Experimental approaches to uncertainty: Communicating the unquantifiable

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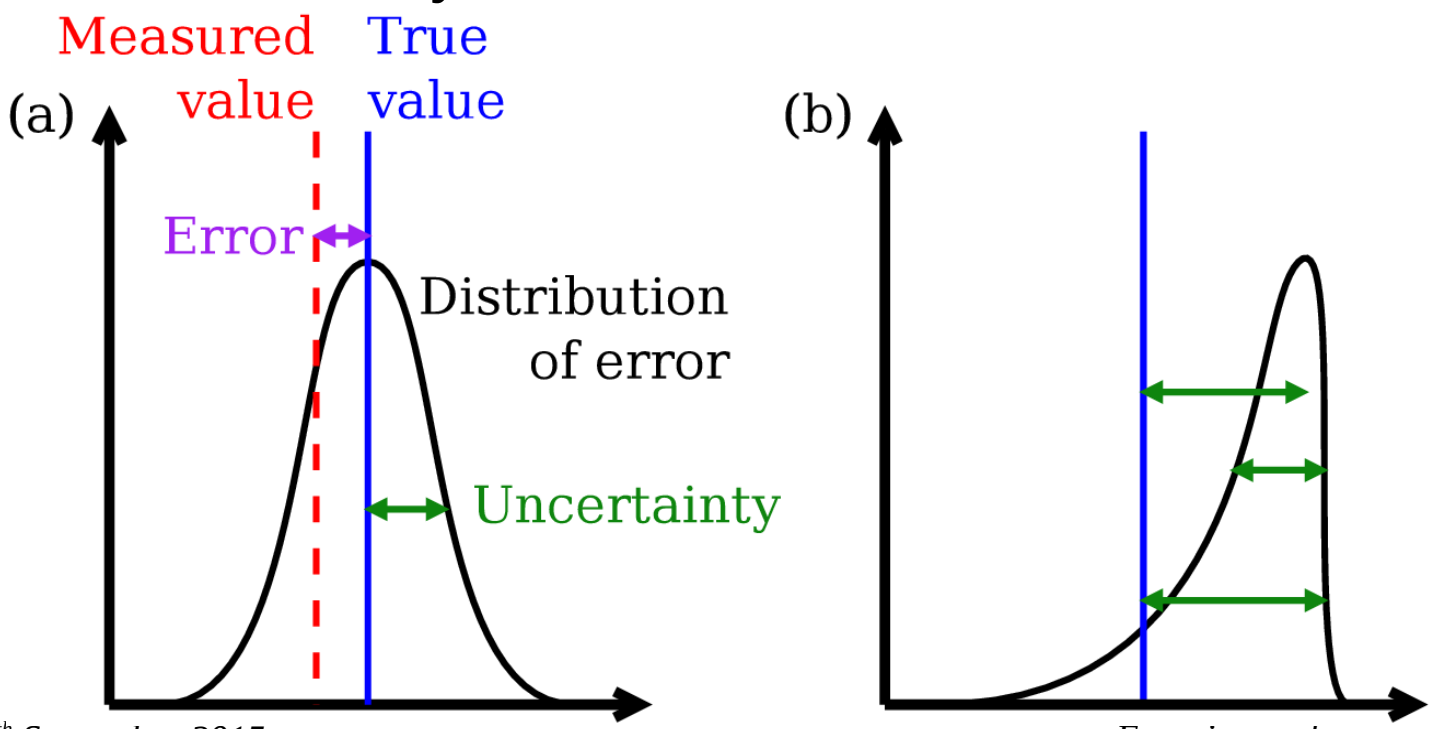
Representing uncertainty

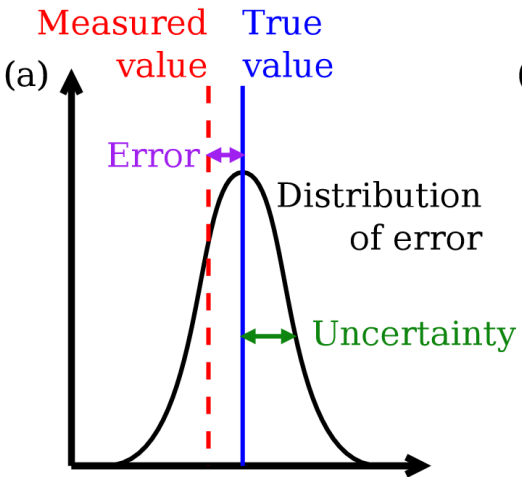
a) Typical understanding of uncertainty as the width of the distribution of error around the measurand. This is generally accurate for random errors.

b) The 'uncertainty' of a systematic error can be more complex as the distribution of error is asymmetric with non-zero mean.



Classifying sources of error

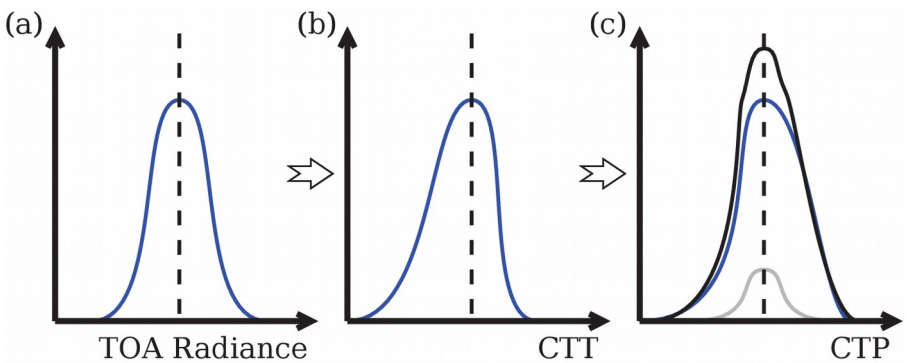
- Intrinsic sources of error
  - Measurement
    - Statistical variation in measurand or detector
    - e.g. dark current, radiometric calibration
  - Parameter
    - Uncertainty in auxiliary information used
    - e.g. spectroscopic data, meteorological profiles
  - Both also known as “parametric errors”



- Generally well-represented by traditional techniques for calculating uncertainty.

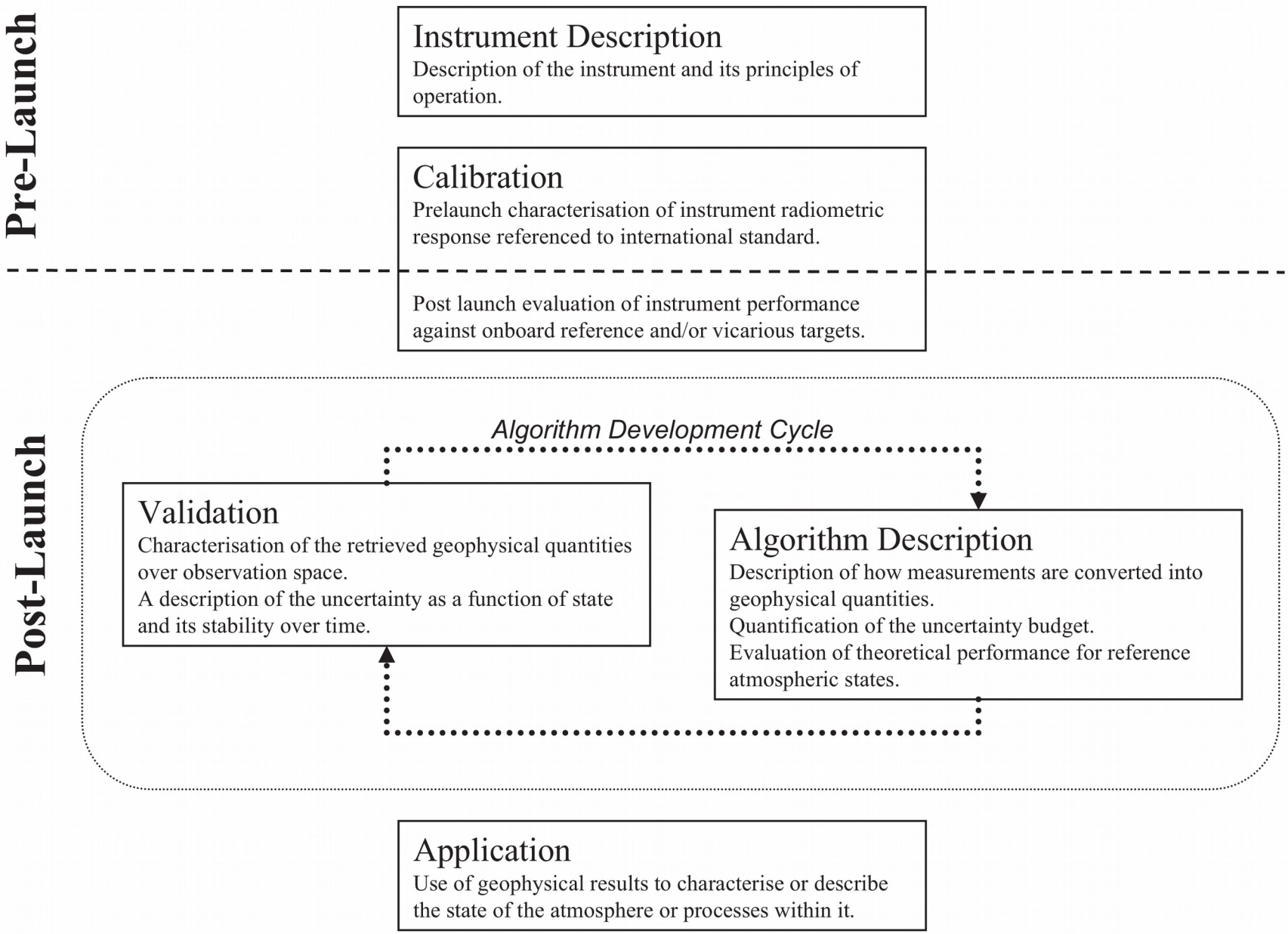
Classifying sources of error

- Structural errors, resulting from choices made in the measurement and analysis systems
  - Approximation
    - Simplifications and approximations in calculations
    - e.g. using a LUT or plane-parallel atmosphere
  - System
    - Physically meaningful assumptions
    - e.g. choice of aerosol optical model
  - Resolution
    - Finite sampling of a constantly varying system
    - e.g. fair-weather bias, MODIS “bow-tie effect”



- Potentially non-linear and circumstantial.
  Thus, the source of error affects how it needs to be reported to users.

Communicating with scientific community



Communicating with users

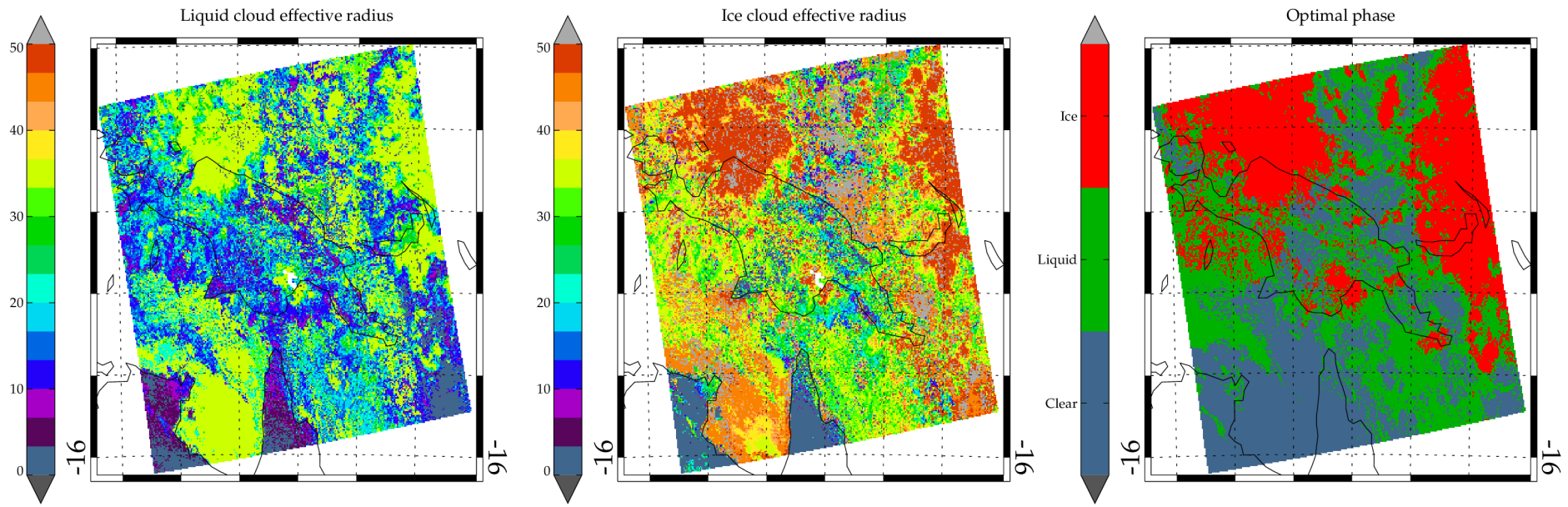
- Important to clarify the difference between what is measured and what the user wants to know.
  - For example, satellites only sample one time of day but users may need observations at other times.
    - For SST, in situ observations indicate the diurnal cycle is somewhat predictable so empirical corrections may be useful.
    - For cloud, data indicates the diurnal cycle is highly circumstantial so a single observation is not representative of an entire day.
- A quantity can be adjusted to meet a user's needs but
  - The transformation will introduce additional uncertainty and
  - The new quantity may not meet other user's needs.
- We prefer to report only the measured value and provide secondary support (i.e. communication) to produce transformations as needed.

Communicating with users

- Many satellite products require significant assumptions to constrain their analysis.
  - Some simplify the problem, introducing approximation errors
    - e.g. neglecting multiple scattering
  - Others are physical constraints, introducing system errors
    - e.g. classifying land type into finite, idealised categories
  - In either case, it isn't obvious how to quantify the uncertainty

Ensemble techniques

- Ensemble techniques can better communicate uncertainties resulting from such errors.
  - A “multi-model” ensemble of analyses with differing assumptions and approximations.
  - A “multi-run” ensemble of analyses with different constraints.



System maturity

CORE-CLIMAX System Maturity Matrix

Maturity	SOFTWARE READINESS	METADATA	USER DOCUMENTATION	UNCERTAINTY CHARACTERISATION	PUBLIC ACCESS, _x000D_FEEDBACK, UPDATE	USAGE
1	Conceptual development	None	Limited scientific description of the methodology available from PI	None	Restricted availability from PI	None
2	Research grade code	Research grade	Comprehensive scientific description of the methodology, report on limited validation, and limited product user guide available from PI; paper on methodology is sumitted for peer-review	Standard uncertainty nomenclature is idenitified or defined; limited validation done; limited information on uncertainty available	Data avaliable from PI, feedback through scientific exchange, irregular updates by PI	Research: Benefits for applications identified_x000D_DSS: Potential benefits identified
3	Research code with partially applied standards; code contains header and comments, and a README file; PI affirms portability, numerical reproducibility and no security problems	Standards defined or identified; sufficient to use and understand the data and extract discovery metadata	Score 2 + paper on methodology published; comprehensive validation report available from PI and a paper on validation is submitted; comprehensive user guide is available from PI; Limited description of operations cocept available from PI	Score 2 + standard nomenclature applied; validation extended to full product data coverage, comprehensive information on uncertainty available; methods for automated monitoring defined	Data and documentation publically available from PI, feedback through scientifc exchange, irregular updates by PI	Research: Benefits for applications demonstrated._x000D_DSS: Use occuring and benefits emerging
4	Score 3 + draft software installation/user manual available; 3rd party affirms portability and numerical reproducibility; passes data providers security review	Score 3 + standards systematically applied; meets international standards for the data set; enhanced discovery metadata; limited location level metadata	Score 3 + comprehensive scientific description available from data provider; report on inter comparison available from PI; paper on validation published; user guide available from data provider; comprehensive description of operations concept available from PI	Score 3 + procedures to establish SI traceability are defined; (inter)comparison against corresponding CDRs (other methods, models, etc); quantitative estimates of uncertainty provided within the product characterising more or less uncertain data points; automated monitoring partially implemented	Data record and documentation available from data provider and under data provider's version control; Data provider establishes feedback mechanism; regular updates by PI	Score 3 + _x000D_Research: Citations on product usage in occurring_x000D_DSS: societal and economical benefits discussed
5	Score 4 + operational code following standards, actions to achieve full compliance are defined; software installation/user manual complete; 3rd party installs the code operationally	Score 4+ fully compliant with standards; complete discovery metadata; complete location level metadata	Score 4 + comprehensive scientific description maintained by data provider; report on data assessment results exists; user guide is regularly updated with updates on product and validation; description on practical implementation is available from data provider	Score 4 + SI traceability partly established; data provider participated in one inter-national data assessment; comprehensive validation of the quantitative uncertainty estimates; automated quality monitoring fully implemented (all production levels)	Score 4 + soure code archived by Data Provider; feedback mechanism and international data quality assessment are considered in periodic data record updates by Data Provider	Score 4+_x000D_Research: product becomes reference for certain applications_x000D_DSS: Societal and economic benefits are demonstrated
6	Score 5 + fully compliant with standards; Turnkey System	Score 5 + regularly updated	Score 5 + journal papers on product updates are and more comprehensive validation and validation of quantitative uncertainty estimates are published; operations concept regularly updated	Score 5 + SI traceability established; data provider participated in multiple inter-national data assessment and incorporating feedbacks into the product development cycle; temporal and spatial error covariance quantified; Automated monitoring in place with results fed back to other accessible information, e.g. meta data or documentation	Score 5 + source code available to the public and capability for continuous data provisions established (ICDR)	Score 5 + _x000D_Research: Product and its applications becomes references in multiple research field_x000D_DSS: Influence on decision and policy making demonstrated

- Designed for judging the suitability of an algorithm for operational use and it's uptake by the community.
- Does not measure the science value, i.e. if the product extracts all the information available or addresses the needs of users.
- We are concerned that using these to publicly evaluate products could mistake data with a short/long heritage as in/accurate.

Summary

- Uncertainty must represent the non-linear and circumstantial nature of errors often dominant in satellite products.
- Communication of uncertainty to users should be tailored to
  - The data available to calculate and validate the uncertainty,
  - The underlying cause of the error, and
  - A broad range of users' needs.
- As the distribution of these errors is not always well understood, data producers must engage in a dialogue with data users to work towards useful estimates.
  - This can include ensemble techniques, quality assurance, qualitative descriptions.
  - This is complimented, not replaced, by validation activities.

Questions and comments?

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Atmospheric Measurement Techniques Discussions
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Known and unknown unknowns: ~~the application of ensemble techniques to~~ uncertainty estimation in satellite remote sensing ~~data~~

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Uncertainty

- Uncertainty is a vital component of data as it provides
  - a means of efficiently and consistently communicating the strengths and limitations of data to users, and
  - a metric with which to compare different data sets.
- Uncertainty should be
  - Universal: calculated in a manner applicable to all data;
  - Internally consistent: derived from the same information as the data and not draw on external validation data;
  - Transferable: of use to users for various purposes.

Ensemble Techniques

- Consider estimating the volume of a bucket, knowing only its mass.
- Shape is assumed but different assumptions produce different errors.
- The magnitude of error due to that assumption depends on the underlying state and other parameters of the retrieval.