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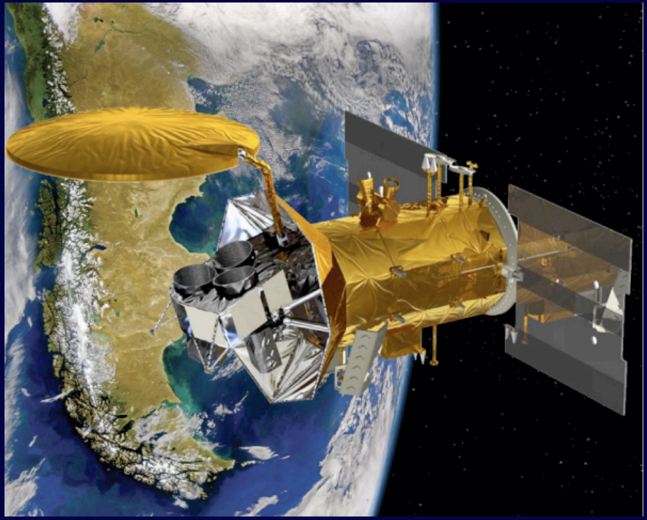
# Formal Uncertainty Assessment in Aquarius Salinity Retrieval Algorithm

T. Meissner



Aquarius Cal/Val Meeting
Santa Rosa
March 31/April 1, 2015

# Outline

1. Background/Philosophy
2. Developing an Algorithm for Assessing Formal Uncertainties
    - Level 2
    - Level 3
3. Physical Error Model
    - Description of Major Components
4. Results
    - Formal Versus Empirical Uncertainties

# Aquarius L3 Performance

## Triple Collocation Series

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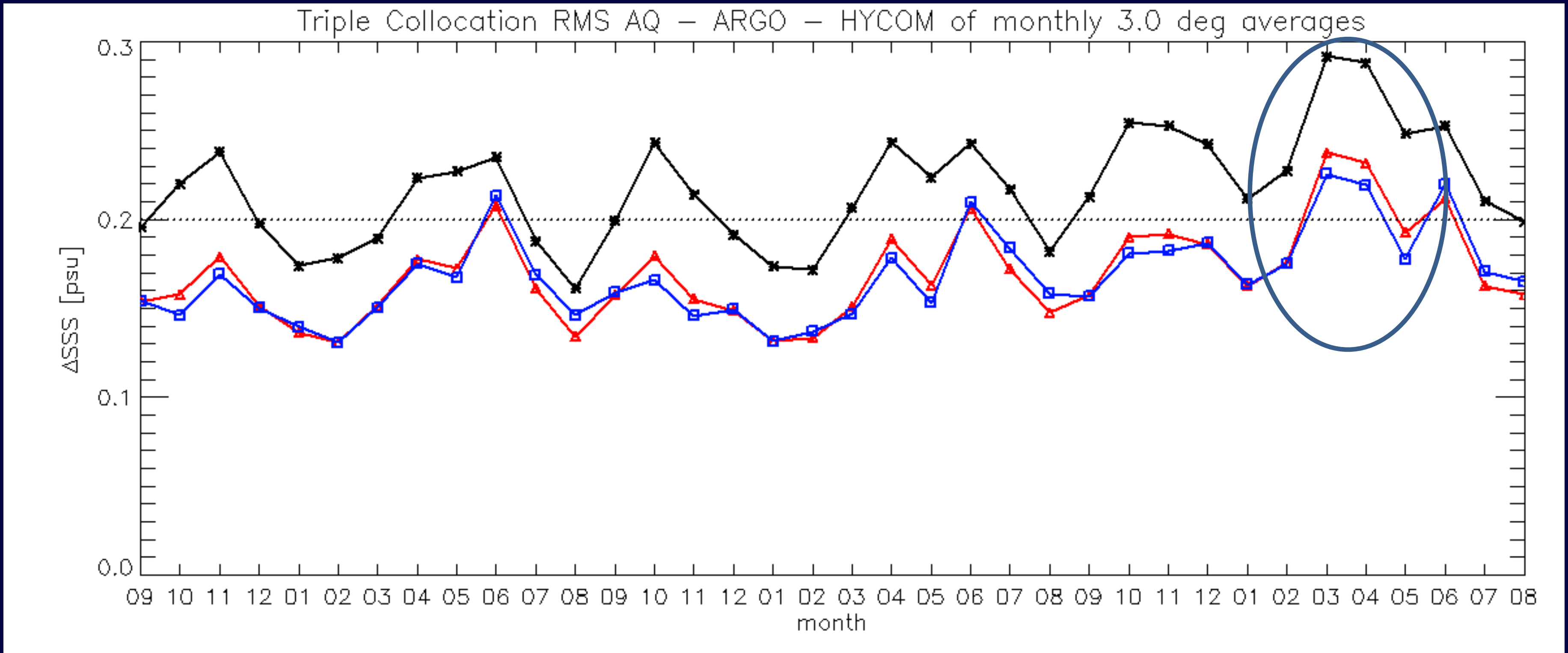


| | V3.0 | V3.0 bias adjusted | V3.4 (new GMF) |
|---|---|---|---|
| RMS | 0.220 | 0.170 | 0.172 |

open ocean, very strict Q/C (cold water, high winds, RFI mask, …)

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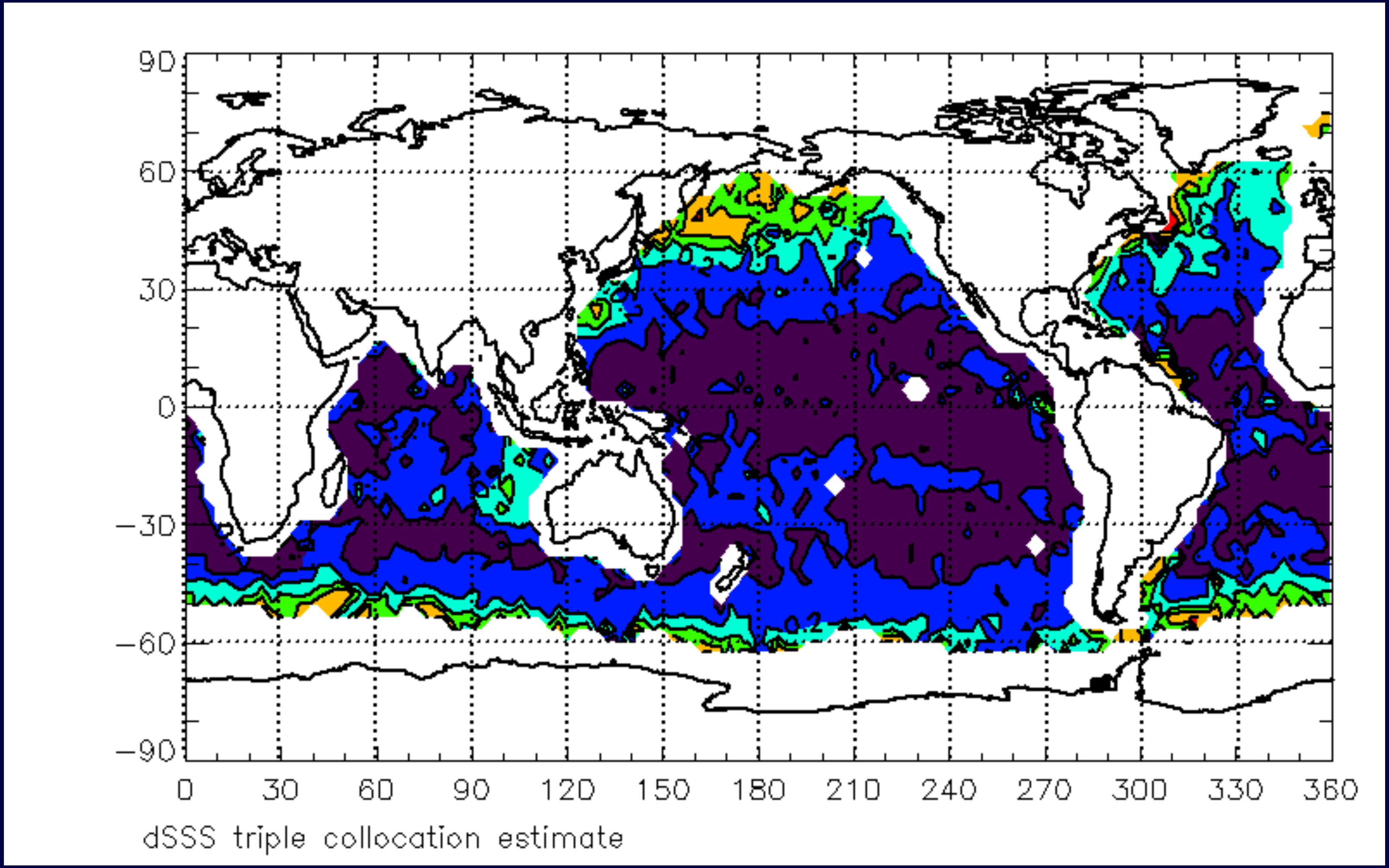
# Aquarius L3 Performance
## Triple Collocation Map




open ocean, very strict Q/C (exclude cold water, high winds, RFI mask, …)

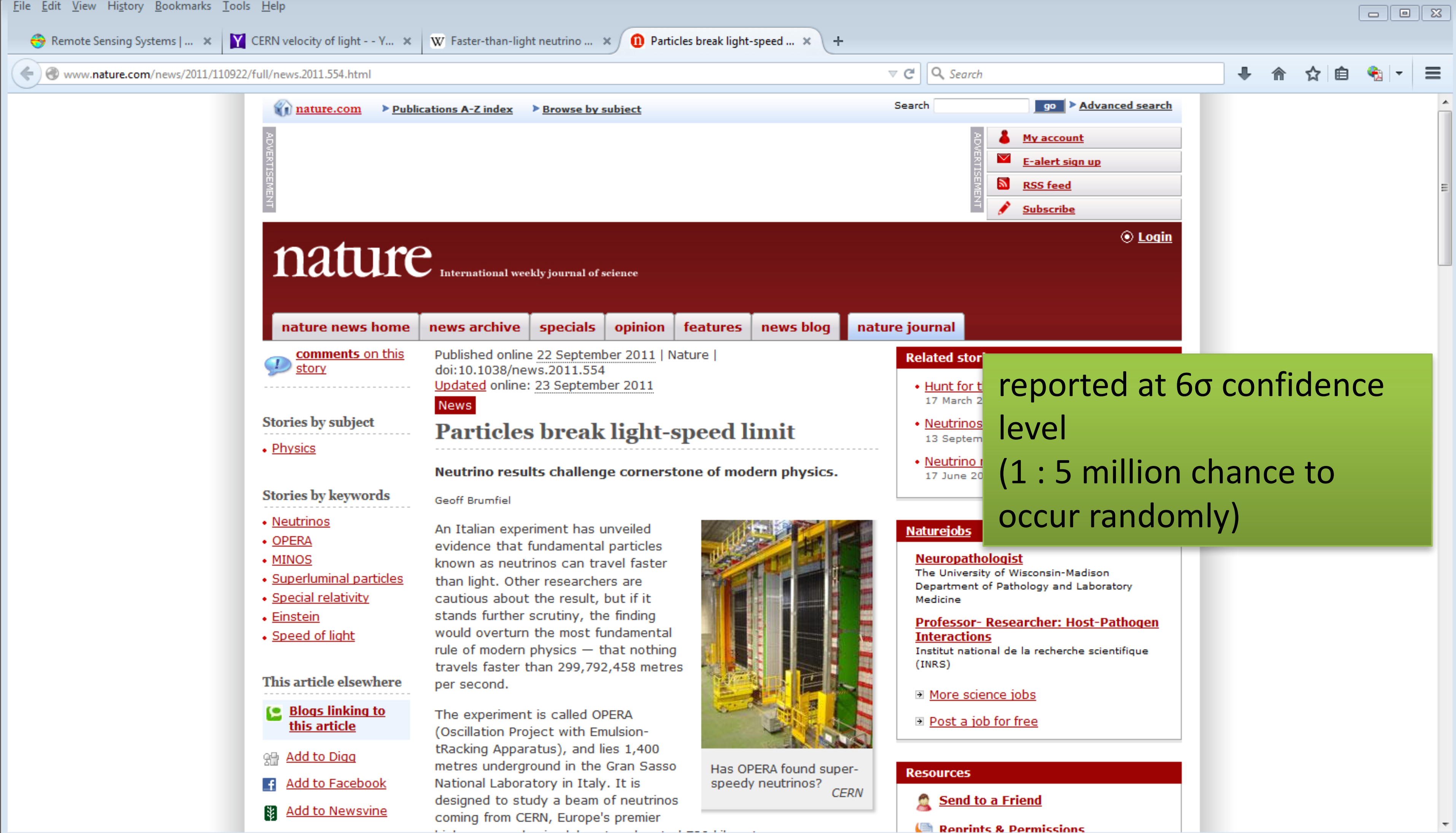
# Uncertainty Estimates
## Purpose

- Any meaningful physical measurement has a value and an uncertainty (error bar).
  - Required nowadays for many studies (ROSES calls).
  - Not easy. Not straightforward. Reality is far behind.
- Important for ocean modeling who use Aquarius salinity as input in their model.
  - Determines relative weight of observation in assimilation.
- Creating L3 maps.
  - Appropriate weighting of L2 observations.
- Identifying degraded conditions.
- Uncertainty estimates are needed for both L2 and L3.
- Aquarius has only few channels and essentially only one observation (salinity).
- But it also has lots of error sources that need to be considered!

# Uncertainty Estimates

## Formal Method in a Nutshell

- Formal parameter in the physical salinity retrieval algorithm: λ.
  - NEDT, SST auxiliary field, wind speed (roughness correction), galaxy, moon, land, RFI, …
  - Independent.
- Physical model for uncertainty Δλ.
  - Physical retrieval has physical error.
  - Can be scene dependent.
  - **Must be realistic! NOT worst case!**
  - Error model is developed off-line.
  - Not always straightforward and unequivocal.
  - Some components are based on SSS input from ground truth.
- Run perturbed retrieval for L2 salinity *S*
  - Separate for each parameter λ.
  - **Determine derivative:** $\frac{\partial S}{\partial \lambda} = \frac{S(\lambda+\epsilon)-S(\lambda-\varepsilon)}{2\epsilon}$.
  - Depends on scene: SST, wind speed, wind direction, ….
- Uncertainty in S due to error in λ: $\Delta S_\lambda = \left|\frac{\partial S}{\partial \lambda} \cdot \Delta\lambda\right|$.
- Total uncertainty: $(\Delta S)^2 = \sum_\lambda (\Delta S_\lambda)^2$ .
- Compare with empirical error: ARGO, HYCOM, PMEL, ….



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Published online 22 September 2011 | Nature | doi:10.1038/news.2011.554
Updated online: 23 September 2011

News

# Particles break light-speed limit

**Neutrino results challenge cornerstone of modern physics.**

Geoff Brumfiel

An Italian experiment has unveiled evidence that fundamental particles known as neutrinos can travel faster than light. Other researchers are cautious about the result, but if it stands further scrutiny, the finding would overturn the most fundamental rule of modern physics — that nothing travels faster than 299,792,458 metres per second.

Has OPERA found super-speedy neutrinos? *CERN*

The experiment is called OPERA (Oscillation Project with Emulsion-tRacking Apparatus), and lies 1,400 metres underground in the Gran Sasso National Laboratory in Italy. It is designed to study a beam of neutrinos coming from CERN, Europe's premier

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# Neutrinos not faster than light

**ICARUS experiment contradicts controversial claim.**

Geoff Brumfiel

16 March 2012 | Corrected: 19 March 2012

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Neutrinos obey nature's speed limit, according to new results from an Italian experiment. The finding, posted to the preprint server arXiv.org, contradicts a rival claim that neutrinos could travel faster than the speed of light.

Neutrinos are tiny, electrically neutral particles produced in nuclear reactions. Last September, an experiment called OPERA turned up evidence

Top story

**Ethiopian jawbone may mark dawn of humankind**

A 2.8-million-year-old mandible and a digital model of a key fossil paint a complicated picture of the genus Homo.

# Random versus Systematic Errors

- Observed Aquarius salinity errors

| | SSS AQ – HYCOM 1.44 sec σ (L2) | average # for monthly 1 deg average | $\frac{\sigma(L2)}{\sqrt{N}}$ | σ (L3) (triple collocation analysis) |
|---|---|---|---|---|
| V3.0 | 0.40 | 70 | 0.05 | 0.23 |
| V3.4 | 0.35 | | 0.04 | 0.17 |

- L3 errors do not reduce when averaging over 3 months.
- At L2 random and systematic errors are roughly of the same size.
- Most of the error observed at L3 is not a random error and does not reduce with $^1/_{\sqrt{N}}$ .
- Physical error model needs to distinguish between random and (quasi - ) systematic errors.
  - **Need to estimate systematic and random errors.**
  - Propagate differently from L2 to L3.
  - Random errors: Get reduced by $^1/_{\sqrt{N}}$ .
  - Quasi-systematic errors: Stay constant over time scales of 1 week – 3 months and within 100 – 150 km.

# Error Propagation + Correlations

- Independent random errors at L2 are added in the rms sense: $(\Delta S)^2 = \sum_{\lambda}(\Delta S_{\lambda})^2$.
- Independent systematic errors at L2:
  - Conservative method: Add absolute values.
  - Standard method: Can be of either sign. Treat them like random errors (add rms). I have adopted this method.
- Correlations need to be taken into account in perturbed retrievals. For example:
  - NEDT: V-pol and H-pol independent. When performing the perturbed retrieval, they are treated as two separate parameters $\lambda$ and perturbed independently.
  - Error in galaxy: V-pol and H-pol are not independent. There is only one independent parameter, say the V-pol component $TA_{gal,v\text{-}pol}$. When performing the perturbed retrieval, only the V-pol gets perturbed and the H-pol is calculated from the perturbed V-pol.

# Error Propagation in L3 Averaging

- Assume we have $N$ observations:
  $S_i, i = 1, \ldots N$, which have all the same random error $(\Delta S)_{ran}$ and the same systematic error $(\Delta S)_{sys}$.
- Estimation theory: **Best estimate** (maximum probability) is the mean:

$$\bar{S} = \frac{1}{N}\sum_{i=1}^{N} S_i$$

- **Standard deviation of the mean** (uncertainty of the average):

$$(\Delta\bar{S})_{ran} = \sqrt{\sum_{i=1}^{N}\left[\frac{\partial\bar{S}}{\partial S_i}\cdot\left(\Delta S_{i,ran}\right)\right]^2} = \frac{(\Delta S)_{ran}}{\sqrt{N}}$$

- Total **systematic error**:

$$(\Delta\bar{S})_{sys} = \frac{1}{N}\sum_{i=1}^{N}\left|(\Delta S)_{i,sys}\right| = (\Delta S)_{sys}$$

- This can be straightforwardly generalized if the errors of the single observations are not equal or if a weighted average is taken.
- Consider optimum weighting in L3 averaging:
  Weight by inverse variance (square error).

# Uncertainty Parameters included

| λ | Type (ran/sys) | |
|---|---|---|
| NEDT (V, H, S3) | ran | all 3 polarizations are treated independently<br>calculated in count to TA algorithm<br>apply front end losses<br>divide by $\sqrt{(\# \text{ of obs in } 1.44 \text{ sec})}$ |
| wind speed / roughness correction | ran + sys | see error model |
| wind direction (auxiliary) | ran | 10 deg random error in NCEP |
| SST (auxiliary) | sys | WindSat – Reynolds weekly |
| IU coupling | sys | see error model |
| galactic reflection | sys | see error model<br>V-pol and H-pol are correlated |
| lunar reflection | sys | |
| land contamination | sys | |
| sea ice contamination | sys | |
| RFI | sys | treated on SSS level |

# Uncertainty Parameters neglected/not considered

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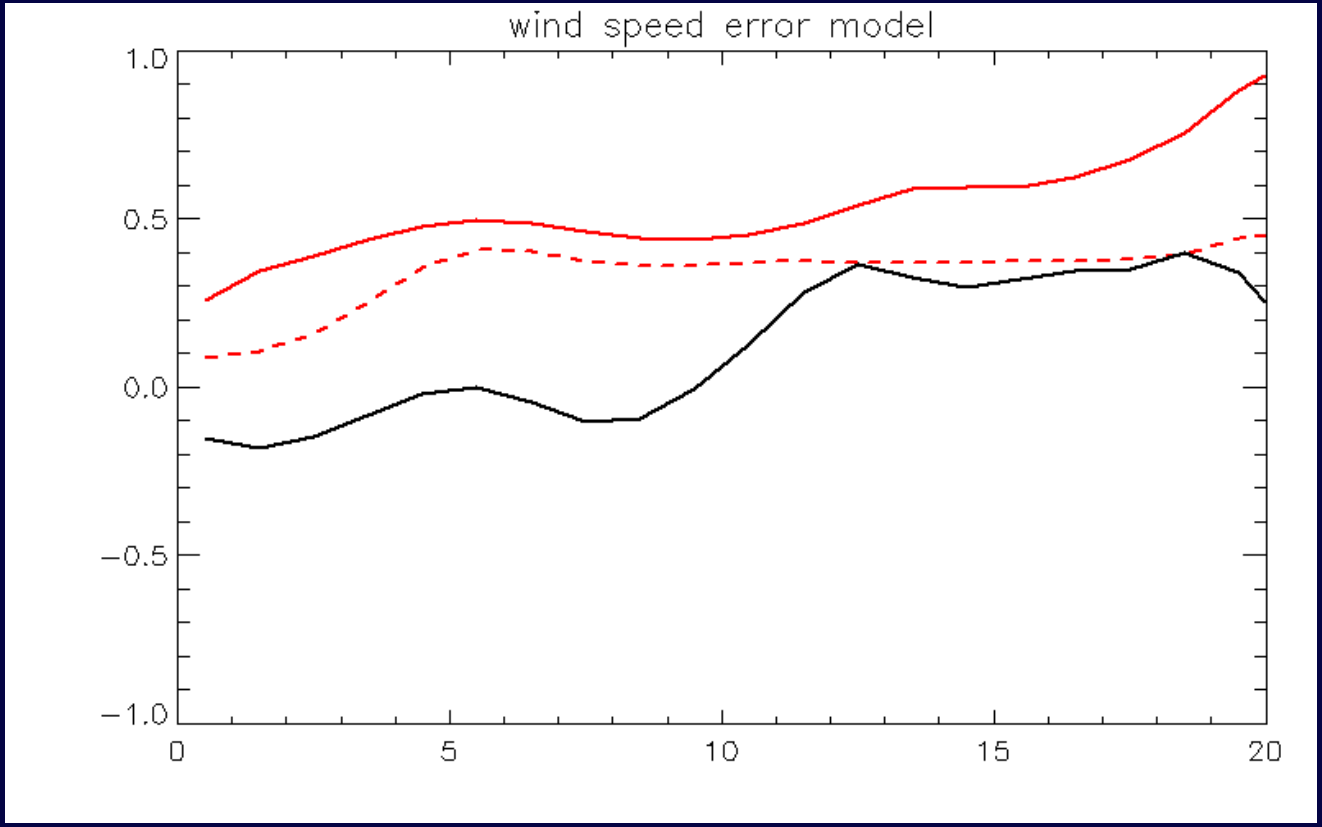
| λ | Type(ran/sys) | |
|---|---|---|
| EIA / pointing | ran | small. estimated from difference between nominal (nadir) and actual pointing |
| APC | ran + sys | not considered (beside IU coupling) assumed to be calibrated correctly to ocean RTM |
| calibration system | ran + sys | |
| RTM: dielectric, $O_2$ ,wind emissivity | sys | assumed that the SST dependent biases are corrected |
| atmosphere: $O_2$ | sys | small. estimated sensitivity of SSS to atmospheric temperature error at most 0.05 psu/K. |
| atmosphere: water vapor | | signal itself is already small |
| atmosphere: rain, cloud | sys | sizeable in very heavy rain (0.2 psu too fresh at 10 mm/h)<br>not accessible as long as only NCEP cloud water is used in L2 algorithm |
| sun | sys | signal itself is already small |
| direct galactic | sys | not considered |

# Error Model

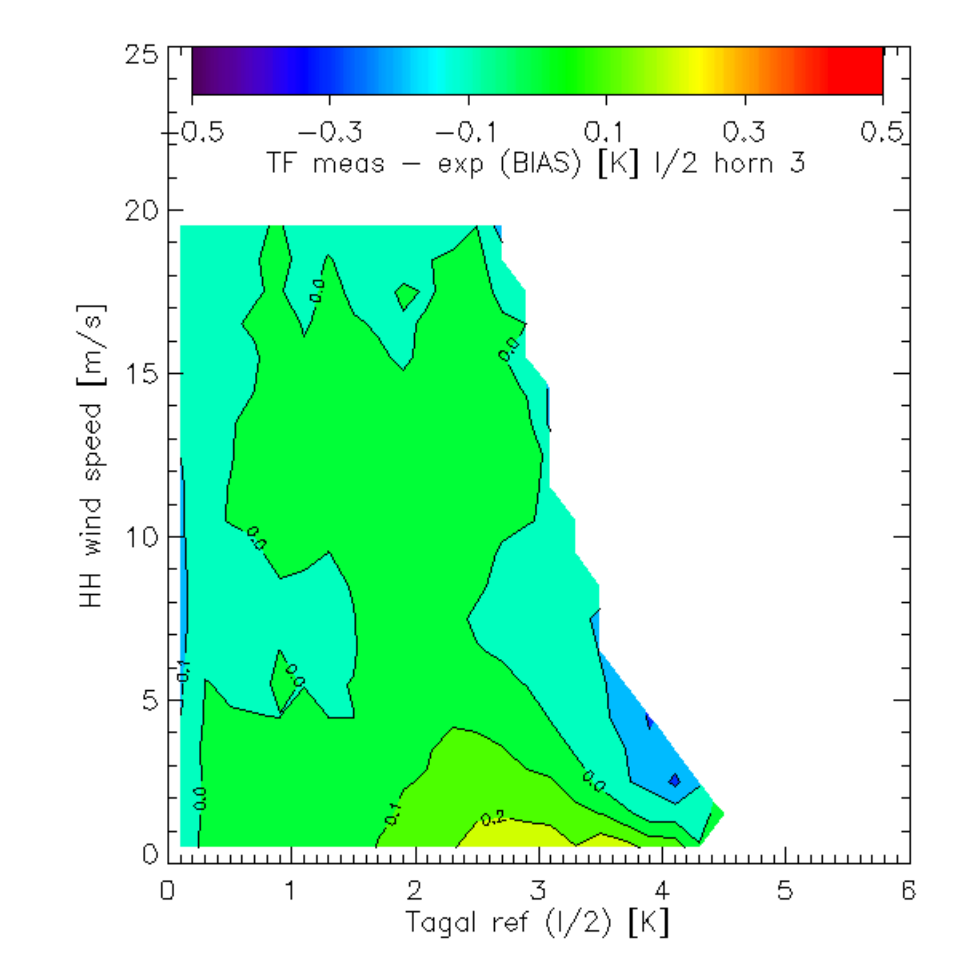
## Wind Speed / Roughness Correction




Black line: systematic component (AQ HHH – WindSat).
Red Line: random component (AQ HHH – WindSat). Divide by $\sqrt{2}$.
Red dashes: random error model for AQ HHH wind speed (
$K_P$ value for $\sigma_{0HH}$, NEDT for TBH, error in NCEP background field, wind direction, …).

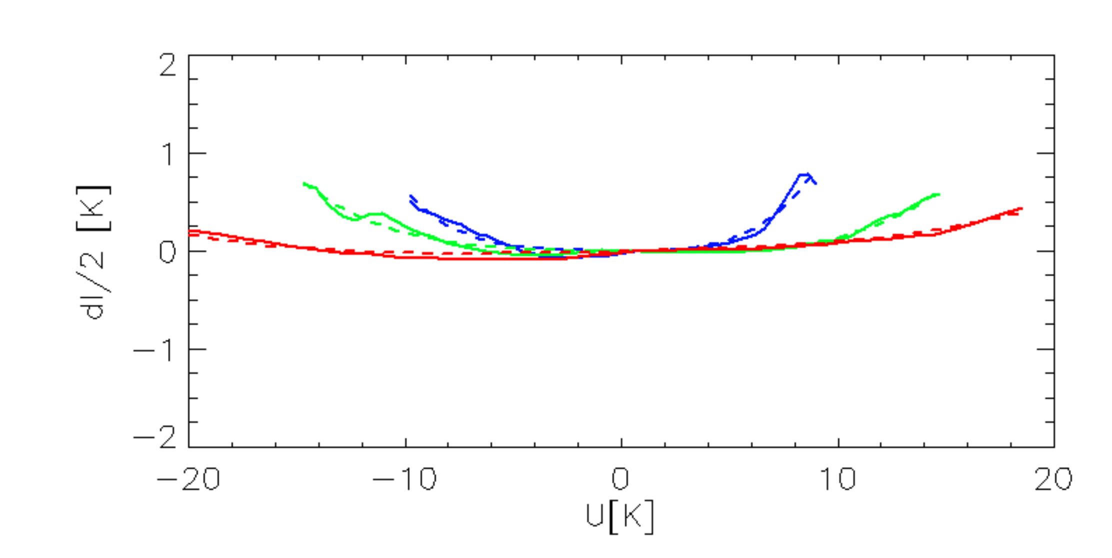
# Error Model
## Reflected Galaxy





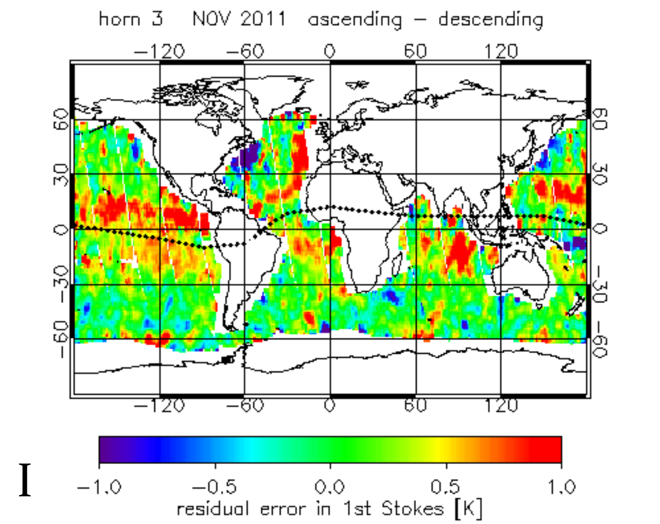

TA measured – expected.
Based on ground truth (HYCOM).

# Error Model
## IU Coupling




horn 1 horn 2 horn 3

non-linear relation.
can NOT be absorbed in APC IU couplings.
TB measured – expected.
Based on ground truth (HYCOM).
Consider to correct in L2 algo.

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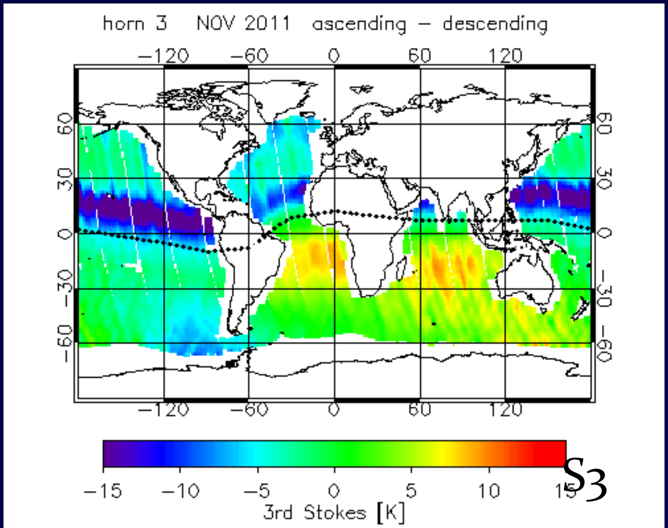
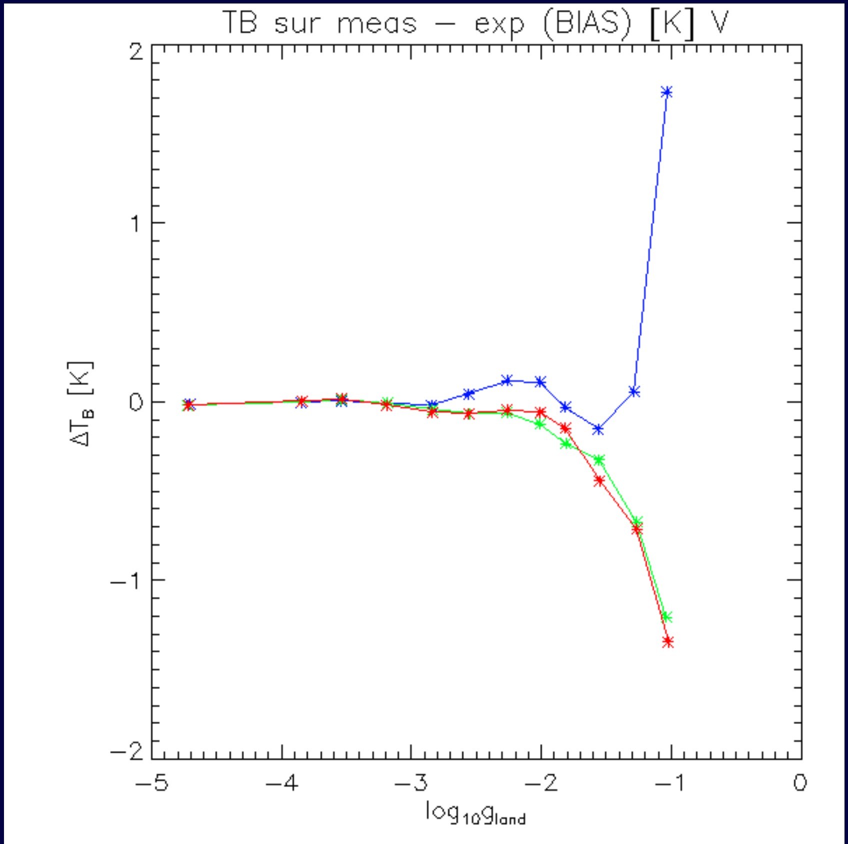
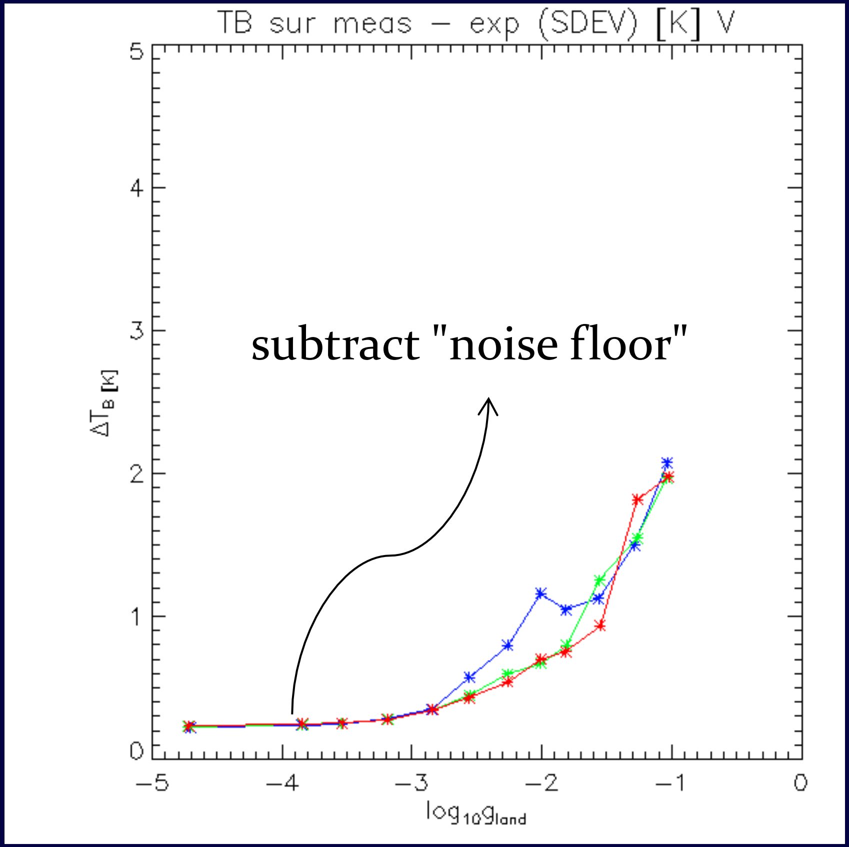



S3

# Error Model
## Land Contamination

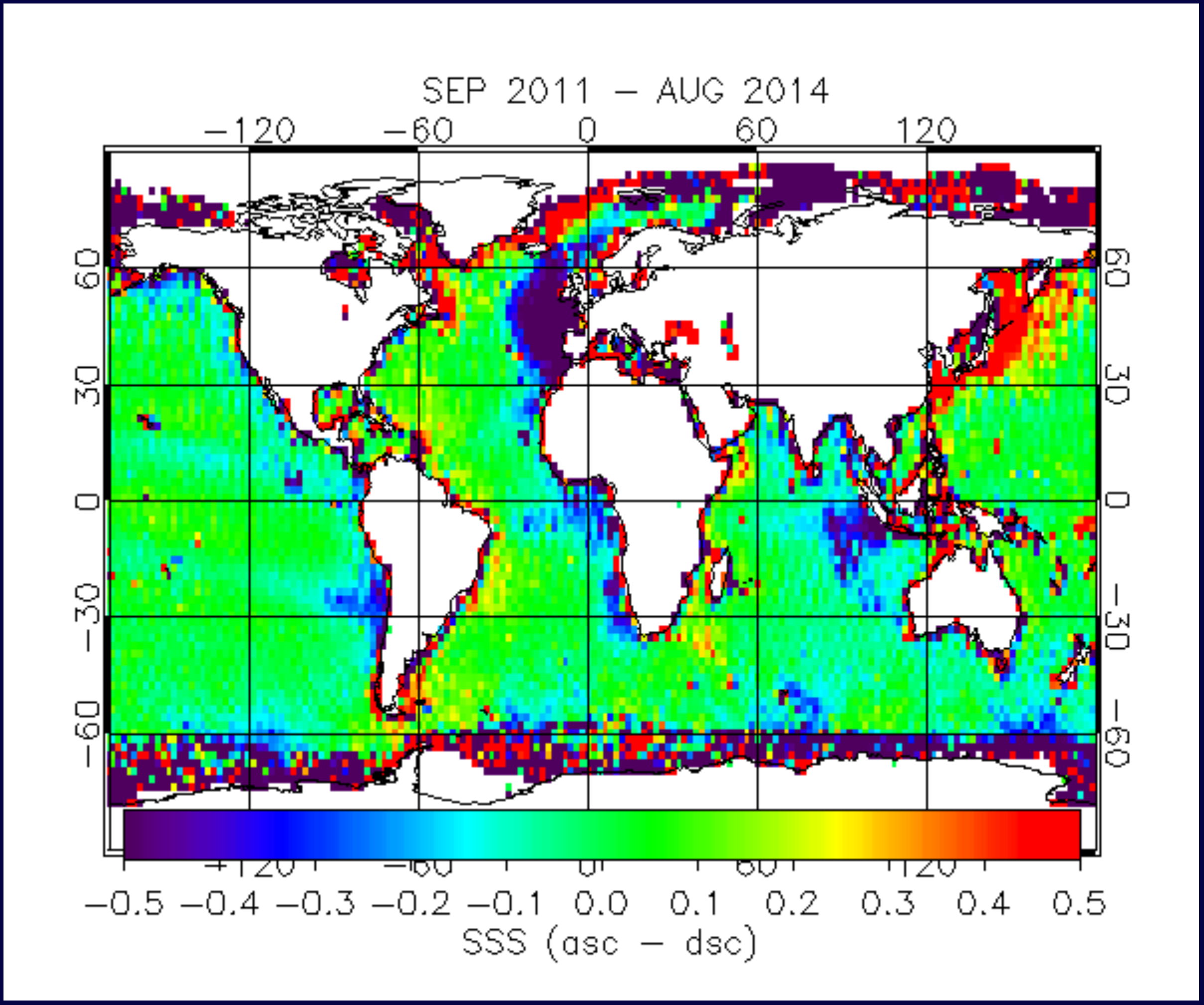
horn 1 horn 2 horn 3




TB measured – expected. Based on ground truth (HYCOM).
Total RMS treated as systematic error.
V/H –pols correlated in perturbed retrievals.

# Error Model
## Estimated Undetected RFI

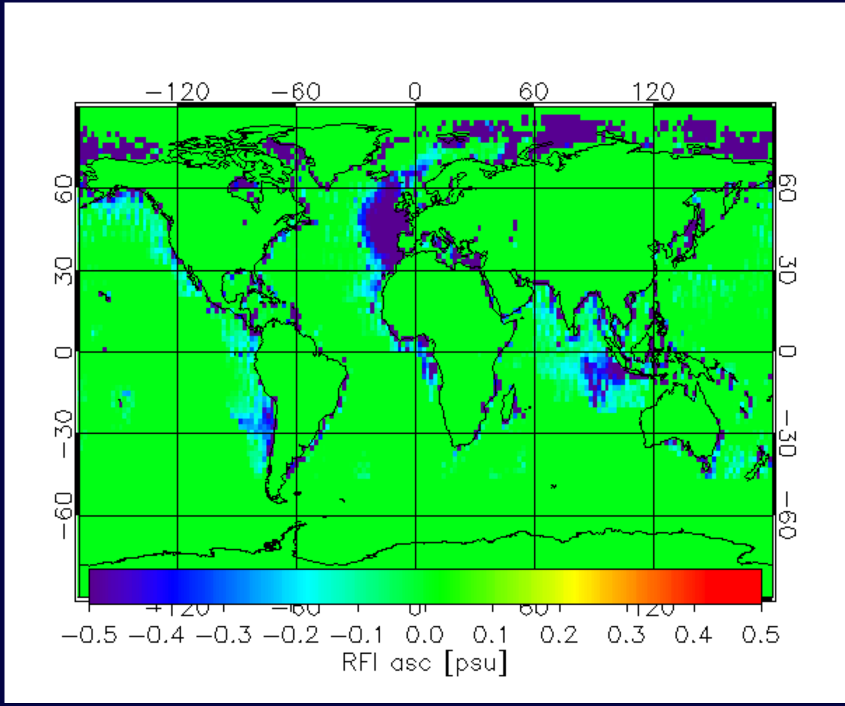


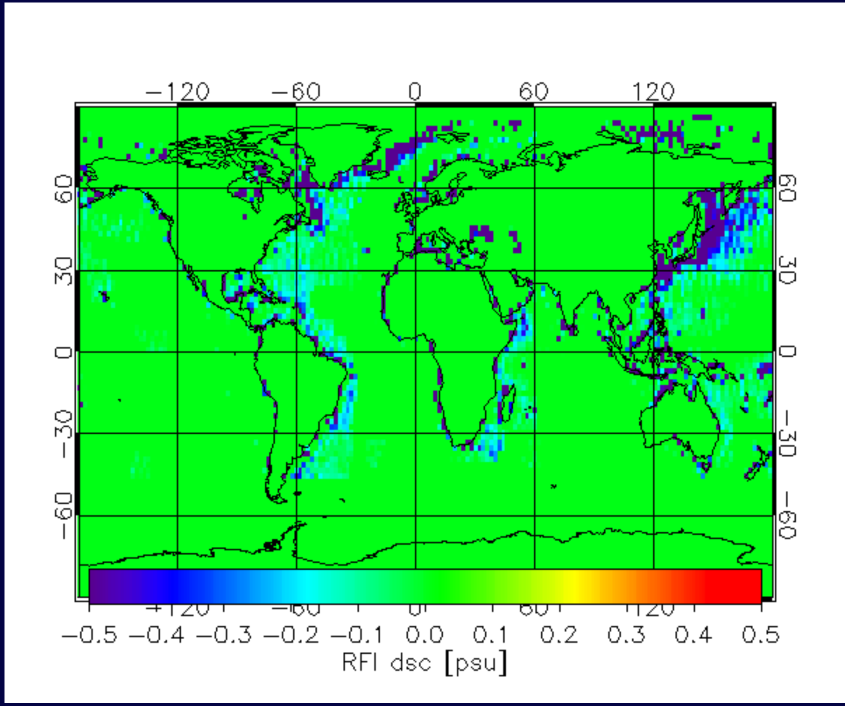

3-year Aquarius SSS ascending - descending

# Error Model

## Estimated Undetected RFI

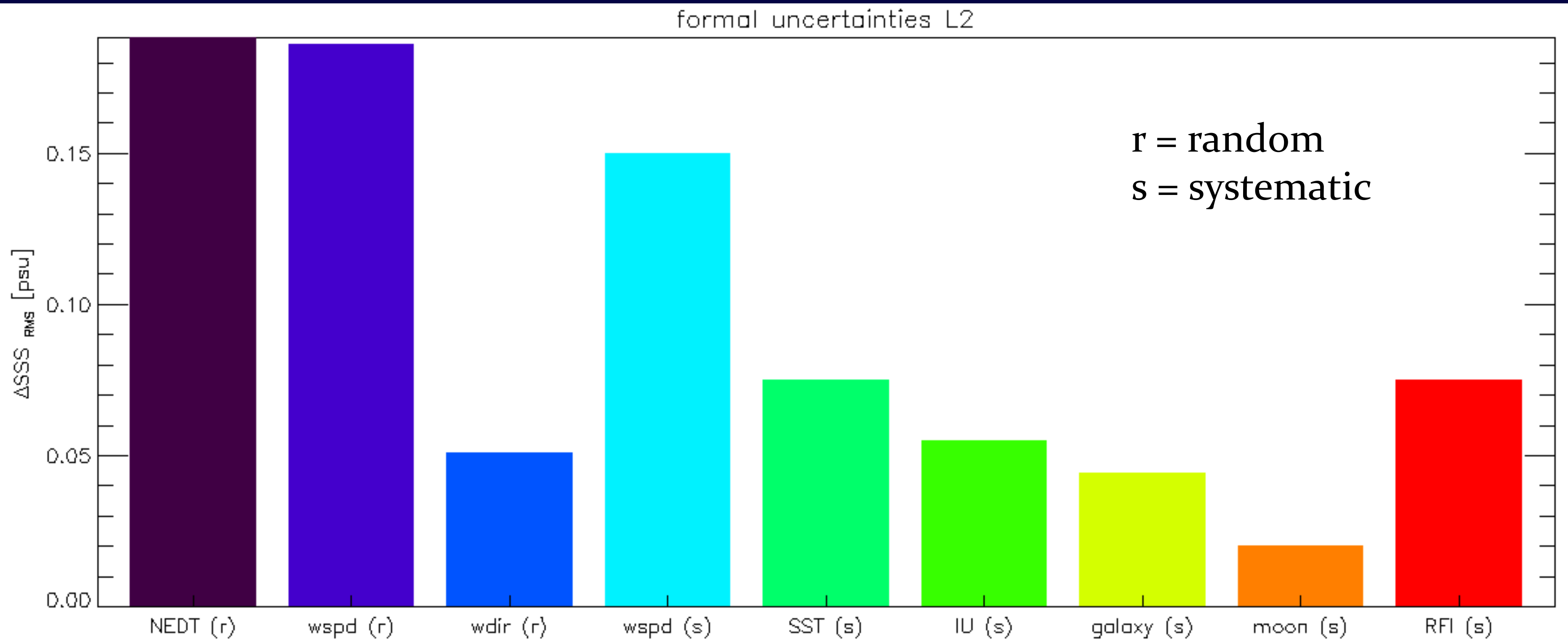
in vicinity of RFI (TF – TA peak hold)
SSS (asc – dsc) < 0:  RFI in ascending swath
SSS (asc – dsc) > 0:  RFI in descending swath
treated as systematic error for retrieved SSS




V3.0/V3.4 use this to mask out undetected RFI.

# Formal Errors L2



# Formal Errors L3

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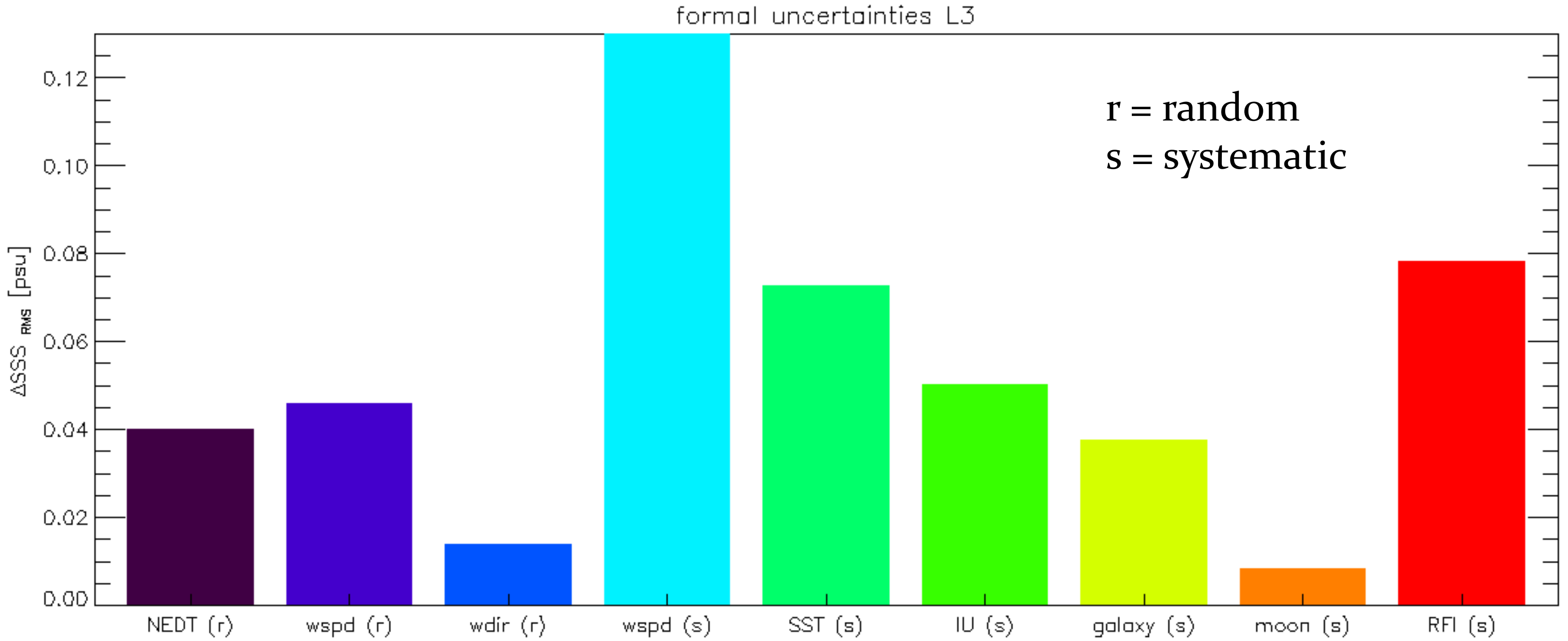
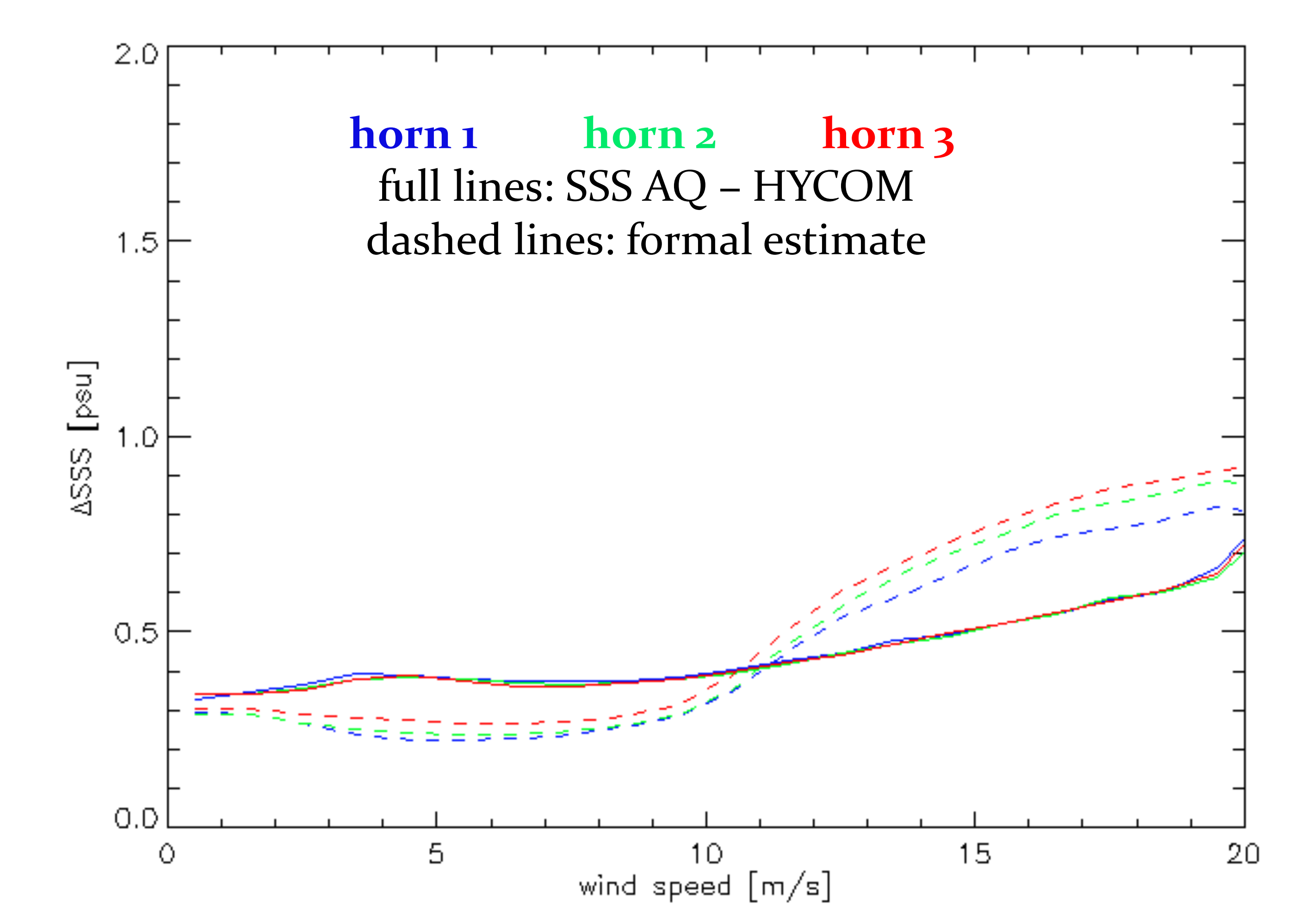
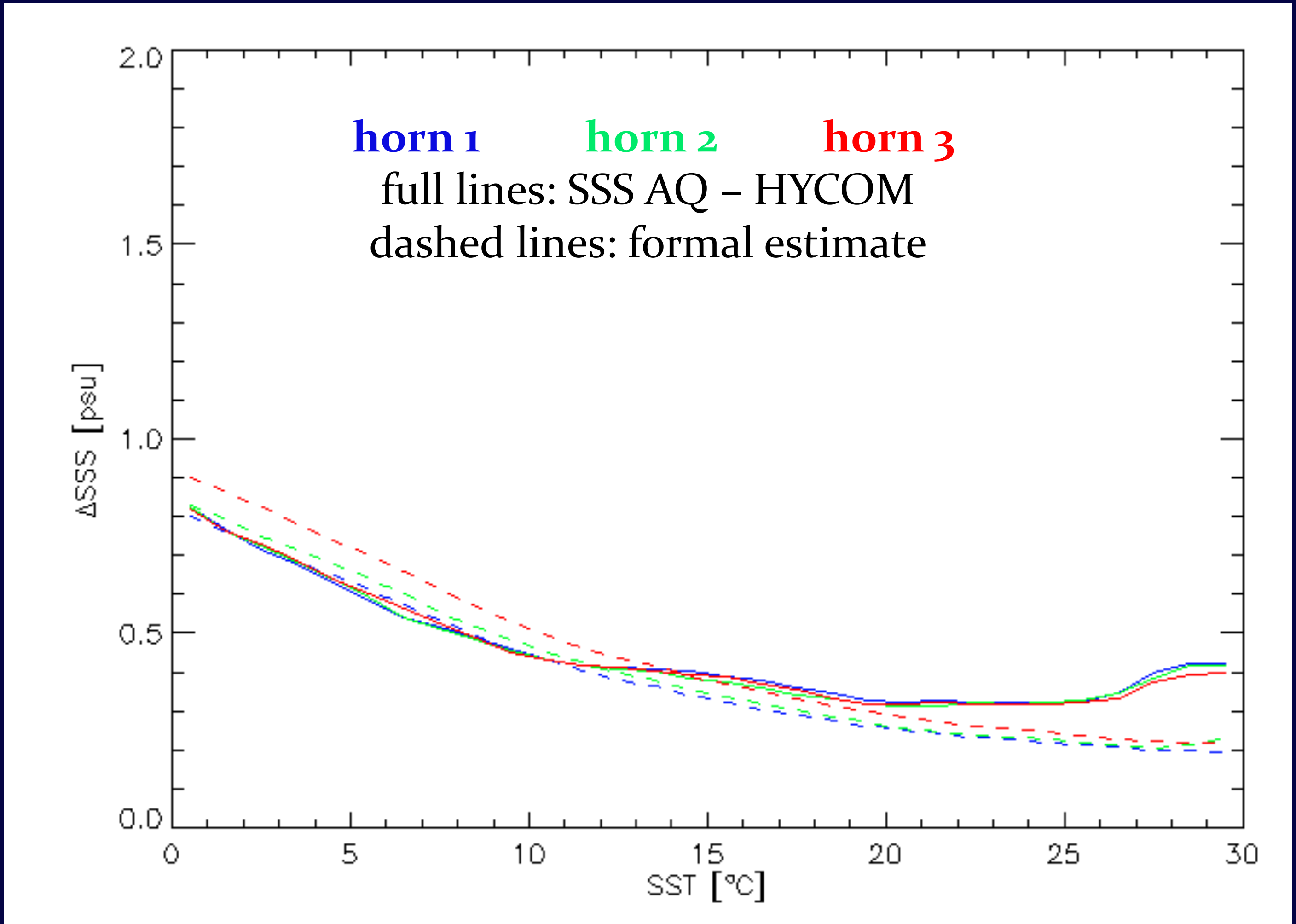


# Estimated L2 Uncertainty

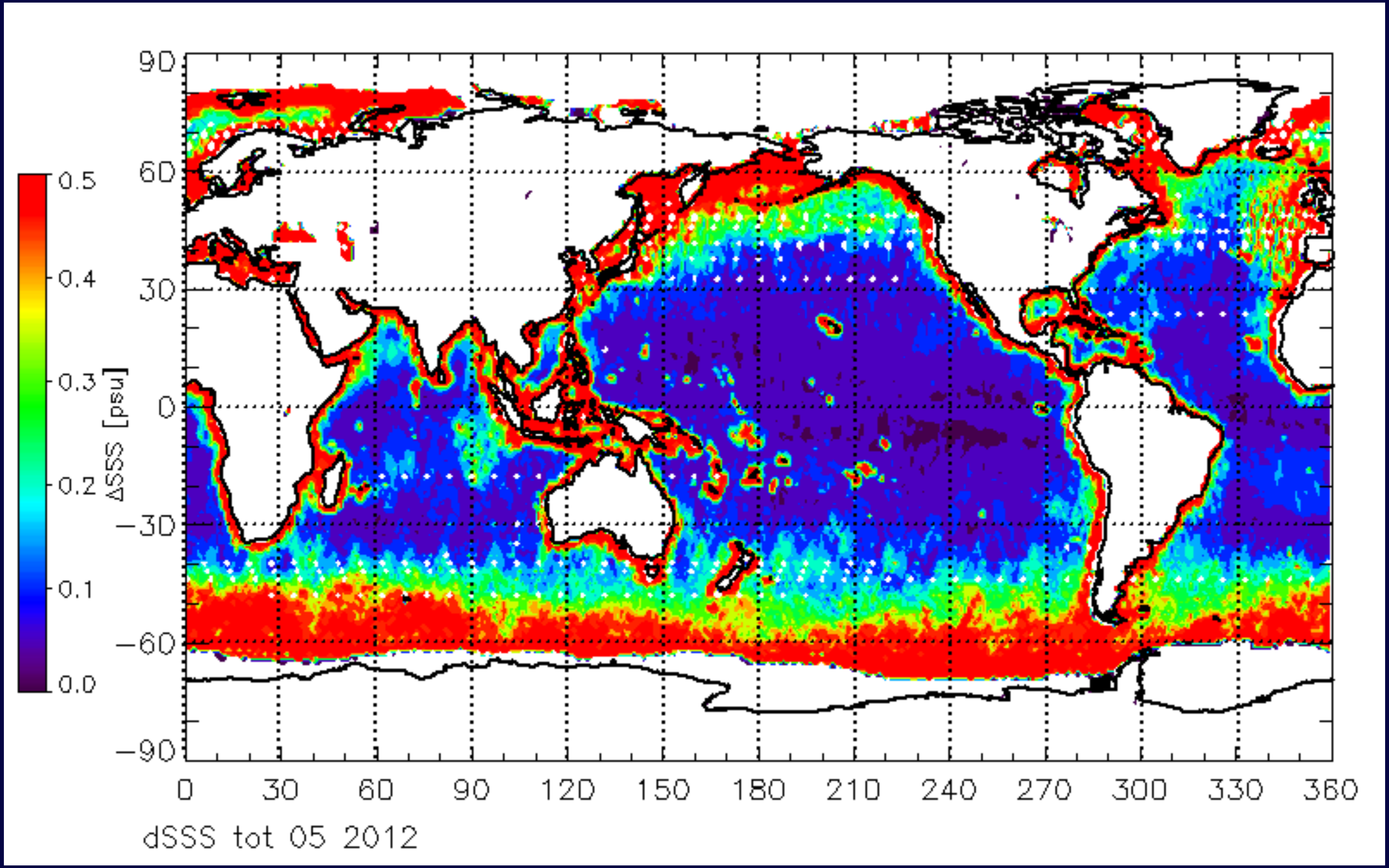
## stratified with wind speed



# Estimated L2 Uncertainty
## stratified with SST



# Estimated L3 Uncertainty



# Estimated L3 Uncertainty

## formal versus empirical: time series open ocean + strict Q/C

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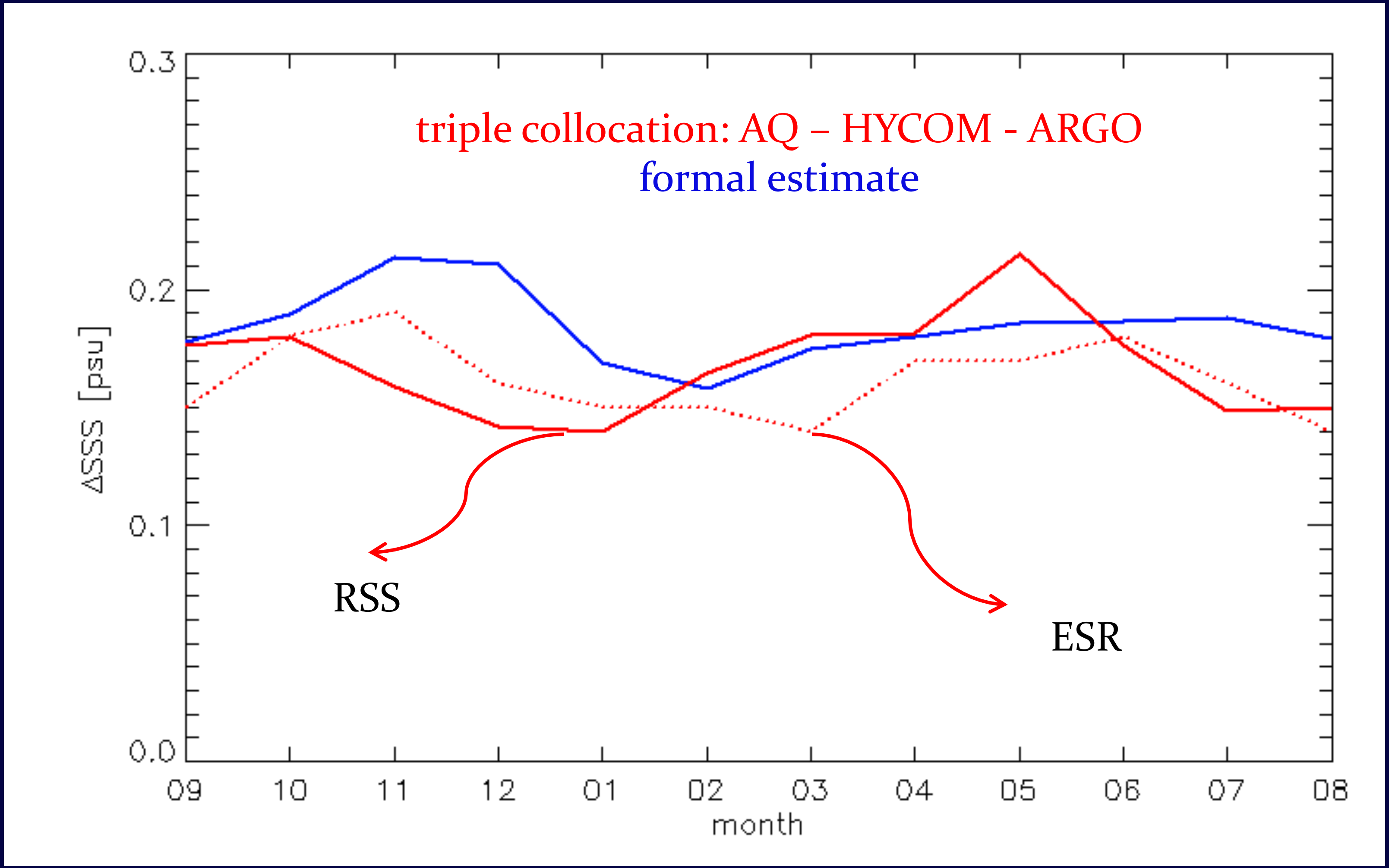
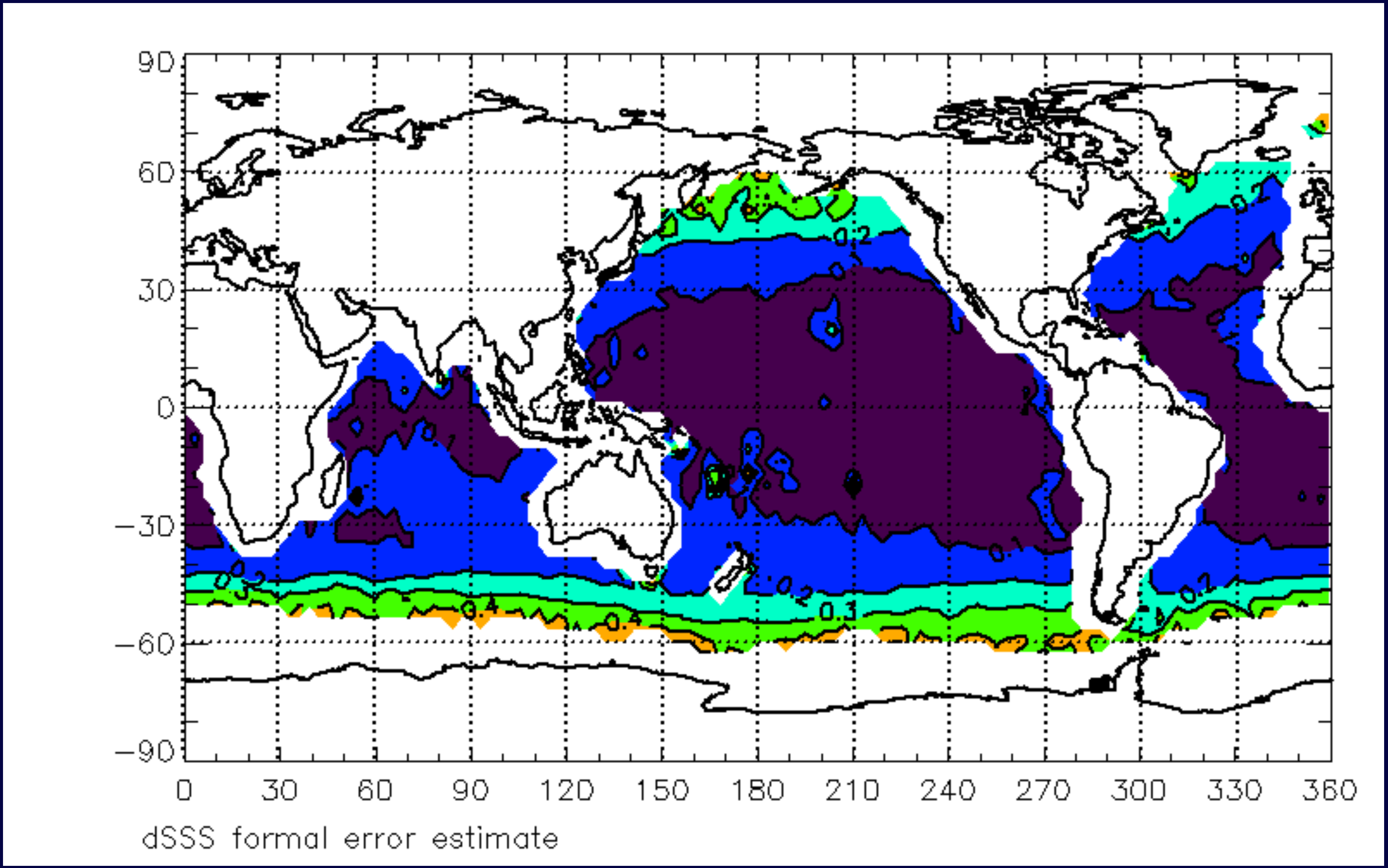
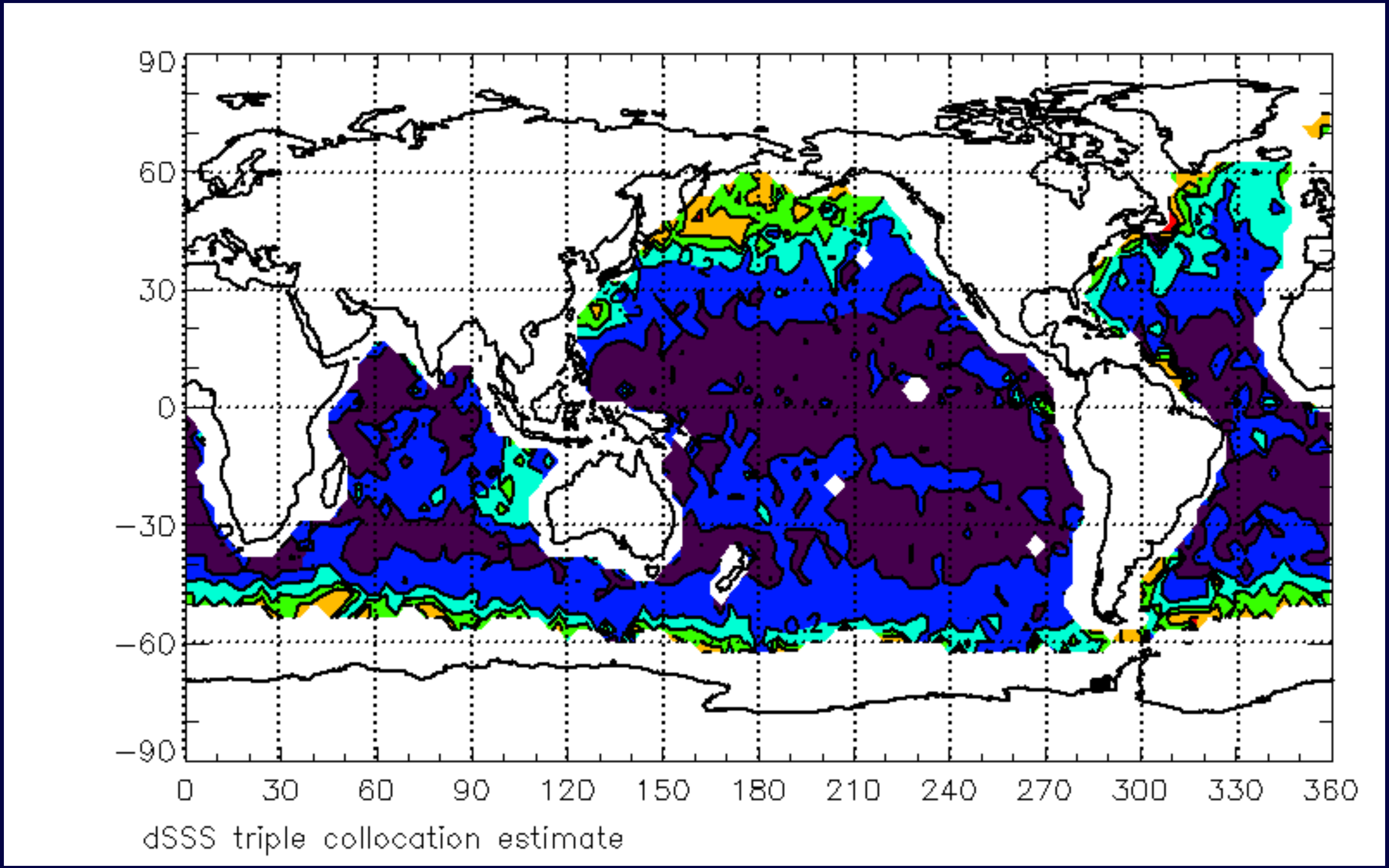


# Estimated L3 Uncertainty
## open ocean + strict Q/C



# Empirical L3 Uncertainty

## triple collocation map (AQ – HYCOM – ARGO)

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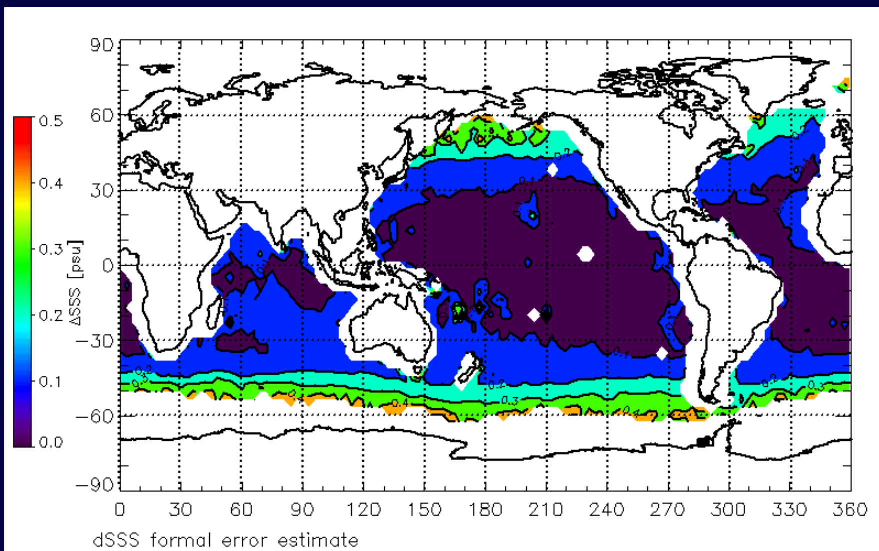
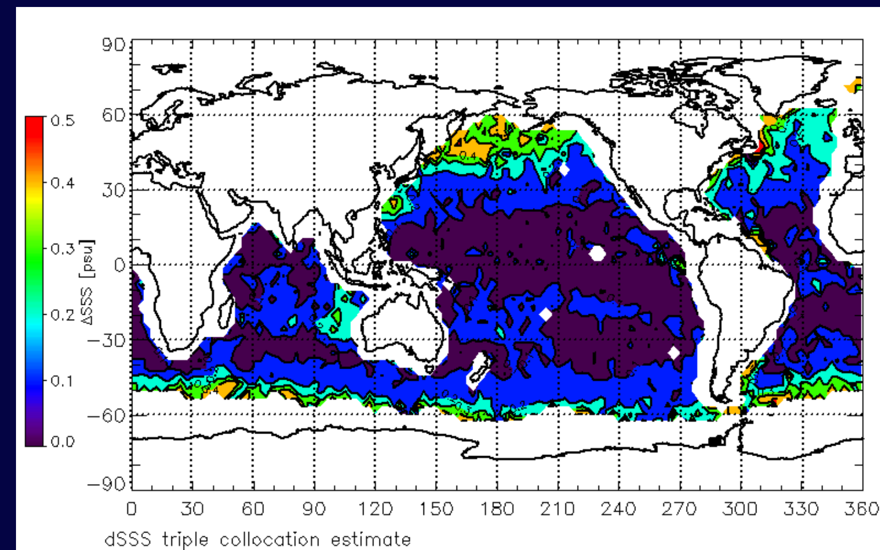
# Estimated L3 Uncertainty
## formal versus empirical map




- Possible cancellation or enhancement of systematic errors in certain regions.
- For example: errors in wind speed and auxiliary fields.
- Improving one source for systematic errors (e.g. auxiliary SST) does not necessarily show as an improvement everywhere.

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# Summary and Reflections

- We have derived an algorithm for estimating formal uncertainties to our physical Aquarius salinity retrieval algorithm.
- 2 major components:
    1. Physical error model for each component of the salinity retrieval.
    2. Running perturbed retrievals: sensitivity of SSS to the various parameters.
- The physical error model is developed off line.
    - Will be delivered as collection of look-up tables.
    - Some components need information from ground truth salinity (HYCOM)
    - Tied to physical components of retrieval algorithm.
- Keep track of uncertainty in each parameter.
- Essential to separate random and systematic uncertainties.
    - Propagate differently when forming L3 averages form L2 observations.
- Results for both L2 and L3 uncertainty estimate compare very well with empirical uncertainty estimates from ground truth.
    - Triple collocation