New physically based sea surface temperature retrievals for NPP VIIRS

Andy Harris, Prabhat Koner

CICS, ESSIC, University of Maryland

Activities

- **Data**
  - VIIRS & MODIS L1B
  - VIIRS & MODIS GHRSST SST
  - NCEP GFS
  - Aerosol climatology (CMIP5)
- **Working with matchups**
  - Time-space matches with *in situ*
  - iQUAM data (drifting & moored buoys)
  - Allows quantitative assessment of algorithm adjustments
- **Channel selection**
  - Check observed BTs against output from CRTM
  - For now, only use channels which agree "well"
    - *Ad hoc* bias correction risks corrupting signal, or distorting physical model
    - Best to identify and fix issues at source
    - Experiments with GOES indicate bias correction can degrade retrieval

Physical Retrieval

- **Reduces the problem to a local linearization**
  - Dependent on ancillary data (NWP) for an initial guess
  - More compute-intensive than regression – not an issue nowadays
    - Especially with fast RTM (*e.g.* CRTM)
- **Widely used for satellite sounding**
  - More channels, generally fewer (larger) footprints
- **Start with a simple reduced state vector**
  - $\boldsymbol{x} = [\mathrm{SST}, \mathrm{TCWV}]^{\mathrm{T}}$
  - *N.B.* Implicitly assumes NWP profile shape is more or less correct
- **Selection of an appropriate inverse method**
  - Ensure that satellite measurements are contributing to signal
  - Avoid excessive error propagation from measurement space to parameter space
    - If problem is ill-conditioned

History of Inverse Model

- **Forward model:** $\mathbf{Y} = \mathbf{K}\mathbf{X}$
- **Simple Inverse:** $\mathbf{X} = \mathbf{K}^{-1}\mathbf{Y}$ **(measurement error)**

- **Legendre (1805) Least Squares:**

$$\mathbf{X} = \mathbf{X}_{ig} + (\mathbf{K}^{\mathbf{T}}\mathbf{K})^{-1}\mathbf{K}^{\mathbf{T}}(\mathbf{Y}_{\delta} - \mathbf{Y}_{ig})$$

- **MTLS:** $\mathbf{X} = \mathbf{X}_{ig} + (\mathbf{K}^{\mathbf{T}}\mathbf{K} + \lambda\mathbf{R})^{-1}\mathbf{K}^{\mathbf{T}}(\mathbf{Y}_{\delta} - \mathbf{Y}_{ig})$

- **OEM:** $\mathbf{X} = \mathbf{X}_{\mathbf{a}} + (\mathbf{K}^{\mathbf{T}}\,\mathbf{S}_{\mathbf{e}}^{-1}\mathbf{K} + \mathbf{S}_{\mathbf{a}}^{-1})^{-1}\mathbf{K}^{\mathbf{T}}\mathbf{S}_{\mathbf{e}}^{-1}\,(\mathbf{Y}_{\delta} - \mathbf{Y}_{\mathbf{a}})$

Uncertainty Estimation

Physical retrieval

Normal LSQ Eqn: $\Delta x = (K^T K)^{-1} K^T \Delta y \quad [= G\Delta y]$

MTLS modifies gain: $G' = (K^T K + \lambda I)^{-1} K^T$

Regularization strength: $\lambda = (2 \log(\kappa)/\|\Delta y\|)\sigma^2_{end}$

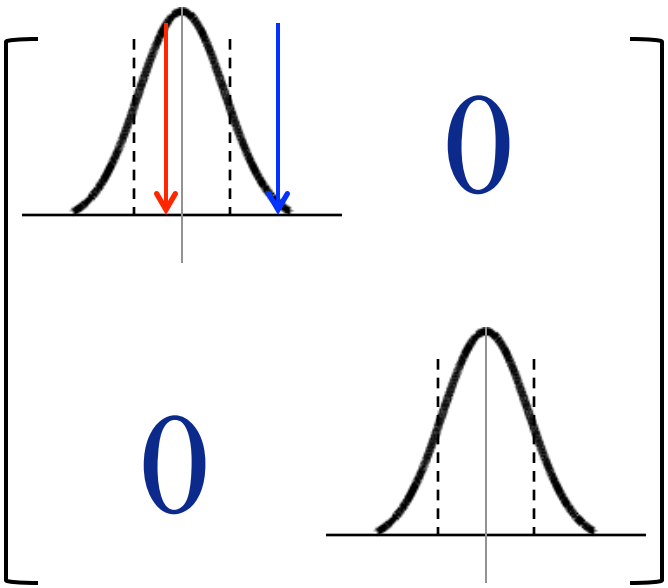
(σ^2_{end} = lowest singular value of $[K\ \Delta y]$)

Total Error

$$\|e\| = \|(MRM - I)\Delta x\| + \|G'\|\langle\|(\Delta y - K\Delta x)\|\rangle$$

N.B. **Includes TCWV as well as SST**

"Optimized" OE

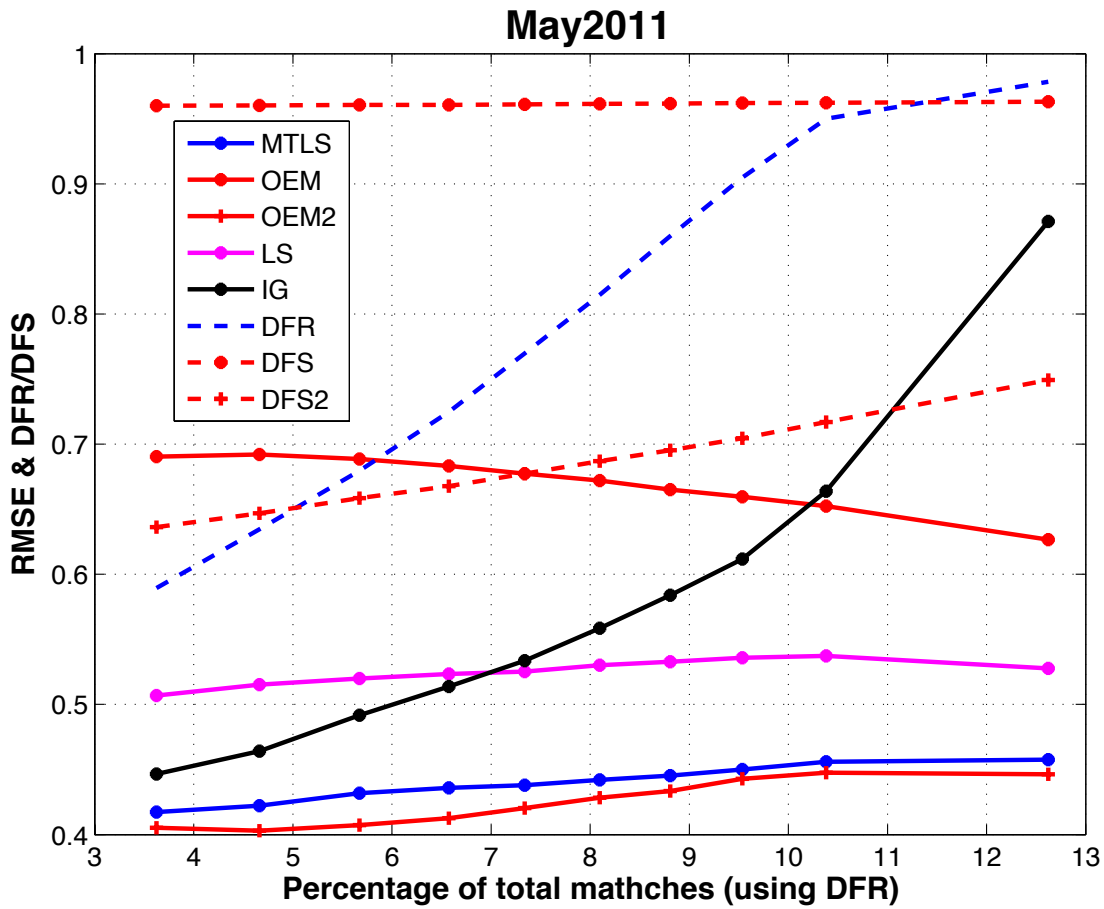
- $[S_e]$, S_a = 

σ^2 is an overestimate…

…or an underestimate

- **Perform experiment – insert "true" SST error into S_a^{-1}**
  - Can only be done when truth is known, *e.g.* with matchup data

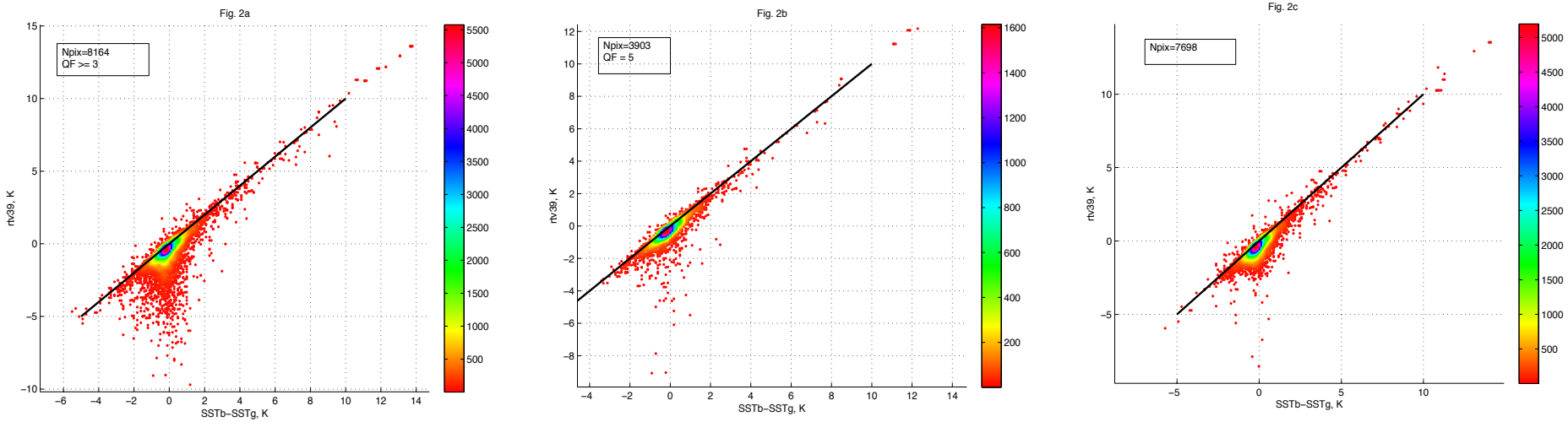
DFS/DFR and Retrieval error



- Retrieval error of OEM higher than LS
- More than 75% OEM retrievals are degraded w.r.t. *a priori* error
- DFR of MTLS is high when *a priori* error is high
- The retrieval error of OEM is good when *a priori* SST is perfectly known, but DFS of OEM is much lower than for MTLS

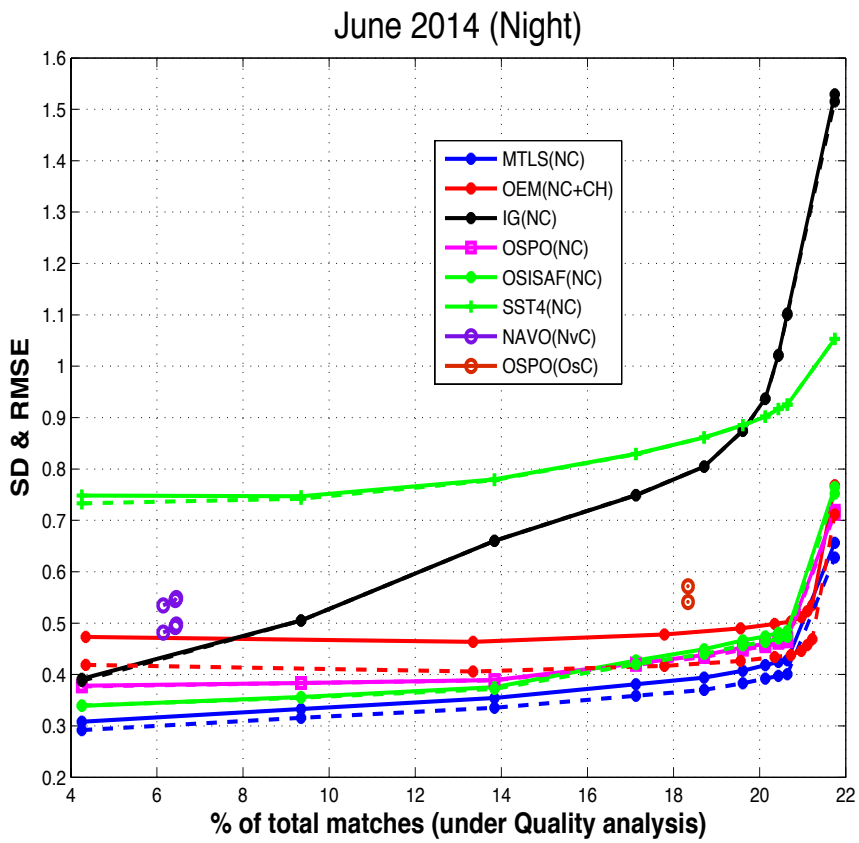
Improved cloud detection

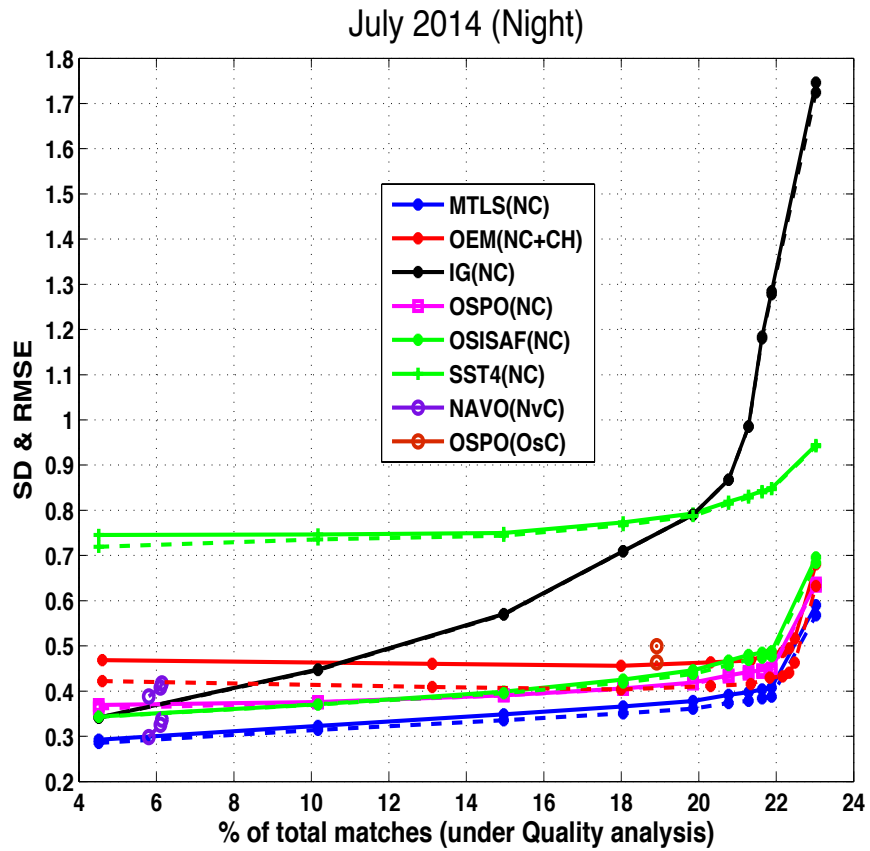
- **Use a combination of spectral differences and RT**
  - Envelope of physically reasonable clear-sky conditions
- **Spatial coherence (3×3)**
- **Also check consistency of single-channel retrievals**
- **Flag excessive TCWV adjustment & large MTLS error**



- **Almost as many as GHRSST QL3+, but with greatly reduced leakage**

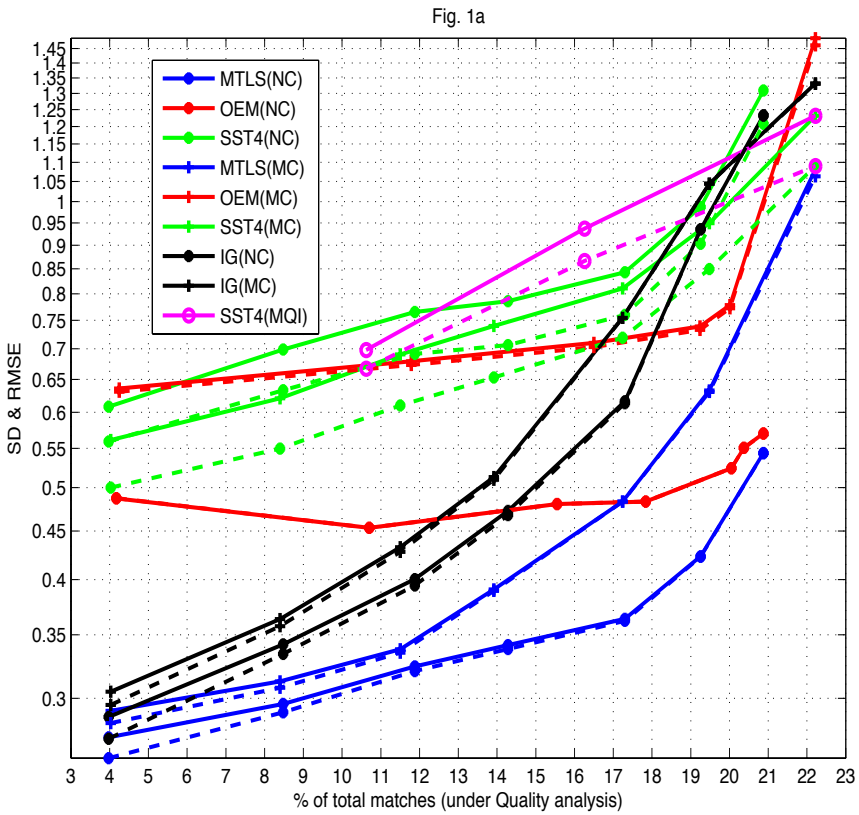
VIIRS Initial Results

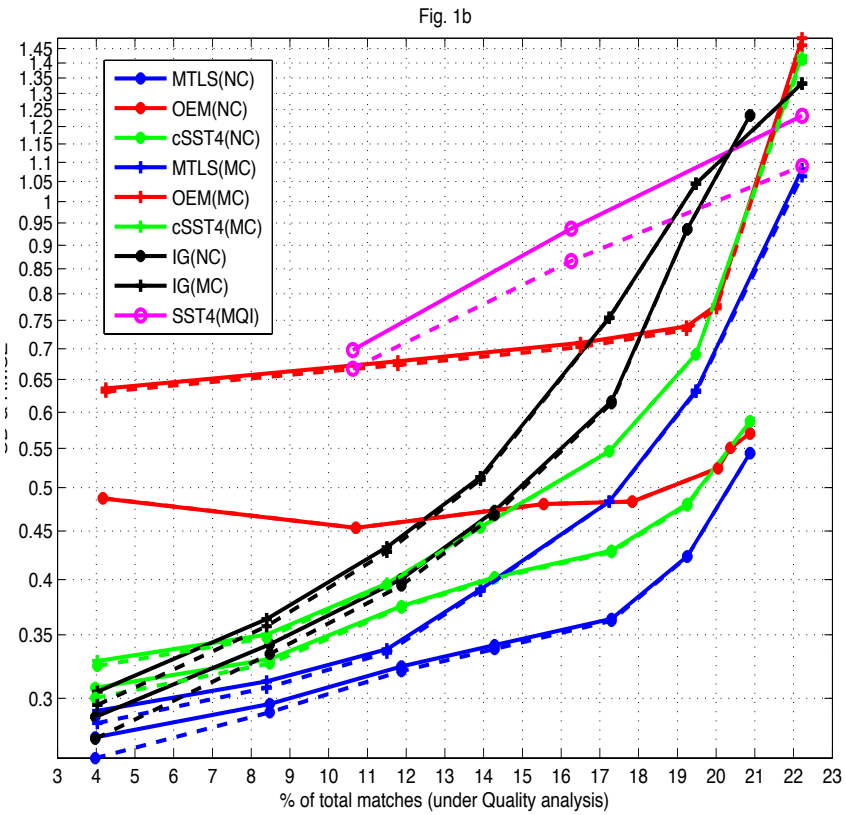




- **Data are ordered according to MTLS error**
  - Reliable guide for regression as well as MTLS
  - Trend of initial guess error is expected

MODIS Initial Results





- **Note improvement from discarding MTLS error "last bin"**
  - Irrespective, MTLS is quite tolerant of cloud scheme
- **Recalculated SST4 coefficients produce quite good results**

Status & Plans

- **"Initial cut" MTLS shows promise with VIIRS**
  - Well-calibrated instrument, with reliable* fast RTM available
  - Error calculation useful quality indicator
  - MODIS offers more possibilities
- **Cloud detection can be aided by RTM**
  - "Single-channel" retrieval consistency, MTLS error calculation
- **Plans**
  - Take advantage of SIPS!
    - Liaise w/ RSMAS on matchups
  - Take advantage of differing length scales to reduce atmospheric noise
  - Perhaps combine with sounder for more local atmospheric information
  - Refine fast RTM, iteration
  - Tropospheric aerosols…

Backup slides

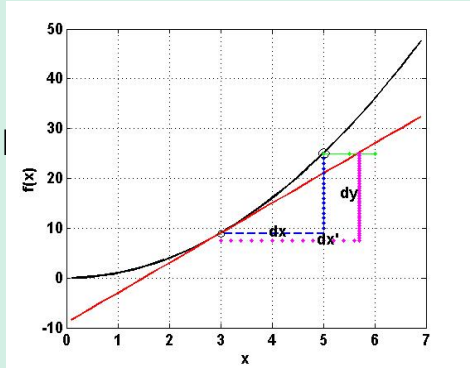
Deterministic & Stochastic

Determinitic

MTLS/RTLS/Tikhonov: Single pixel

$$d\mathbf{X} = \mathbf{K}^{-1} d\mathbf{Y}$$

measurement error



Lengendre (1805)
Least Squares:

$$\mathbf{X}_{ls} = \mathbf{X}_{ig} + (\mathbf{K}^{\mathbf{T}}\mathbf{K})^{-1}\mathbf{K}^{\mathbf{T}} d\mathbf{Y}_{\delta}; \quad dY_{\delta} = \mathbf{Y}_{\delta} - \mathbf{Y}_{ig}$$

Last 30~40 years: $\delta X \le \kappa\, \delta E;\ \kappa = \mathbf{cond}(\mathbf{K})$

$$\mathbf{X}_{rg} = \mathbf{X}_{ig} + (\mathbf{K}^{\mathbf{T}}\mathbf{K} + \lambda \mathbf{R})^{-1}\mathbf{K}^{\mathbf{T}} d\mathbf{Y}_{\delta}$$

$$= X_{ig} + K_{ps}^{inv}\ dY_{\delta}$$

MTLS: $[\mathbf{u}\ \sigma\ \mathbf{v}] = [\mathbf{K} \quad d\mathbf{Y}_{\delta}]; \quad \mathbf{R} = \mathbf{I}$

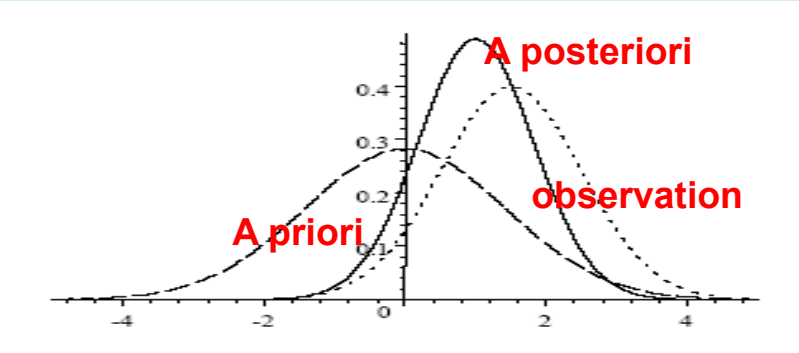
$$\lambda = (2\log(\kappa) / \left\| d\mathbf{Y}_{\delta} \right\|^2)\, \sigma_{end}^2$$

Total Error: $\left\| \mathbf{X}_{true} - \mathbf{X}_{mtls} \right\|$

$$\left\| (\mathbf{K}_{ps}^{inv}\ \mathbf{K} - \mathbf{I}) \mathbf{X}_{true} \right\| + \left\| \mathbf{K}_{ps}^{inv} (d\mathbf{Y}_{\delta} - \mathbf{K}\mathbf{x}_{mtls}) \right\|$$

Stochastic/Probabilistic

OEM: A set of measurement



$$\mathbf{X}_{oem} = \mathbf{X}_{ig} + (\mathbf{K}^{\mathbf{T}}\mathbf{S}_e^{-1}\mathbf{K} + \mathbf{S}_a^{-1})^{-1}\mathbf{K}^{\mathbf{T}} d\mathbf{Y}_{\delta}$$

Low confidence for pixel retrieval
Chi-Square test:

$$\chi_{resd} = \mathbf{K}\mathbf{X}_{oem} - d\mathbf{Y}_{\delta}$$

$$\chi = \chi_{resd}^{T} (\mathbf{S}_e (\mathbf{K}^{\mathbf{T}}\mathbf{S}_a\mathbf{K} + \mathbf{S}_e)^{-1}\mathbf{S}_e)^{-1} \chi_{resd}$$

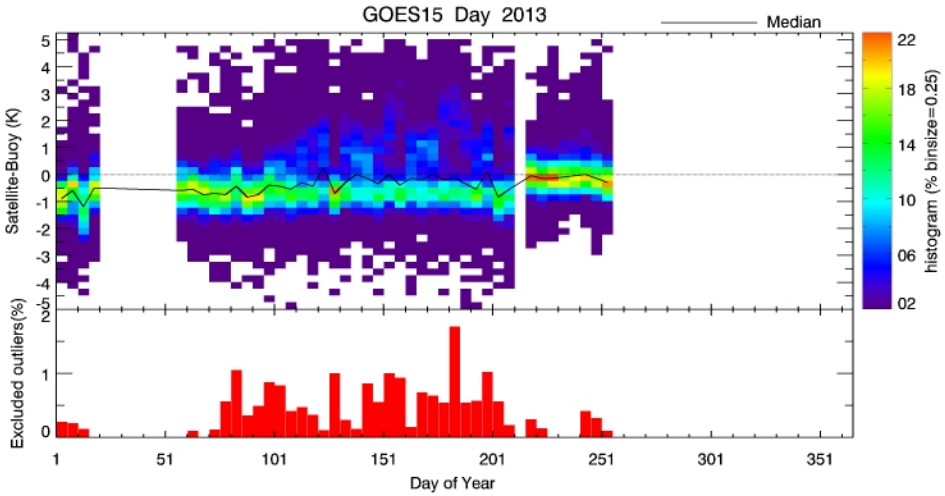
Regression: A set of measurement
Historical heritage in SST retrieval using Window channels.
Coefficient Vector/matrix: **C** $X_{reg} = \mathbf{C}\ \mathbf{Y}_{\delta}$

Main concerns: Correlation & Causation

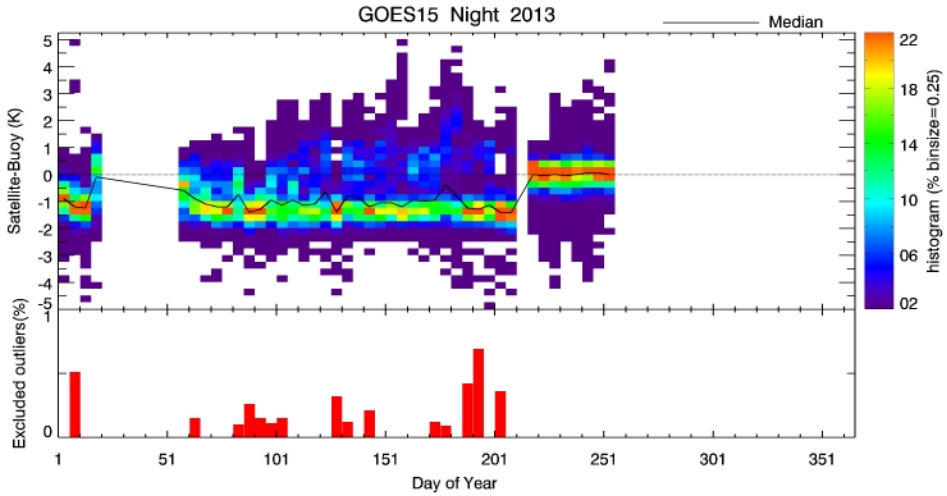
Recent update to Geo-SST

- **Physical retrieval based on Modified Total Least Squares**
- **Improved bias and scatter *cf.* previous regression-based SST retrieval**

GOES-15



Daytime



Nighttime

How sensitive is retrieved SST to true SST?

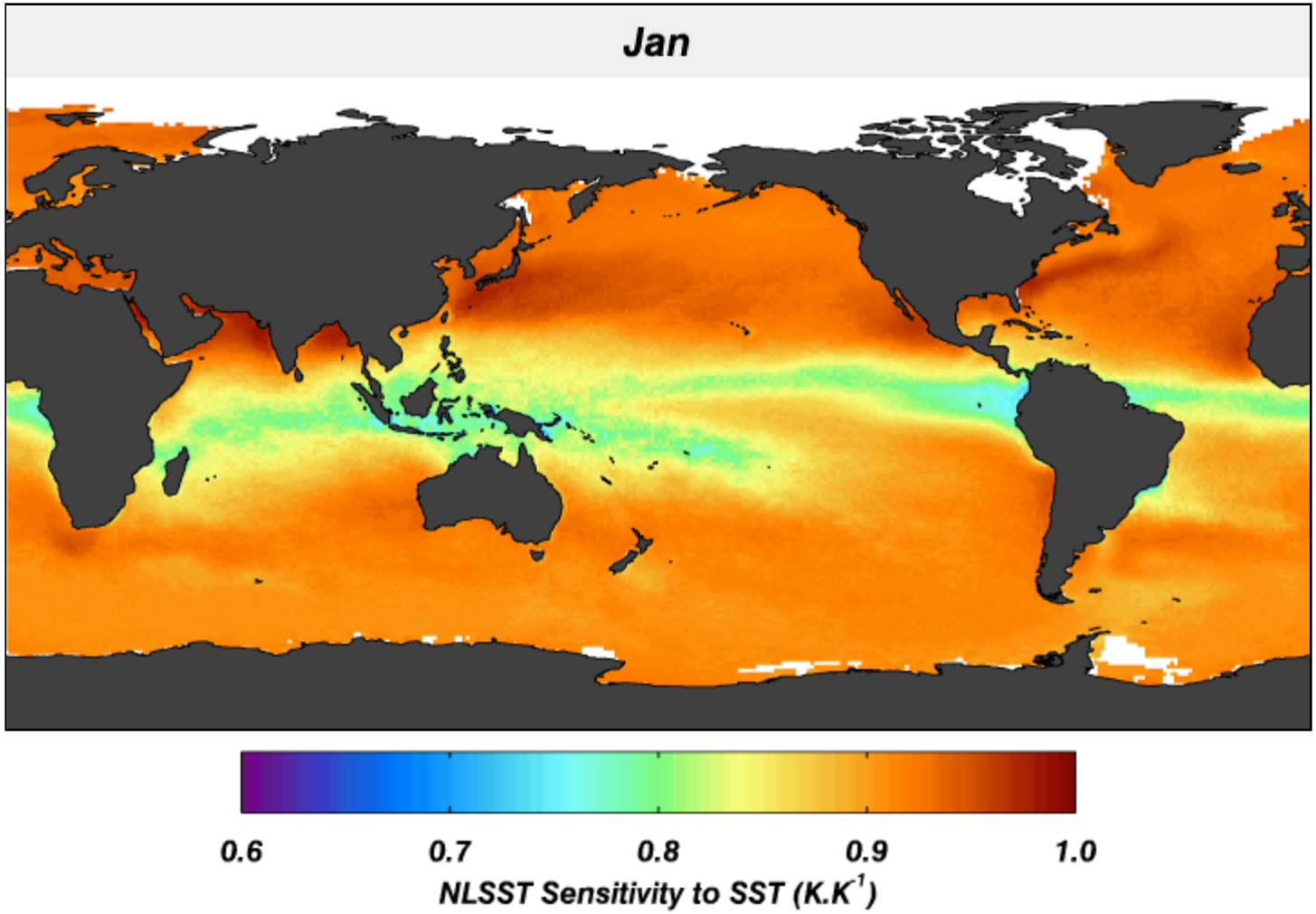
- If SST changes by 1 K, does retrieved SST change by 1 K?
- CRTM provides tangent-linear derivatives $\partial T_{11} / \partial SST_{\text{true}}$ $\partial T_{12} / \partial SST_{\text{true}}$

Response of **NLSST algorithm** to a change in **true SST** is…

$$\partial NLSST / \partial SST_{\text{true}} = \left(a_1 + a_2 \times SST_{bg} + a_3 \times \{\sec(ZA) - 1\}\right) \times \partial T_{11} / \partial SST_{\text{true}} - \left(a_2 \times SST_{bg} + a_3 \times \{\sec(ZA) - 1\}\right) \times \partial T_{12} / \partial SST_{\text{true}}$$

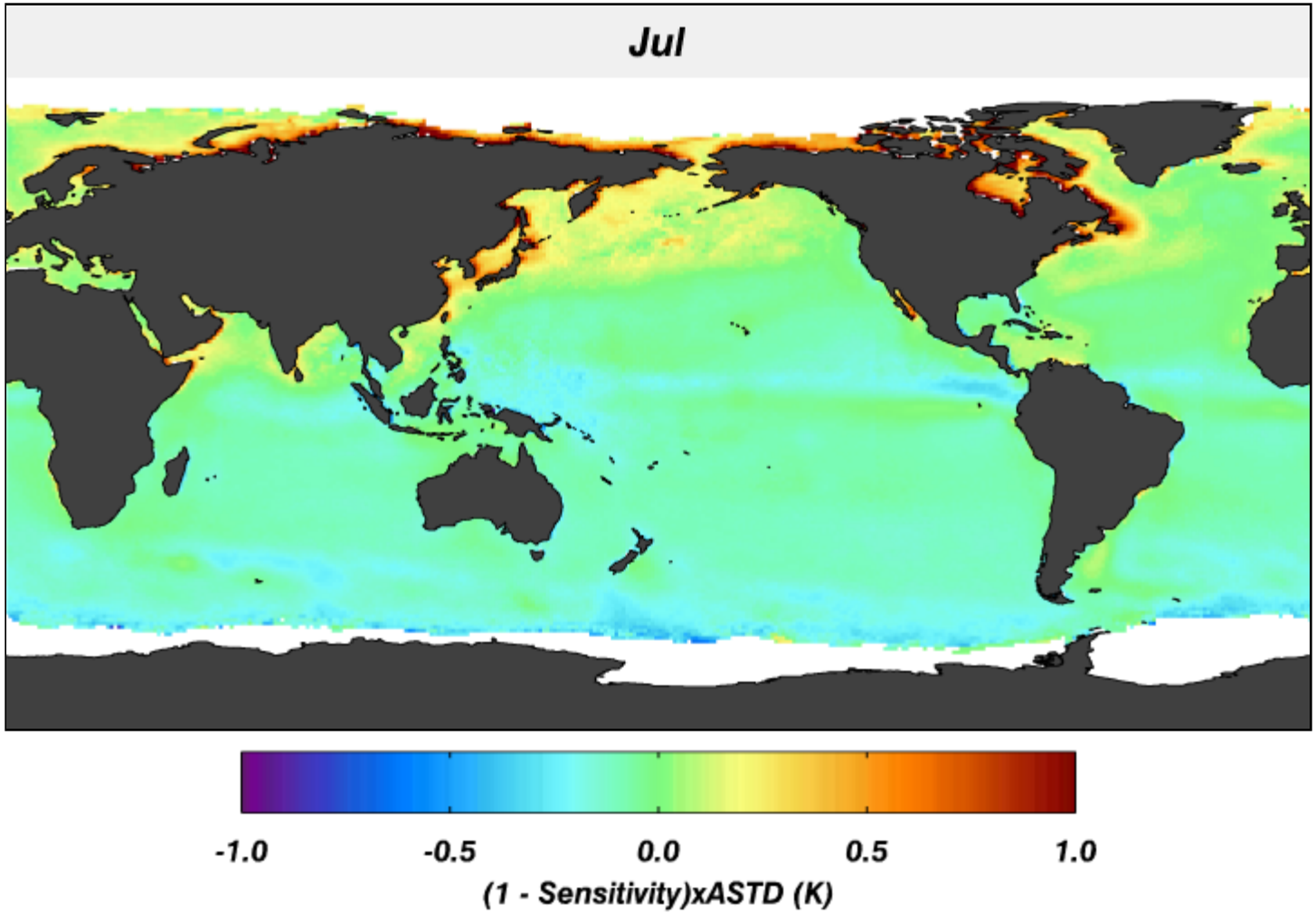
Merchant, C.J., A.R. Harris, H. Roquet and P. Le Borgne, Retrieval characteristics of non-linear sea surface temperature from the Advanced Very High Resolution Radiometer, Geophys. Res. Lett., **36**, L17604, 2009

Sensitivity to true SST

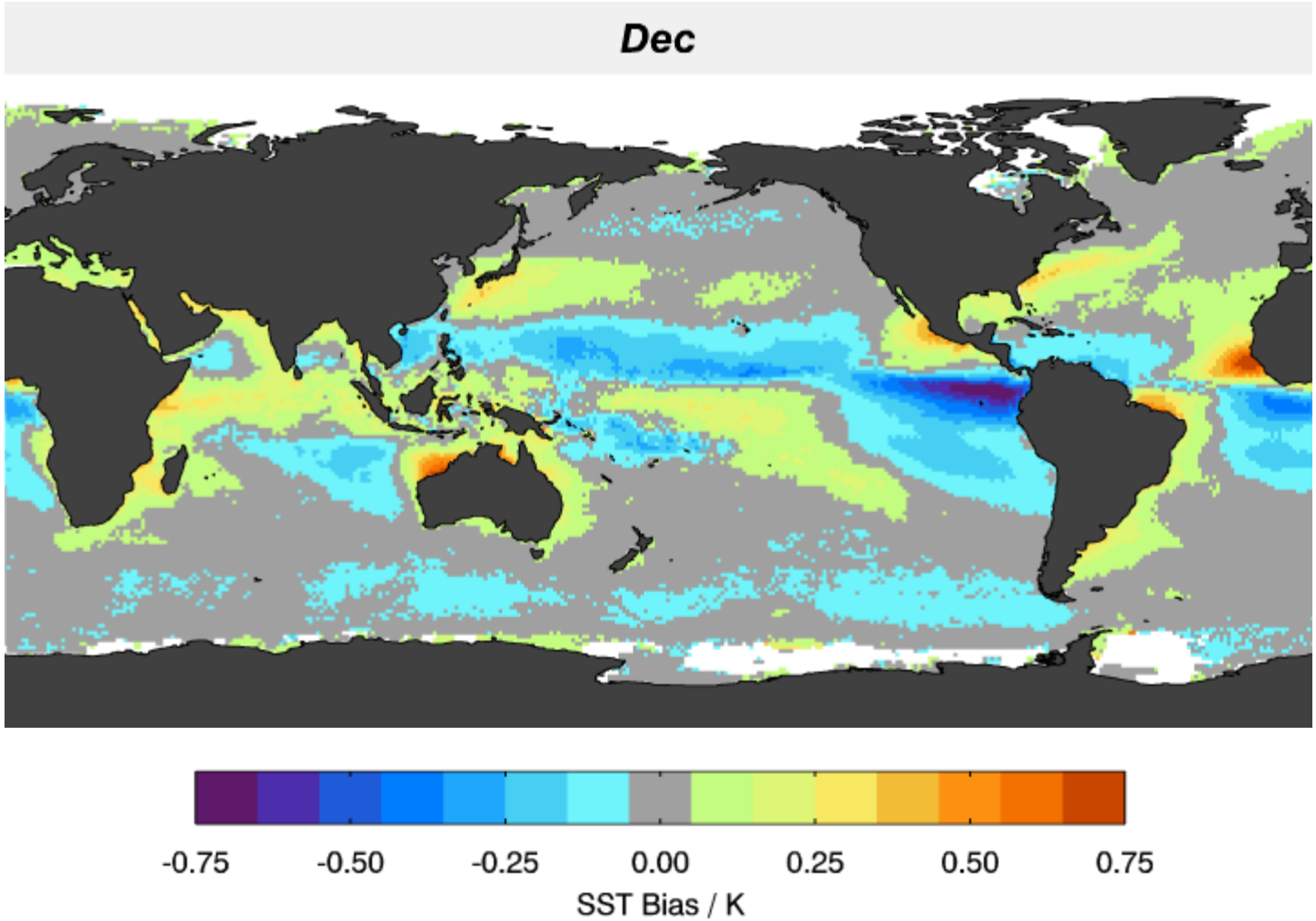


Sensitivity often <1 and changes with season

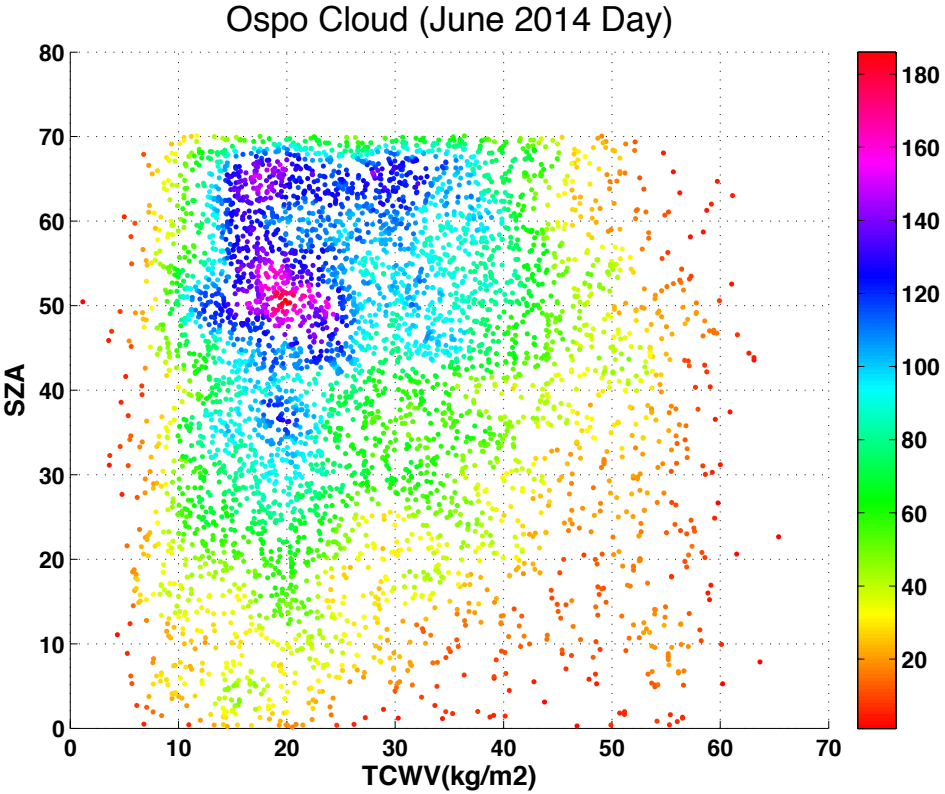
Sensitivity to true SST
Air – Sea Temperature Difference

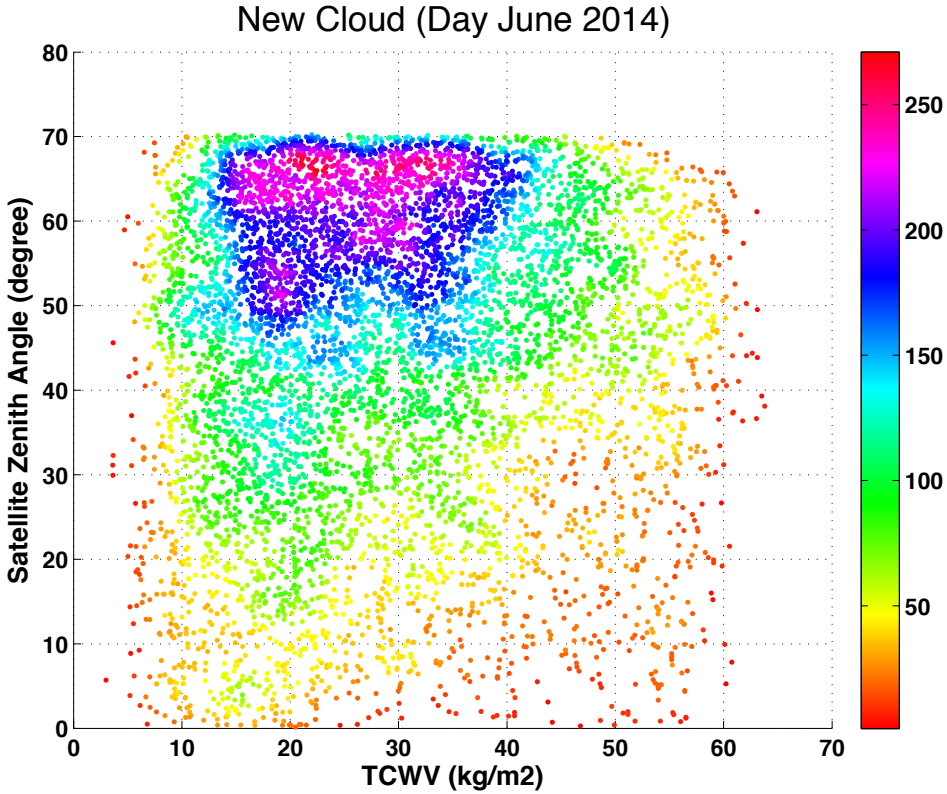


Seasonal Geographic Distribution of Bias



Characteristics of different cloud detections





- The data coverage of new cloud (NC) 50% more than OSPO
- # cloud free pixels for high SZA is sparse – maybe OSPO & OSI-SAF regression form are not working for this regime

- There is no physical meaning from RT for a regression variable of SSTg multiplied with (T11-T12).