Welcome! 👋

Mentimeter Survey

Code: 5322 5551

Today’s Exercises

comet-toolkit.org/user-guide/training/lps

WiFi Details
SSID: LPS2025
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Hello! 👋

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Mentimeter Survey

Code: 5322 5551

Today's Exercises

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📋Today's Agenda

1. **Presentation: CoMet Toolkit Introduction**
   - □ *What is CoMet?*
   - □ *Uncertainty 101*
   - □ *Tools Intro*
2. **Exercises**
   - □ **punpy** basics with in-situ type data
   - □ **obsarray** basics with EO type data
3. **"Real-life" Examples**

Today's Exercises

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The CoMet Toolkit – Uncertainties made easy

Pieter De Vis, Sam Hunt, Astrid Zimmermann, Maddie Stedman

National Physical Laboratory

LPS hands-on tutorial - 22/06/2025

Presentation Outline

1. CoMet Toolkit Introduction

- □ *Motivation & Overview*
- □ *Uncertainties 101*
- □ *CoMet Packages*
  - **punpy**
  - **obsarray**
- □ *Application examples*

Today's Exercises

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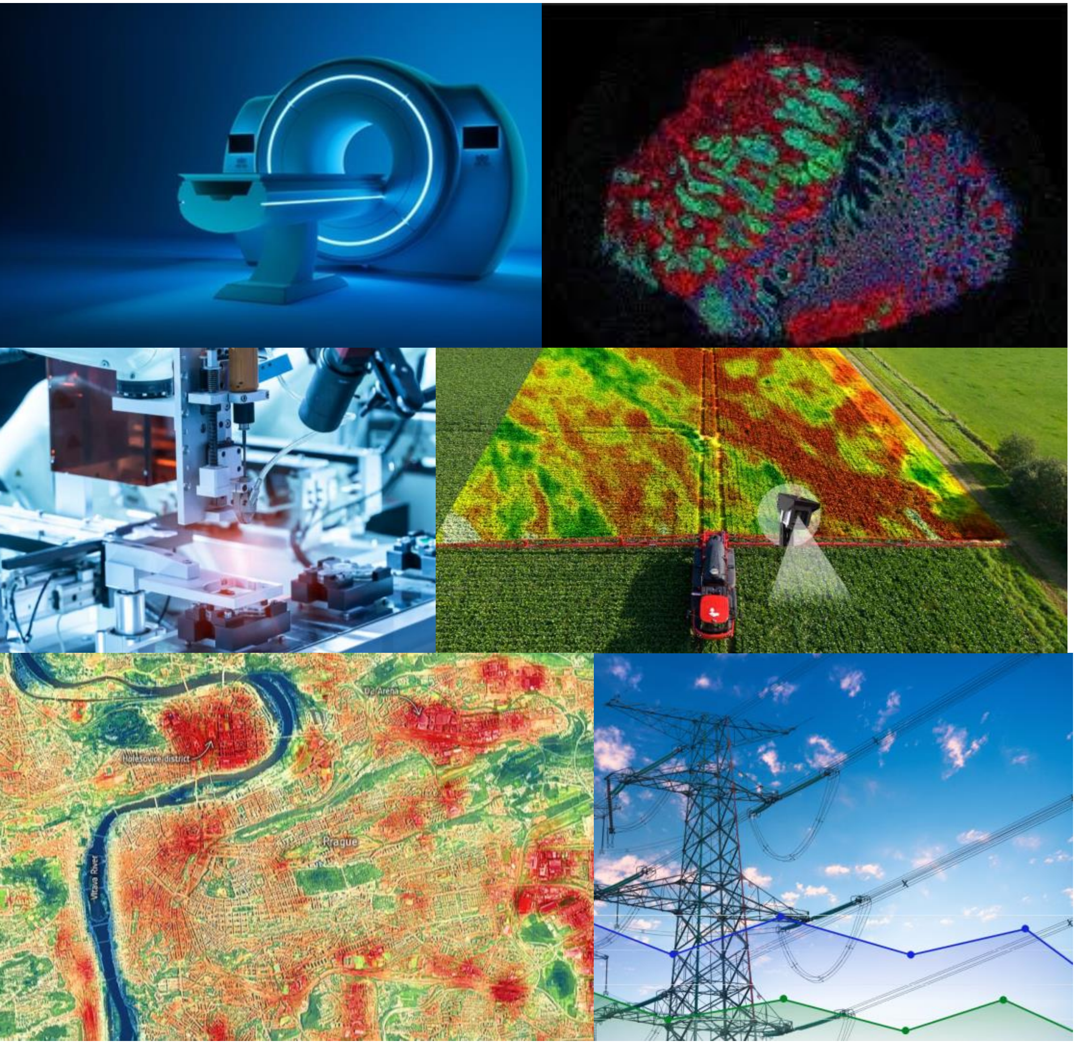
Measurements in Society



- 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

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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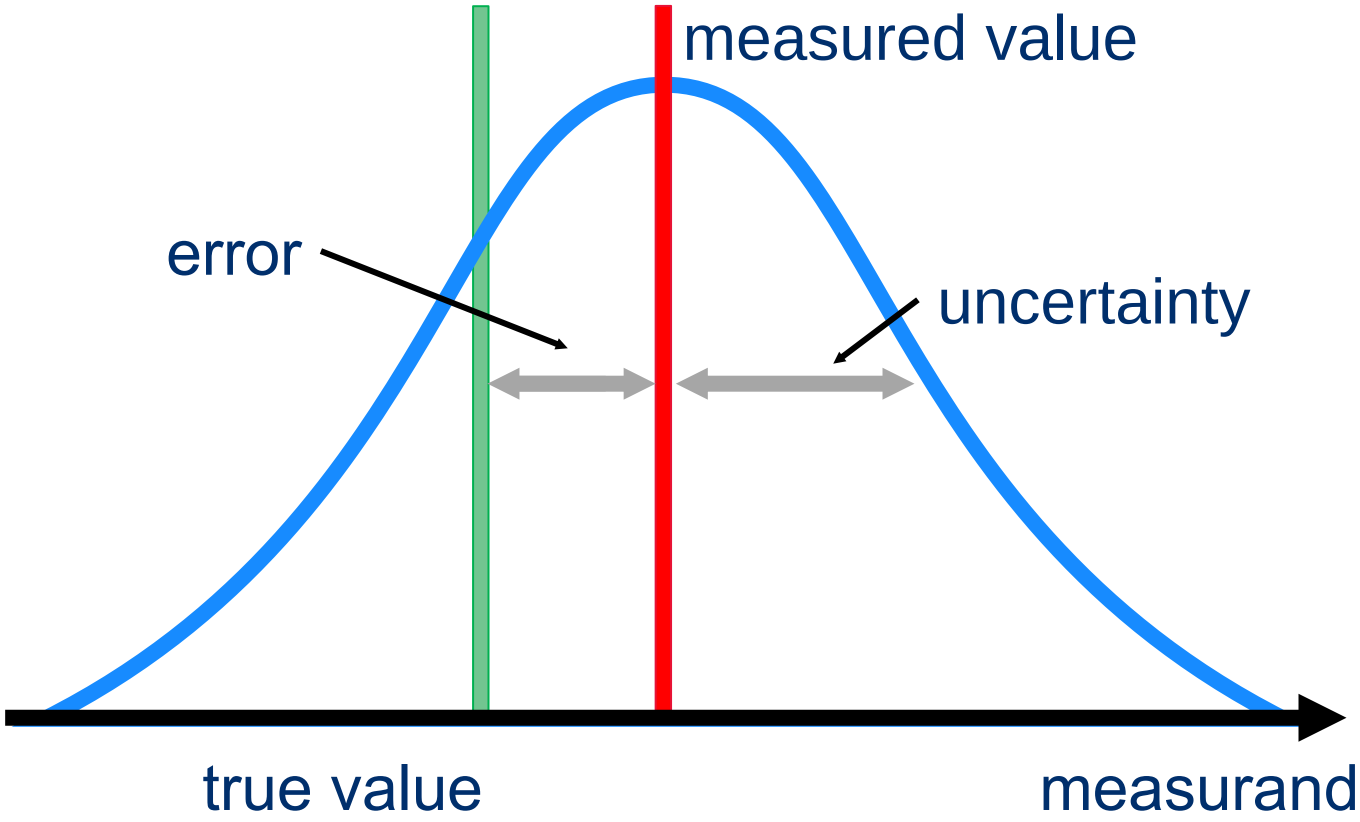
🔍 Uncertainties 101



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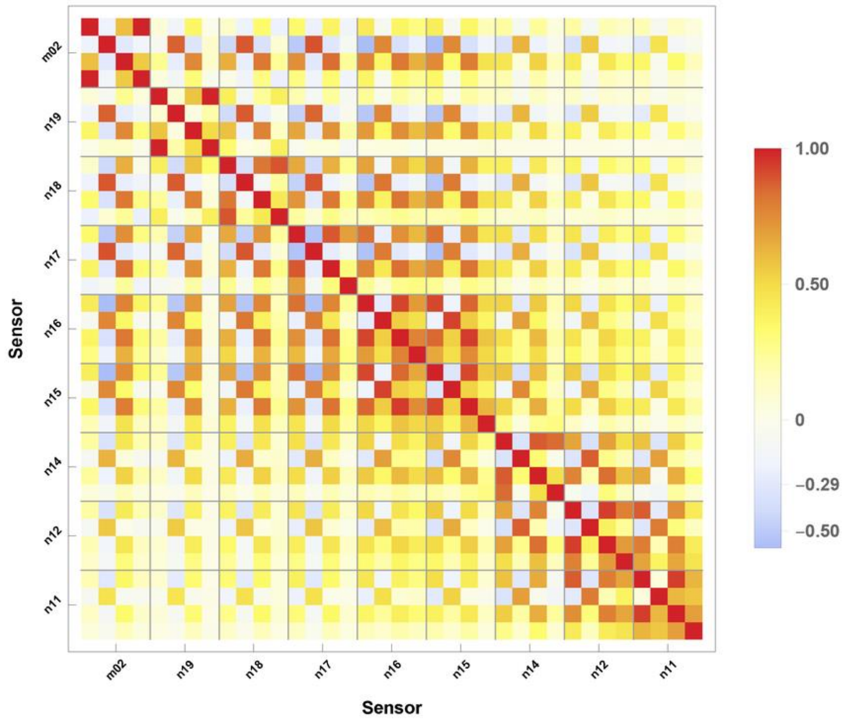
🔍 Error Correlation

🔎 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 off – affecting retrieval uncertainty
- □ Misleading confidence in trends



Error correlation matrix from Giering et al. 2019

🔍 Error Correlation

🔎 What is Error Covariance?

Combines error correlation and uncertainty

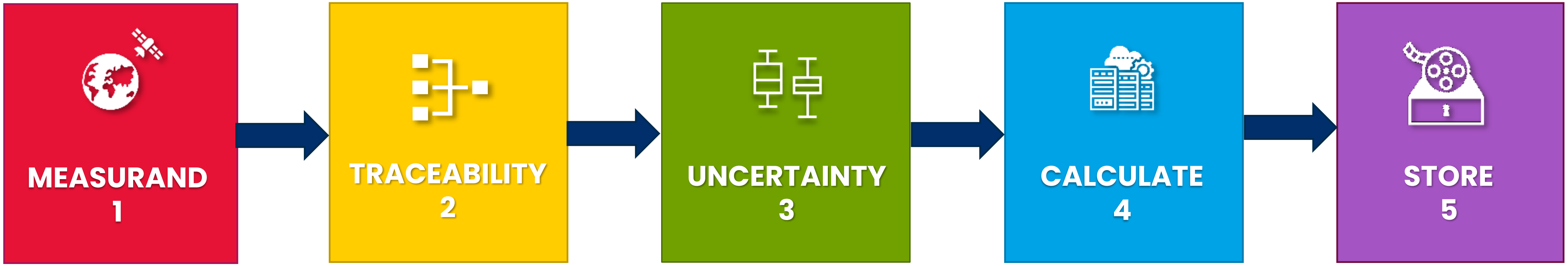
$$\boldsymbol{S} = \boldsymbol{U}\ \boldsymbol{R}\ \boldsymbol{U}^T$$

🤷 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

A Metrological Approach

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



MEASURAND 1

TRACEABILITY 2

UNCERTAINTY 3

CALCULATE 4

STORE 5

Define the measurand and measurement function

Establish the traceability with a diagram

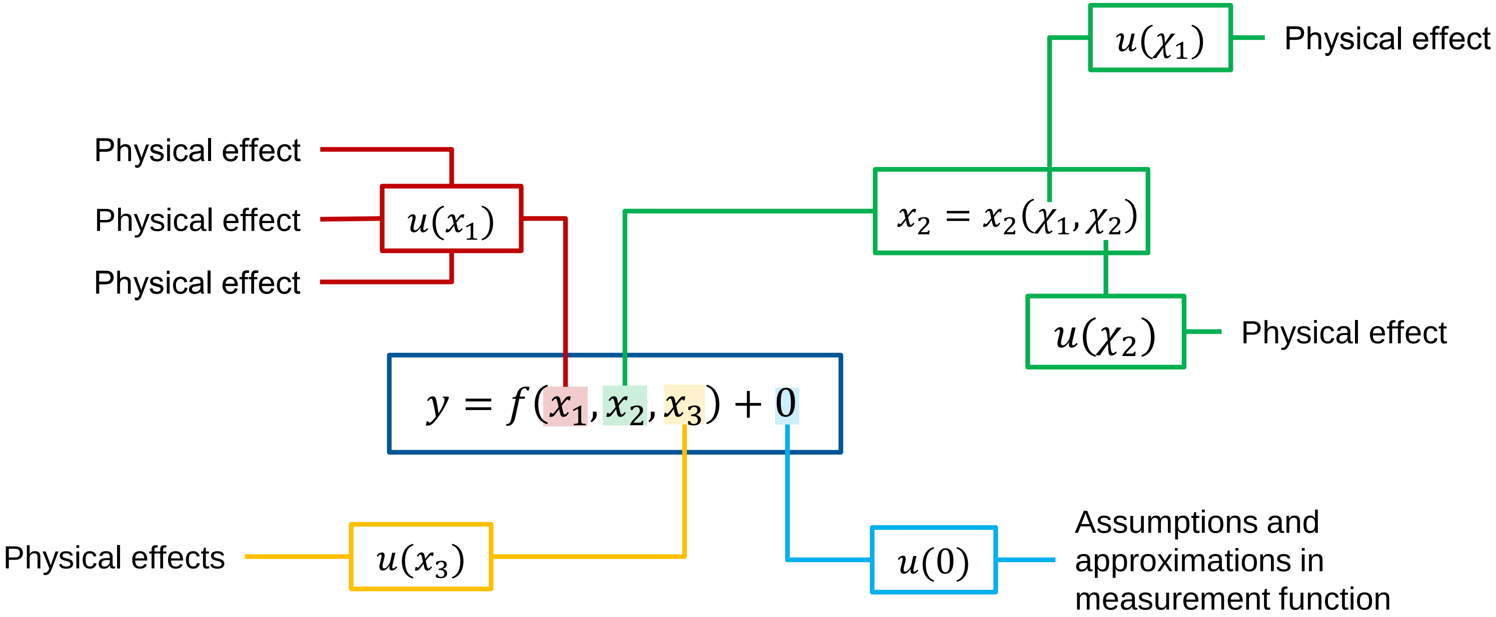
Evaluate each source of uncertainty and fill in an effects table

Calculate the data product and uncertainties

Record information for users

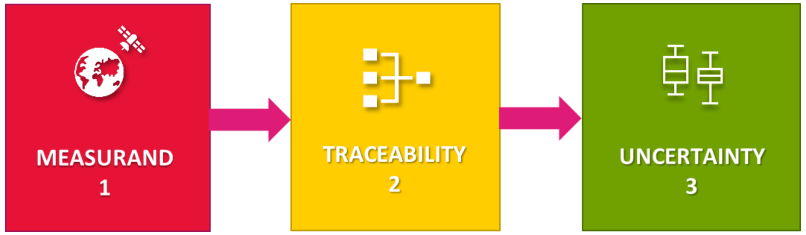
MEASURAND
1

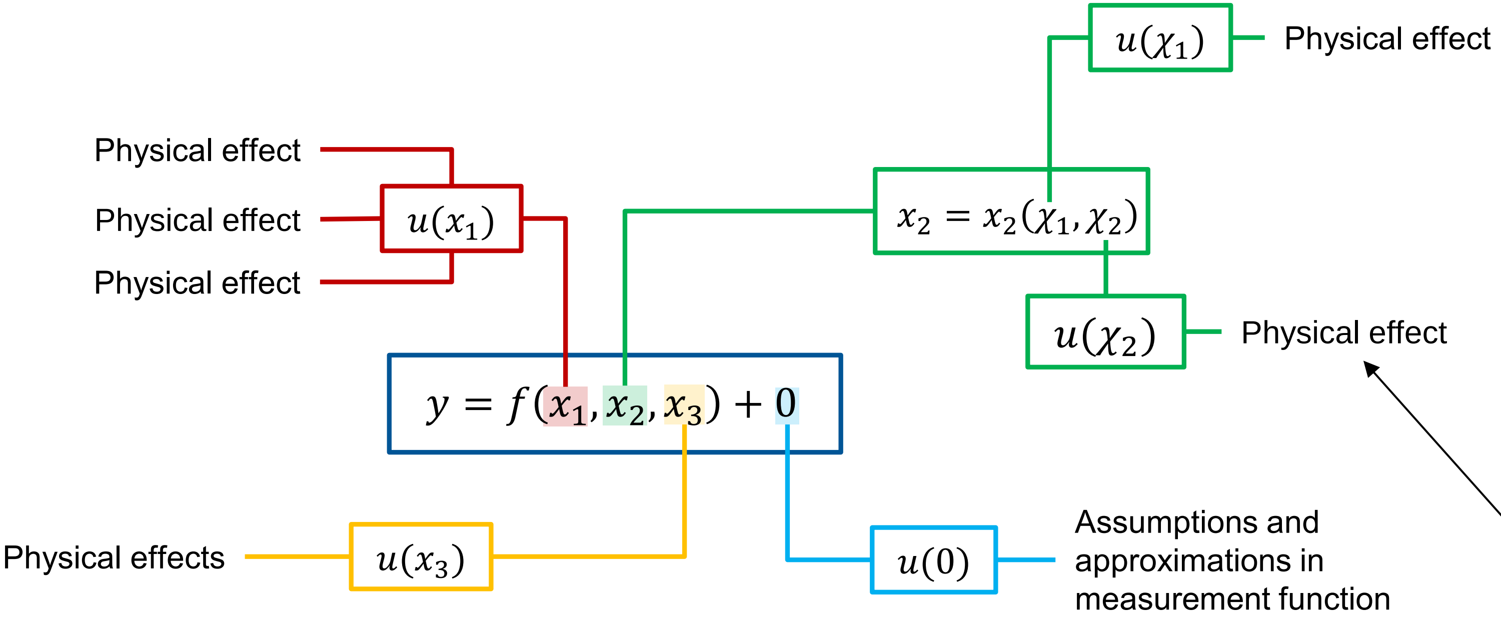
$$\boxed{y = f(x_1, x_2, x_3) + 0}$$

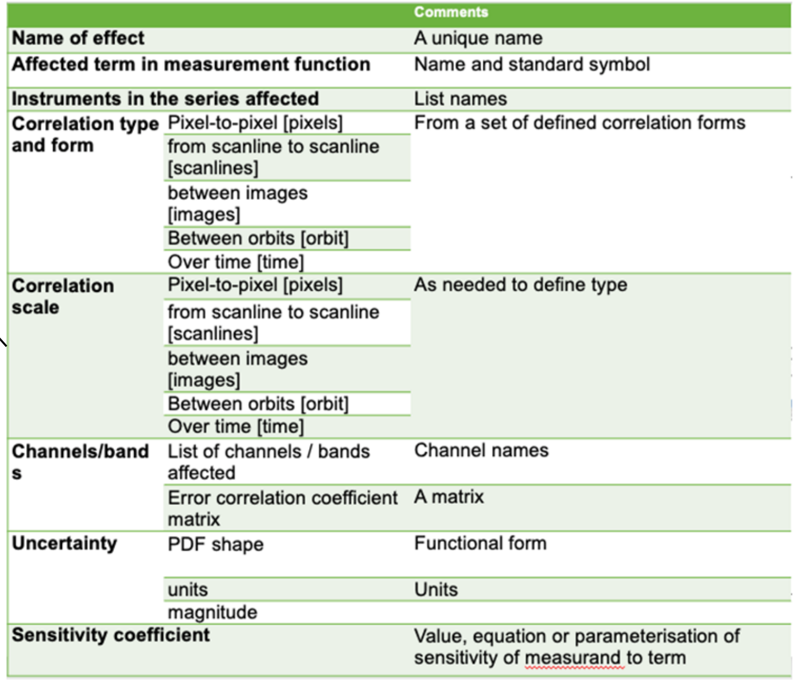


$y = f(x_1, x_2, x_3) + 0$

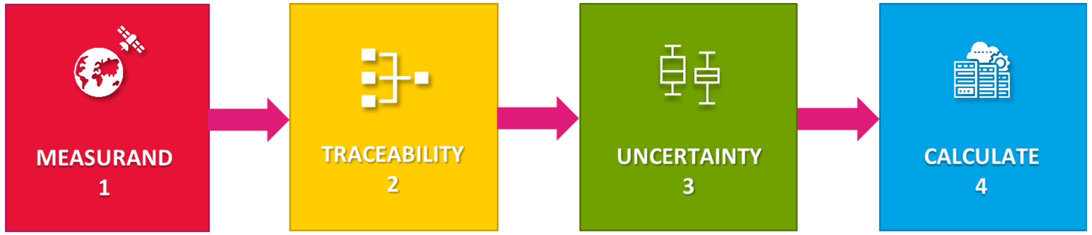
$x_2 = x_2(\chi_1, \chi_2)$







		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



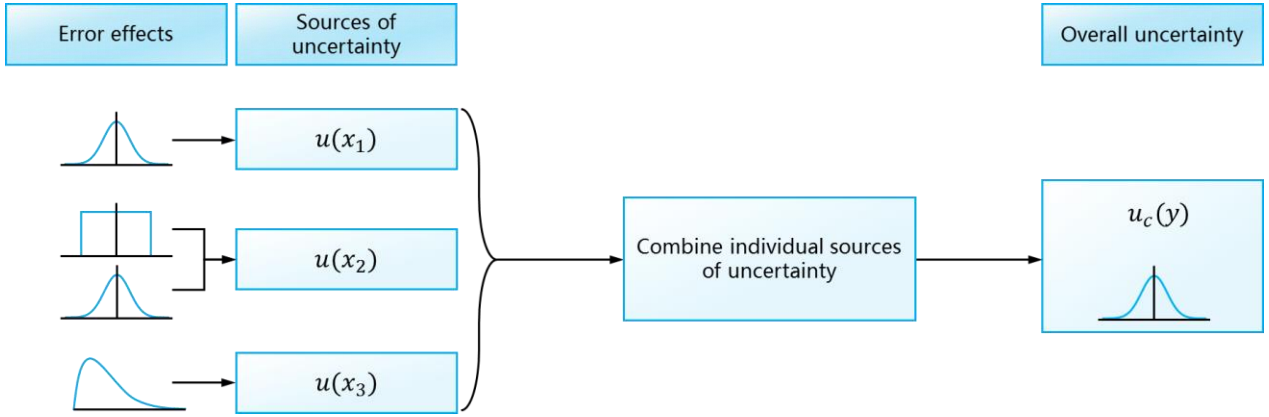
MEASURAND 1

TRACEABILITY 2

UNCERTAINTY 3

CALCULATE 4

punpy



Error effects

Sources of uncertainty

Overall uncertainty

$u(x_1)$

$u(x_2)$

$u(x_3)$

Combine individual sources of uncertainty

$u_c(y)$

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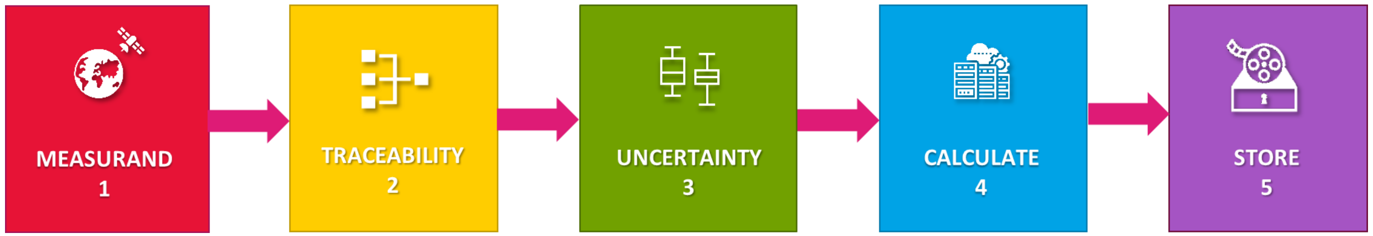
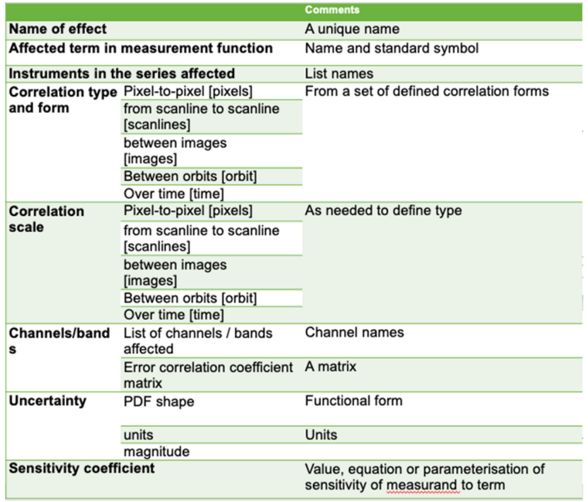


obsarray



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	Over time [time]	
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	between images [images]	
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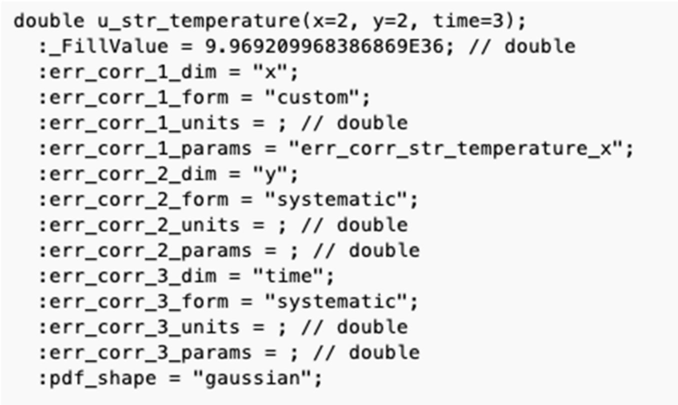

```
double u_str_temperature(x=2, y=2, time=3);
  :_FillValue = 9.969209968386869E36; // double
  :err_corr_1_dim = "x";
  :err_corr_1_form = "custom";
  :err_corr_1_units = ; // double
  :err_corr_1_params = "err_corr_str_temperature_x";
  :err_corr_2_dim = "y";
  :err_corr_2_form = "systematic";
  :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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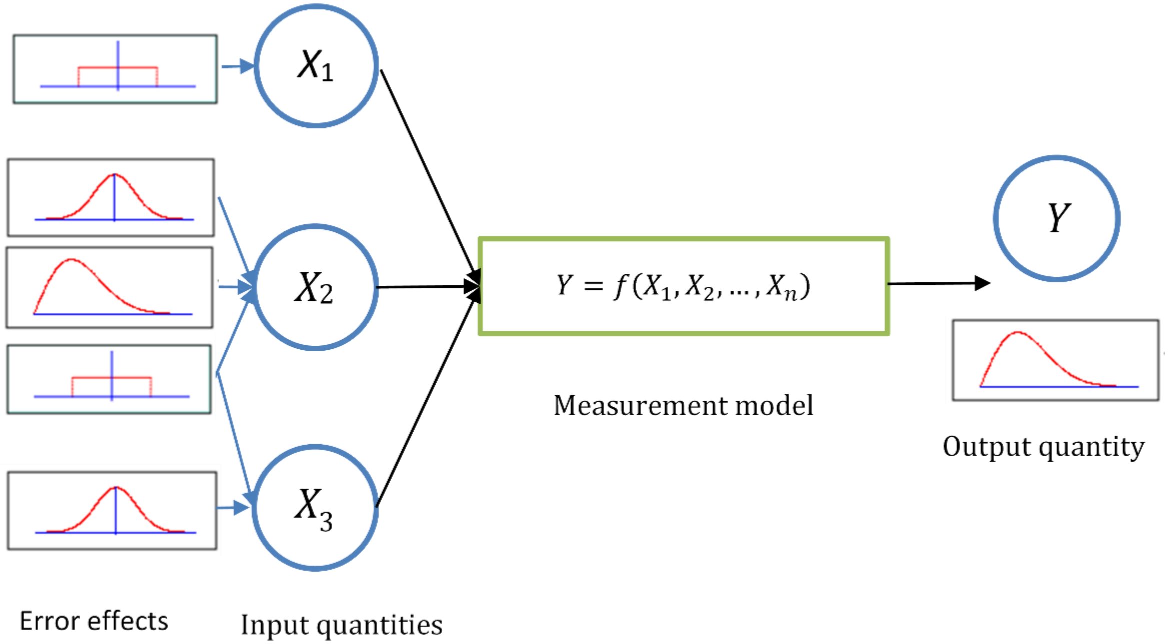
Propagating Uncertainties with punpy

- ❑ 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

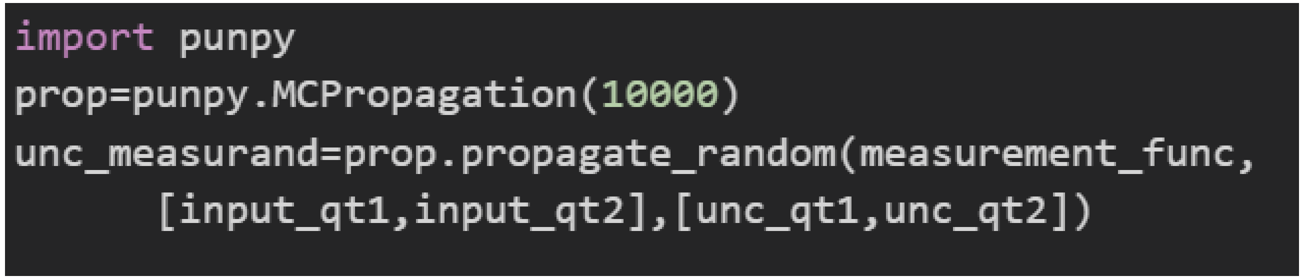
- ❑ ***Monte Carlo*** and ***Law of Propagation of uncertainties*** methods available



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])
```

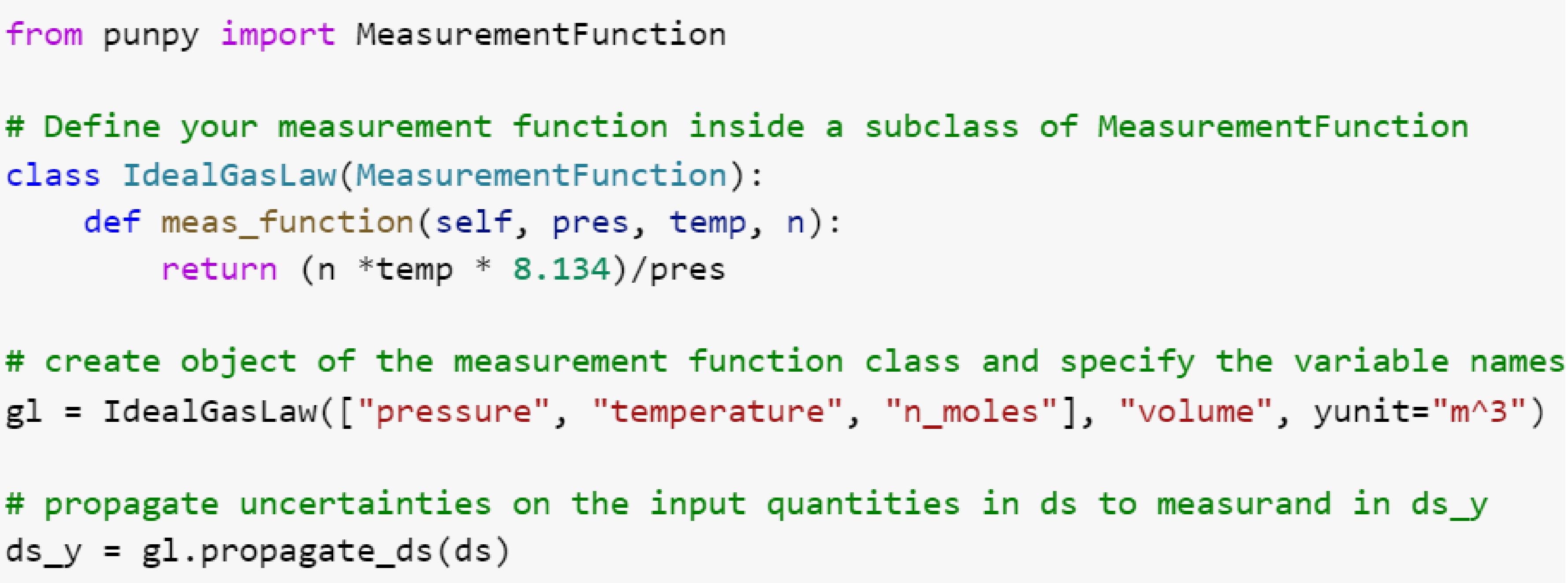
❑ **Measurement function** are defined as python functions that take arrays as input quantities and return an array as measurand

❑ Many optional **keywords** for flexible functionality

- *return_corr*
- *Corr_between*
- *Repeat_dims*
- *Parallel_cores*
- *Output_vars*
- …

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)
```

CoMet Packages:

obsarray

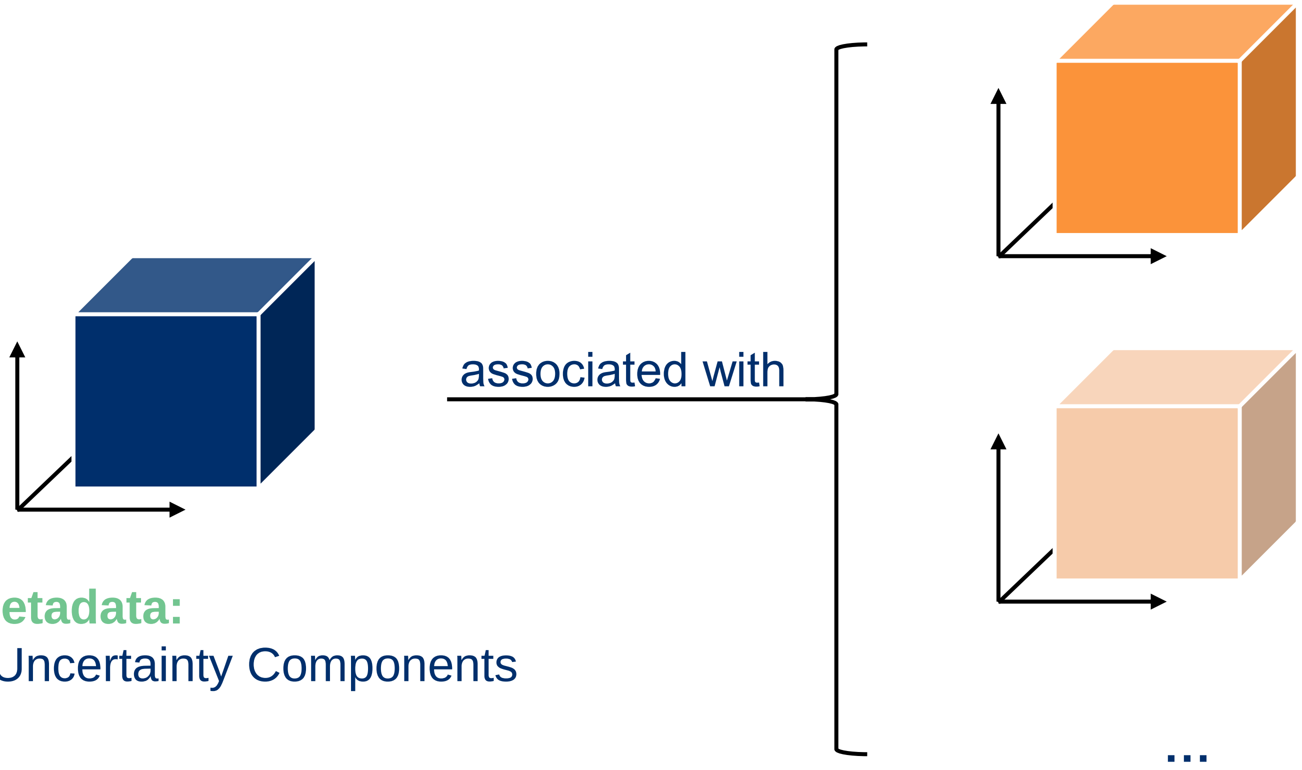
UNC Specification

obsarray

Uncertainty Variable Metadata

Observation Variables

Uncertainty Variables



associated with

...

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

Metadata:
- Uncertainty Components

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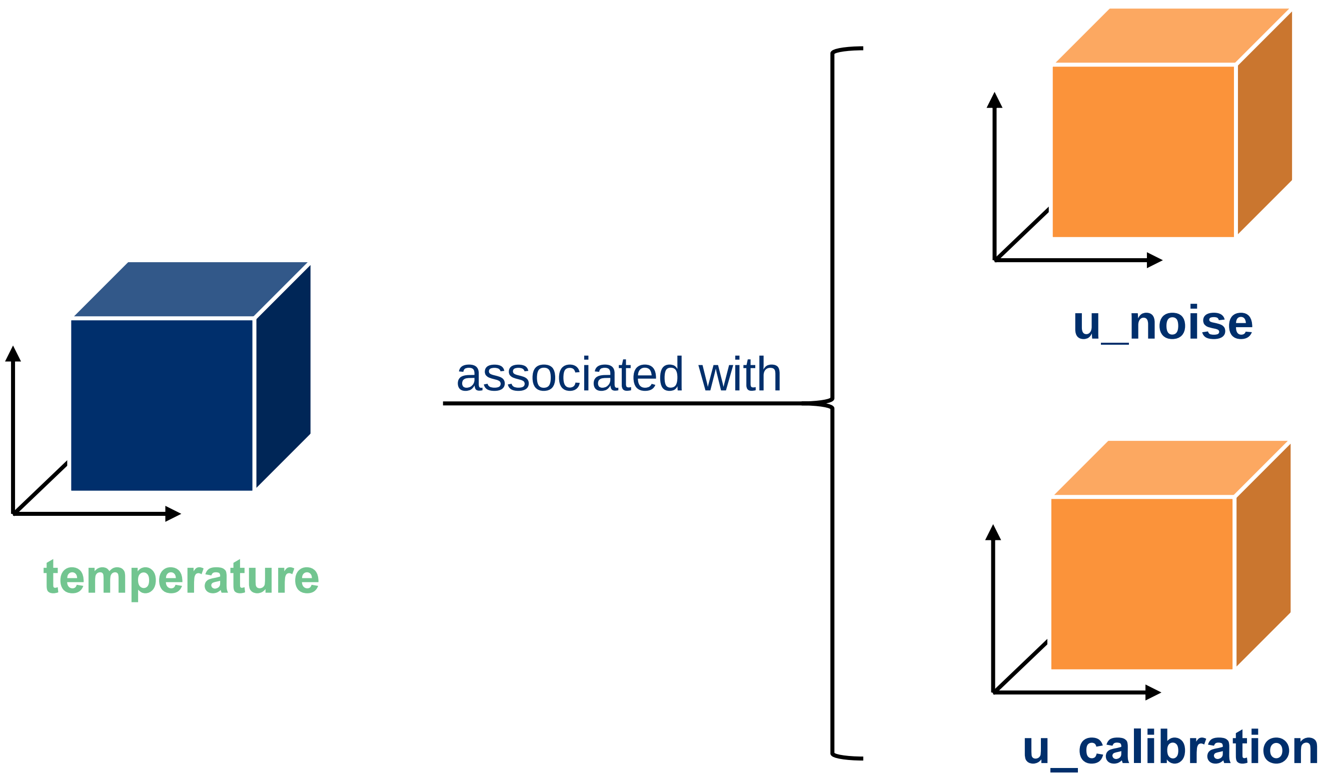
UNC Specification

Example – Temperature Dataset

Observation Variables

Uncertainty Variables



Metadata:

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

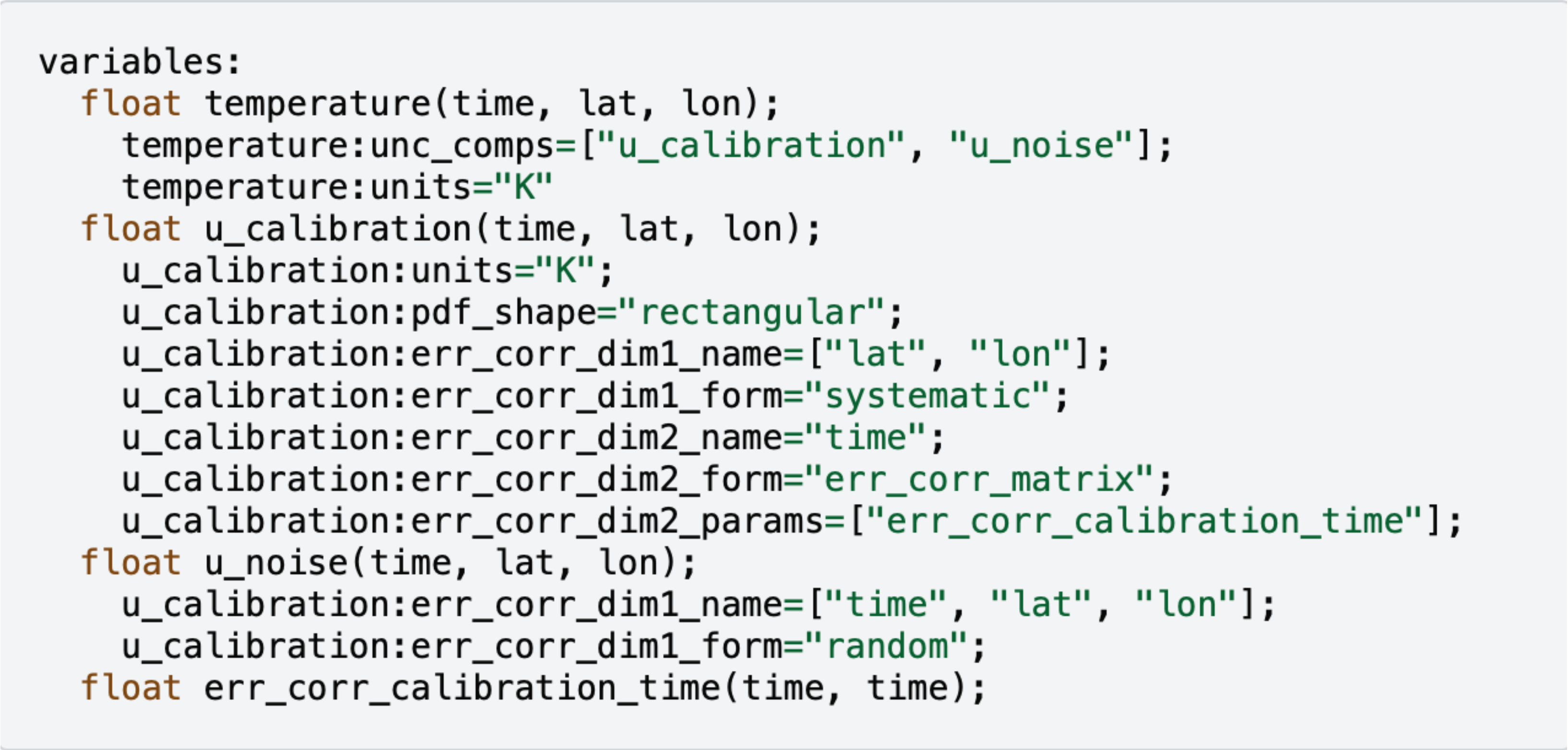
Metadata:

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

📃UNC Specification

obsarray

🌡Example – Temperature Dataset



```
variables:
  float temperature(time, lat, lon);
    temperature:unc_comps=["u_calibration", "u_noise"];
    temperature:units="K"
  float u_calibration(time, lat, lon);
    u_calibration:units="K";
    u_calibration:pdf_shape="rectangular";
    u_calibration:err_corr_dim1_name=["lat", "lon"];
    u_calibration:err_corr_dim1_form="systematic";
    u_calibration:err_corr_dim2_name="time";
    u_calibration:err_corr_dim2_form="err_corr_matrix";
    u_calibration:err_corr_dim2_params=["err_corr_calibration_time"];
  float u_noise(time, lat, lon);
    u_calibration:err_corr_dim1_name=["time", "lat", "lon"];
    u_calibration:err_corr_dim1_form="random";
  float err_corr_calibration_time(time, time);
```

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obsarray

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!

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CoMet Application Examples

punpy

obsarray

comet_maths

CoMet Toolkit in Action

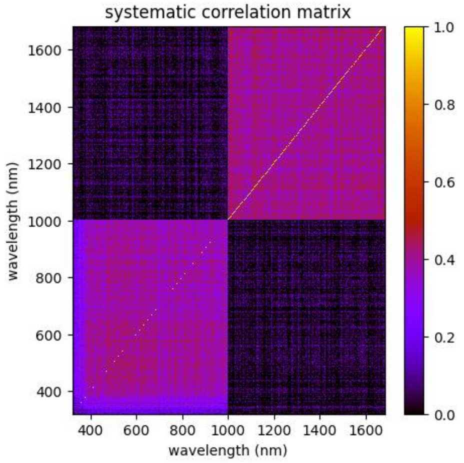
- Validated against **NIST** uncertainty engine:

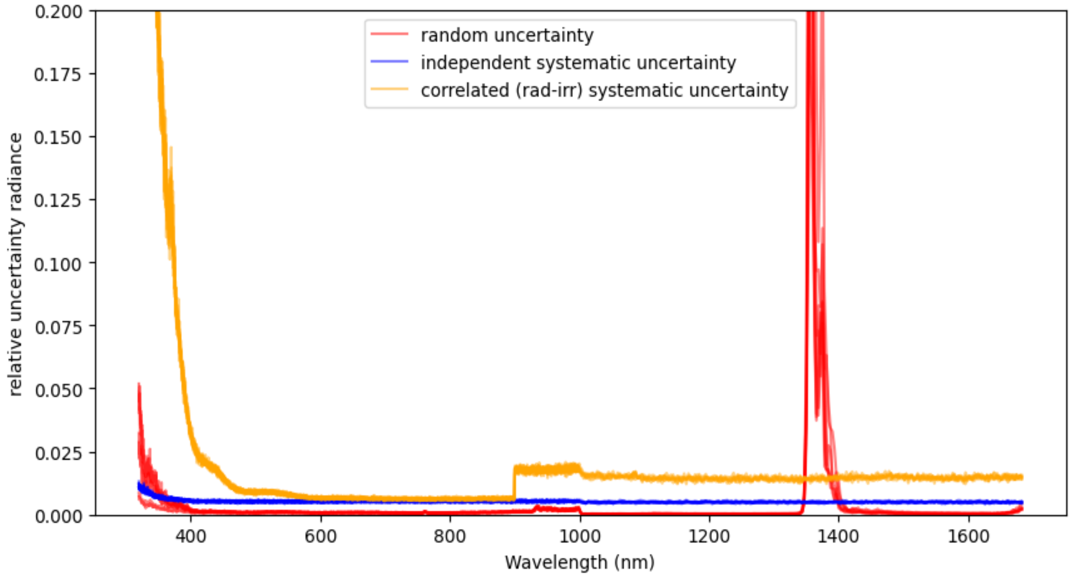
  https://colab.research.google.com/github/comet-toolkit/comet_training/blob/main/NIST_example.ipynb

- *CoMet* is used in various other projects, such as **QA4EO**, **HYPERNETS**, **CHIME L2**, **FLEX** validation, **TRUTHS** science studies, **LIME**, **FRM4SOC**, **RPV4PICS**

- **Example** from *hypernets_processor*:

  Hypernets is an automated network of in-situ instruments measuring reflectance for L2 satellite validation





🎉 CoMet Release

□ V1.0 of Comet toolkit has been released as **open source** toolkit:

- www.comet-toolkit.org
- github.com/comet-toolkit

□ Accompanied by training material (**Jupyter** notebooks hosted on google colab):

- www.comet-toolkit.org/examples

□ Documentation & ATBD for individual tools:

- obsarray.readthedocs.io/en/latest/
- punpy.readthedocs.io/en/latest/
- comet-maths.readthedocs.io/en/latest/

📈Outlook

❑ **Current release** will be presented De Vis & Hunt (in prep)

❑ 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!

❑ This has been our first step into this way of working, **many more ideas in a roadmap** to building up a comprehensive set of tools

- e.g. retrieval tool/optimisation, BRDF tool, Look-up tables for faster processing, etc.

✅ Summary

□ The **CoMet toolkit** is an open-source software project to develop Python tools for the handling of error-covariance information in the analysis of measurement data

□ This toolkit is based on **robust metrology**, and makes dealing with complexities of uncertainties much easier

□ Includes **obsarray**, **punpy** **&** **comet_maths** as initial offering, to be extended

□ These tools are already being used operationally in various projects (e.g. Hypernets)

Exercises

□ Please go to www.comet-toolkit.org/user-guide/training/

Mentimeter

Today's Exercises

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