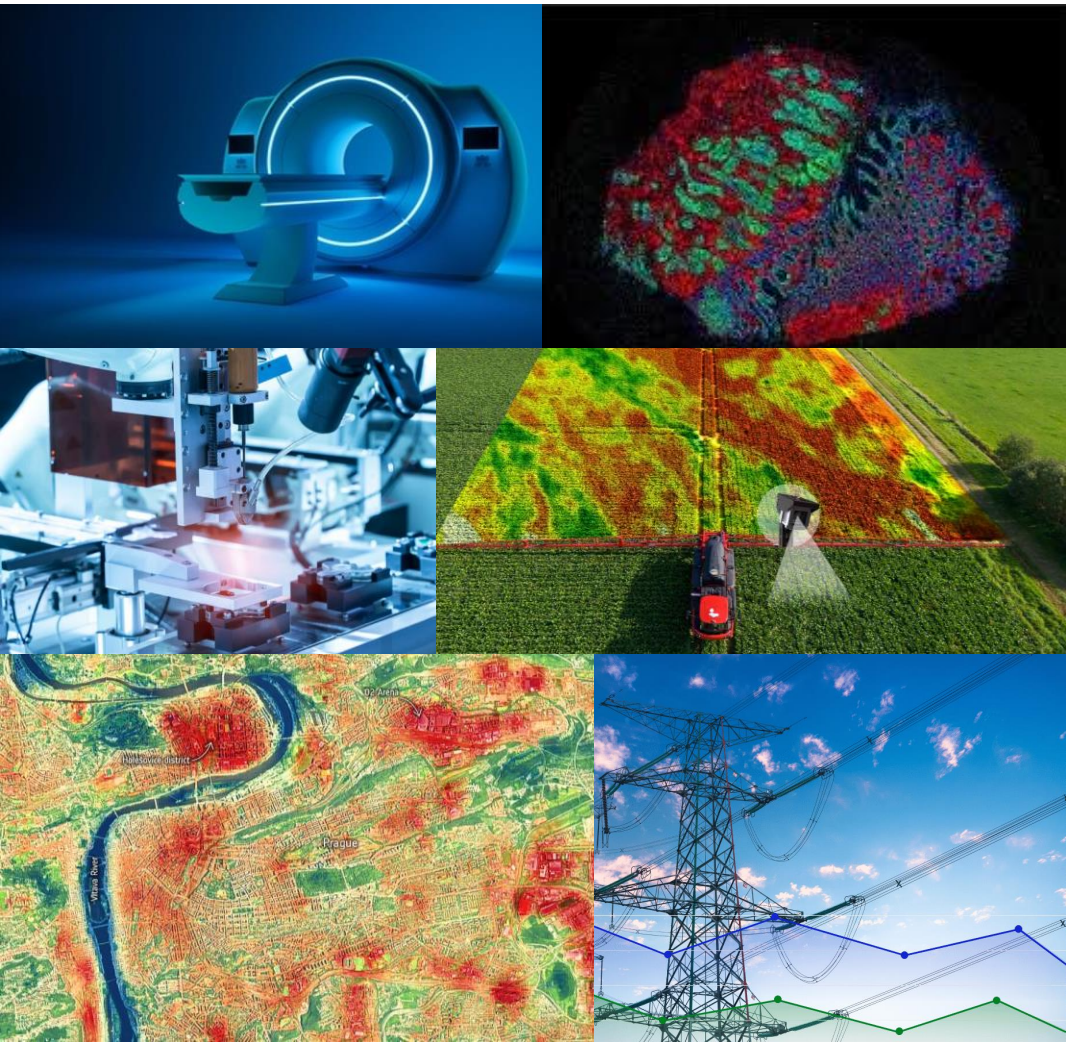




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Measurements in Society



- 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

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CoMet Toolkit

punpy

Propagation UNcertainties in Python

obsarray

Handling uncertainty and error-covariance in datasets

comet_maths

CoMet mathematical algorithms and interpolation tools

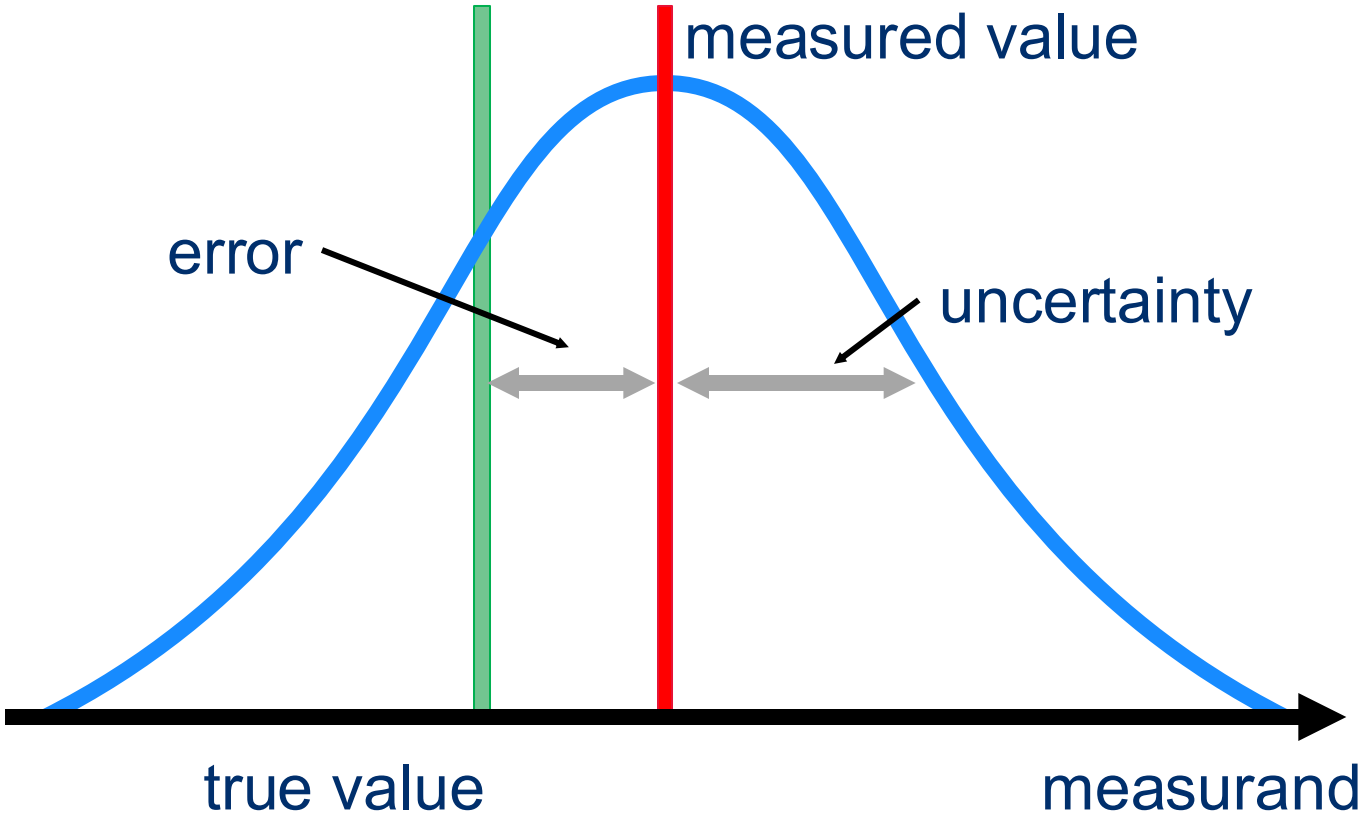
UNC Specification

Uncertainty metadata naming conventions

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Uncertainties 101



A Metrological Approach

Uncertainties are evaluated and expressed following ***QA4EO*** *Five Steps*, a framework which employs the principles of metrology.



Define the measurand and measurement function

Establish the traceability with a diagram

Evaluate each source of uncertainty and fill in an effects table

Calculate the data product and uncertainties

Record information for users

QA4EO

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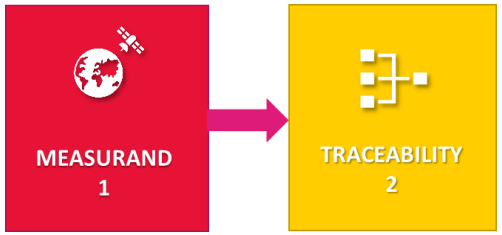
Fiduceo

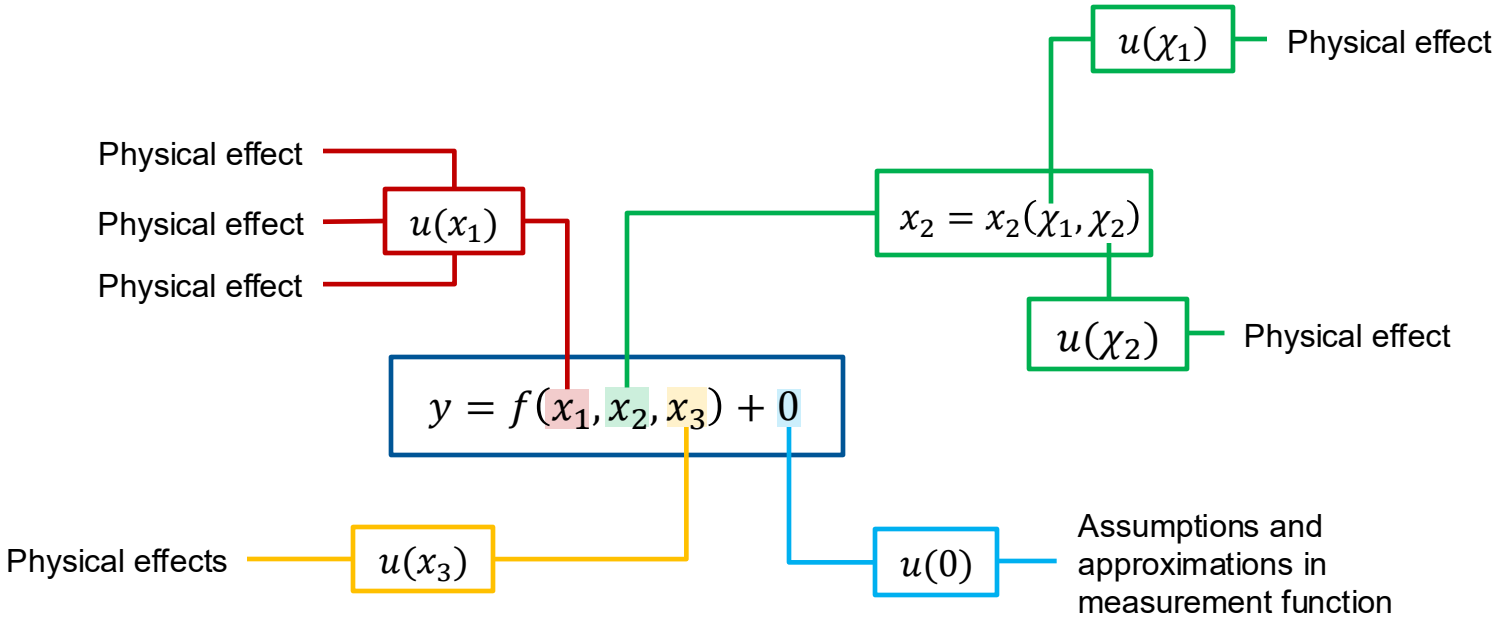
MEASURAND
1

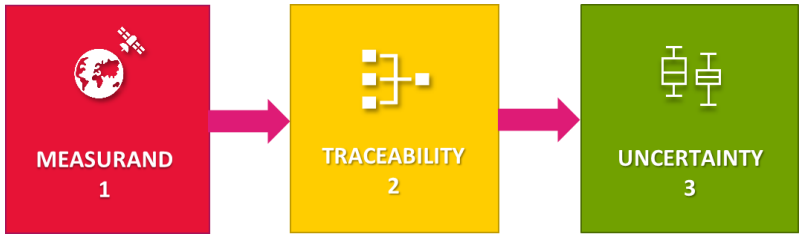
$$y = f(x_1, x_2, x_3) + 0$$

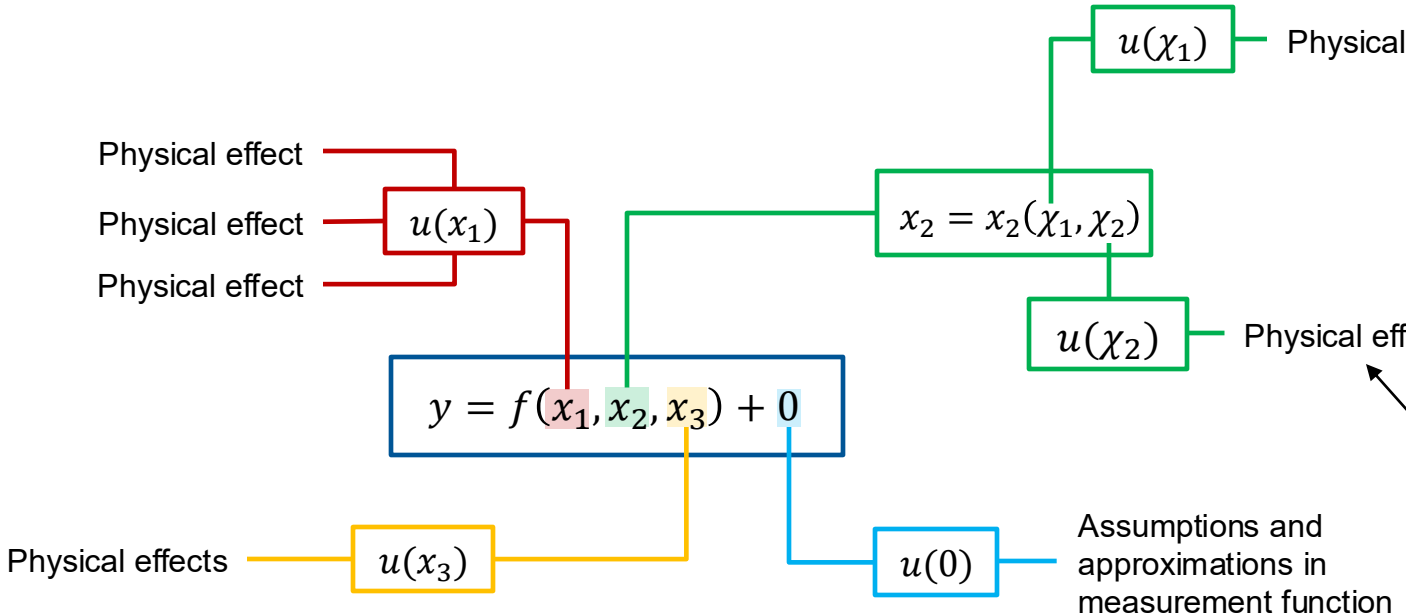
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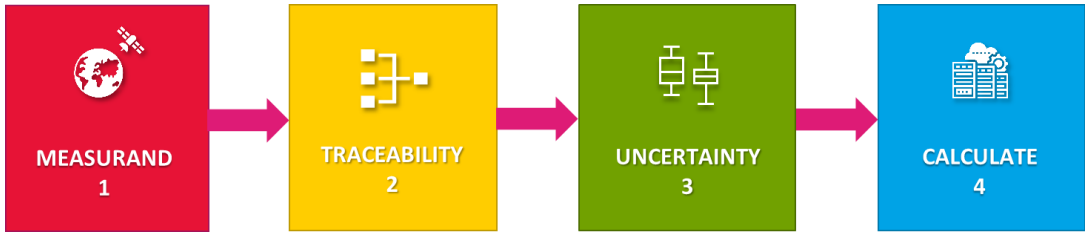

MEASURAND
1
TRACEABILITY
2


$u(\chi_1)$
Physical effect
Physical effect
Physical effect
Physical effect
$u(x_1)$
$x_2 = x_2(\chi_1, \chi_2)$
$u(\chi_2)$
Physical effect
$y = f(x_1, x_2, x_3) + 0$
Physical effects
$u(x_3)$
$u(0)$
Assumptions and approximations in measurement function



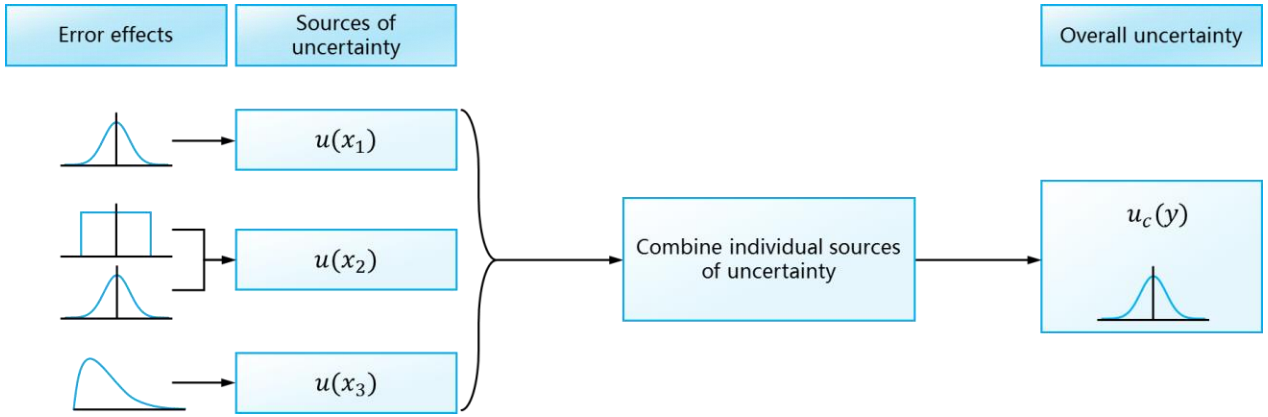


		Comments
Name of effect		A unique name
Affected term in measurement function		Name and standard symbol
Instruments in the series affected		List names
Correlation type and form	Pixel-to-pixel [pixels]	From a set of defined correlation forms
	from scanline to scanline [scanlines]	
	between images [images]	
	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	Units
	magnitude	
Sensitivity coefficient		Value, equation or parameterisation of sensitivity of measurand to term





punpy

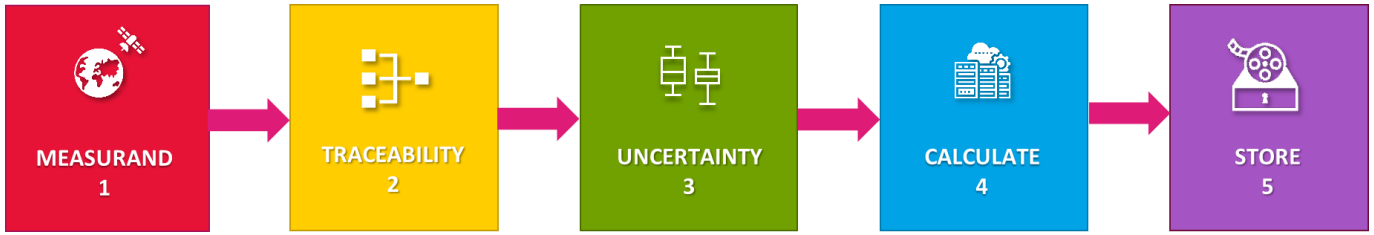


- Monte Carlo (MC)
  - ❑ Draw random input samples
  - ❑ Correlate samples
  - ❑ Run samples through measurement function
  - ❑ Calculate statistics

- Law of Propagation of Uncertainty (LPU)
  - ❑ $u^2(y) = \sum_{i=1}^{N} c_i^2 u^2(x_i) + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} c_i c_j u(x_i, x_j).$
  - ❑ $S_y = J^T S_x J$

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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	Units
	magnitude	
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";
```

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CoMet Packages:

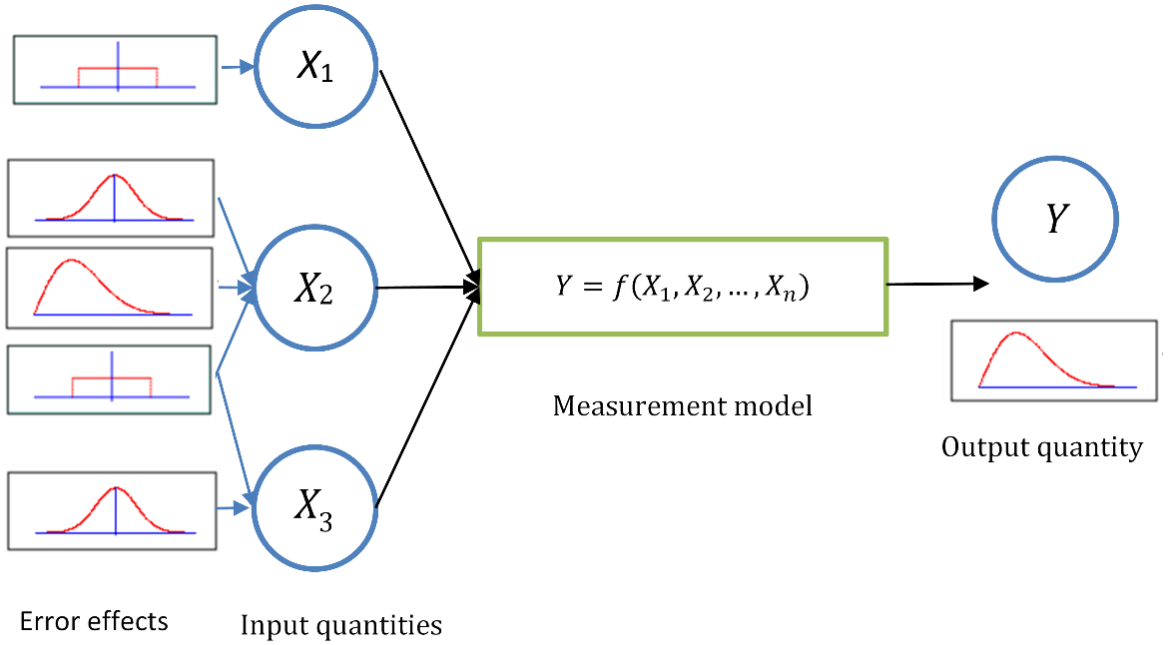


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Propagating Uncertainties with punpy

- 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



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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*
  - *…*

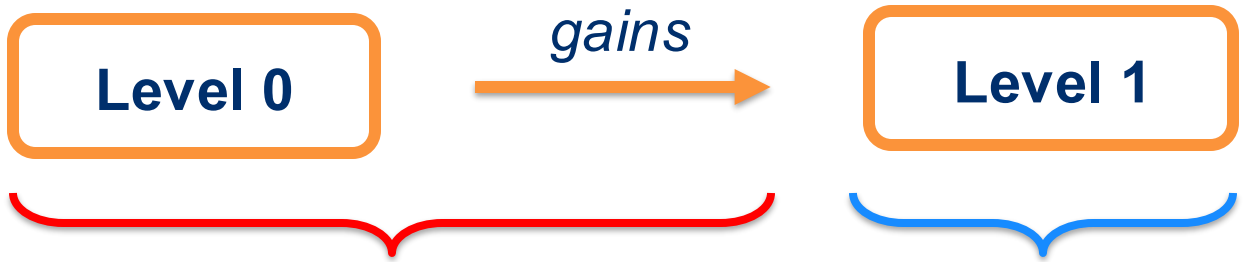
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Exercise 1

Please go to https://www.comet-toolkit.org/user-guide/training/imperial2026/

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



Measurement function → $f(L0, gains)$

Input values → $L0, gains$

Input uncertainties → $u(L0), u(gains)$

L1 uncertainties → punpy

$L1$

$u(L1)$

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The CoMet Toolkit – Error Correlation

Maddie Stedman, Sam Hunt, Pieter De Vis, Rasma Ormane

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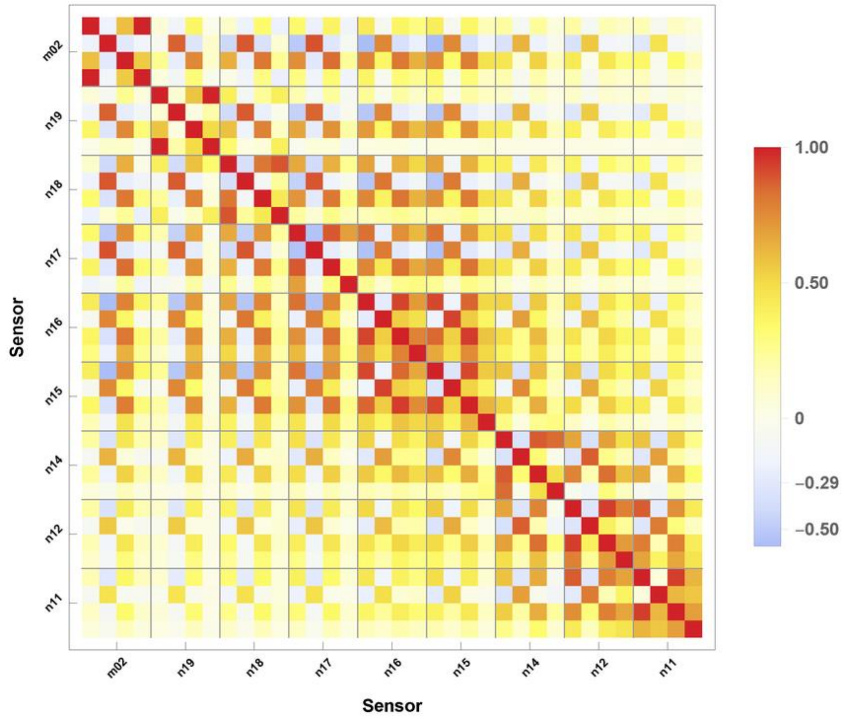
Error Correlation

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.

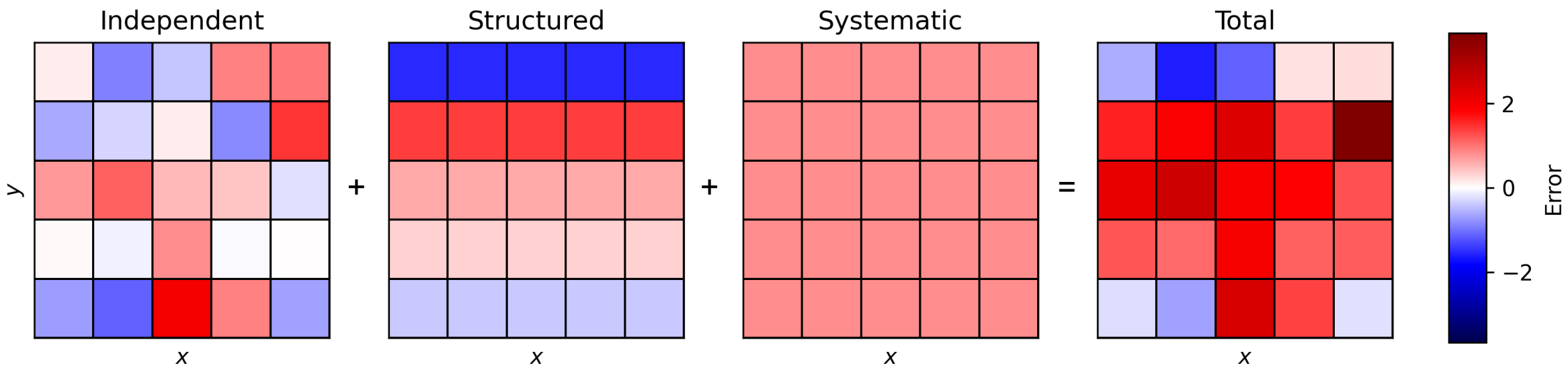
Why does it Matter?

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

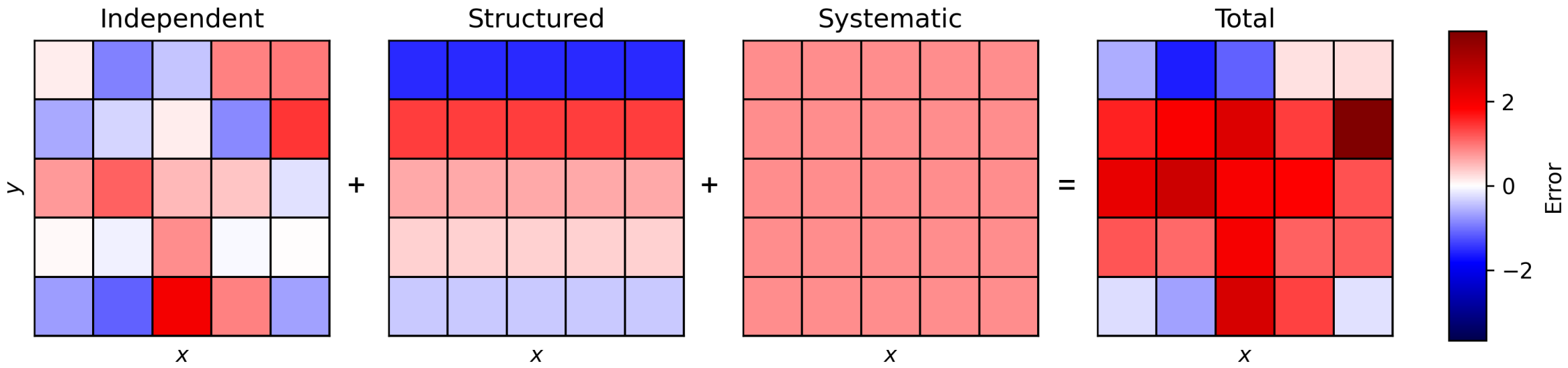


Error correlation matrix from Giering et al. 2019

ND Datasets & Error-Correlation



ND Datasets & Error-Correlation



Examples

Noise from detector

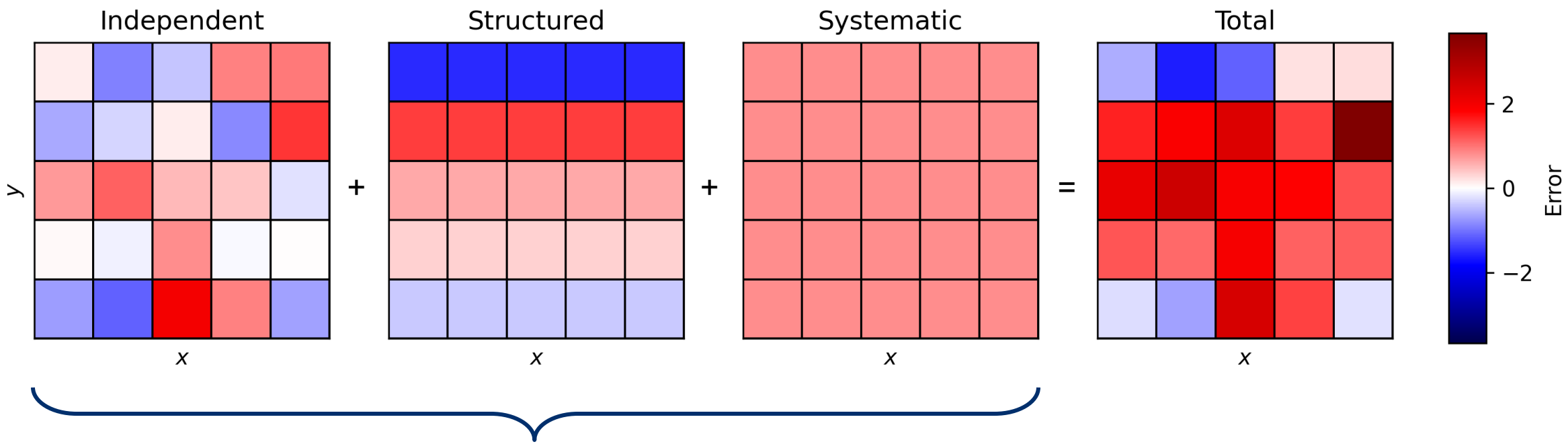
Periodically updated correction

Pre-flight calibration error

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ND Datasets & Error-Correlation

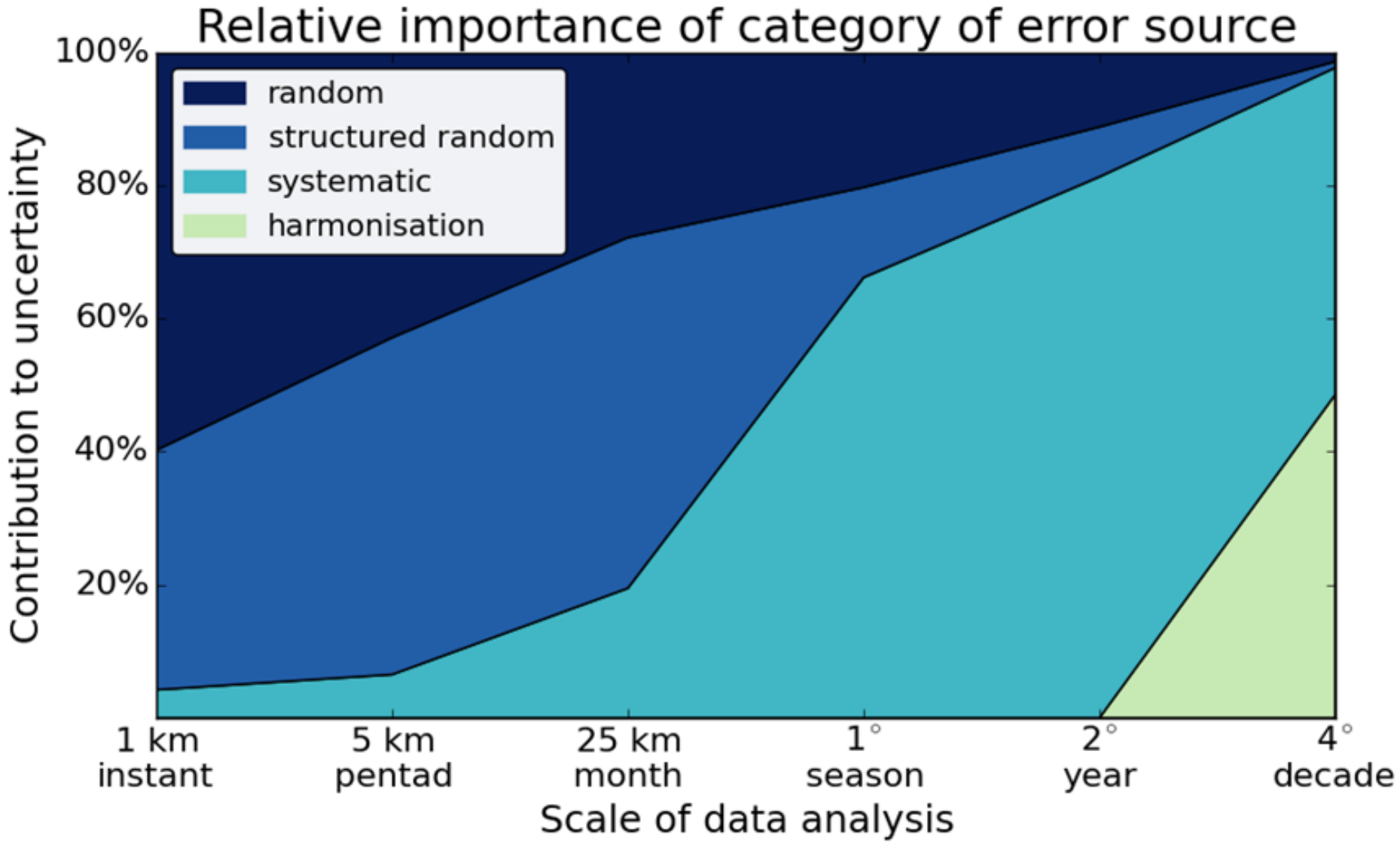


All three effects have the **same uncertainty** (u=1)
BUT a very **different behaviour** in the overall dataset!
This matters!

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Why does error-correlation matter?



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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

$$\begin{bmatrix} r_{1,1} & r_{2,1} & r_{3,1} & r_{4,1} & r_{5,1} & r_{6,1} & \cdots \\ r_{1,2} & r_{2,2} & r_{3,2} & & & & \\ r_{1,3} & r_{2,3} & r_{3,3} & & & & \\ r_{1,4} & & & \ddots & & & \\ r_{1,5} & & & & & & \\ r_{1,6} & & & & & & \\ r_{1,7} & & & & & & \\ r_{1,8} & & & & & & \\ \vdots & & & & & & \end{bmatrix}$$

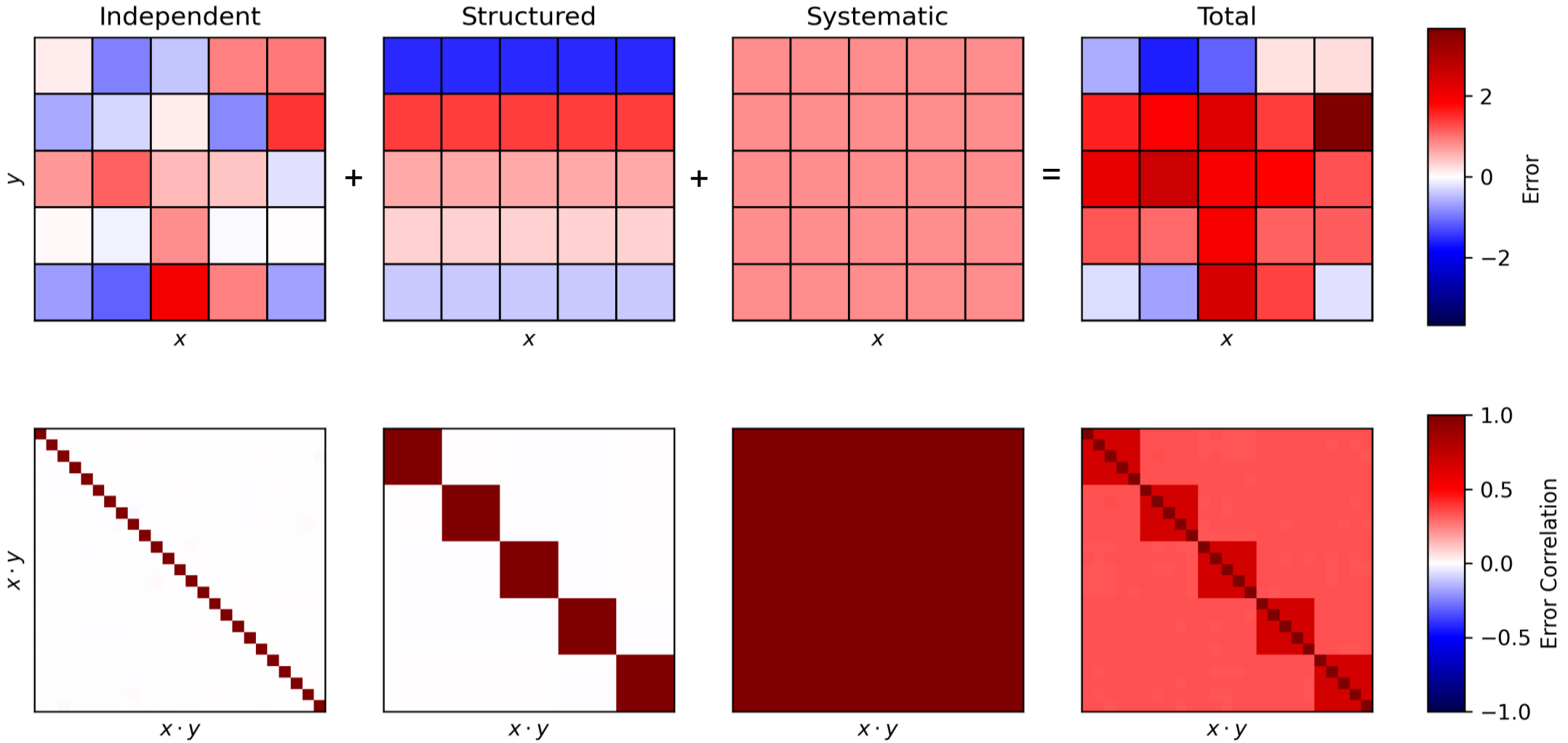
Pixels

Cross-pixel error-correlation

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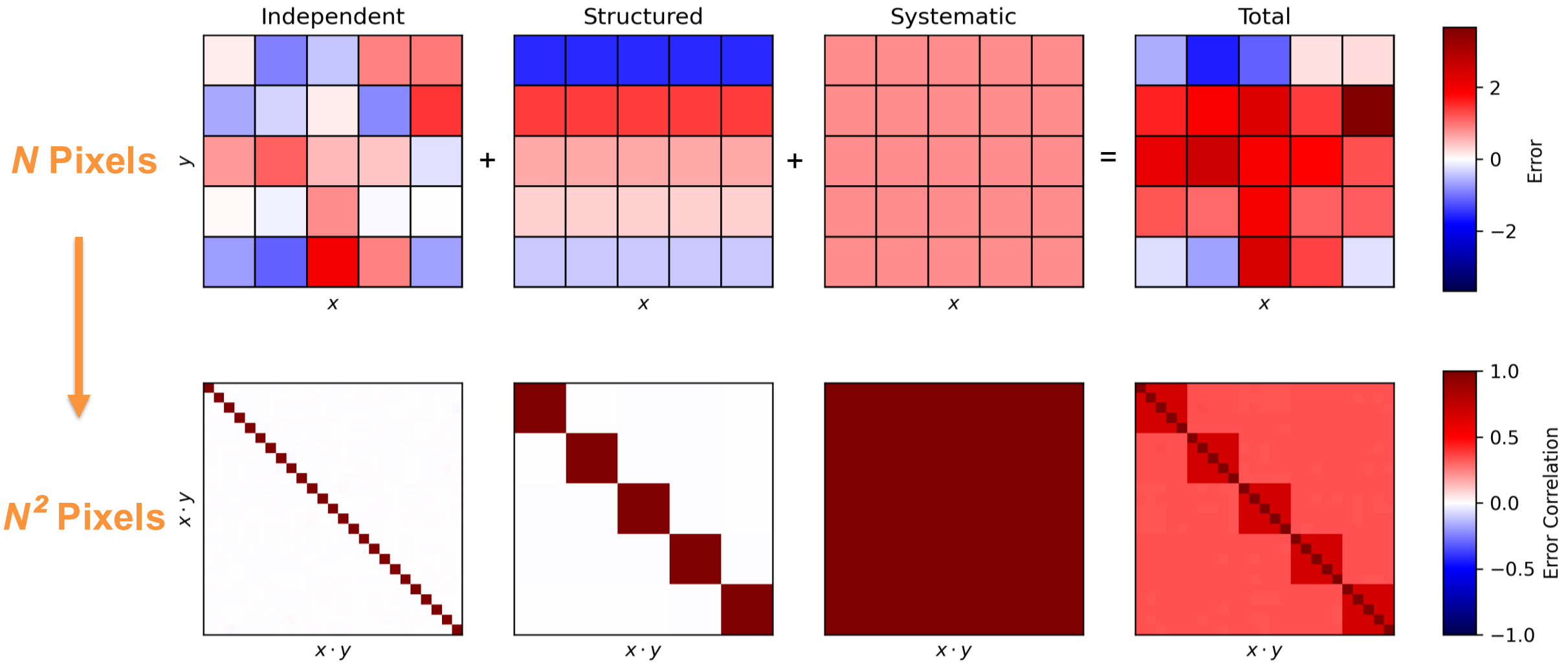
ND Datasets & Error-Correlation



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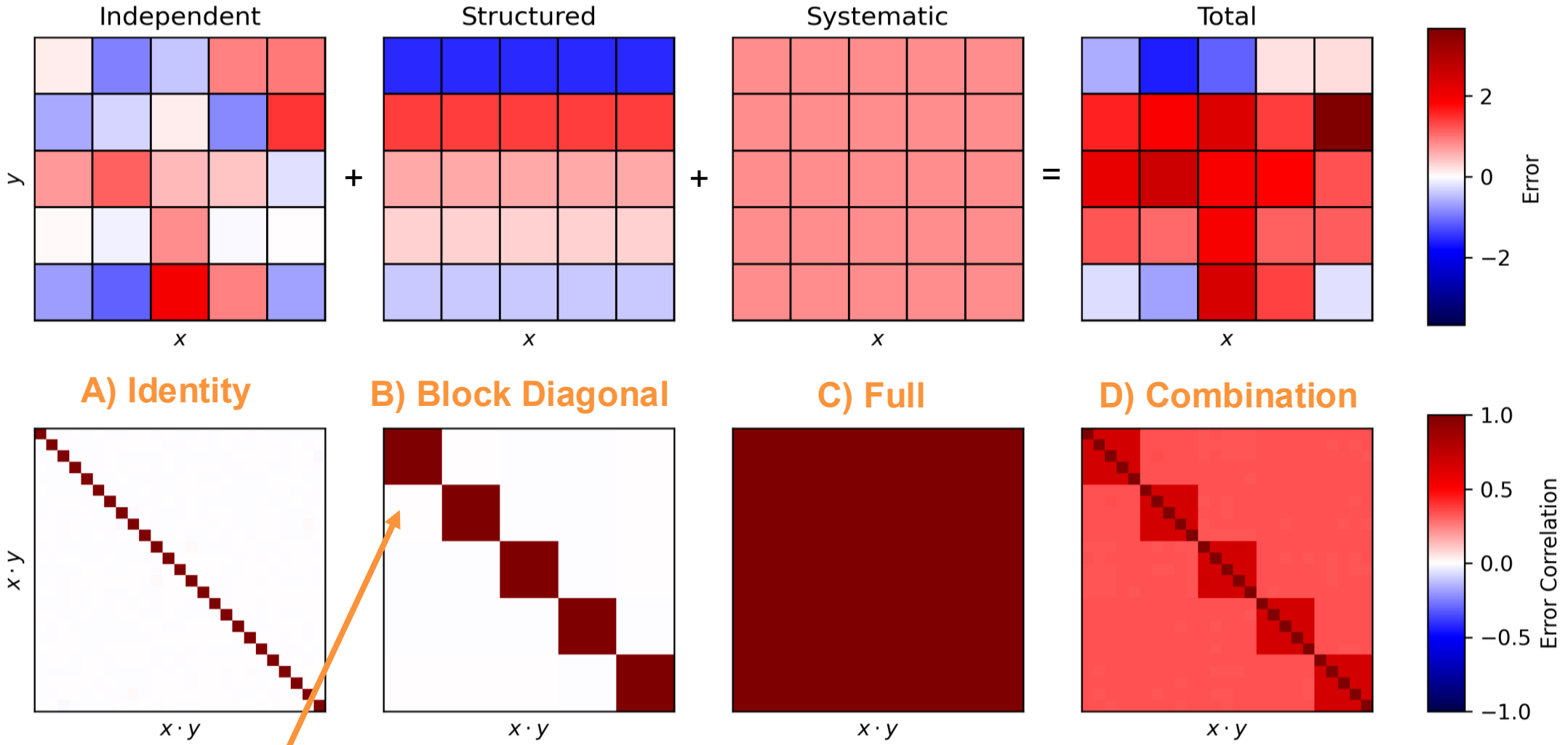
ND Datasets & Error-Correlation



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ND Datasets & Error-Correlation

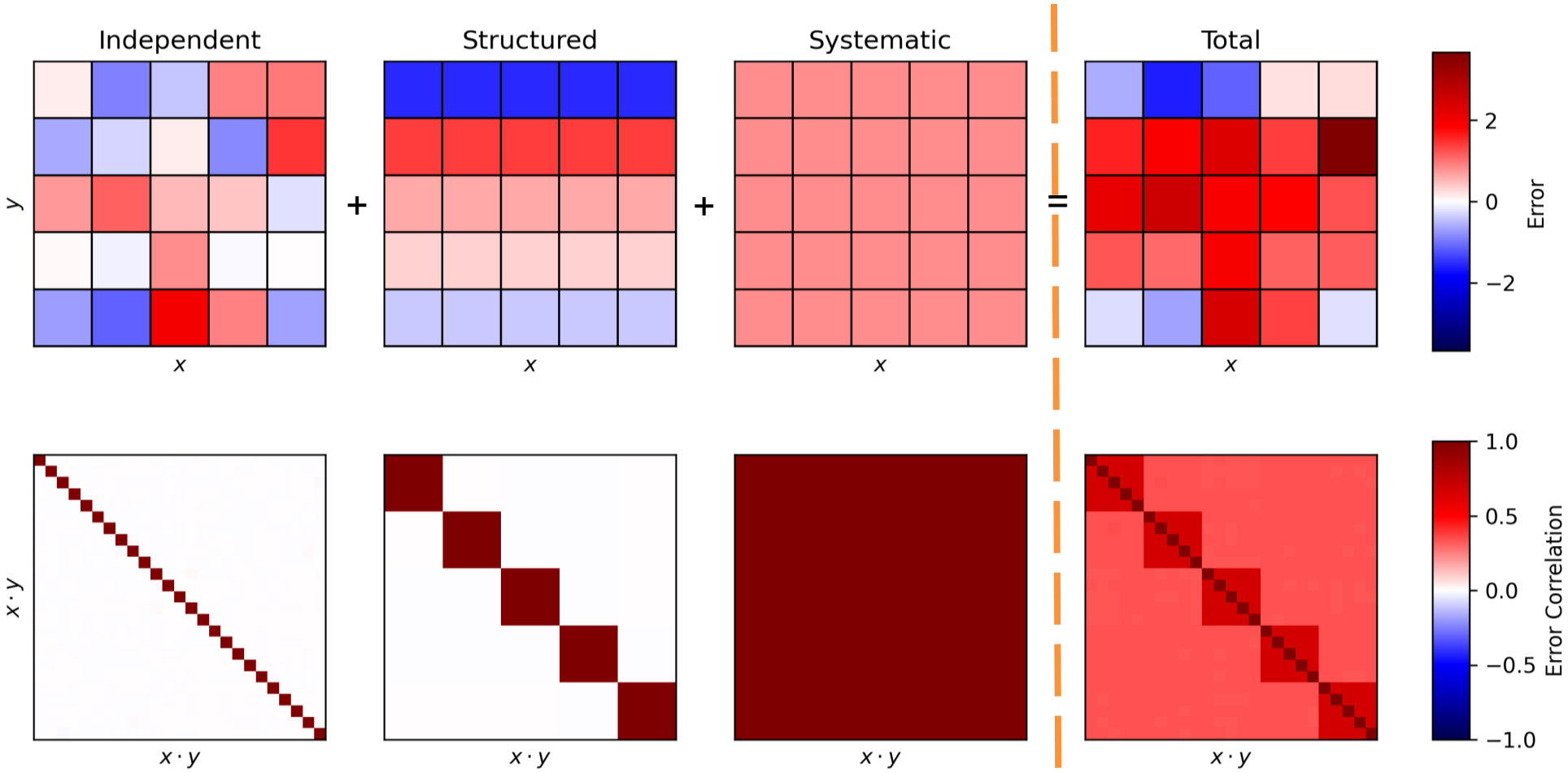


Sub-matrices for systematic error-correlation within row

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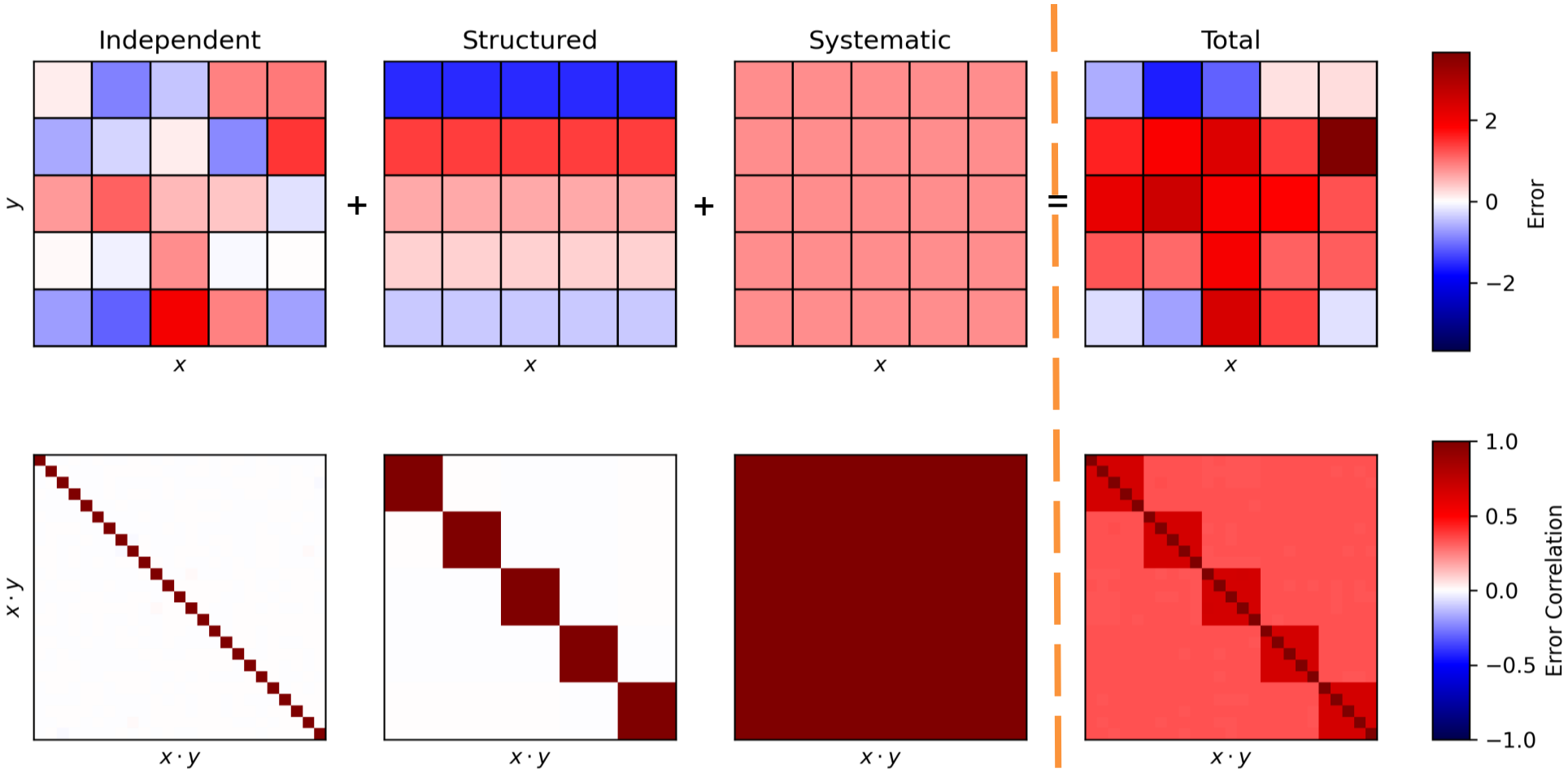
ND Datasets & Error-Correlation



✓ *Simply parameterizable*

✓ *Parameterizable via other terms*

ND Datasets & Error-Correlation



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

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

Error Correlation

What is Error Covariance?

Combines error correlation and uncertainty

$$S = U\,R\,U^T$$

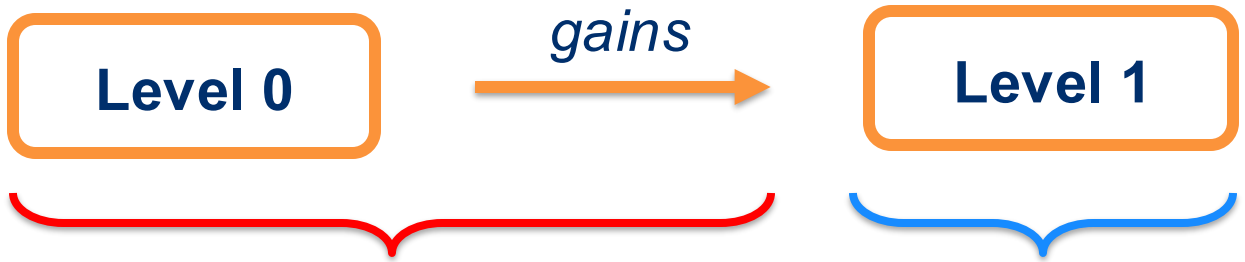
Random, systematic and structured uncertainty

- 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/imperial2026/

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



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

Input values → $L0, gains$

Random uncertainties → $u_r(L0), u_r(gains)$

Systematic uncertainties → $u_s(L0), u_s(gains)$

$L1$ $corr$

$u_r(L1)$ cov

$u_s(L1)$

$u_t(L1)$

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The CoMet Toolkit – UNC & obsarray

Maddie Stedman, Sam Hunt, Pieter De Vis, Rasma Ormane

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UNC

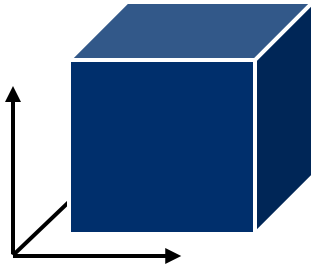
🔎 What is UNC?

- ❑ *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
  - **JCGM 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

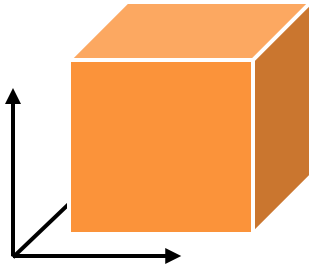
Observation Variables



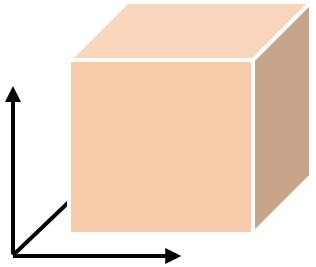
Metadata:
- Uncertainty Components

associated with

Uncertainty Variables



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

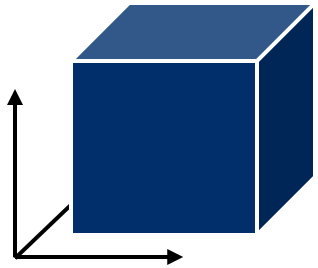


…

UNC Specification

Example – Temperature Dataset

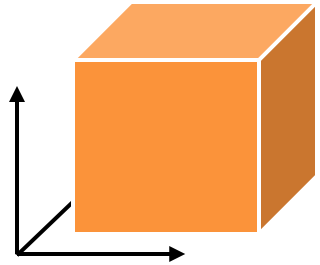
Observation Variables



temperature

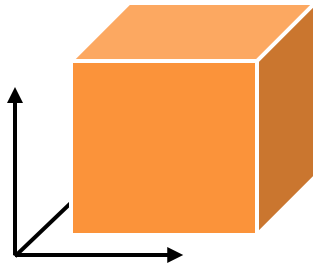
associated with

Uncertainty Variables



u_noise

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



u_calibration

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

```python
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

punpy

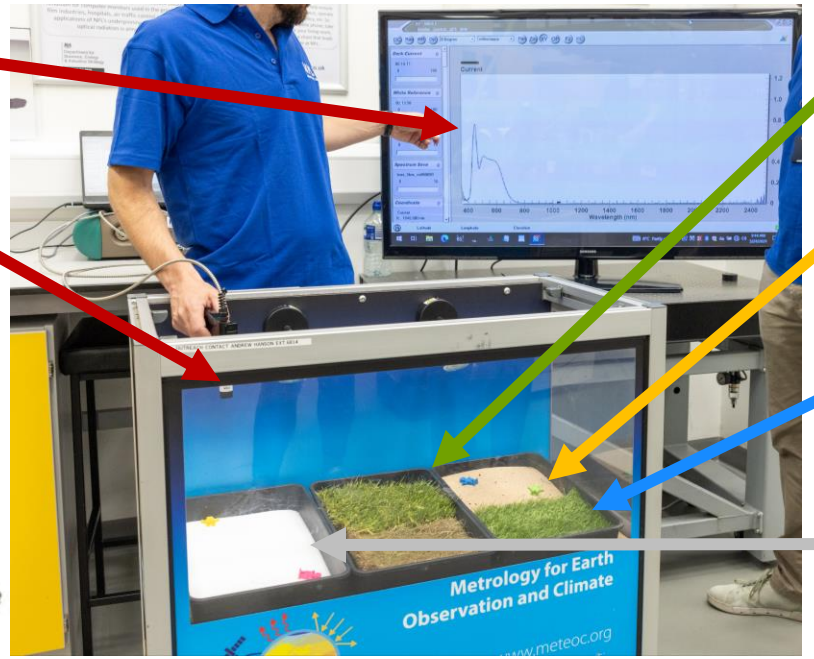
Please go to https://www.comet-toolkit.org/user-guide/training/imperial2026/

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

Spectrum

Spectrometer





Vegetation

Sand

Astro-turf

White reference

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Exercise 4

Please go to https://www.comet-toolkit.org/user-guide/training/imperial2026/

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)
- ❑ **Analyse** depending on application (temporal correlation)

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The CoMet Toolkit – Wrap-up

Maddie Stedman, Sam Hunt, Pieter De Vis, Rasma Ormane

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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**

LUNAR IRRADIANCE MODEL OF ESA

HYPERNETS

DTE-S2GOS

FDR4ATMOS

RPV4PICS

GRUAN

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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/

MetEOR

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Thank you for your attention!

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