Understanding and Estimating Uncertainty in Ocean Colour Remote Sensing Data and Derived Products

Co-Chairs

Part I: Kevin Turpie (UMBC), Emmanuel Boss (U. Maine),

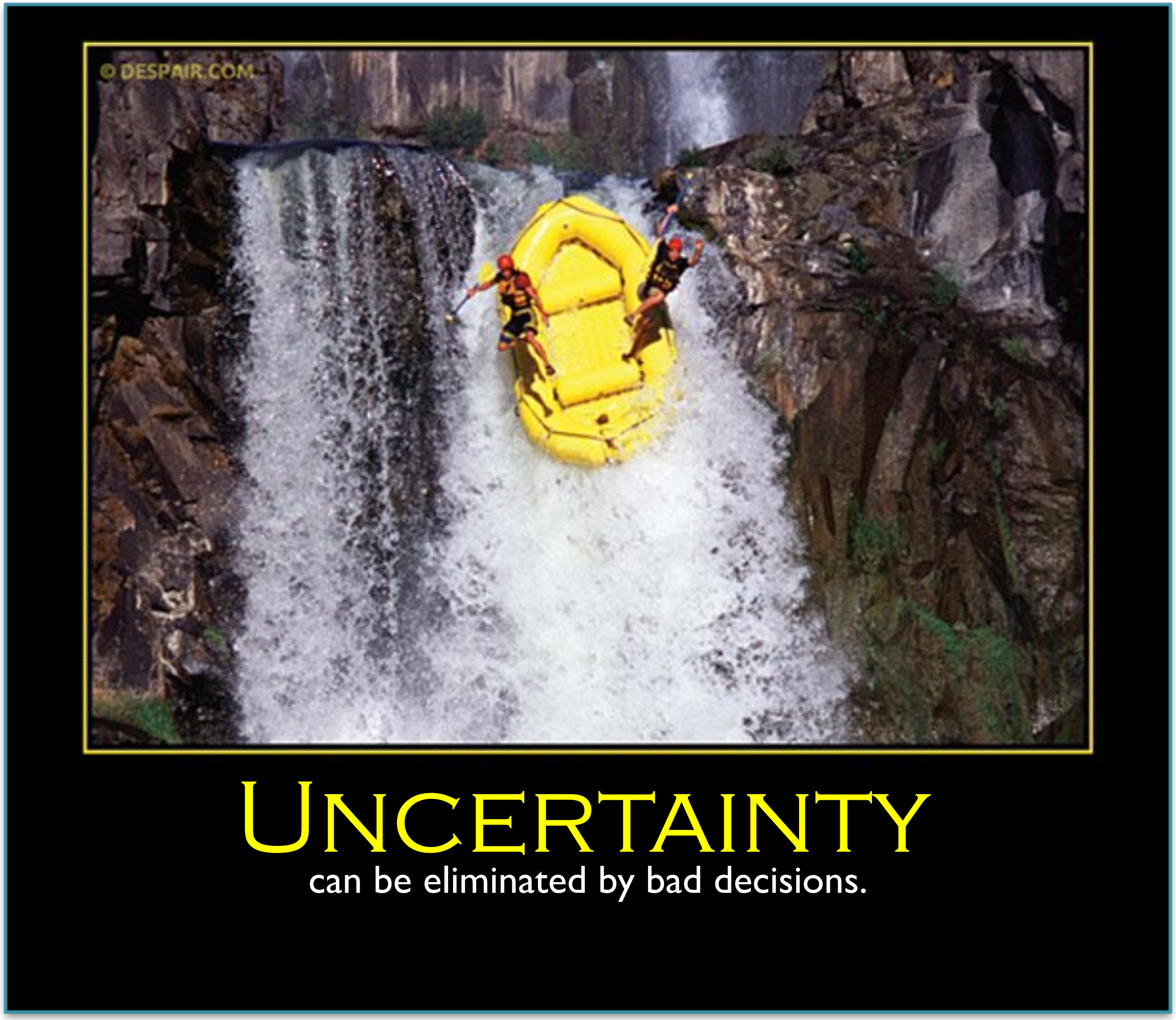
Part II: Stéphane Maritorena (UCSB), Frédéric Melin (JRC ISPRA),

Part III: Jeremy Werdell (NASA GSFC)

International Ocean Colour Science Meeting II

San Francisco, California USA

16 June 2015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UNCERTAINTY
can be eliminated by bad decisions.

AGENDA

Part I: *Theory and overview*

14:30-14:45	**Uncertainty definitions and theory** Kevin Turpie (UMBC)
14:45-14:50	**IOCCG/CEOS/GCOS context** Frédéric Mélin (JRC ISPRA)

Part II: *Surface reflectance uncertainty estimation methods*

14:50-15:00	**Synthesis of published methods and collocation approach** Frédéric Mélin (JRC ISPRA)
15:00-15:10	**Uncertainties from the Bayesian method** Robert Frouin (UCSD)
15:10-15:20	**Uncertainty propagation** Philippe Goryl (ESA)
15:20-15:30	**Neural networks and Rrs uncertainty** Roland Doerffer (Helmholtz Zentrum Geesthacht)

Part III: *Derived product uncertainty methods*

15:30-15:40	**Status report on in situ uncertainties** Emmanuel Boss (U. Maine)
15:40-15:50	**Overview of methods for remotely-sensed IOP uncertainties** Suhyb Salama (U. Twente)
15:50-16:00	**Spatial, temporal, and content considerations for Level-3 uncertainties** Tim Moore (U. New Hampshire)

16:00-17:15	**Moderated Community Discussion**

OBJECTIVES

- Attempt to overview some of what has been done for satellite data product uncertainty.
- Look at research directions.
- Discuss the path forward.
- Discussion questions developed thanks to input from:

Carsten Brockmann	Samantha Lavender
Janet Campbell	ZhongPing Lee
Stephanie Dutkiewicz	Hubert Loisel
Bryan Franz	Antoine Mangin
Robert Frouin	Tim Moore
Philippe Goryl	Griet Neukermans
Watson Gregg	Cecile Rousseaux
Stephanie Henson	Kevin Ruddick
Chuanmin Hu	Suhyb Salama
Cedric Jamet	Shubha Sathyendranath
Ewa Kwiatkowska	Giuseppe Zibordi

QUESTIONS FOR DISCUSSION:

Coordinating and Integrating Efforts

- **Gaps** - What information is currently not sufficiently characterized, but that would be helpful for the derivation of uncertainty estimates?

- **Coordination** - How does the community coordinate and integrate disparate efforts and results?

- **Pros and Cons** - What are the pros and cons of the techniques used to derive uncertainties?

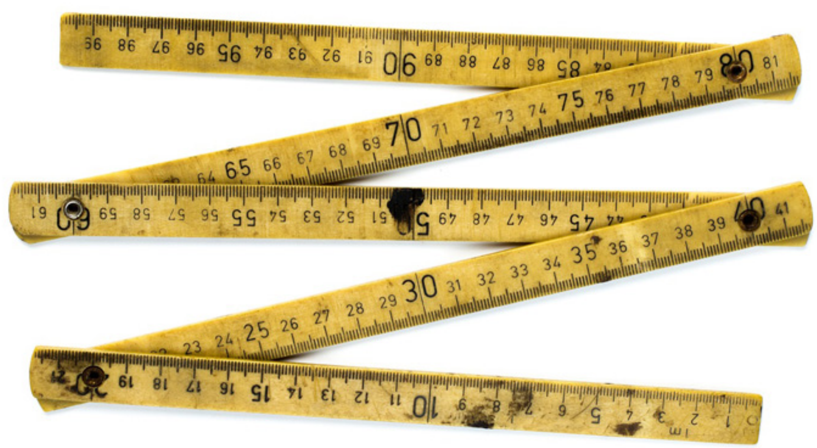
QUESTIONS FOR DISCUSSION:

Standardizing Methods and Metrics

- **Cross Mission** - How do we standardize data quality metrics and their derivation across multiple missions?

- **Types of Uncertainty** - What are the types of uncertainty statistics that are associated with data measurement types?

- **Choice of Metrics** - Which specific metrics do we use to quantify uncertainties?



QUESTIONS FOR DISCUSSION:

Determining Uncertainty Estimation Quality

- **Verify or Validate Uncertainty** - Can we validate, or perhaps verify, uncertainty estimates and to what extent is good enough?

- **Validation Satellite Data** - How do we achieve traceability from *in situ* data uncertainties to satellite products?

IOCS Posters on Uncertainty:

Poster No.	First Name	Last Name	Title
5	William	Balch	Predicting the Iceberg from its Tip: Resolving Integrated, Water-Column Particle Biogeochemistry Using Measurements from just the Upper Optical Depth
7	Brian	Barnes	Dependence of satellite ocean color data products on viewing angles: A comparison between SeaWiFS, MODIS, and VIIRS
17	Carsten	Brockmann	Visualisation and Processing Support of Uncertainties in SNAP - ESA's Sentinel Toolbox
22	Joaquin	Chaves	Ocean color algorithm uncertainty evaluation using Monte Carlo computational methods
24	Jacek	Chowdhary	Case studies for polarimetric airborne remote sensing observations of coastal waters: atmospheric correction for aerosols and thin cirrus clouds.
25	Emanuele	Ciancia	Integration of Satellite Data and In-Situ Measurements for Coastal Water Quality Monitoring: The Ionian Sea Case Study
37	Stephanie	Dutkiewicz	Numerical model laboratory for exploring uncertainty in satellite derived chlorophyll-a
39	Lian	Feng	Effects of cloud adjacency on TOA radiance and ocean color products: A statistical assessment
64	Thomas	Jackson	Utilising Optical Water Classification for Pixel-By-Pixel Assignment of Uncertainties in a Merged Ocean-Colour Product.
77	Samantha	Lavender	An Ensemble Approach to Atmospheric Correction Over Optically Complex Waters
83	Soo Chin	Liew	Uncertainty Estimates in the Retrieval of Water Depth and Turbidity in Turbid Coastal Waters Using Very High Resolution Satellites Data
86	Hubert	Loisel	Impact of the temporal binning algorithm on ocean color products: application to the SeaWiFS time period
93	Morgaine	McKibben	Merging glider and ocean color data to accurately estimate phytoplankton biomass in Oregon's coastal waters
95	Frederic	Melin	Uncertainty Estimates for Remote Sensing Reflectance Derived from the Comparison Between Missions
99	Curtis	Mobley	Improved Sea Surface Reflectance Calculations Using Fully Resolved Sea Surfaces and Polarized Ray Tracing
126	M.S.	Salama	Uncertainties of Sentinel-3-OLCI Ocean Colour Products: Simulation based on APEX Acquisitions
132	Sergio	Signorini	Preliminary Assessment of Satellite Spatial Resolution Required to Capture Spatial Dynamics of Phytoplankton and CDOM across Estuaries and Adjacent Coastal Ocean
152	Jianwei	Wei	An Empirical Approach for Quality Screening of The Satellite Ocean Color Data
156	Pengwang	Zhai	Assessing the Uncertainty of the Ocean Water Bidirectional Reflectance Model

Further Reading:

NIST TM-1297 Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results, 1994.

JCGM 100:2008 Evaluation of measurement data — Guide to the expression of uncertainty in measurement (GUM), Bureau International des Poids et Mesures (BIPM), 2008.

JCGM 200:2008 International vocabulary of metrology — Basic and general concepts and associated terms (VIM), Bureau International des Poids et Mesures (BIPM), 2008.

Kubáček, L., Nonlinear error propagation law, Applications in Mathematics, No. 5, 329-345, 1996.

Kubáček, L., Tesaříkova, E., Linear error propagation law and nonlinear functions, Acta Univ. Palacki. Olomuc., Fac. rer. nat., Mathematica 49, 2, 69–82, 2010.

Melin, F., Franz, B.A., Chapter 6.1 – Assessment of Satellite Ocean Colour Radiometry and Derived Geophysical Products, in Experimental Methods in the Physical Sciences, Vol. 47., Elsevier Inc., 2014.
http://dx.doi.org/10.1016/B978-0-12-417011-7.00020-9

Mowrer, H.T., Congalton, R.G., *Quantifying Spatial Uncertainty in Natural Resources,* Anne Arbor Press, Chelsea, MI, 2007.

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Uncertainty Definitions and Theory

Kevin Turpie, UMBC/JCET

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Other Types of Uncertainty:

Type A uncertainty can be estimated statistically.
Type B uncertainty cannot. This will not be overviewed.

- However, data product meta data should provide or point to information describing measurements exactly.
- User should be able to estimate what additional Type B uncertainty arises when applied to her or his application.
- Also not covered in this talk is inclusion of classification uncertainties (e.g., Phytoplankton Functional Types, Flags) (Type A) in the meta data.
  - — Error (or Confusion) Matrix.
  - — Kappa Statistics.
  - — Not a pixel-by-pixel statistic.
  - — Similar techniques for spectral endmembers.

Fundamental Principle of Remote Sensing:

- Start with basics for Type A uncertainties. Let…

Z_0 be an observable quantity.

Z_{rs} be a remote measurement of Z_0 from different location (or time).

$\varepsilon = Z_{rs} - Z_0$ is the <u>remote sensing measurement error</u> (i.e., the difference between the "true" quantity and measured quantity).

U is some measure of the typical size of ε.

The fundamental principle of remote sensing is simply that

$$\frac{U}{|Z_o|} \ll 1$$

In other words, the Fundamental Principle of Remote Sensing is that ε is typically, very small – ideally, sufficiently small enough to answer a specific science question. This provides a framework that unifies several concepts.

Fundamental Principle of Remote Sensing:

- How do we determine that ε is sufficiently small?

We first need some measure U of the the typical size of ε.

U could be represented, for instance, with the following statistics:

$u = |\beta| + \sigma$ is the **measurement uncertainty** in Z_{rs}, where,

$\beta = \mathrm{E}\varepsilon$ is the **bias** (systematic measurement error) in Z_{rs}, and

$\sigma = \sqrt{\mathrm{Var}\,\varepsilon}$ is the **standard deviation** (random measurement error) in Z_{rs}.

Of course, there are other metrics*, but these are useful for discussion.

* e.g.: median error, mean absolute difference or interquartile range.

FUNDAMENTAL PRINCIPLE OF REMOTE SENSING:

- How do we determine that ε is sufficiently small?

We need to show that the uncertainty is smaller than some tolerance pertinant to our science question.

For instance, we may wish to show that

$$\frac{u}{|Z_o|} < r_0 \qquad \text{or} \qquad u < d_0 = r_0 |Z_o|$$

where,

r_0 is the relative threshold criterion (tolerance) and

d_0 is the absolute threshold criterion (tolerance) for the total uncertainty.

Similarly, criteria could be set for the error bias and standard deviation individually.

Validation and Components of Uncertainty:

- It is also useful to consider the quantities that contribute to ε.

First, define the *validation measurement* as follows

$$Z_0^* = Z_0 + \varepsilon_{in} + \varepsilon_s$$

So, a validation measurement has an instrument error ε_{in} and an error ε_s that depends on scaling and sampling differences (inc. time displacement) between the satellite data and *in situ* measurements.

In practice, we substitute the validation measurement for Z_0 as a "close" estimate.

Thus, in reality, we get the validation error

$$\varepsilon_{val} = Z_{rs} - Z_0^* = \varepsilon + \varepsilon_{in} + \varepsilon_s$$

→ ε_{in} and ε_s can cause the measurement uncertainty to be overestimated.

Validation and Components of Uncertainty:

- Next we consider that Z_{rs} is derived from several sources of information. The quantity Z_{rs} can be described as a function of inputs

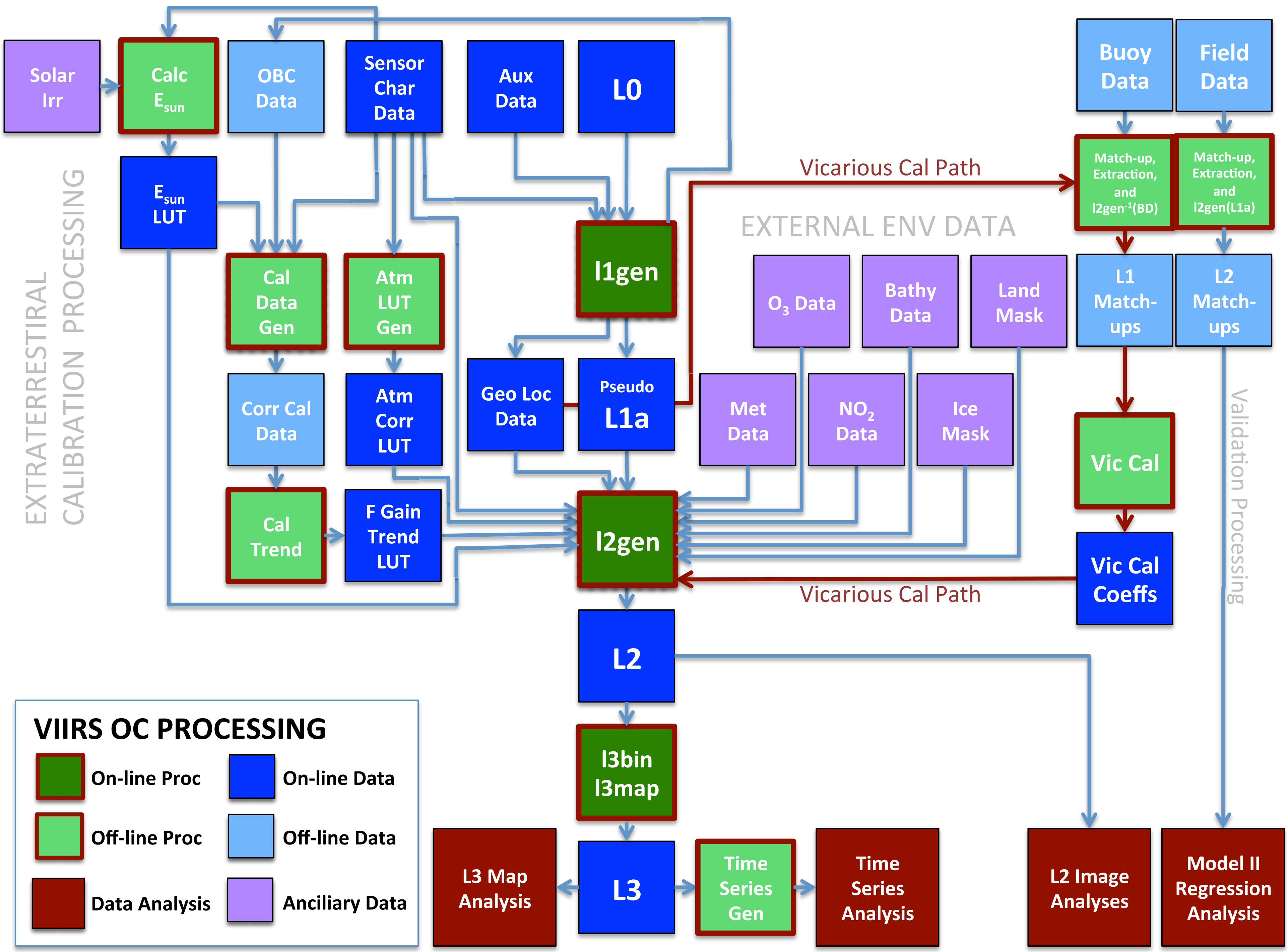
$$Z_{rs} = f(x)$$

f(x) is the remote sensing model and x is vector of input values

$$x = \left[\; x_{sat}; \quad x_{aux}; \quad x_{char}; \quad x_{anc} \; \right]$$

which is a composite of the following vectors:
x_{sat}, containing the TOA radiometric measurements made by the sensor.
x_{aux}, containing the geometric and calibration data for measurements.
x_{char}, containing the prelaunch characteristics of the sensor.
x_{anc}, containing environmental (anciliary) data use to retrieve Z_{rs}.

All of these sources of information have their own associated error, which we will call ε_{dat}, a vector containing all the input errors.



Solar Irr
Calc E_{sun}
OBC Data
Sensor Char Data
Aux Data
L0
E_{sun} LUT
Cal Data Gen
Atm LUT Gen
l1gen
Corr Cal Data
Atm Corr LUT
Geo Loc Data
Pseudo L1a
Cal Trend
F Gain Trend LUT
l2gen
L2
l3bin l3map
L3
L3 Map Analysis
Time Series Gen
Time Series Analysis
EXTRATERRESTIRAL CALIBRATION PROCESSING
Vicarious Cal Path
EXTERNAL ENV DATA
O_3 Data
Bathy Data
Land Mask
Met Data
NO_2 Data
Ice Mask
Buoy Data
Field Data
Match-up, Extraction, and l2gen^{-1}(BD)
Match-up, Extraction, and l2gen(L1a)
L1 Match-ups
L2 Match-ups
Vic Cal
Vic Cal Coeffs
Vicarious Cal Path
Validation Processing
L2 Image Analyses
Model II Regression Analysis
VIIRS OC PROCESSING
On-line Proc
On-line Data
Off-line Proc
Off-line Data
Data Analysis
Anciliary Data

Validation and Components of Uncertainty:

- We can assume that the function f is a perfect representation of Z_0, i.e., $f(x) = Z_0$ whenever $\varepsilon_{dat} = 0$.

Thus we can describe a **Perfect Model Error (PME)** as

$$Z_{rs} - Z_0 = f(x + \varepsilon_{dat}) - Z_0 = f(x) + \varepsilon_{PME} - Z_0 = \varepsilon_{PME}$$

Validation and Components of Uncertainty:

- However, the function f is not necessarily a perfect representation of Z_0, so even with perfect data as input, so it has its own **Inherent Model Error (IME)**.

To first order approximation, we thus have

$$Z_{rs} – Z_0 = f(x + \varepsilon_{dat}) + \varepsilon_{IME} – Z_0$$

$$Z_{rs} – Z_0 = \varepsilon_{PME} + \varepsilon_{IME}$$

Thus the validation error has four components

$$\varepsilon_{val} = \varepsilon_{PME} + \varepsilon_{IME} + \varepsilon_{in} + \varepsilon_s$$

Components of Uncertainty:

- In considering the IME, we would prefer to assume the the algorithm is dealing with inputs of the same scale on which it was parameterize.

  However, for a nonlinear model, the function of an average does not equal the average of the function, thus we have an aggregation bias

$$\varepsilon_{agg} = f(\bar{x}) - \overline{f(x)} \simeq \frac{1}{2} E\left[(x - \bar{x})^T H(\bar{x})(x - \bar{x})\right]$$

  where H is the Hessian for a single dependent variable of f(x).

  Thus, validation error can be rewritten as a sum of five components :

$$\underbrace{\varepsilon_{val}}_{\text{Known match-up difference.}} = \underbrace{\varepsilon_{PME} + \varepsilon_{IME} + \varepsilon_{agg}}_{\text{Algorithm errors – could be estimated.}} + \underbrace{\varepsilon_{in} + \varepsilon_{s}}_{\textit{In situ} \text{ errors – could be reduced.}}$$

In situ errors – could be reduced.

Algorithm errors – could be estimated.

Known match-up difference.

Components of Uncertainty:

Imperfect Model Error (ε_{IME}) Estimate

- RS models (e.g., f(x)) are essentially composite functions of models.
- Uncertainty for individual components can be mined from literature.
- Collective algorithm error statistics can be estimated using uncertainty propagation theory.
- Empirical models have uncertainty statistics build-in (e.g., regression residuals)
- Can be comparable to ε_{PME} and **must be included in an estimate of ε.**

Components of Uncertainty:

- **Perfect Model Error (ε_{IME}) Estimate**

Delta Method

(Kubáček and Tesaříkova 2010)

$$E\,\varepsilon_{PME} = E\,f(x+\varepsilon_{dat}) - f(u) = \frac{1}{2}\begin{bmatrix} Tr(F_1\Sigma_x) \\ Tr(F_2\Sigma_x) \\ \vdots \\ Tr(F_n\Sigma_x) \end{bmatrix}$$

Hessian for function output

Covariance matrixe for ε_{dat}

Jacobian matrix for f(x)

$$\Sigma_f = Var(f(x+\varepsilon_{dat})) = F\Sigma_x F^T + \frac{1}{2}\begin{bmatrix} Tr(F_1\Sigma_x F_1\Sigma_x) & Tr(F_1\Sigma_x F_2\Sigma_x) & \cdots & Tr(F_1\Sigma_x F_1\Sigma_x) \\ Tr(F_2\Sigma_x F_1\Sigma_x) & Tr(F_2\Sigma_x F_2\Sigma_x) & & \vdots \\ \vdots & & \ddots & \vdots \\ Tr(F_1\Sigma_x F_1\Sigma_x) & \cdots & \cdots & Tr(F_n\Sigma_x F_n\Sigma_x) \end{bmatrix}$$

- Requires tests for linearity and convergence. Nonlinearity requires more terms.

(for nonlinear models see Kubáček 1996)

- Jacobian and Hessian matrices must be approximated numerically.
- Build statistical model of ε_{PME} as a function of x.

Components of Uncertainty:

Perfect Model Error (ε_{IME}) Estimate (cont.)

Monte Carlo Simulation

Steps:

1. Repeatedly simulate ε_{dat} using a random number generator and model.

2. For each instance of ε_{dat}, calculated $\varepsilon_{PME} = f(x+\varepsilon_{dat})-f(x)$.

3. Accumulate statistics of ε_{PME}.

4. Build statistical model of ε_{PME} as a function of x.

- Requires a model of ε_{dat}.
- Can be accurate, but is computationally expensive.
- Approach is a focus of ESA and NASA efforts for uncertainty products.

Wrap Up:

- Type A uncertainty can be quantified using statistics of systematic and random measurement errors. Type B and classification data uncertainty could be in metadata.

- Other analyses are required for categorical data like flags for classes.

- To first order, validation error can be view as a sum of contributing errors : $\varepsilon_{val} = \varepsilon_{PME} + \varepsilon_{IME} + \varepsilon_{agg} + \varepsilon_{in} + \varepsilon_{s}$.

- This equation unifies sources of Type A uncertainty. It could be perhaps used in a closure study.

- Numerical approximations are possible for ε_{PME}, but require a good model of ε_{dat} and development of a reusable model of ε_{PME} as a function of x.

- ε_{IME} can be comparable in size to ε_{PME} and must be included in any uncertainty estimate.

- Further research and analysis is required to estimate ε_{IME} based on model component uncertainty and propagation of uncertainty with consideration of random vs systematic behavior.

- Estimates ε_{IME} is often already provided in the literature on a component by component basis by the modeler developers.

THANK YOU

And now, let's begin...

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Discussion Questions with Suggested Answers

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QUESTIONS FOR DISCUSSION:

Coordinating and Integrating Efforts

- **Gaps** - What information is currently not sufficiently characterized, but that would be helpful for the derivation of uncertainty estimates?

All uncertainty sources are not fully characterized. E.g., the inherent model error should be considered for most algorithms? Likewise, for sampling/scaling differences between satellite and validation data, intrapixel or pixel coverage should be understood.

Questions for Discussion:

Coordinating and Integrating Efforts

- **Coordination** - How does the community coordinate and integrate disparate efforts and results?

A group (e.g., IOCCG Uncertainty group) could track and organized activity. Suggest supporting a website where a reading list of results, reports and publication can be maintained (including links to documents, where appropriate). Effecacious techniques could be selected by agencies for implementation, if they monitor this site and news.

QUESTIONS FOR DISCUSSION:

Coordinating and Integrating Efforts

- **Pros and Cons** - What are the pros and cons of the techniques used to derive uncertainties?

Global approaches, such as neural networks (NN) or Bayesian techniques, build on all availabe information, but are the results instructive regarding the source of uncertainty?

"Perfect Model" uncertainty using Monte Carlo simulation could be computationally expensive. Taylor/Delta methods can be less expensive computational, but are mathematically and numerically challenging to implement. In either case, a simplified model to describe changes in uncertainty must be constructed.

"Imperfect Model" uncertainty needs more attention. Material can be found in the literature, but it needs careful review and consolidation into complete description.

QUESTIONS FOR DISCUSSION:

Standardizing Methods and Metrics

- **Cross Mission** - How do we standardize data quality metrics and their derivation across multiple missions?

Community surveys and discussions to identify user needs coud, to an extent, help develop a standard for metrics. But, ultimately, this will require a dialogue between agencies generating data products, perhaps facilitated through the IOCCG working group.

QUESTIONS FOR DISCUSSION:

Standardizing Methods and Metrics

- **Types of Uncertainty** - What are the types of uncertainty statistics that are associated with data measurement types?

- **Choice of Metrics** - Which specific metrics do we use to quantify uncertainties?

Typical uncertainty statistics involve single numbers regarding total uncertainty (e.g., RMSE). For some missions (e.g., JPSS), data product performance is stated in accuracy (bias) and precision (variability). The expected skewness of uncertainty for some data products (e.g., log normal) suggests confidence intervals or quartile ranges.

However, the approaches suggested for the previous questions could elucidate which specific metrics are wanted by users.

QUESTIONS FOR DISCUSSION:

Determining Uncertainty Estimation Quality

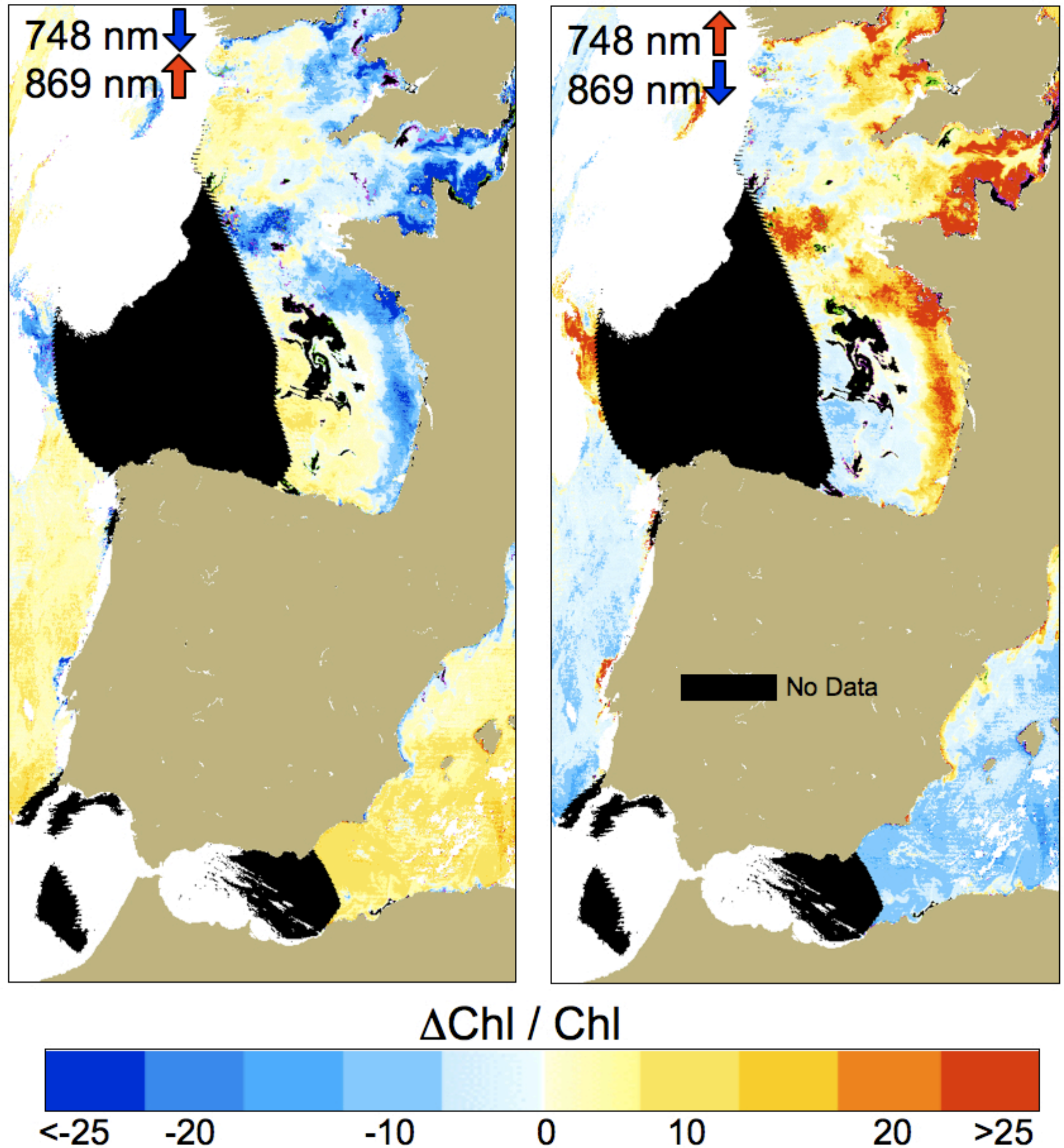
- **Verify or Validate Uncertainty** - Can we validate, or perhaps verify, uncertainty estimates and to what extent is good enough?

- **Validation Satellite Data** - How do we achieve traceability from *in situ* data uncertainties to satellite products?

Ideally, we would want all estimates of uncertainty to fit withing the framework of theory. E.g., summation of all uncertainty components should be comparable to the average difference between the satellite data and *in situ* measurements.

A mismatch may not provide much information as to the cause. Still, perhaps an end-to-end simulation or error budget of all error sources, including *in situ* measurement uncertainty, could be used test how well components uncertainty are estimated.

Effect on Chl of perturbing L_t for each NIR band %0.3 in opposite directions.



(Turpie et al. 2014)