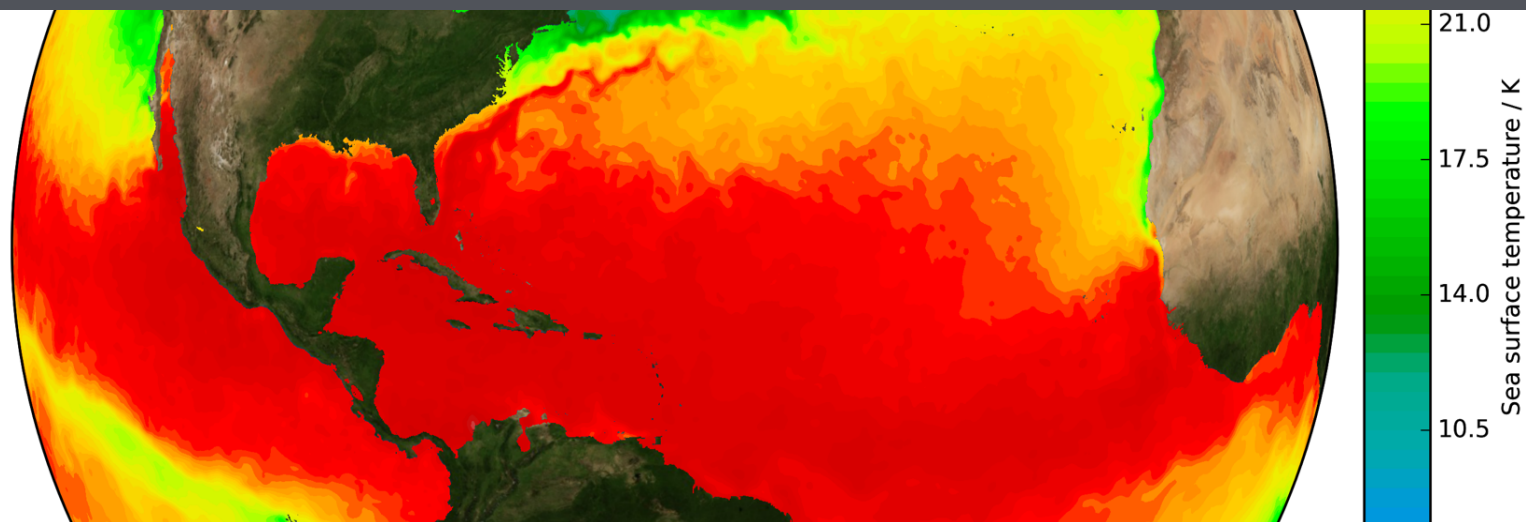


# UNCERTAINTY MODELLING FOR SATELLITE-BASED SST



Chris Merchant, Jon Mittaz\*, Claire Bulgin, Owen Embury  
and Marine Desmons.

Department of Meteorology  
University of Reading

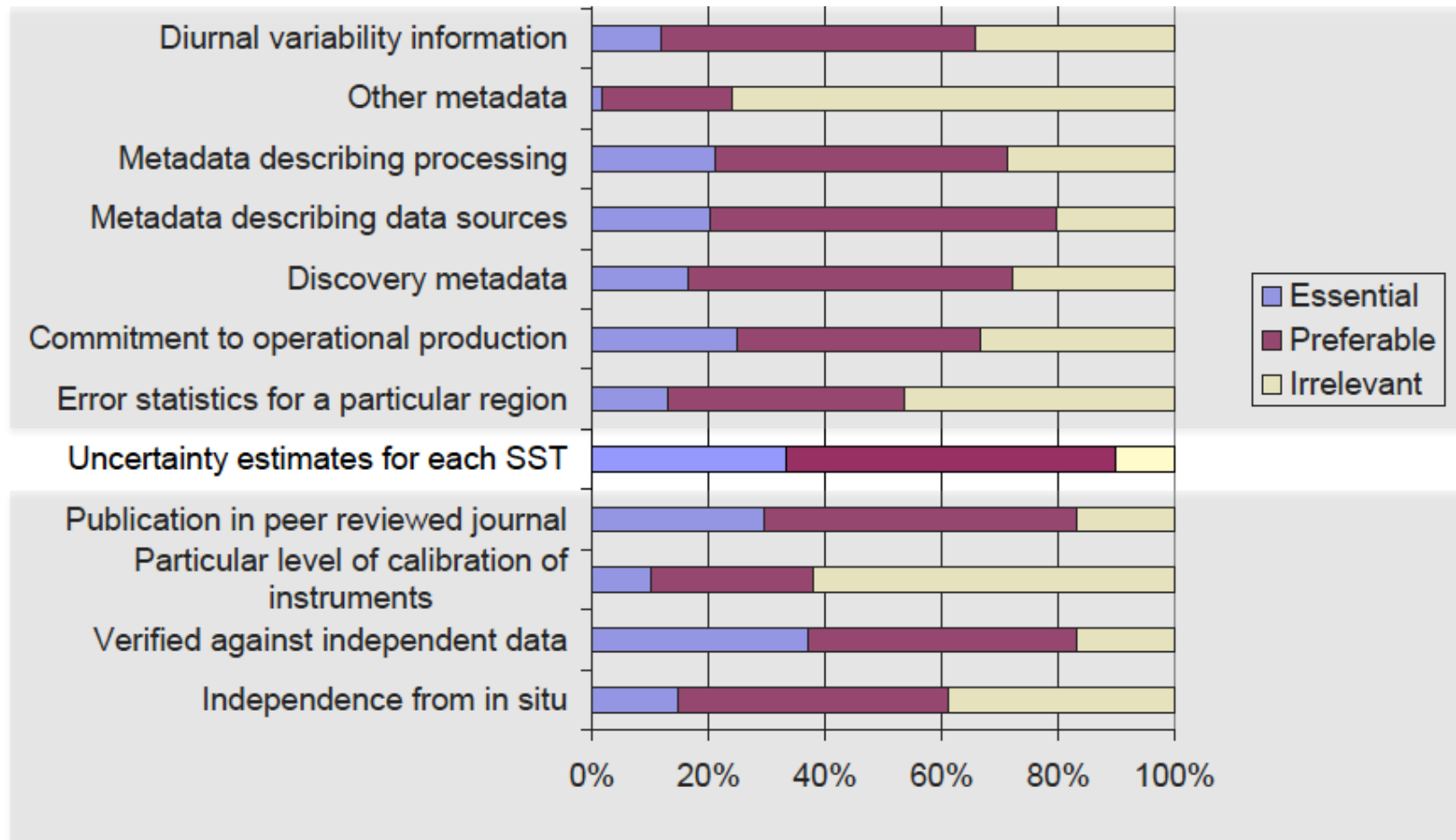
\*and National Physical Laboratory

1

# OBJECTIVES FOR UNCERTAINTY

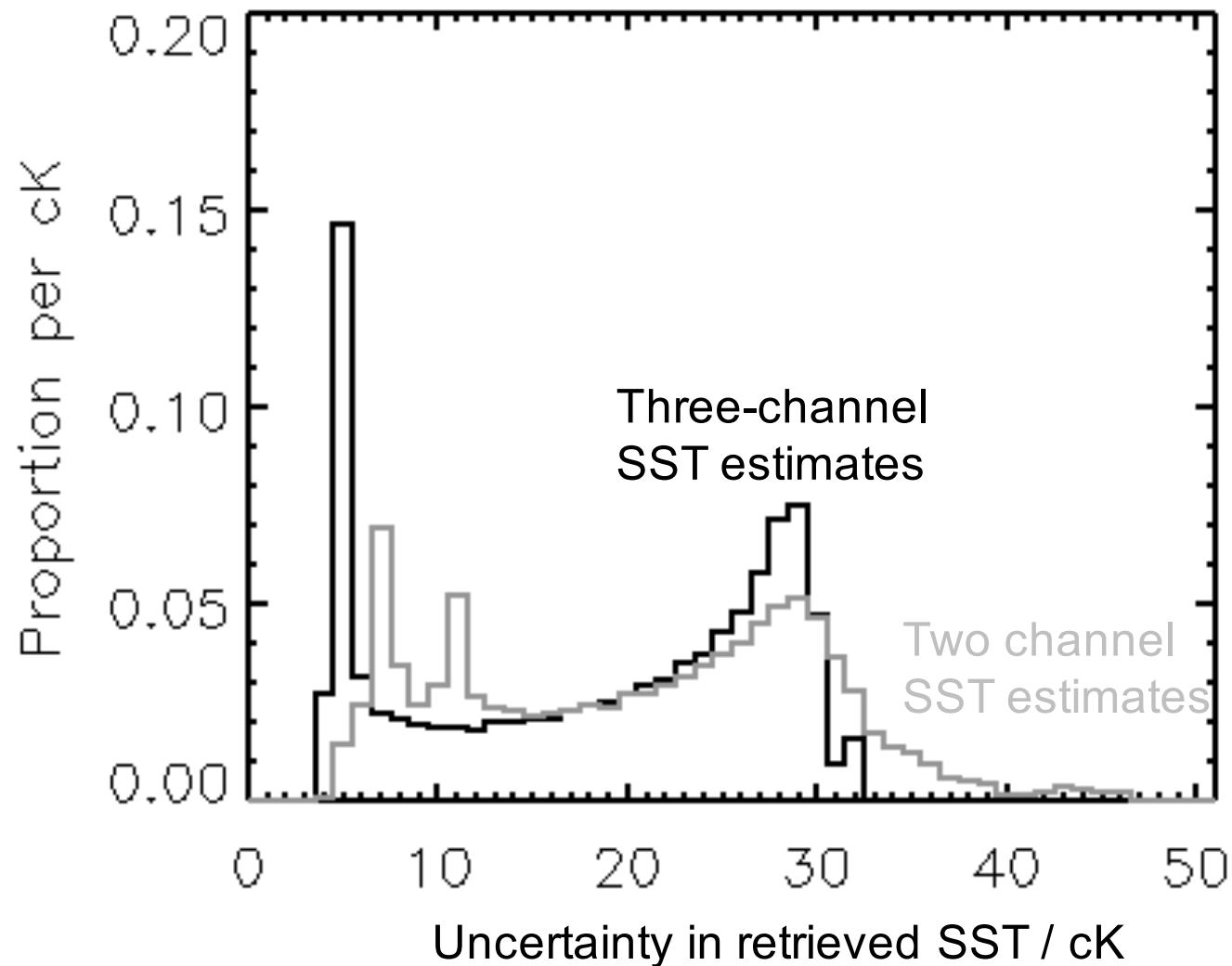
- Satellite datasets should contain sufficient information about uncertainty to
  - distinguish more and less uncertain data
    - per datum
  - propagate uncertainty correctly to higher level datasets
    - such as gridded products and analyses
  - propagate uncertainty to aggregated and derived products
    - products combining datasetswithout over-inflating the data volume
- Give confidence in the uncertainty estimates through validation of them
- Help data users understand and use dataset uncertainties

# USER REQ'MTS (SST)



User requirements survey by UKMO in SST CCI

# Uncertainty varies. This should matter to some users



SST CCI Phase-II



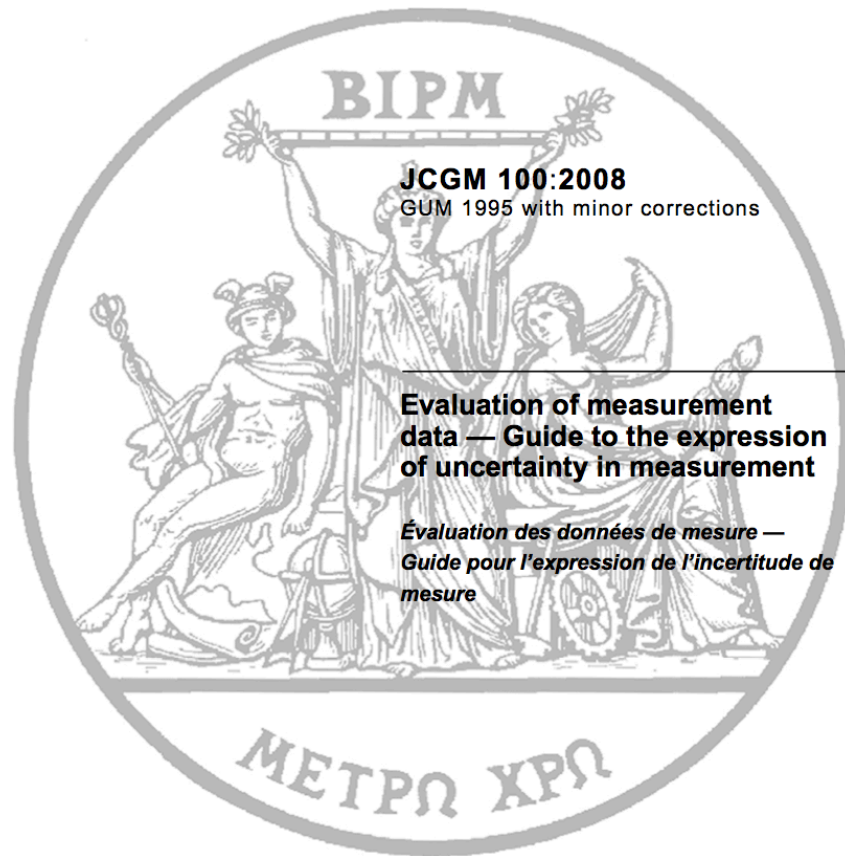
# DEFINITIONS

- Error
  - Concept: How wrong is the measured value?
  - Number: Measured value minus true value
  - We don't know the error, but we should estimate its probability distribution
- Uncertainty
  - Concept: To what degree is the measured value in doubt?
  - Number: e.g., “standard uncertainty” is the SD of the (estimated) error distribution
- Random errors
  - Unpredictable in sign and magnitude
  - Cannot correct
- Systematic errors
  - Predictable in principle, if we had the understanding
  - Not just bias
  - Can learn to correct (and remove)
- Structured random errors
  - (Predictable relationship of error in measured values) x (Random magnitude)
  - Errors are correlated (but, not “correlated uncertainty”)

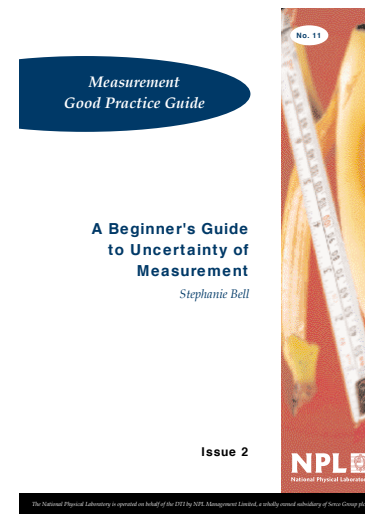
# I PLEAD GUILTY

- I have been on a learning journey – and have published confusing terms along the way!
  - All these terms refer to the same component of uncertainty in satellite SST images
  - “Symmetric pseudo-random **error**”
    - ATBD for Sentinel 3 SLSTR
    - Focus on how errors affect validation statistics
  - “Synoptically **correlated uncertainty**”
    - SST CCI ATBD and Product Specification
    - Focus on the origin in synoptic variability of atmosphere
  - “Uncertainty from spatio-temporally correlated effects”
    - Focus on general statistical nature of effect
- It is worth adopting (and extending) the language of measurement experts

# GUM IS RECOMMENDED



[www.bipm.org/en/publications/guides/gum.html](http://www.bipm.org/en/publications/guides/gum.html)



# UNCERTAINTY CASCADE

detector, amplifier, digitisation, non-linearity ...

**L0**



radiance calibration, geolocation ...

**L1b**



retrieval ambiguity, geophysical definition ...

**L2**



spatio-temporal sampling, correlated errors ...

**L3**

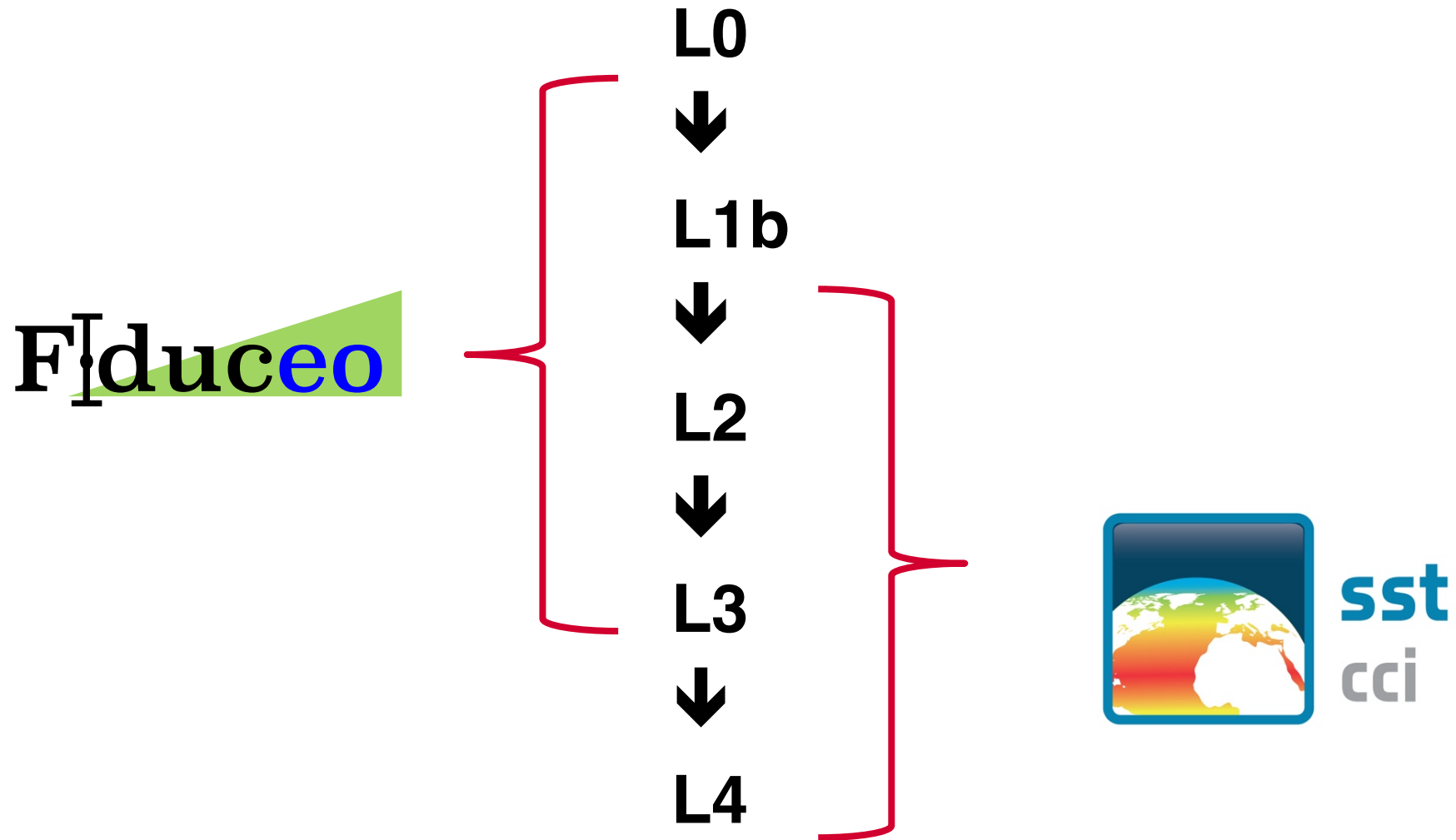


extra-/interpolation, smoothing

**L4**



# UNCERTAINTY CASCADE



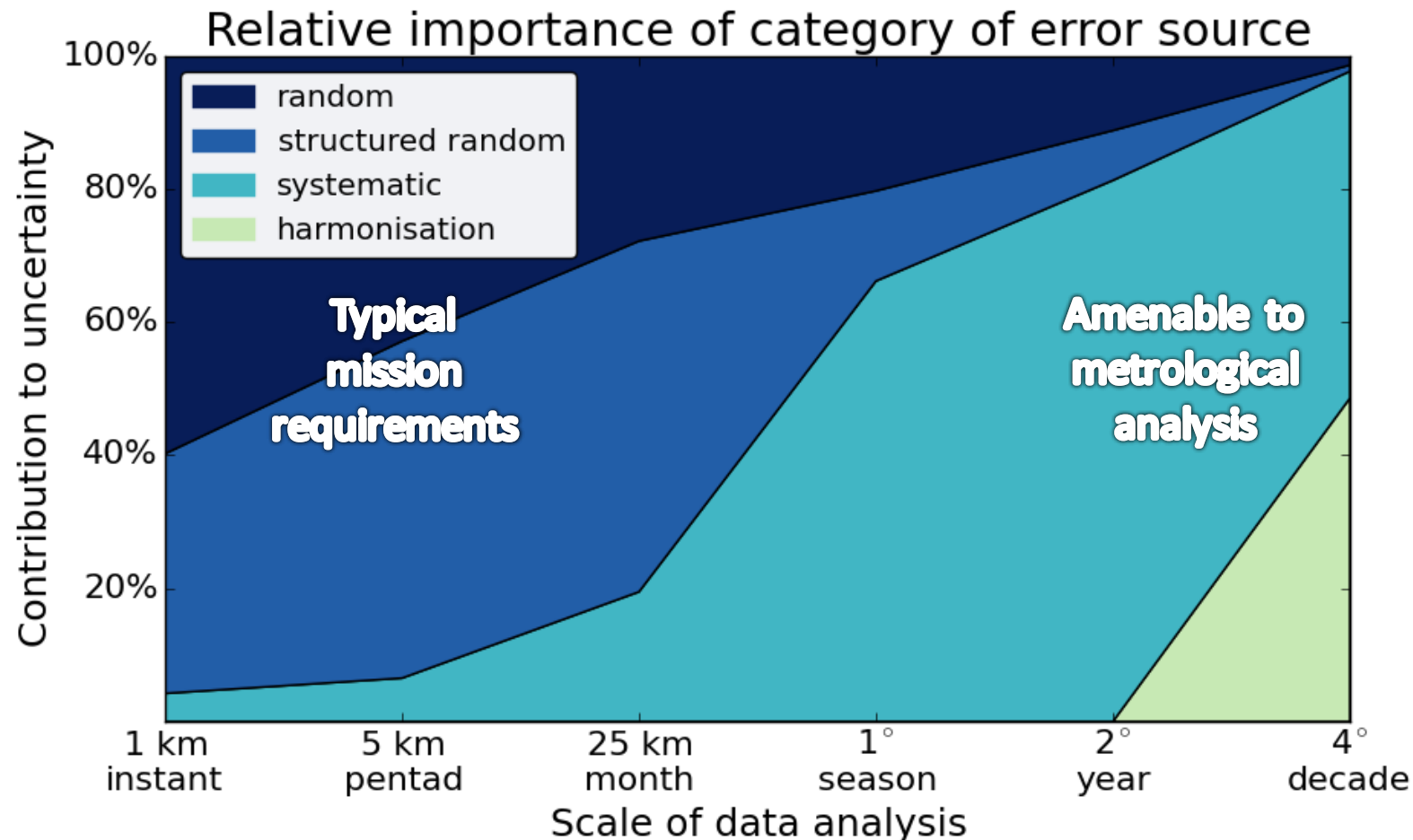
# FIDUCEO



- **Key idea:** develop a widely applicable basis for the **metrology of Earth observation** including historical satellite missions
- The **motivation** is to establish “uncertainty-quantified” evidence base for long-term climate and environmental change from EO systems
- Project runs March 2015 to February 2019

# Why a metrological approach?

## Why consider **all** sources of uncertainty?



If you compare two measurements on different space-time scales the dominant sources of uncertainty in that difference change.

See blog article <http://www.fiduceo.eu/node/237>

# FIDUCEO FCDRs (Yr 1 & 2)

| DATASET           | NATURE                                                                               | POSSIBLE USES                                                                 |
|-------------------|--------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|
| AVHRR FCDR        | Harmonised infra-red radiances and best available reflectance radiances, 1982 - 2016 | SST, LSWT, aerosol, LST, phenology, cloud properties, surface reflectance ... |
| HIRS FCDR         | Harmonised infra-red radiances, 1982 - 2016                                          | Atmospheric humidity, NWP re-analysis, stratospheric aerosol ...              |
| MW Sounder FCDR   | Harmonised microwave BTs for AMSU-B and equivalent channels, 1992 – 2016             | Atmospheric humidity, NWP re-analysis ...                                     |
| Meteosat VIS FCDR | Improved visible spectral response functions and reflectance 1982 to 2016            | Albedo, aerosol, NWP re-analysis, cloud, wind motion vectors,...              |

# FIDUCEO CDRs (Yr 3 & 4)

| DATASET                         | NATURE                                                 | USE                                                                              |
|---------------------------------|--------------------------------------------------------|----------------------------------------------------------------------------------|
| <b>Surface Temperature CDRs</b> | <b>Ensemble SST and lake surface water temperature</b> | Climate science ... model evaluation, re-analysis, derived/synthesis products .. |
| UTH CDR                         | From HIRS and MW, 1992 - 2016                          | Sensitive climate change metric, re-analysis ...                                 |
| Albedo and aerosol CDRs         | From M5 – 7 (1995 – 2006)                              | Climate forcing and change, health ...                                           |
| Aerosol CDR                     | 2002-2012 aerosol for Europe and Africa from AVHRR     | Climate forcing and change, health ...                                           |

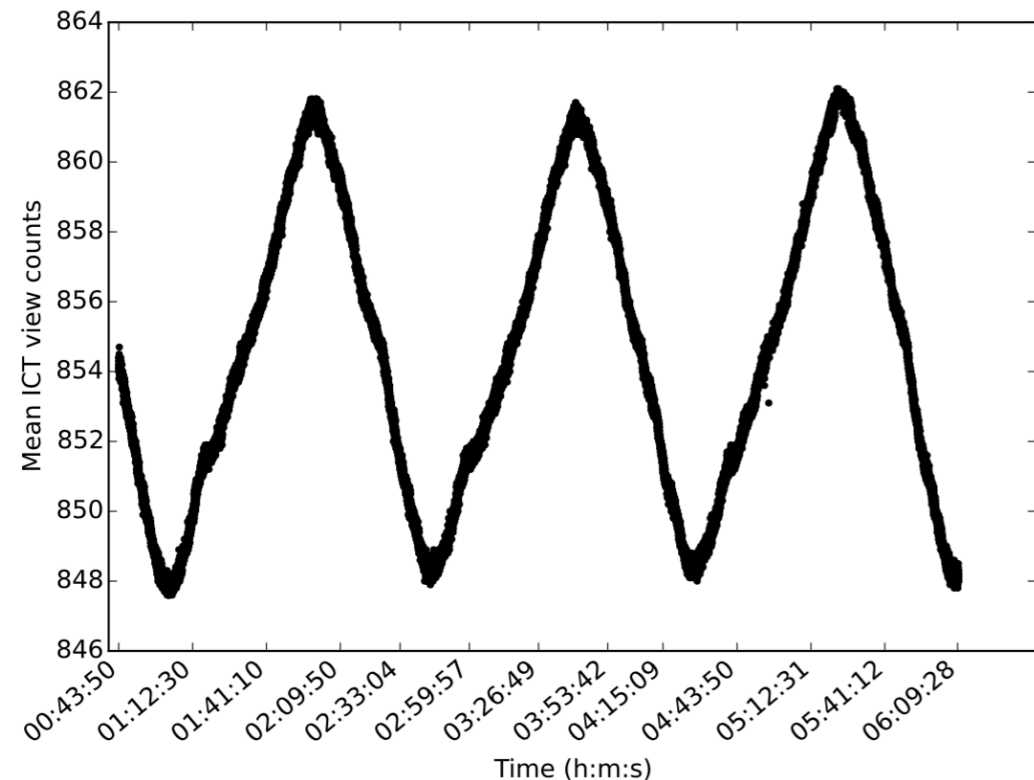
# Example: AVHRR noise effects

Generally quoted  
as “0.12 K” NEDT

Can look at NEDT  
on internal calibration  
target (ICT)

Counts standard deviation

But non-stationary



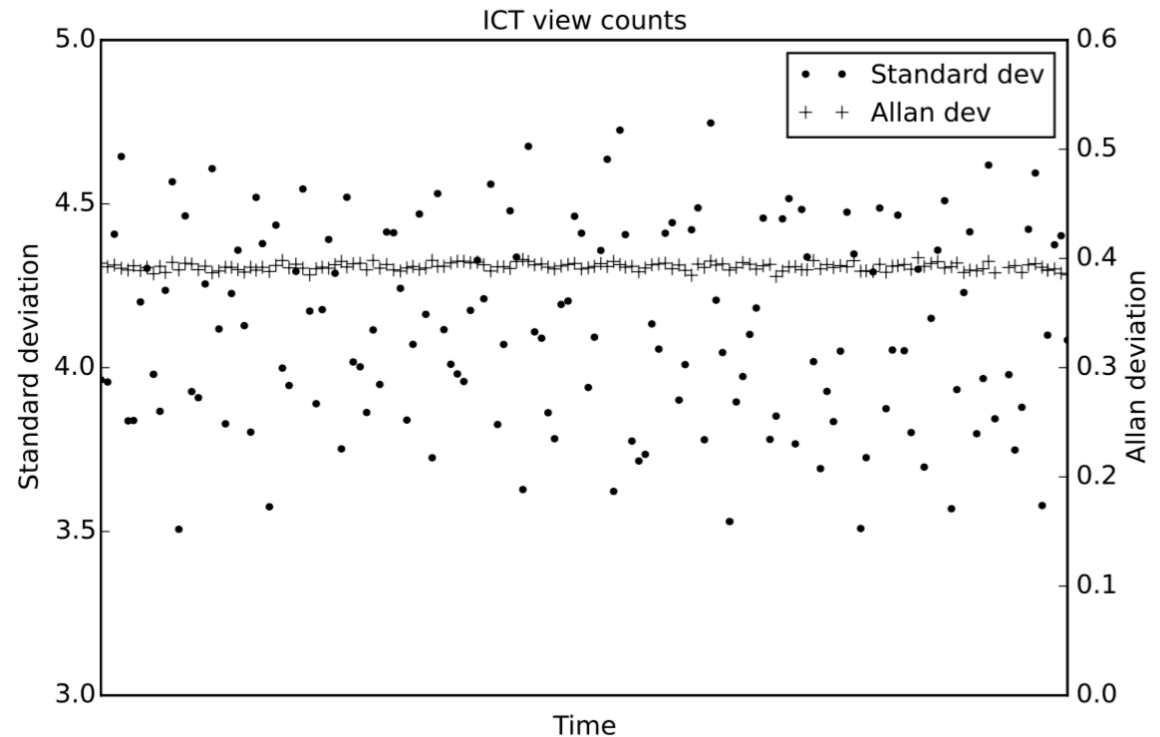
Three orbits of AVHRR ICT counts, NOAA-19

# Example: AVHRR noise effects

Generally quoted as “0.12 K” NEDT

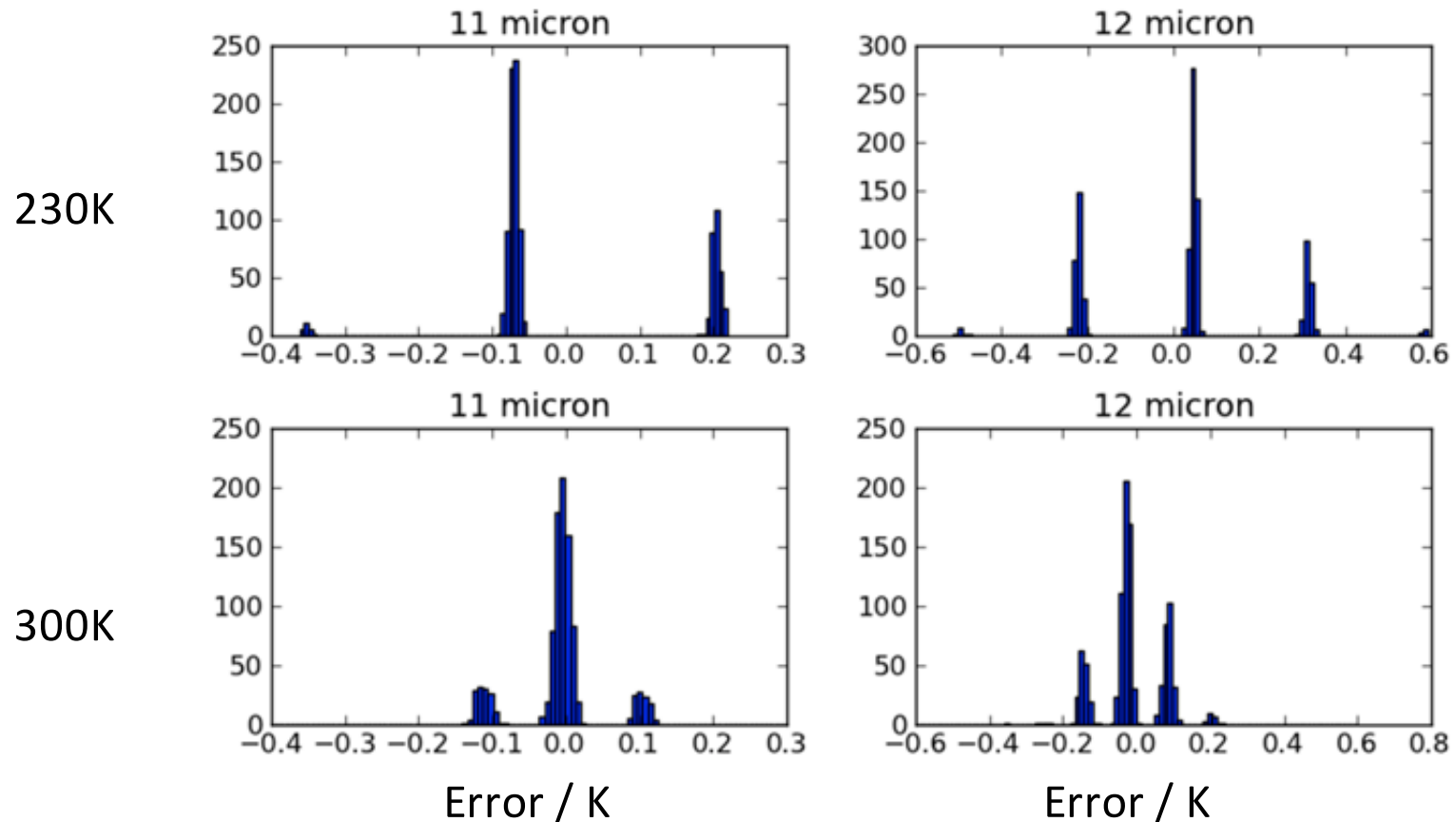
Metrologists use “Allan variances” to analyse noise in non-stationary series

True NEDT  $\sim 0.05$  K



Counts standard deviation, calculated two ways

# Error PDFs for random effects

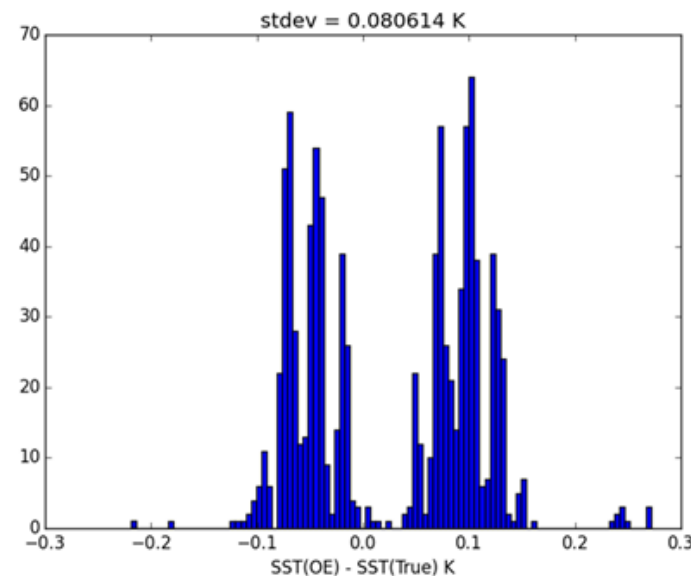
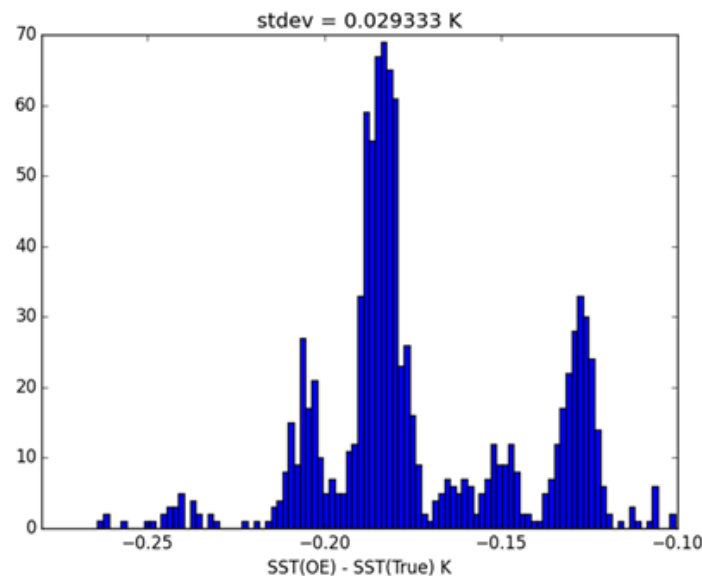


Accounts for: (1) noise and digitization in pixel (random)  
(2) noise/digitization in calibration (structured random)



# Propagation to SST Error PDFs

Monte-Carlo simulation for individual SST retrievals

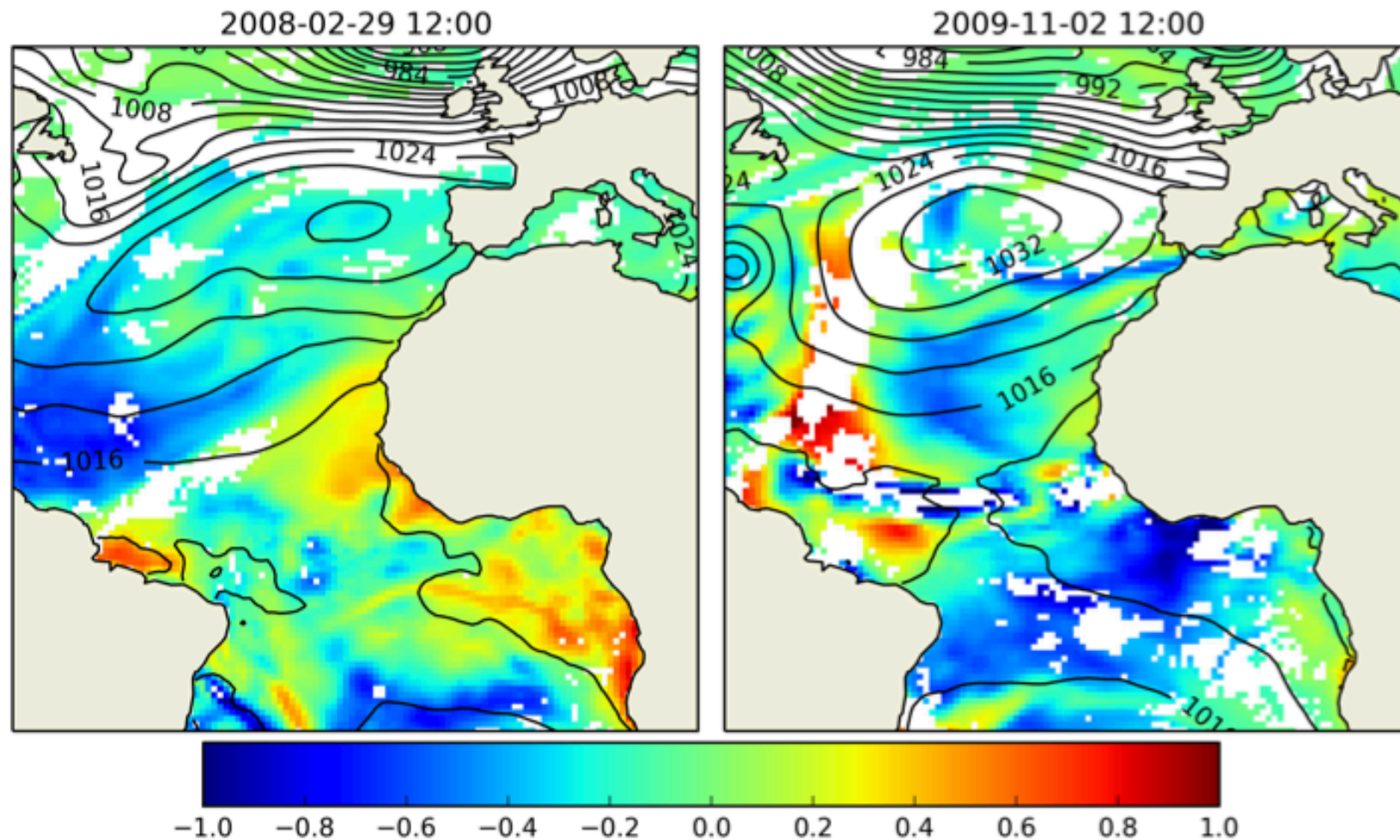


Highly non-Gaussian error distribution

Spread is dominated by propagation of random effect from L1

Non-zero mean dominated by SST retrieval effects (new in L2)

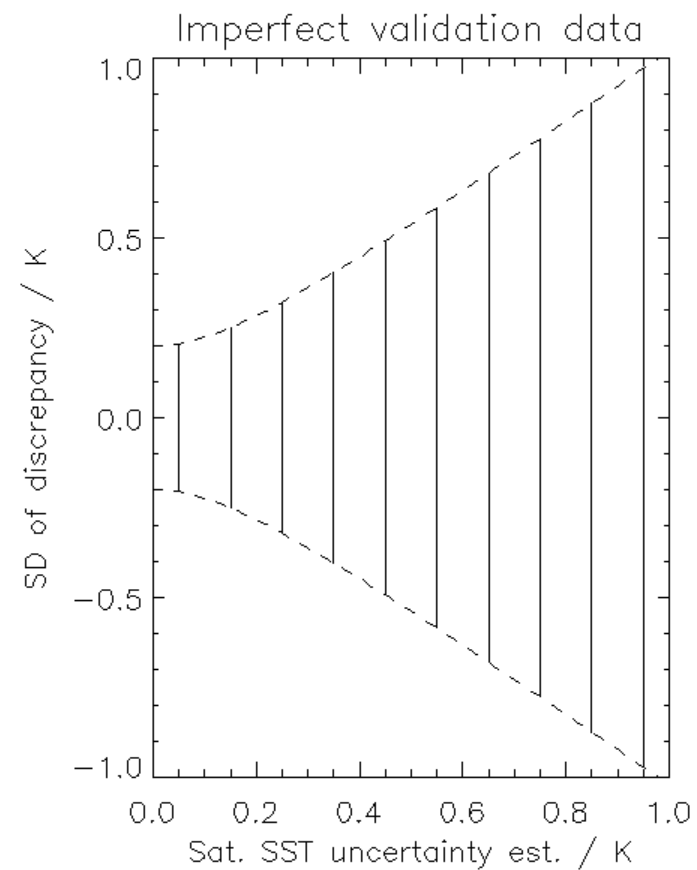
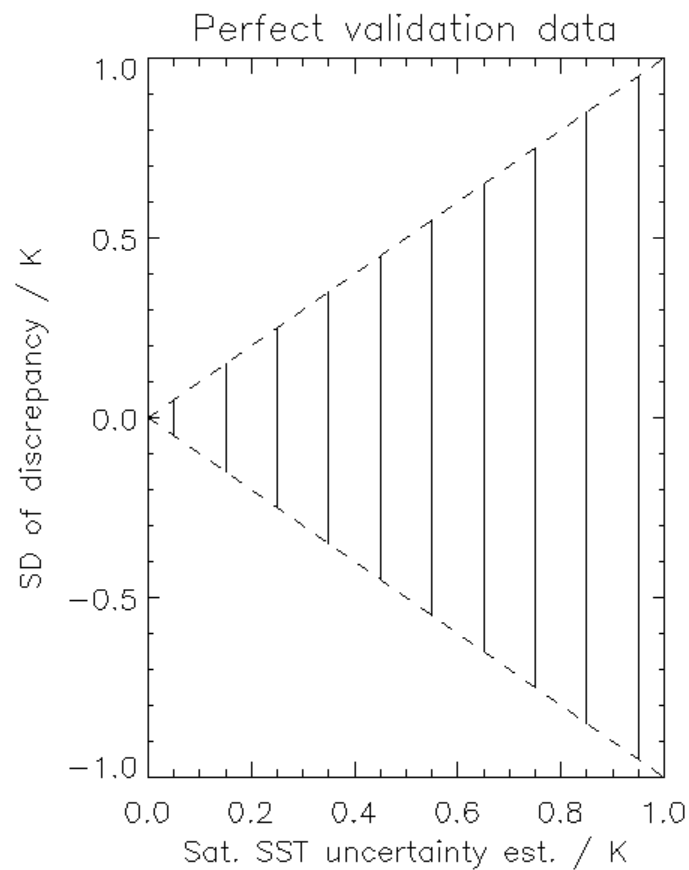
# Simulation of retrieval error



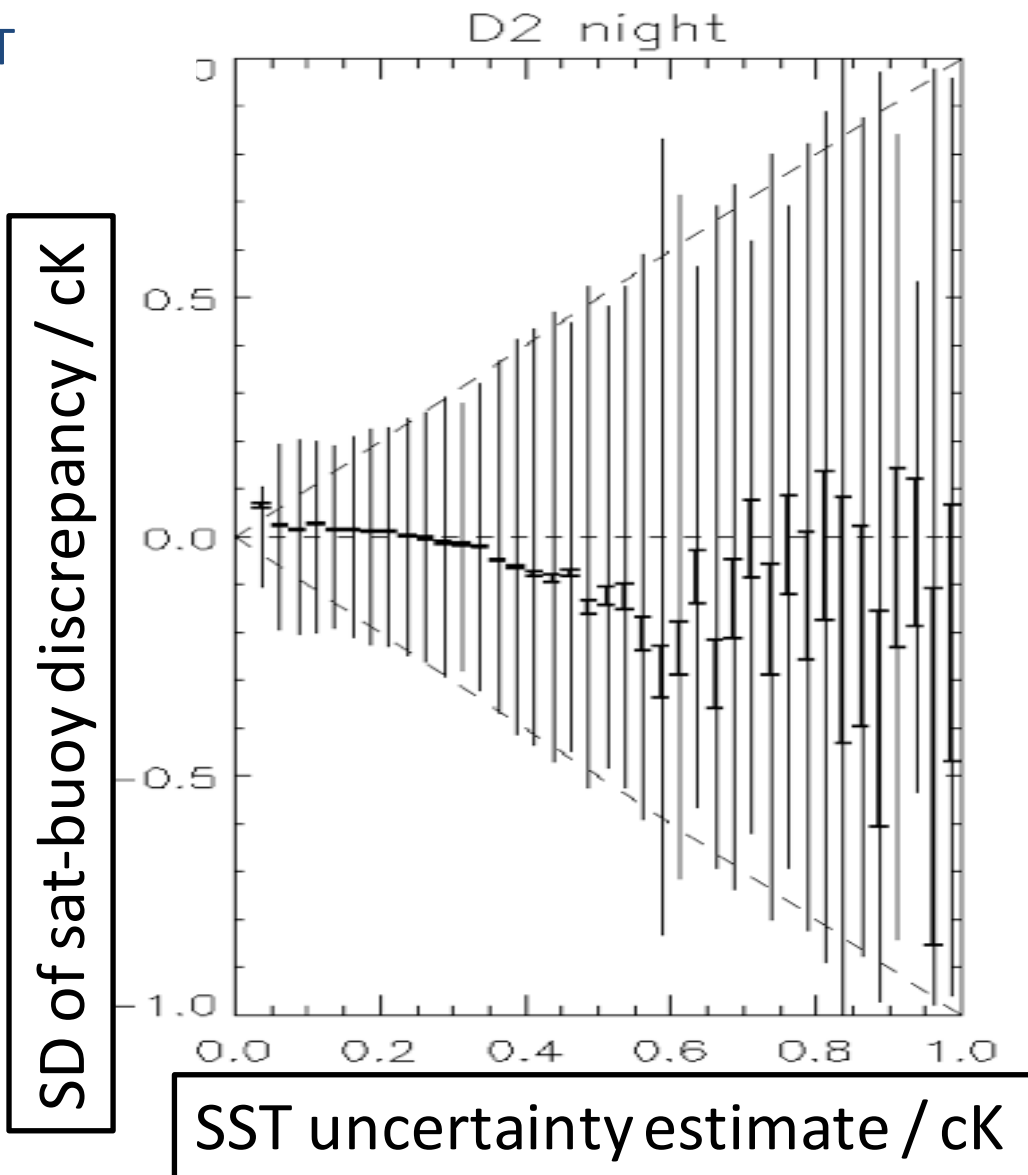
Optical Radiometry for Ocean Climate Measurements (EMPS Vol 47) Chapter 4.3

# How to validate uncertainty?

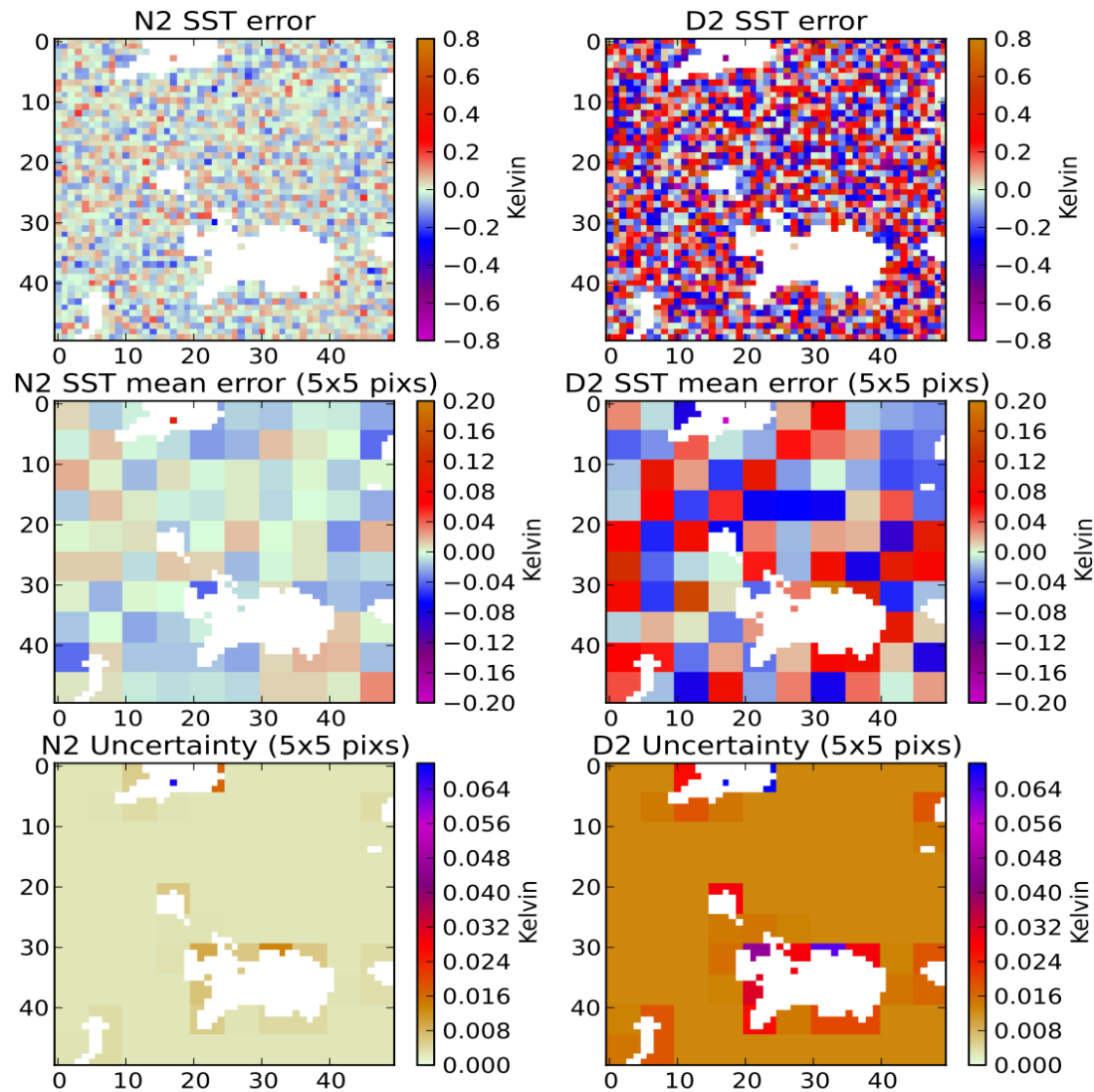
Given drifter calibration uncertainty  $\sim 0.2$  K



AATSR D2 SST  
based on  
coefficients  
0.1 deg cells



# Noise propagation to L3 Gridded Products



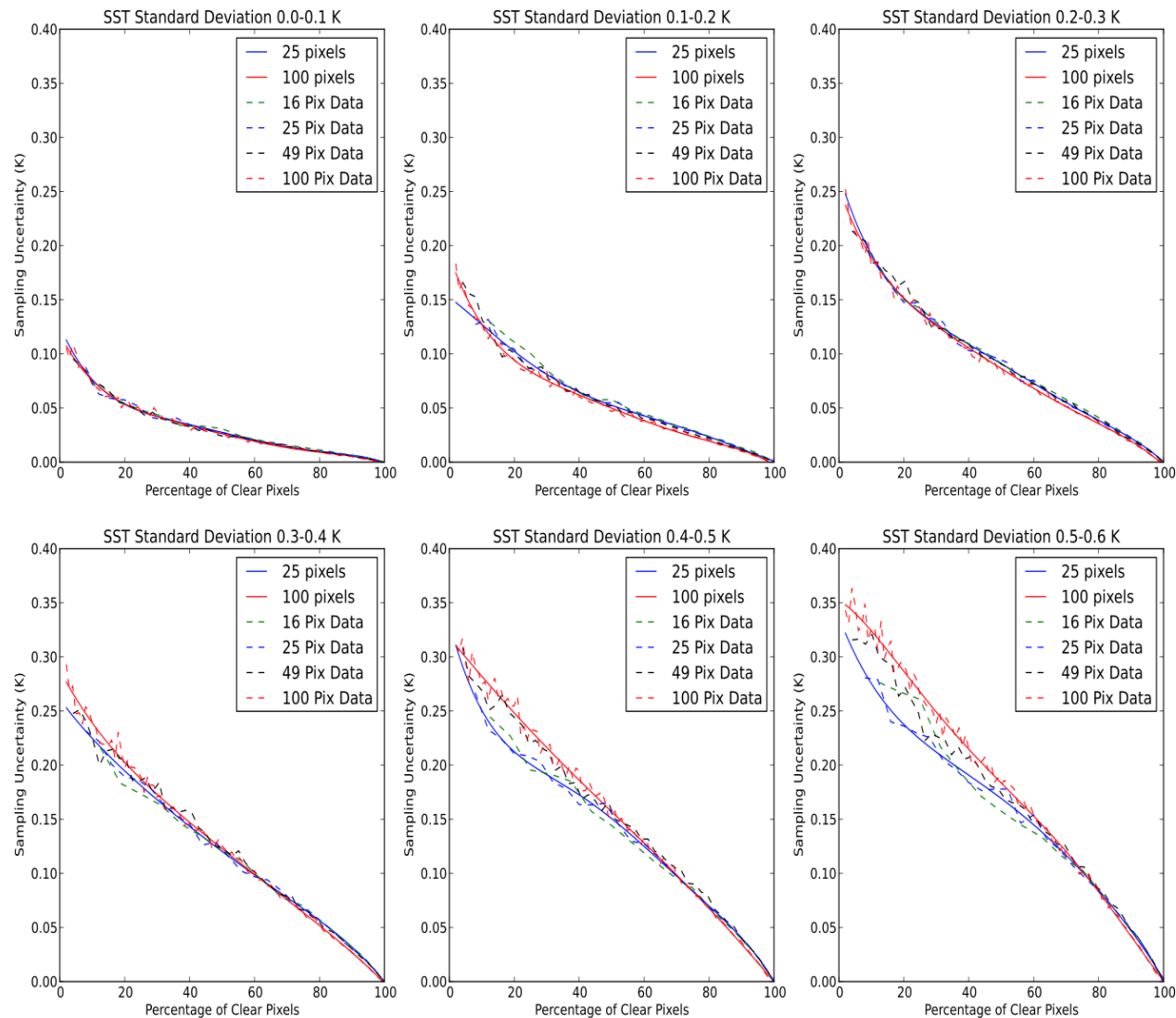
Many SST users want data at 0.05 degrees or coarser so we generate gridded products:

- Uncertainty from random effects reduces as  $1/\sqrt{n}$ .

Bulgin et al., 2016, RSE.

**[10.1016/j.rse.2016.02.022](https://doi.org/10.1016/j.rse.2016.02.022)**

# Sampling Uncertainty in L3 Products



- Sampling uncertainties are introduced where the gridded domain is not fully observed (eg. partially cloud covered).
- These uncertainties can be modeled as a function of domain size, clear sky percentage and SST variability.



# How these uncertainties are communicated in SST CCI products

| Name                                                                                                                    | Long Name                                                            | Type       |
|-------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|------------|
|  20030904091826-ESACCI-L3U_GHR...      | 20030904091826-ESACCI-L3U_GHR SST-SSTskin-AATSR-LT-v02.0-fv0...      | Local File |
|  adjustment_uncertainty                | Time and depth adjustment uncertainty                                | [lon][lat] |
|  l2p_flags                             | L2P flags                                                            | [lon][lat] |
|  large_scale_correlated_uncertainty    | Uncertainty from errors likely to be correlated over large scales    | [lon][lat] |
|  lat                                   | Latitude                                                             | —          |
|  lat_bnds                              | Latitude cell boundaries                                             | —          |
|  lon                                   | Longitude                                                            | —          |
|  lon_bnds                              | Longitude cell boundaries                                            | —          |
|  quality_level                         | quality level of SST pixel                                           | [lon][lat] |
|  sea_surface_temperature               | sea surface skin temperature                                         | [lon][lat] |
|  sea_surface_temperature_depth         | sea surface temperature at 0.2 m                                     | [lon][lat] |
|  sses_bias                             | SSES bias estimate                                                   | [lon][lat] |
|  sses_standard_deviation               | SSES standard deviation                                              | [lon][lat] |
|  sst_depth_total_uncertainty         | Total uncertainty in sea surface temperature depth                   | [lon][lat] |
|  sst_dtime                           | time difference from reference time                                  | [lon][lat] |
|  synoptically_correlated_uncertainty | Uncertainty from errors likely to be correlated over synoptic scales | [lon][lat] |
|  time                                | reference time of sst file                                           | —          |
|  time_bnds                           | Time cell boundaries                                                 | —          |
|  uncorrelated_uncertainty            | Uncertainty from errors unlikely to be correlated between SSTs       | [lon][lat] |
|  wind_speed                          | 10m wind speed                                                       | [lon][lat] |



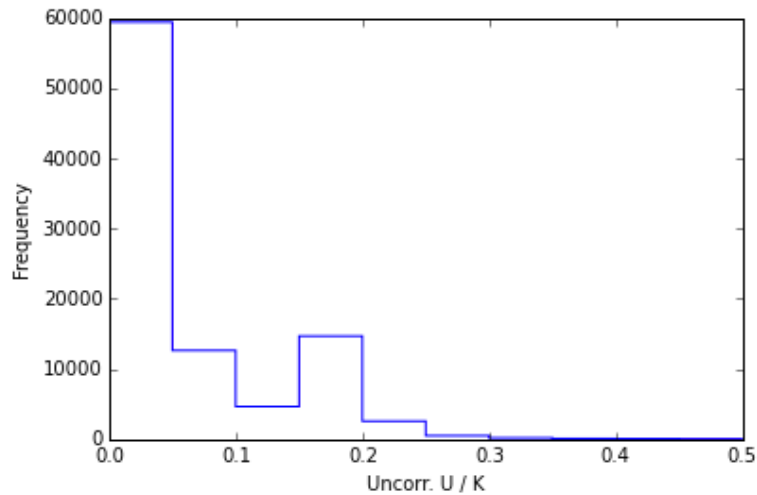
# How these uncertainties are communicated in SST CCI products

| Name                                                                                                                    | Long Name                                                            | Type       |
|-------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|------------|
|  20030904091826-ESACCI-L3U_GHR...      | 20030904091826-ESACCI-L3U_GHR SST-SSTskin-AATSR-LT-v02.0-fv0...      | Local File |
|  adjustment_uncertainty                | Time and depth adjustment uncertainty                                | [lon][lat] |
|  l2p_flags                             | L2P flags                                                            | [lon][lat] |
|  large_scale_correlated_uncertainty    | Uncertainty from errors likely to be correlated over large scales    | [lon][lat] |
|  lat                                   | Latitude                                                             | —          |
|  lat_bnds                              | Latitude cell boundaries                                             | —          |
|  lon                                   | Longitude                                                            | —          |
|  lon_bnds                              | Longitude cell boundaries                                            | —          |
|  quality_level                         | quality level of SST pixel                                           | [lon][lat] |
|  sea_surface_temperature               | sea surface skin temperature                                         | [lon][lat] |
|  sea_surface_temperature_depth         | sea surface temperature at 0.2 m                                     | [lon][lat] |
|  sses_bias                             | SSES bias estimate                                                   | [lon][lat] |
|  sses_standard_deviation               | SSES standard deviation                                              | [lon][lat] |
|  sst_depth_total_uncertainty         | Total uncertainty in sea surface temperature depth                   | [lon][lat] |
|  sst_dtime                           | time difference from reference time                                  | [lon][lat] |
|  synoptically_correlated_uncertainty | Uncertainty from errors likely to be correlated over synoptic scales | [lon][lat] |
|  time                                | reference time of sst file                                           | —          |
|  time_bnds                           | Time cell boundaries                                                 | —          |
|  uncorrelated_uncertainty            | Uncertainty from errors unlikely to be correlated between SSTs       | [lon][lat] |
|  wind_speed                          | 10m wind speed                                                       | [lon][lat] |

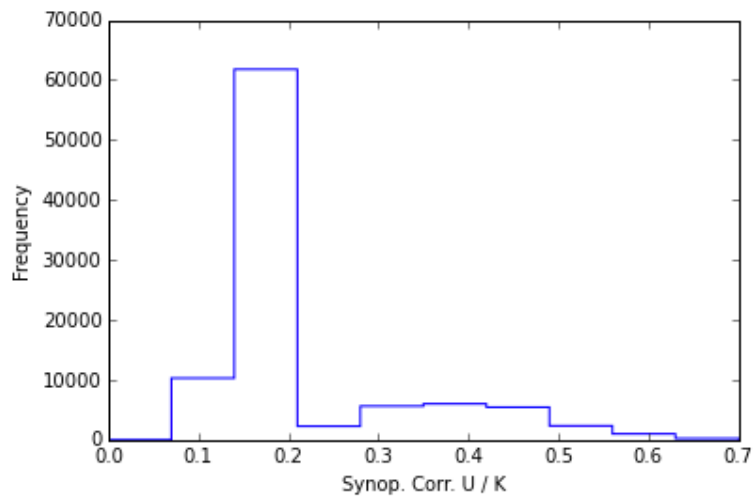




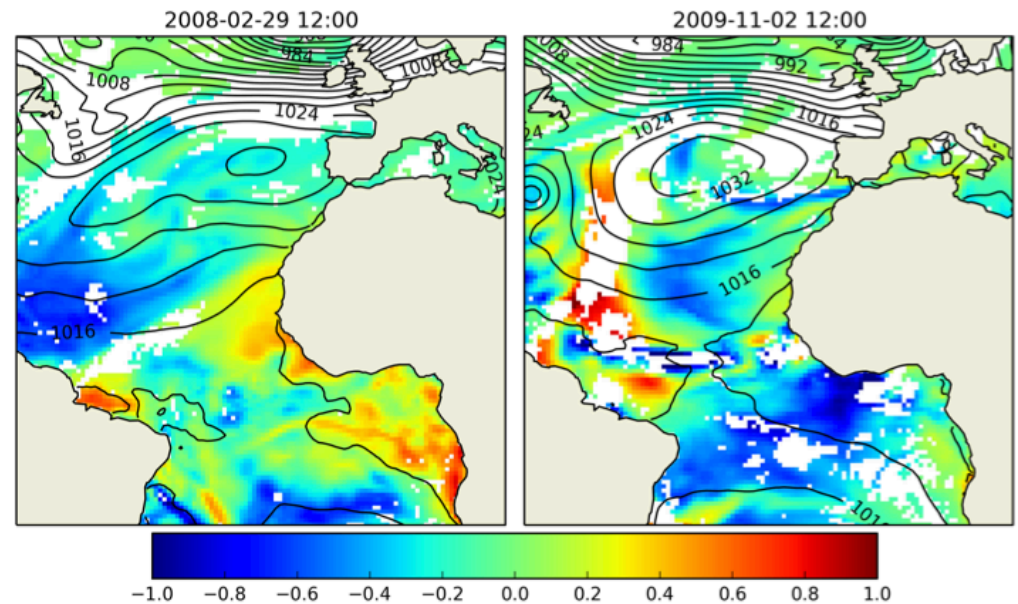
## 'Noise' in SST (uncorrelated)



## Limitations of algorithm (synop. corr.)



## Optical Radiometry for Ocean Climate Measurements (EMPS Vol 47) Chapter 4.3

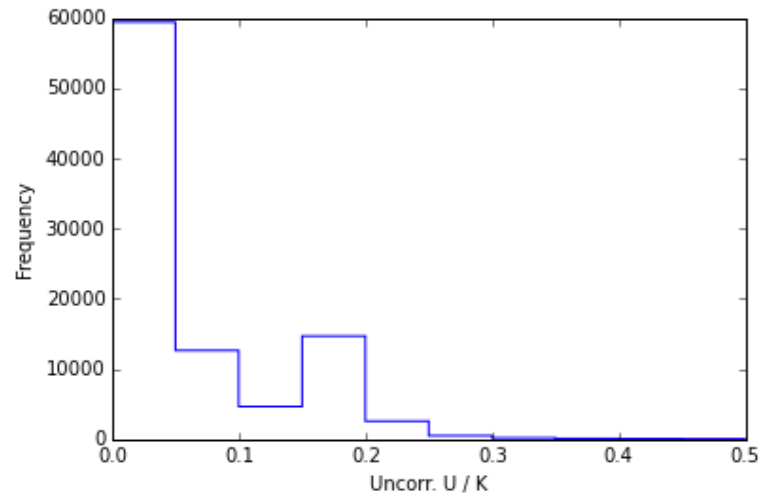


# How these uncertainties are communicated in SST CCI products

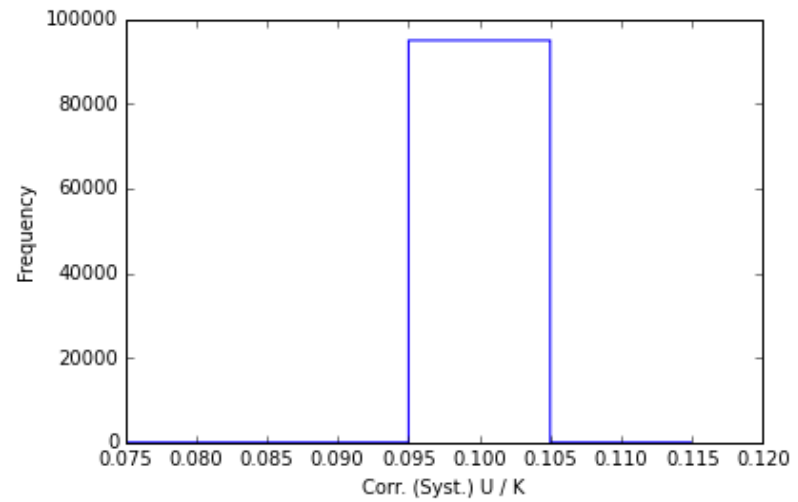
| Name                                                                                                                    | Long Name                                                            | Type       |
|-------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|------------|
|  20030904091826-ESACCI-L3U_GHR...      | 20030904091826-ESACCI-L3U_GHR SST-SSTskin-AATSR-LT-v02.0-fv0...      | Local File |
|  adjustment_uncertainty                | Time and depth adjustment uncertainty                                | [lon][lat] |
|  l2p_flags                             | L2P flags                                                            | [lon][lat] |
|  large_scale_correlated_uncertainty    | Uncertainty from errors likely to be correlated over large scales    | [lon][lat] |
|  lat                                   | Latitude                                                             | —          |
|  lat_bnds                              | Latitude cell boundaries                                             | —          |
|  lon                                   | Longitude                                                            | —          |
|  lon_bnds                              | Longitude cell boundaries                                            | —          |
|  quality_level                         | quality level of SST pixel                                           | [lon][lat] |
|  sea_surface_temperature               | sea surface skin temperature                                         | [lon][lat] |
|  sea_surface_temperature_depth         | sea surface temperature at 0.2 m                                     | [lon][lat] |
|  sses_bias                             | SSES bias estimate                                                   | [lon][lat] |
|  sses_standard_deviation               | SSES standard deviation                                              | [lon][lat] |
|  sst_depth_total_uncertainty         | Total uncertainty in sea surface temperature depth                   | [lon][lat] |
|  sst_dtime                           | time difference from reference time                                  | [lon][lat] |
|  synoptically_correlated_uncertainty | Uncertainty from errors likely to be correlated over synoptic scales | [lon][lat] |
|  time                                | reference time of sst file                                           | —          |
|  time_bnds                           | Time cell boundaries                                                 | —          |
|  uncorrelated_uncertainty            | Uncertainty from errors unlikely to be correlated between SSTs       | [lon][lat] |
|  wind_speed                          | 10m wind speed                                                       | [lon][lat] |



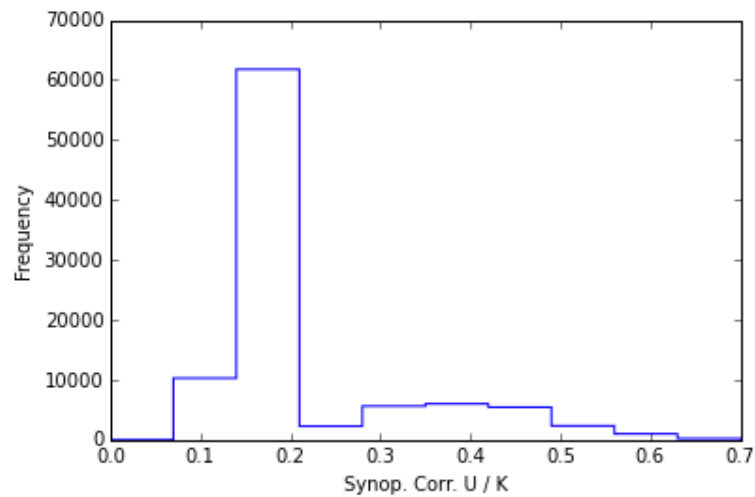
## 'Noise' in SST (uncorrelated)



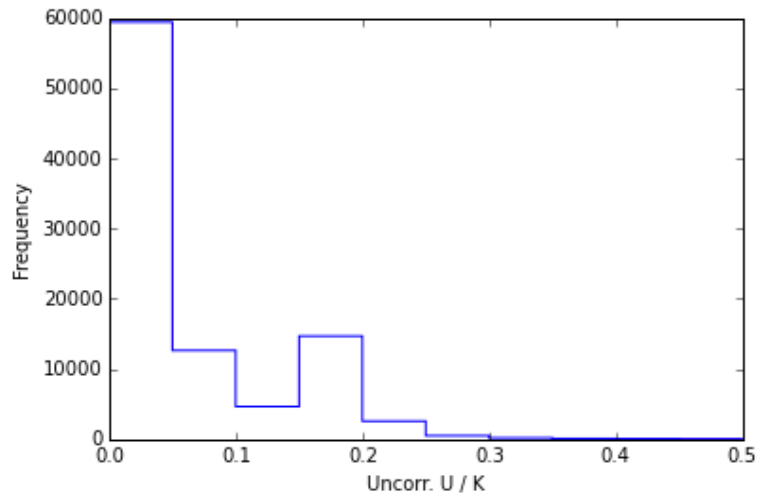
## Systematic (large scale correlated)



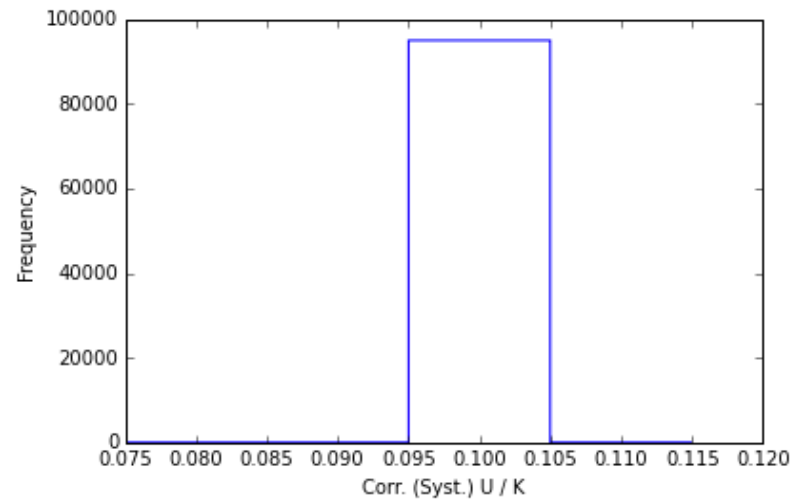
## Limitations of algorithm (synop. corr.)



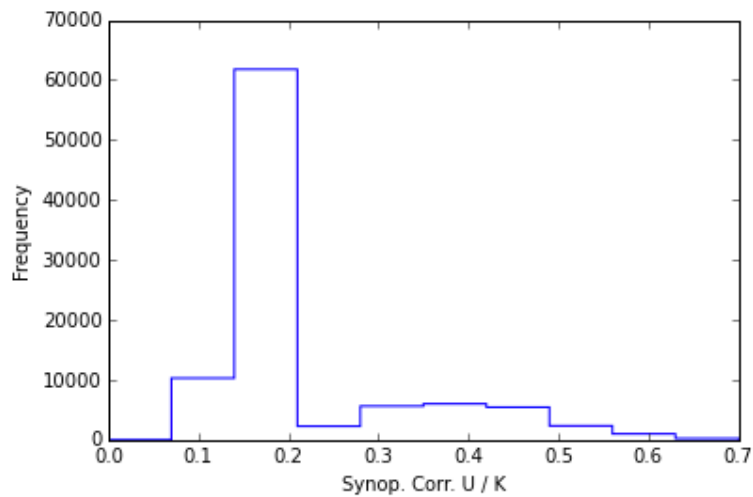
## 'Noise' in SST (uncorrelated)



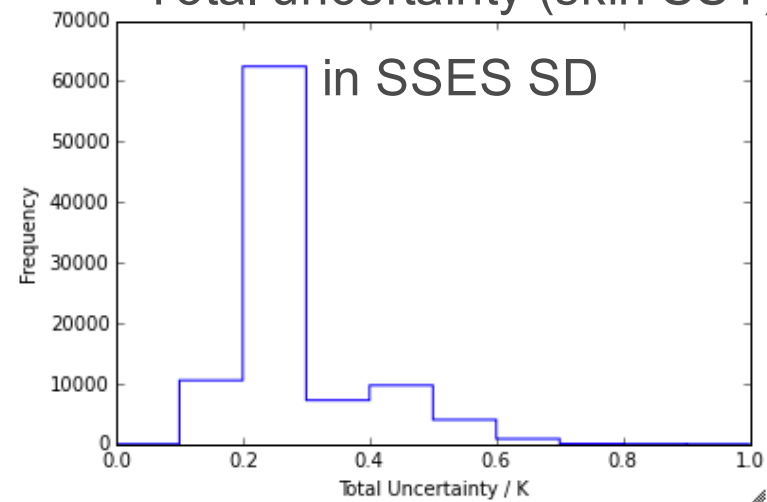
## Systematic (large scale correlated)



## Limitations of algorithm (synop. corr.)



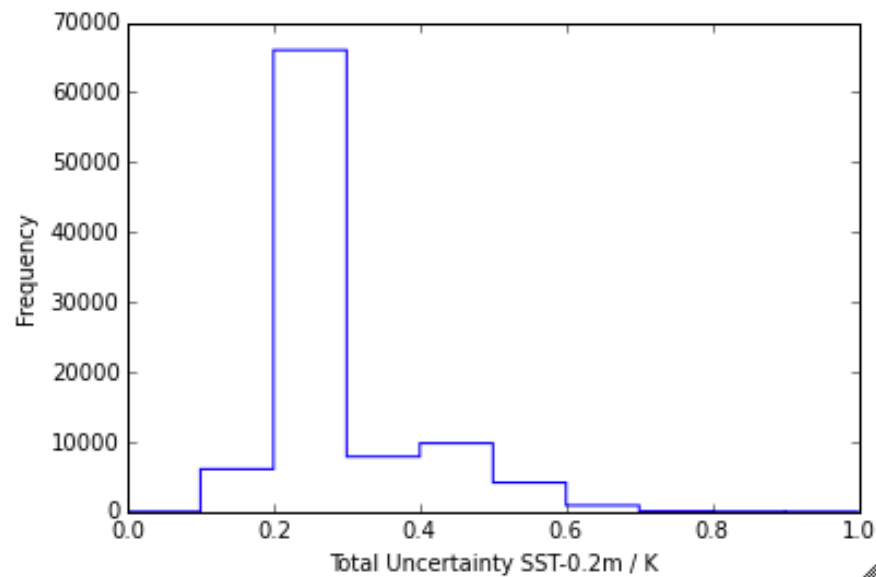
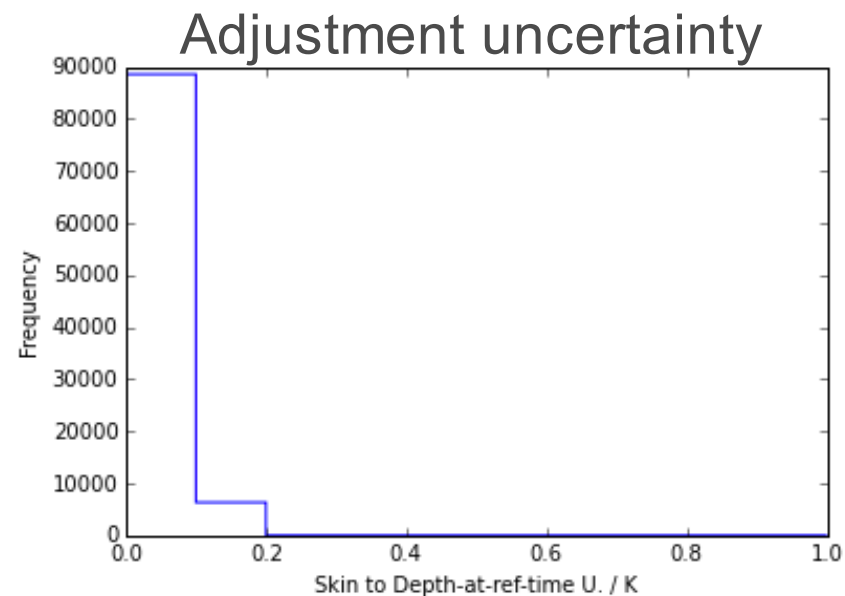
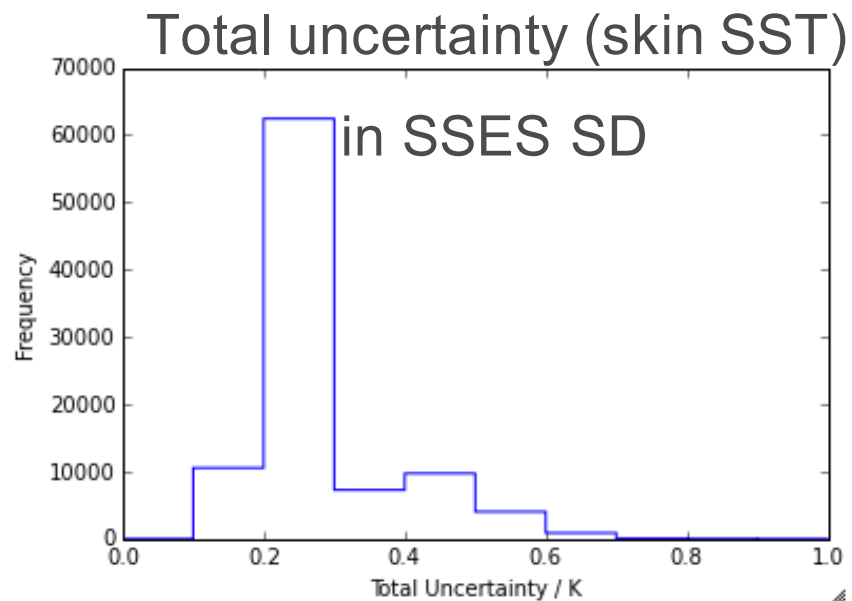
## Total uncertainty (skin SST)



# How these uncertainties are communicated in SST CCI products

| Name                                                                                                                    | Long Name                                                            | Type       |
|-------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|------------|
|  20030904091826-ESACCI-L3U_GHR...      | 20030904091826-ESACCI-L3U_GHR SST-SSTskin-AATSR-LT-v02.0-fv0...      | Local File |
|  adjustment_uncertainty                | Time and depth adjustment uncertainty                                | [lon][lat] |
|  l2p_flags                             | L2P flags                                                            | [lon][lat] |
|  large_scale_correlated_uncertainty    | Uncertainty from errors likely to be correlated over large scales    | [lon][lat] |
|  lat                                   | Latitude                                                             | —          |
|  lat_bnds                              | Latitude cell boundaries                                             | —          |
|  lon                                   | Longitude                                                            | —          |
|  lon_bnds                              | Longitude cell boundaries                                            | —          |
|  quality_level                         | quality level of SST pixel                                           | [lon][lat] |
|  sea_surface_temperature               | sea surface skin temperature                                         | [lon][lat] |
|  sea_surface_temperature_depth         | sea surface temperature at 0.2 m                                     | [lon][lat] |
|  sses_bias                             | SSES bias estimate                                                   | [lon][lat] |
|  sses_standard_deviation               | SSES standard deviation                                              | [lon][lat] |
|  sst_depth_total_uncertainty         | Total uncertainty in sea surface temperature depth                   | [lon][lat] |
|  sst_dtime                           | time difference from reference time                                  | [lon][lat] |
|  synoptically_correlated_uncertainty | Uncertainty from errors likely to be correlated over synoptic scales | [lon][lat] |
|  time                                | reference time of sst file                                           | —          |
|  time_bnds                           | Time cell boundaries                                                 | —          |
|  uncorrelated_uncertainty            | Uncertainty from errors unlikely to be correlated between SSTs       | [lon][lat] |
|  wind_speed                          | 10m wind speed                                                       | [lon][lat] |





Total uncertainty in  
SST<sub>0.2 m</sub>



# How these uncertainties are communicated in SST CCI products

| Name                                                                                                                    | Long Name                                                            | Type       |
|-------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------------------|------------|
|  20030904091826-ESACCI-L3U_GHR...      | 20030904091826-ESACCI-L3U_GHR SST-SSTskin-AATSR-LT-v02.0-fv0...      | Local File |
|  adjustment_uncertainty                | Time and depth adjustment uncertainty                                | [lon][lat] |
|  l2p_flags                             | L2P flags                                                            | [lon][lat] |
|  large_scale_correlated_uncertainty    | Uncertainty from errors likely to be correlated over large scales    | [lon][lat] |
|  lat                                   | Latitude                                                             | —          |
|  lat_bnds                              | Latitude cell boundaries                                             | —          |
|  lon                                   | Longitude                                                            | —          |
|  lon_bnds                              | Longitude cell boundaries                                            | —          |
|  quality_level                         | quality level of SST pixel                                           | [lon][lat] |
|  sea_surface_temperature               | sea surface skin temperature                                         | [lon][lat] |
|  sea_surface_temperature_depth         | sea surface temperature at 0.2 m                                     | [lon][lat] |
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|  sst_dtime                           | time difference from reference time                                  | [lon][lat] |
|  synoptically_correlated_uncertainty | Uncertainty from errors likely to be correlated over synoptic scales | [lon][lat] |
|  time                                | reference time of sst file                                           | —          |
|  time_bnds                           | Time cell boundaries                                                 | —          |
|  uncorrelated_uncertainty            | Uncertainty from errors unlikely to be correlated between SSTs       | [lon][lat] |
|  wind_speed                          | 10m wind speed                                                       | [lon][lat] |



# How should uncertainty be presented?

**“Just give me one number” (60%)**

Total uncertainty (35%)  
Confidence interval (25%)

“Separate out main components of uncertainty” (20%)

“A probability distribution of error would be nice.” (15%)

“Ensemble, please.” (5%)

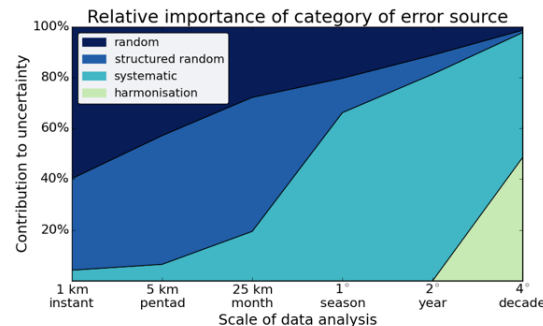
Result of SST CCI  
User Survey, 2010



# How should uncertainty be presented?

Significant request from major users at SST CCI user consultation in 2014 (after discussing uncertainty concepts and issues for two days)

“Ensemble, please.”



# CONCLUSIONS

- Worthwhile to work with metrologists and their defined language for uncertainty in measurement
  - needs some extension: FIDUCEO vocabulary
- Some errors are random or systematic, but structured random errors can't be ignored
  - correlated effects are complex to propagate across scales
  - “slow” effects are most readily captured and understood via ensemble products?
- Uncertainty-quantified Climate Data Record
  - Uncertainty information in product that (i) discriminates more and less certain data, (ii) is validated as being realistic in magnitude and structure, (iii) is traceable back to FCDR uncertainty information (also traceable)
- Still working on
  - Uncertainty propagation across scales
  - Validation of uncertainty – including correlation structures
  - Standardisation of uncertainty in data structures
  - Satellite-based ensemble SST products