# Navigating the unknown: enhancing aquatic remote sensing products through *uncertainty*

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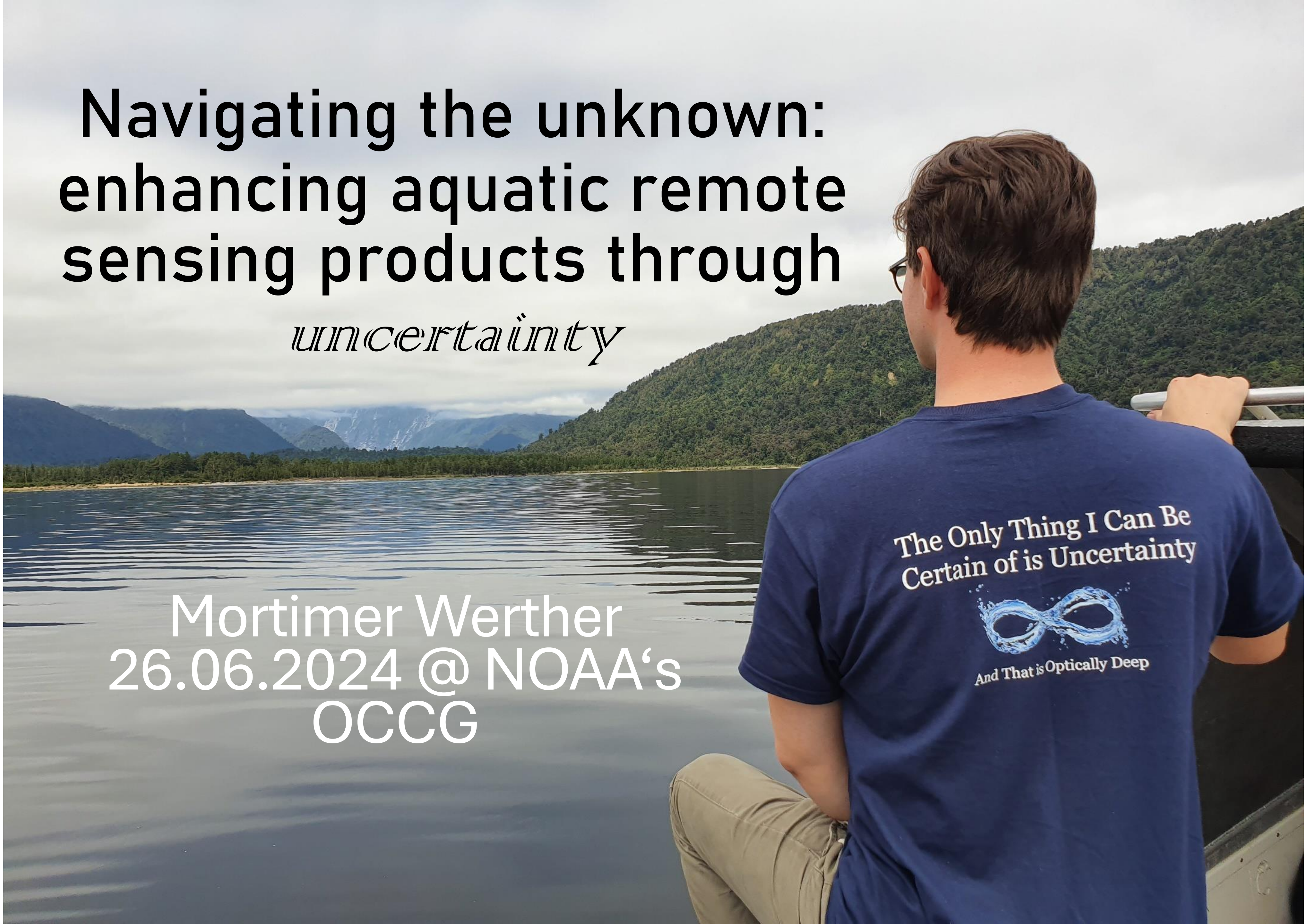


# About me

Eawag
Swiss Federal Institute of Aquatic Science and Technology

PostDoc in the aquatic remote sensing group at EAWAG; Dübendorf, Zurich

My primary research interests include:

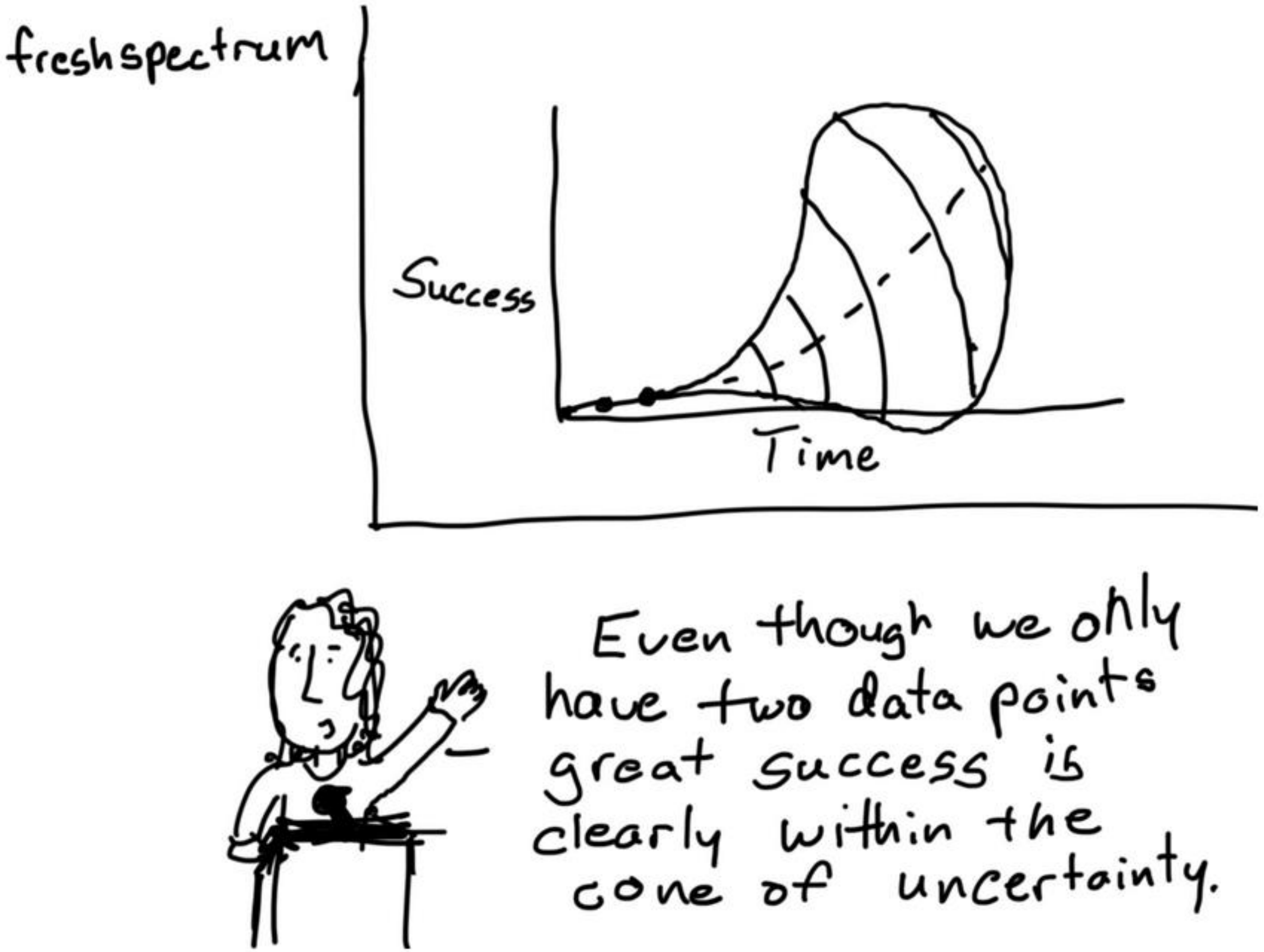
- Aquatic remote sensing of inland and coastal waters
  - IOPs, aquatic optics, phytoplankton, primary production, freshwater ecology
  - RS algorithm development
  - Cal/val of EO products

Work funded through SNSF grant:
*Lake Primary Production using PACE (Lake3P)*

1. Intro
2. Uncertainty: background
3. Practical examples: embracing uncertainty
4. Concluding remarks

# 1. The cone of uncertainty


# The cone of uncertainty




https://freshspectrum.com/cone-of-uncertainty-cartoons/

# The omnipresence of uncertainty in aquatic remote sensing

Atmospheric correction:

$$L_t(\lambda) = L_p(\lambda) + L_r(\lambda) + t(\lambda)L_w(\lambda) + L_a(\lambda)$$

Remote sensing reflectance ($R_{rs}$):

$$R_{rs}(\lambda) = \frac{L_u(\lambda)}{E_d(\lambda)} \propto f/Q \frac{b_b(\lambda)}{a+b_b(\lambda)}$$

$R_{rs}$ uncertainty

E.g.: absorption by phytoplankton:

$$a_{ph}(\lambda) = a(\lambda) - a_w(\lambda) - a_{CDOM+NAP}(443)e^{-S(\lambda-443)}$$

IOP uncertainty

E.g.: primary production (PP) at depth (z) after Lee et al., 1996:

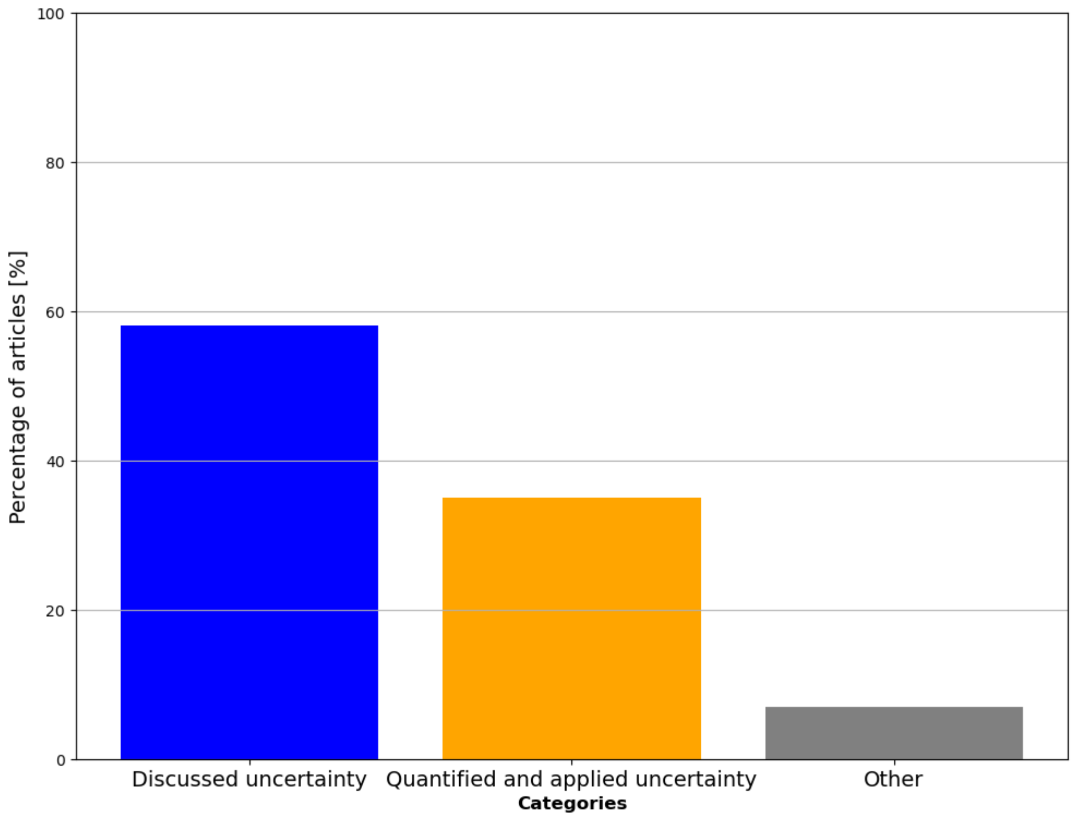
$$pp(z) = \phi_f \int_\lambda a_{ph}(\lambda)E_0(\lambda)d\lambda$$

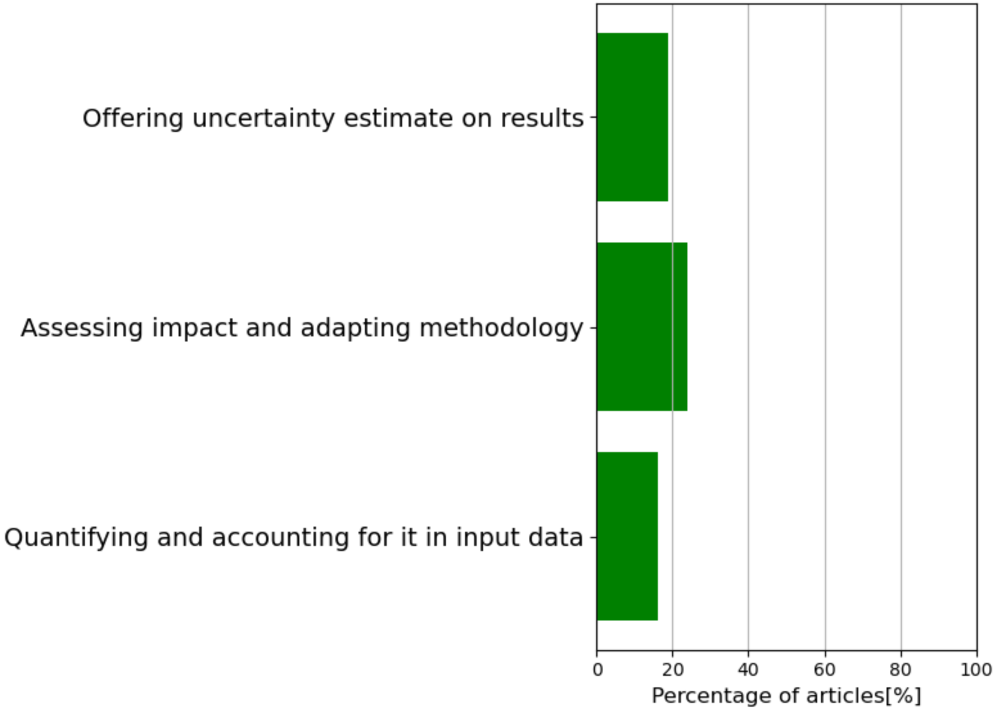
Downstream product uncertainty

# Representation in aquatic remote sensing literature?

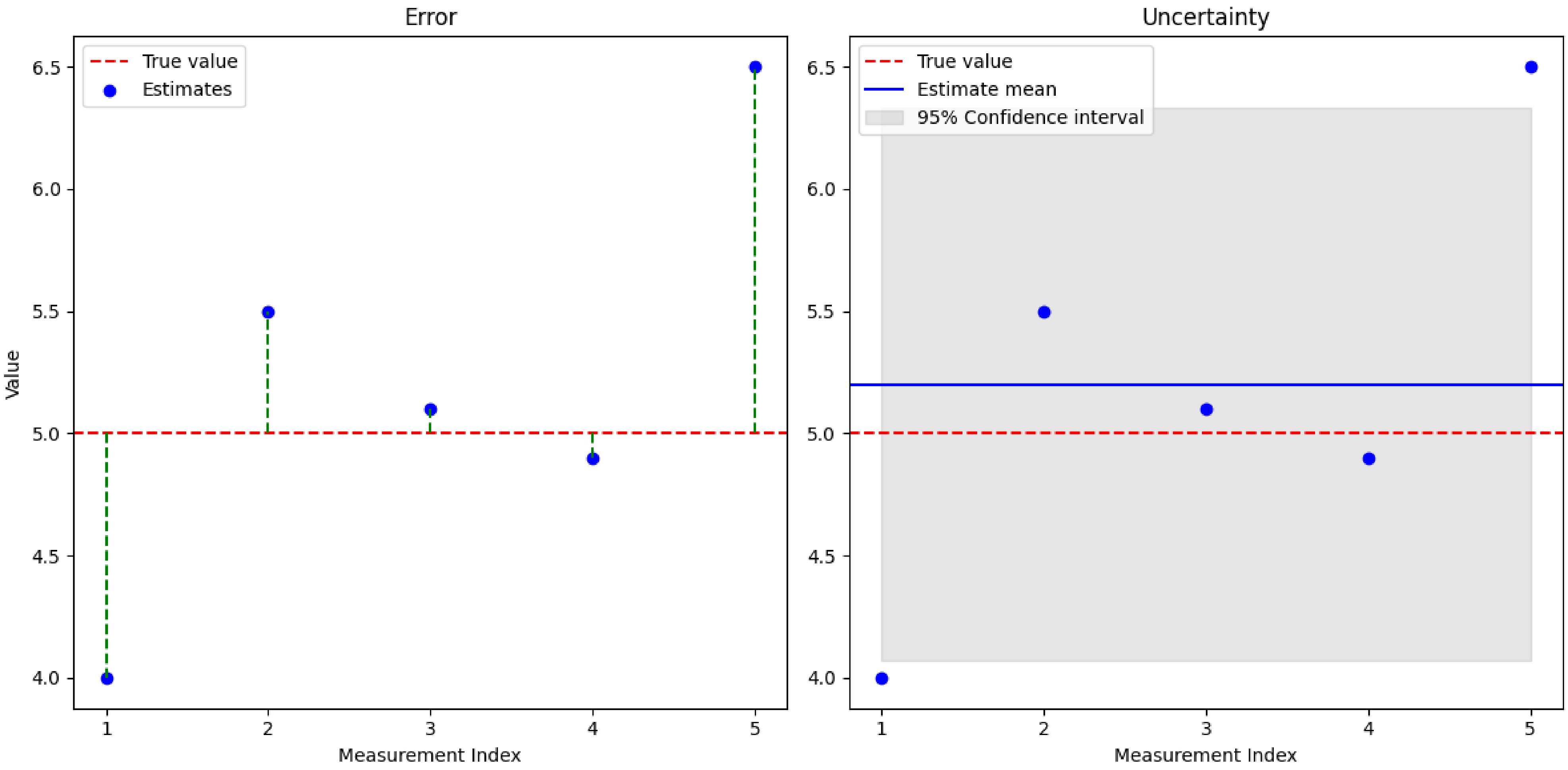
Based on: 100 research articles on aquatic remote sensing published in major journals in 2021–2023 (20 articles per journal) from:

1. Elsevier's *Remote Sensing of Environment* volumes 284 to 290
2. Elsevier's *International Journal of Applied Earth Observation and Geoinformation* volumes 104 to 117
3. MDPI's *Remote Sensing* volumes 15(3) to 15(7)
4. Frontier's *Frontiers in Remote Sensing* volumes 2 to 4
5. IEEE's *IEEE Transactions on Geoscience and Remote Sensing* volumes 60 to 61.



# 2. Uncertainty: Background – Error vs. Uncertainty



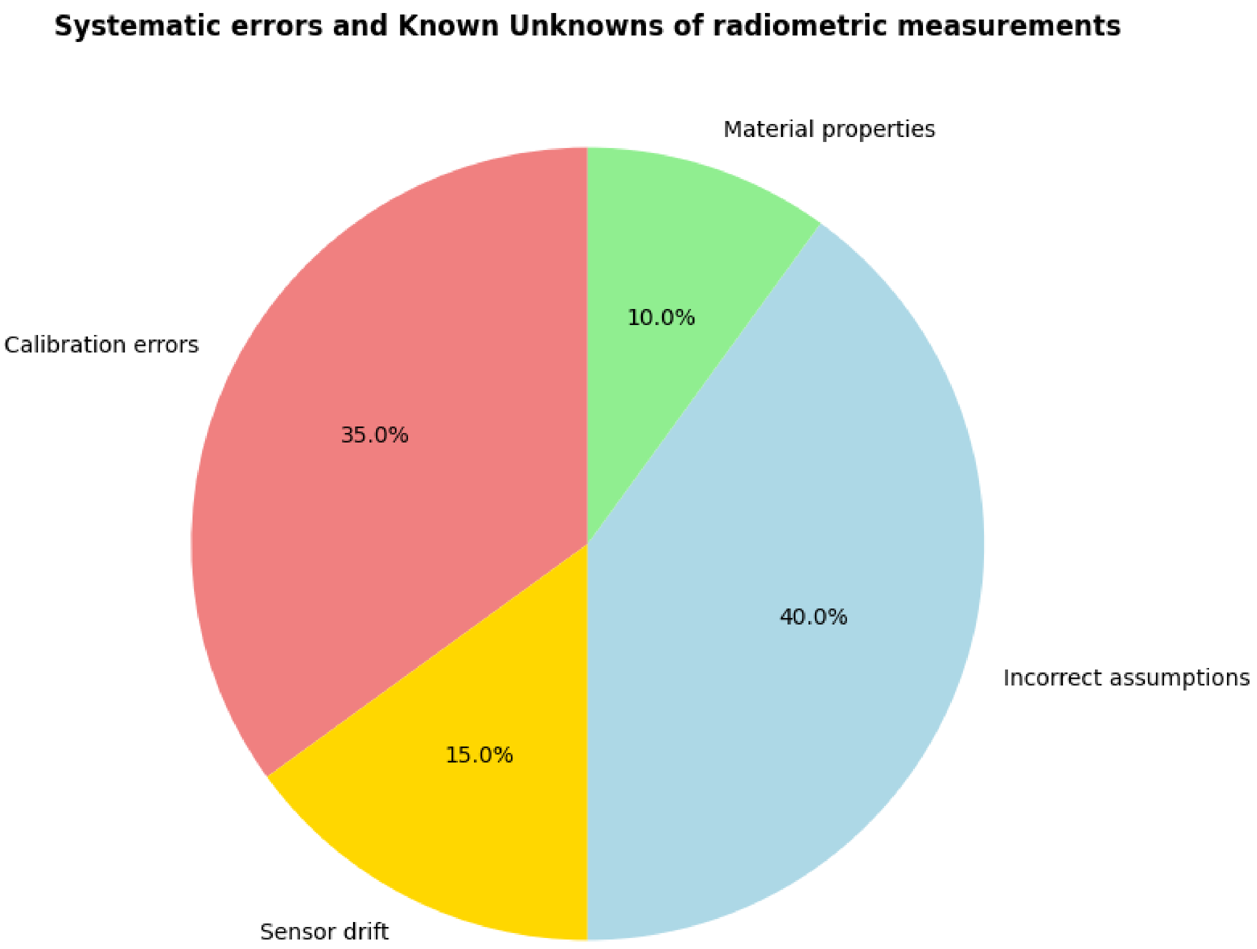
# Error sources

Systematic error: Affects the accuracy of a measurement, i.e. how much an estimated value differs from a "true" reference value.

Random error: Affects the precision of a measurement, i.e. the dispersion between multiple individual measurements of the same quantity, creating an uncertainty on the result.

**IOCCG (2019).** Uncertainties in Ocean Colour Remote Sensing. Mélin F. (ed.), IOCCG Report Series, No. 18, International Ocean Colour Coordinating Group, Dartmouth, Canada.

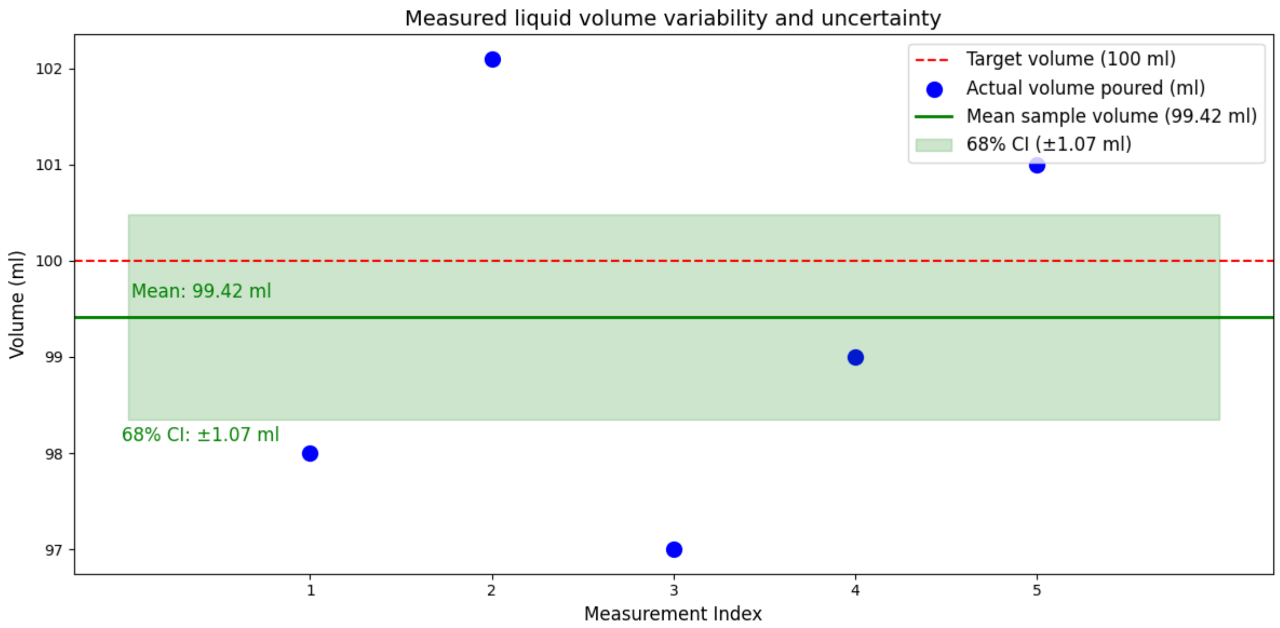
# Systematic error sources: $R_{rs}$ example



# Random error sources

Stems from unpredictable / stochastic variations in a sample, measurement process or data processing, causing uncertainty in individual values. Sources include:

1. Spatial and temporal variability in a sample/pixel
2. Surface glint and wind effects
3. Thermal or photon noise in a sensor
4. Human error



# Analytical uncertainty propagation: Uncorrelated uncertainties

Uncorrelated uncertainties occur with measurements that have independent error sources. For example *in situ* vs satellite-derived radiometric products.

Analytical propagation typically uses derivatives to express the sensitivity of a variable *y* to small changes in a variable *x* due to uncertainty. In the simple case of independent variables with uncorrelated uncertainties, this leads to the familiar sum-of-squares method:

$$\sigma_y^2 = \left(\sigma_{x_1}\frac{\partial y}{\partial x_1}\right)^2 + \left(\sigma_{x_2}\frac{\partial y}{\partial x_2}\right)^2 + \dots$$

# Analytical uncertainty propagation: Correlated uncertainties

Correlated uncertainties arise when measurements share common error sources or are influenced by the same underlying factors.

For this more general case of multiple correlated variables, the Jacobian matrix J is used with $\Sigma_x$, $\Sigma_y$ the covariance matrices for multidimensional variables x, y:

$$\mathbf{\Sigma_y} = \mathbf{J}\mathbf{\Sigma_x}\mathbf{J}^{\mathrm{T}}$$

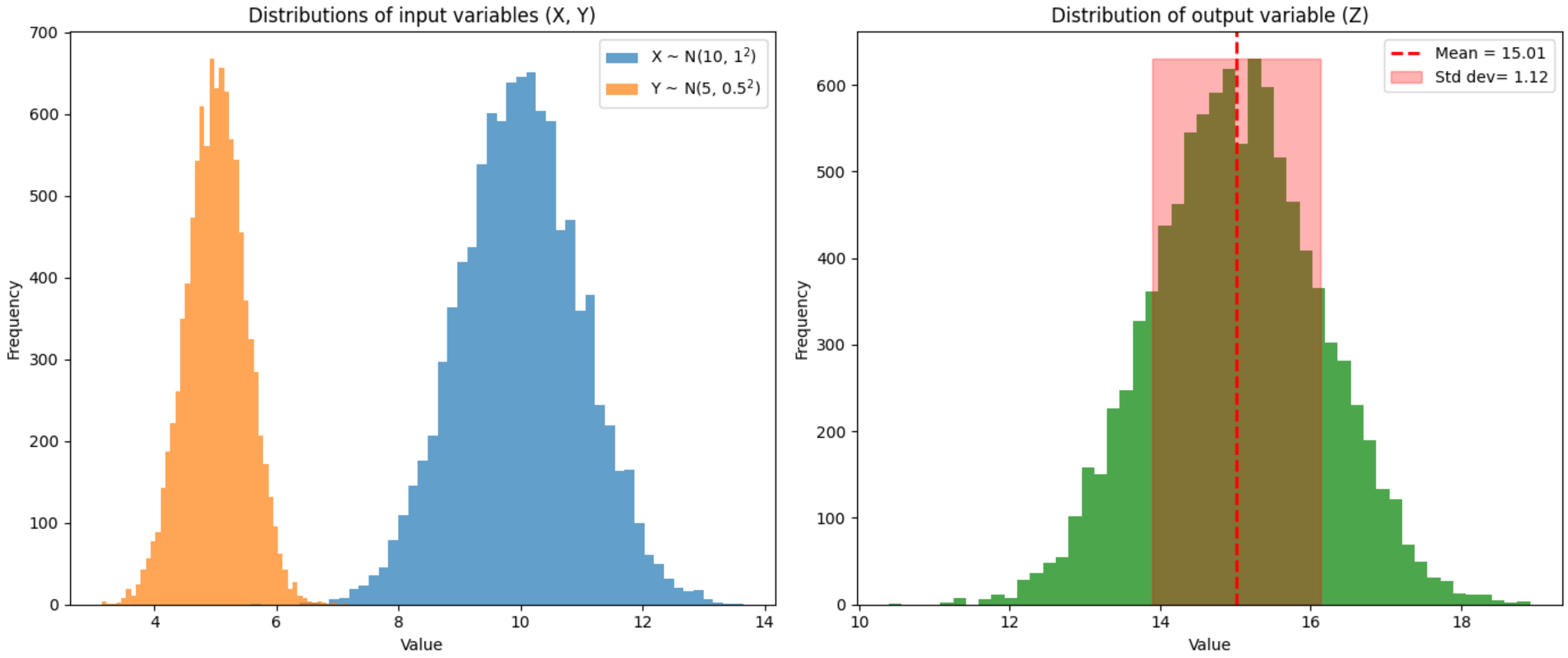
$$\begin{bmatrix} \sigma_{y_1}^2 & \sigma_{y_1 y_2} \\ \sigma_{y_1 y_2} & \sigma_{y_2}^2 \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \frac{\partial y_1}{\partial x_3} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \frac{\partial y_2}{\partial x_3} \end{bmatrix} \begin{bmatrix} \sigma_{x_1}^2 & \sigma_{x_1 x_2} & \sigma_{x_1 x_3} \\ \sigma_{x_1 x_2} & \sigma_{x_2}^2 & \sigma_{x_2 x_3} \\ \sigma_{x_1 x_3} & \sigma_{x_2 x_3} & \sigma_{x_3}^2 \end{bmatrix} \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_2}{\partial x_1} \\ \frac{\partial y_1}{\partial x_2} & \frac{\partial y_2}{\partial x_2} \\ \frac{\partial y_1}{\partial x_3} & \frac{\partial y_2}{\partial x_3} \end{bmatrix}$$

See: Guide to the expression of uncertainty in measurement (GUM) or the IOCCG 2019 report.

# Numerical uncertainty propagation: Monte Carlo simulation

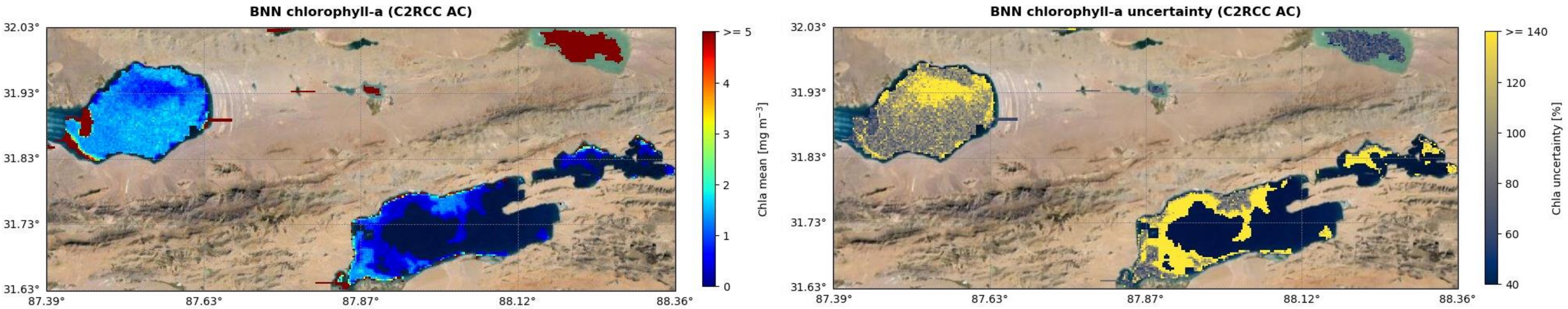
Let's assume we are measuring a physical quantity that depends on two variables, X and Y, where both variables have associated uncertainties. We'll calculate a derived quantity Z as Z = X + Y

- X has a mean of 10 and a standard deviation of 1.
- Y has a mean of 5 and a standard deviation of 0.5.



# 3. Embracing uncertainty: The benefits

*"Embracing uncertainty means **recognizing** its inherent presence, **actively incorporating** it into research and decision-making processes, **leveraging** it as a driving force for innovation and for **gaining** a deeper understanding of aquatic remote sensing models and products."*




Code: https://github.com/mowerther/BNN_2022

… and is more than just providing an uncertainty estimate alongside a RS product

*Werther, M. and Burggraaff, O. (2023): Dive Into the Unknown: Embracing Uncertainty to Advance Aquatic Remote Sensing. J. Remote Sens. 2023;3:0070.*

# Example A: Targeted improvement through uncertainty analysis

… by quantifying the contributions of each input to the overall uncertainty.

Consider the measurements of Chl*a* through a fluorometer for *in situ* data:

$$\mathrm{Chl}a = \frac{F_m}{F_m - 1}(F_o - F_a)F_s\frac{V_{ex}}{V_f}$$

here:

- $V_f$ is the sample volume
- $V_{ex}$ is the extraction volume
- $F_o$ and $F_a$ are the fluorometer readings before and after acidification
- and $F_m$ and $F_s$ are calibration constants

*Which parameter contributes most to the uncertainty in Chla?*

# Example A: Targeted improvement through uncertainty analysis

Consider the following values from an actual experiment:

$F_o$ = 680 ± 2
$F_a$ = 395 ± 2

$V_{ex}$ = 0.0052 ± 0.0001 L, and $V_f$ = 0.2880 ± 0.0005 L

with empirically determined calibration factors:
$F_m$ = 1.95 ± 0.05 and $F_s$ = 0.32 ± 0.02.

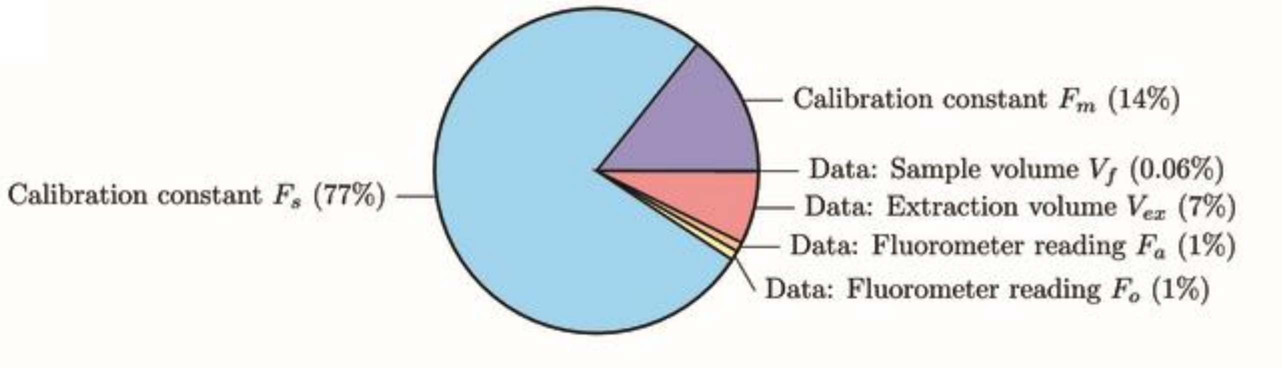
Propagation into $\sigma_{Chla}$ through sum-of-squares analytical method:

$$\left(\frac{\sigma_{\text{Chla}}}{\text{Chla}}\right)^2 = \frac{\sigma_{F_m}^2}{F_m^2(F_m-1)^2} + \frac{\sigma_{F_o}^2+\sigma_{F_a}^2}{(F_o-F_a)^2} + \frac{\sigma_{F_s}^2}{F_s^2} + \frac{\sigma_{V_{ex}}^2}{V_{ex}^2} + \frac{\sigma_{V_f}^2}{V_f^2}$$

Chl*a* = 3.39 ± 0.24 µg $L^{-1}$

# Example A: Targeted improvement through uncertainty analysis

*Which input contributes most to the uncertainty in Chla?*



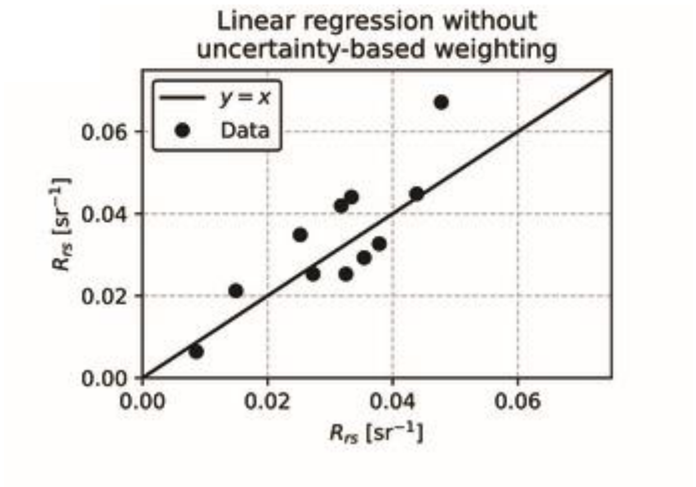

The uncertainty in Chl*a* was dominated (90.1%) by the calibration factors $F_m$ and $F_s$, with only 9.9% coming from measurement uncertainty.

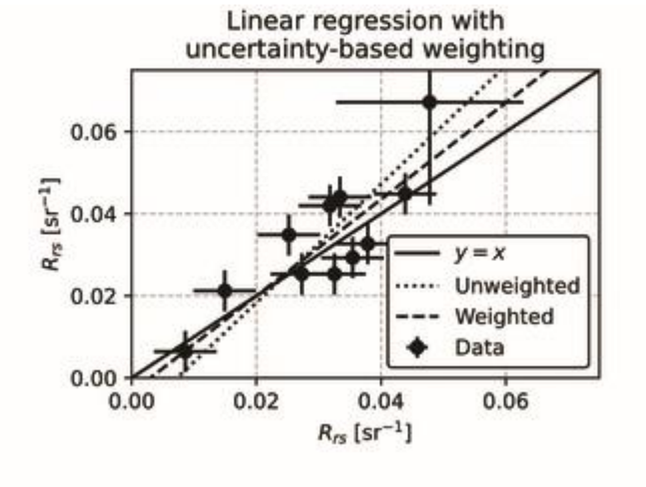
In practical terms: improving the calibration process was more effective for this experiment in reducing uncertainty in Chl*a* than repeated or more precise lab work -> where to spend your time/funding.

# Example B: Validation and match-up analysis

Match-up validation: *in situ* $R_{rs}$ vs. satellite-derived $R_{rs}$

*How different are the values we compare (without knowing the uncertainty associated with them)?*

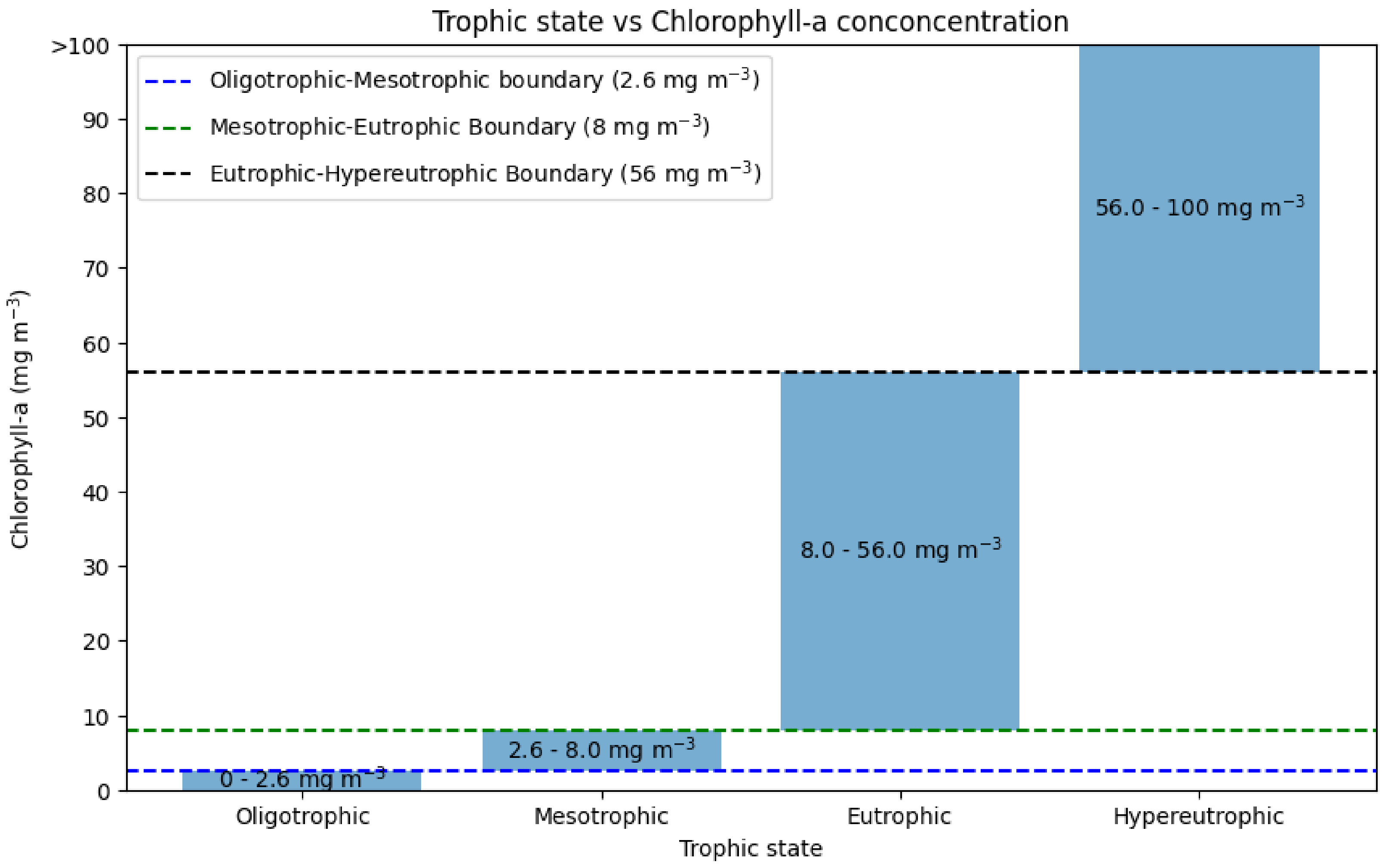



Improved match-up analysis and regression through the application of weights based on uncertainty in *x* and *y* resulted in 2.5 x lower error when compared to unweighted regression.

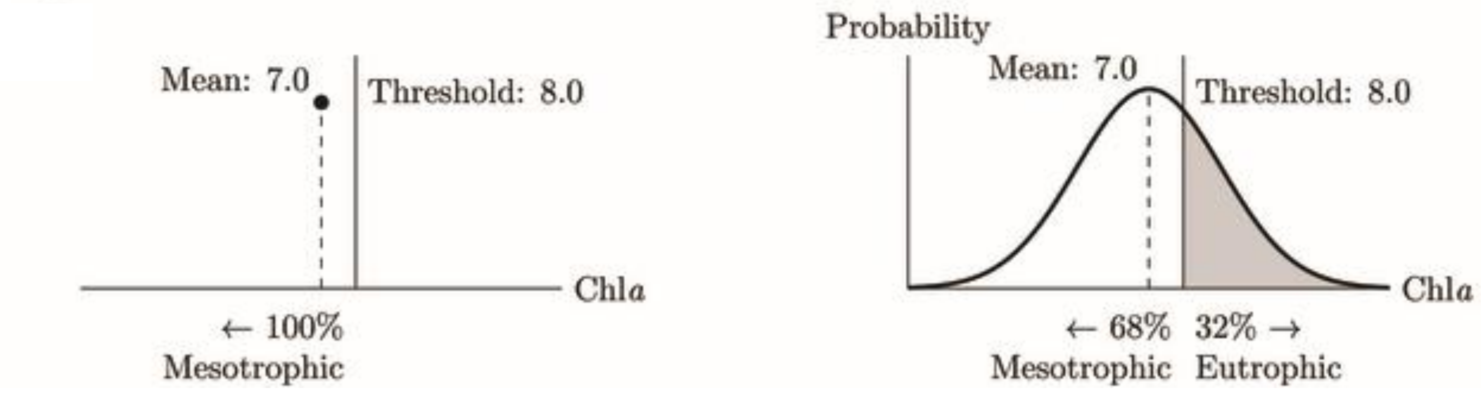
→ **Without quantified uncertainty, findings may be misinterpreted.**

# Example C: Decision-making



# 3. Example C: Decision-making

- Let's assume a Chl*a* value of 7 mg $m^{-3}$ obtained through satellite remote sensing (typical uncertainty for complex waters: 20-100%).
- Here: with an uncertainty of 30% (normally distributed).
- Then the observation results in Chl*a* of 7.0 ± 2.1 mg $m^{-3}$.




Approximately 32% of the associated probability density overlaps with the eutrophic range, indicating a significant probability that the water body is in fact eutrophic.

→ **uncertainty can guide decision-making and forecasting.**

# 3. Example D: Atmospheric correction (AC)

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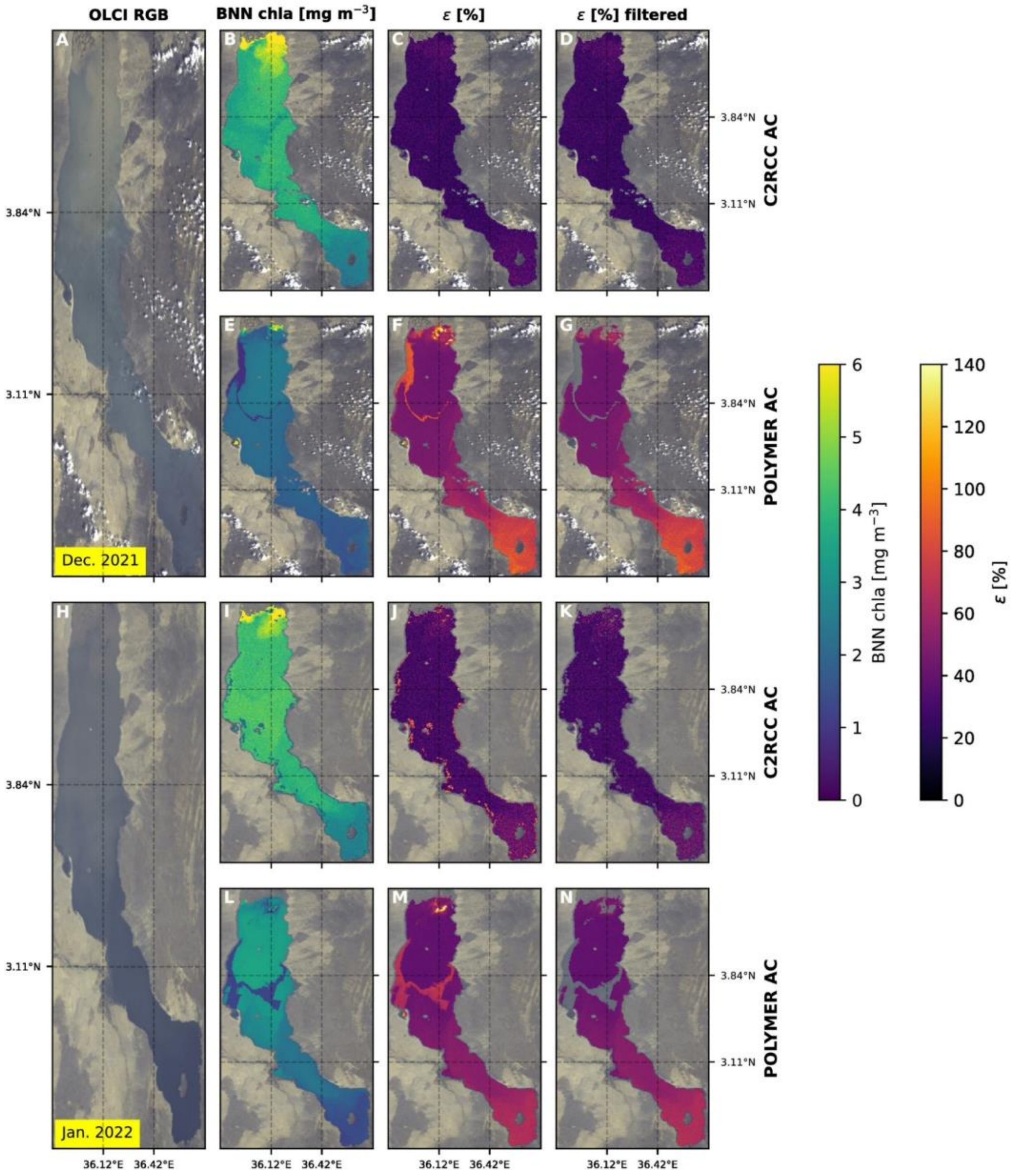
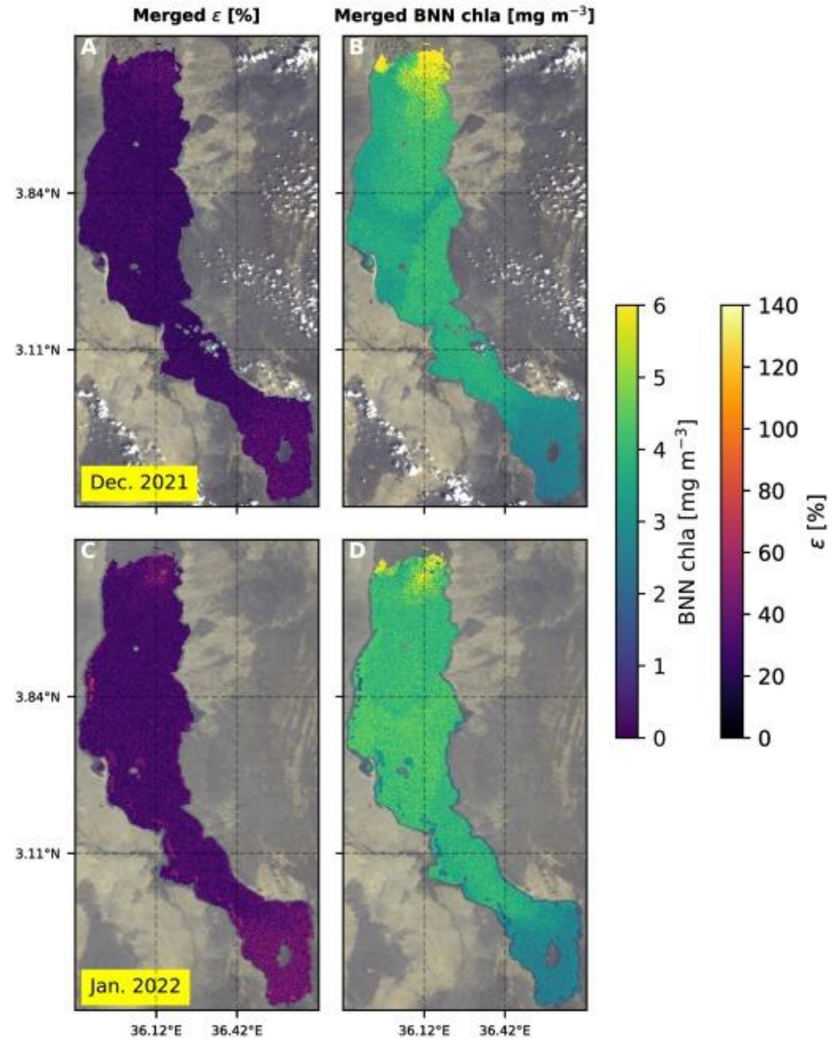



*Werther et al., 2022: A Bayesian approach for remote sensing of chlorophyll-a and associated retrieval uncertainty in oligotrophic and mesotrophic lakes, Rem. Sens. Env. (283), 113295.*



Lake3P

# 3. Example D: AC algorithm selection




→ **let the expressed uncertainty decide for you, when a decision-making criterion is unavailable.**

# 4. Concluding remarks

Uncertainty is inherent in all aspects of aquatic remote sensing, but often remains unaddressed.

The advantages of embracing it are clear -> Uncertainty causes us to challenge our assumptions, refine our models, and enhance methodologies.

However, the journey to understand and effectively managing uncertainty can be a long-term endeavor, and may take years to discover, validate and incorporate into new approaches.

-> Work with uncertainty, rather than against it

Werther, M. and Burggraaff, O. *(2023): Dive Into the Unknown: Embracing Uncertainty to Advance Aquatic Remote Sensing. J. Remote Sens. 2023;3:0070.*

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