A Deterministic Inverse Method for SST Retrieval from VIIRS: Early Results

Andy Harris, Prabhat Koner

CICS, ESSIC, University of Maryland

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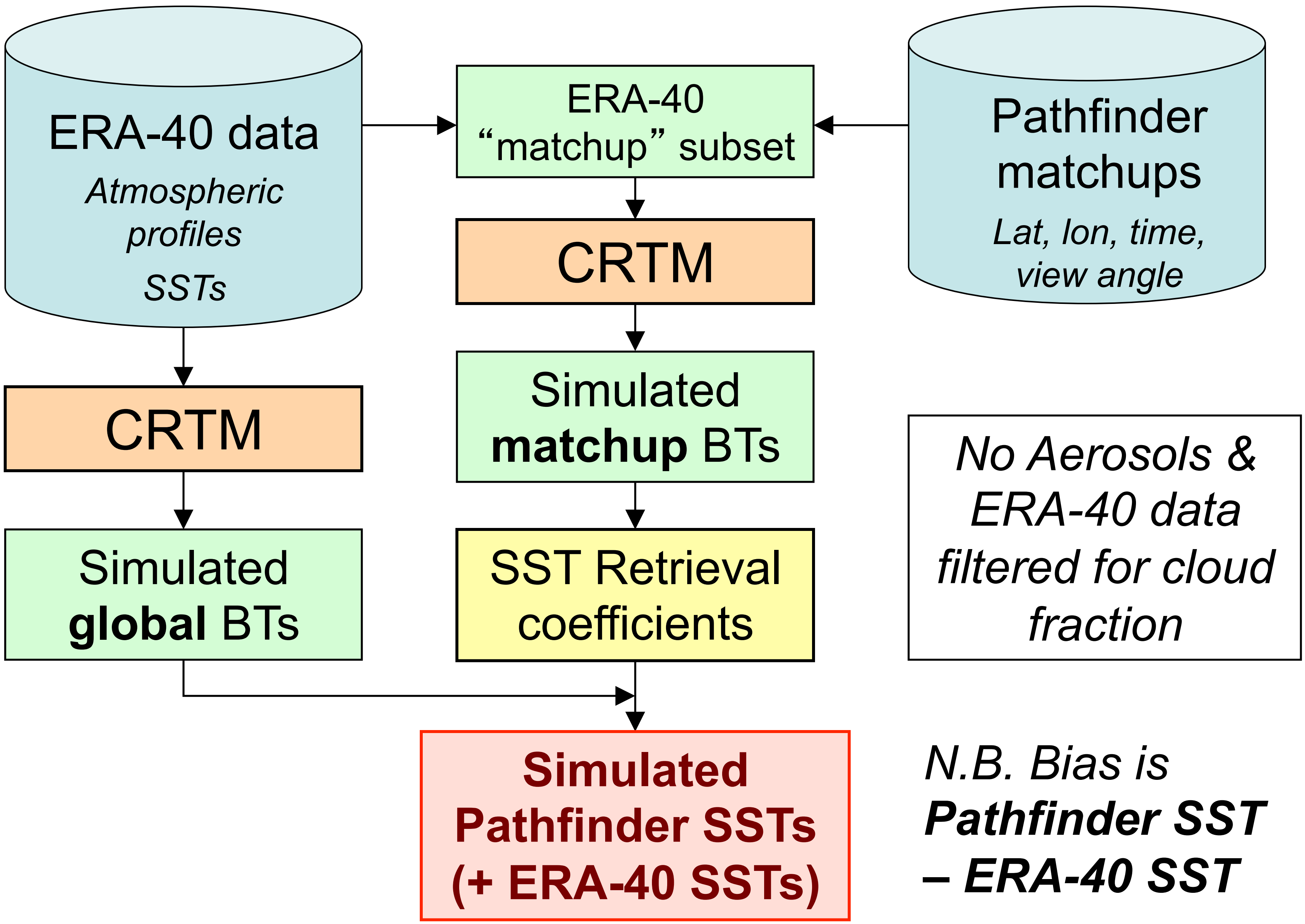
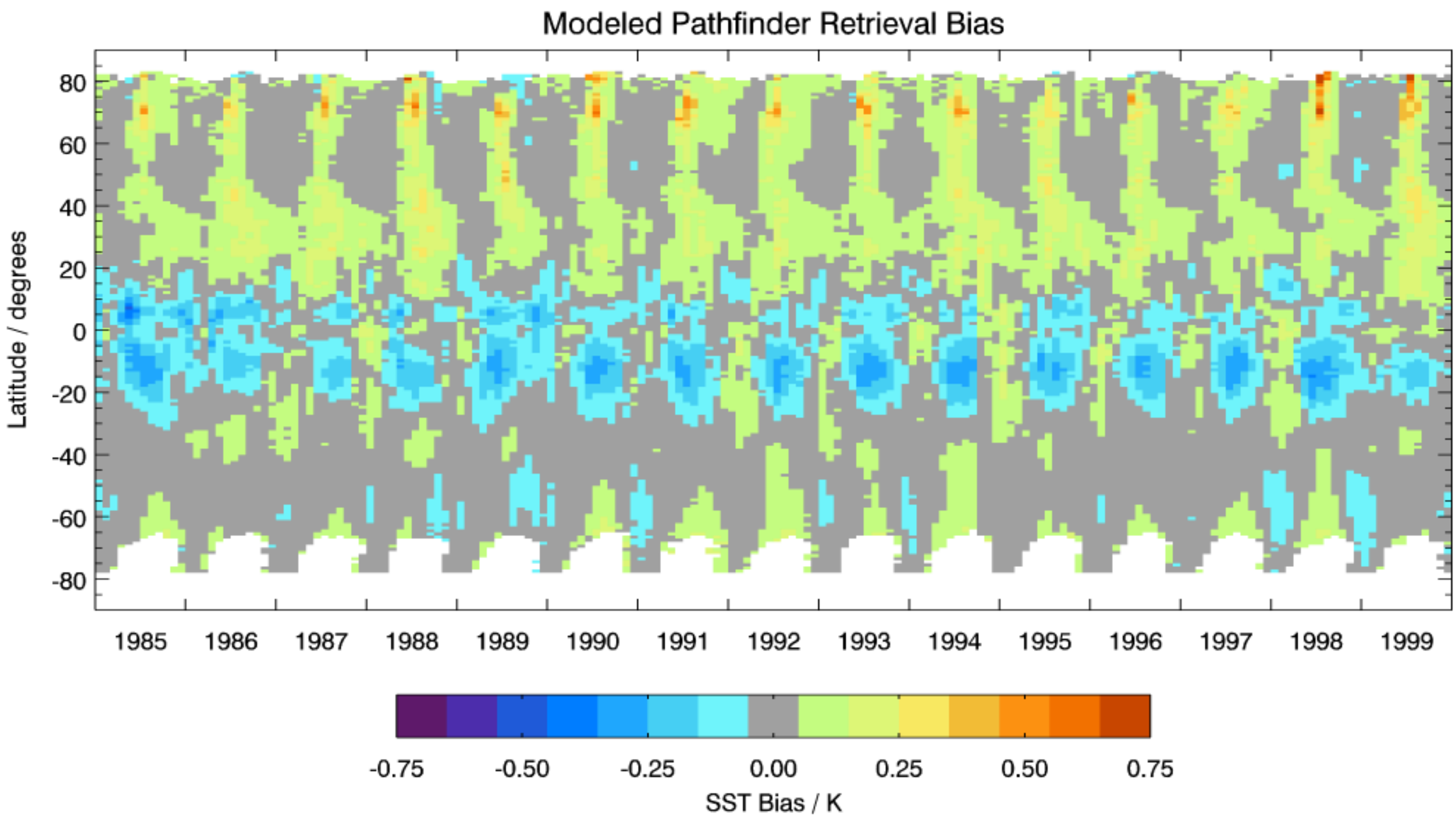
Motivation

- **Previous generation SST algorithms are regression-based**
  - *E.g.* MCSST, NLSST (Pathfinder)
  - Usually employed direct regression of radiances against *in situ* SSTs
  - Ameliorates issues with instrument calibration/characterization
- **Some success for RT-based regression**
  - Primary example (A)ATSR series
  - Well-calibrated and characterized radiometer
  - Dual-view permitted robust retrieval, but fairly narrow swath
- **Regression-based algorithms could result in regional/ seasonal biases**
  - Attempt to characterize global retrieval conditions with only a few coefficients
  - Causes bias if local atmospheric conditions are different from the ensemble mean for the training data

Simulated Pathfinder Retrieval Errors

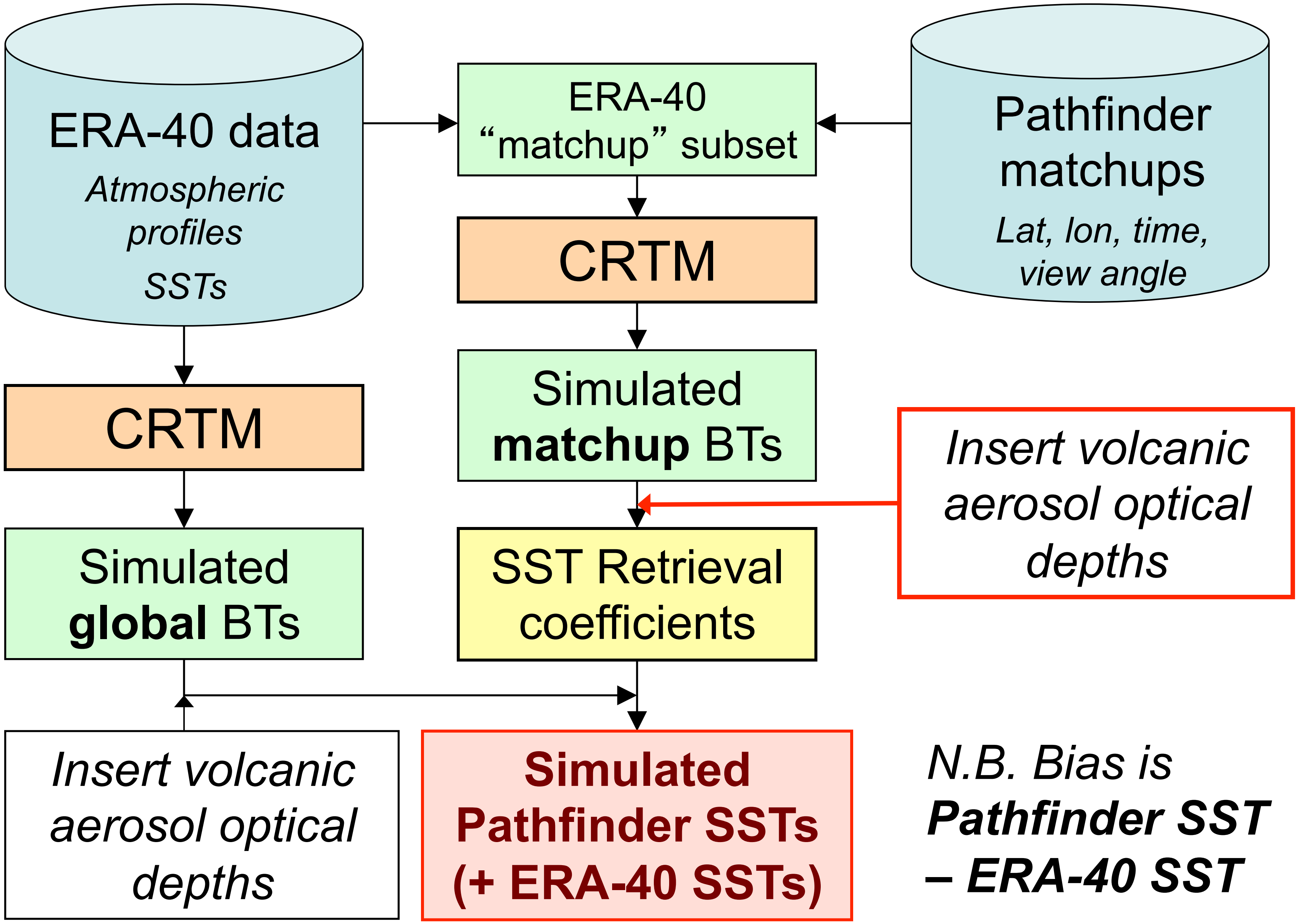


Modeled Pathfinder Bias 1985 – 1999



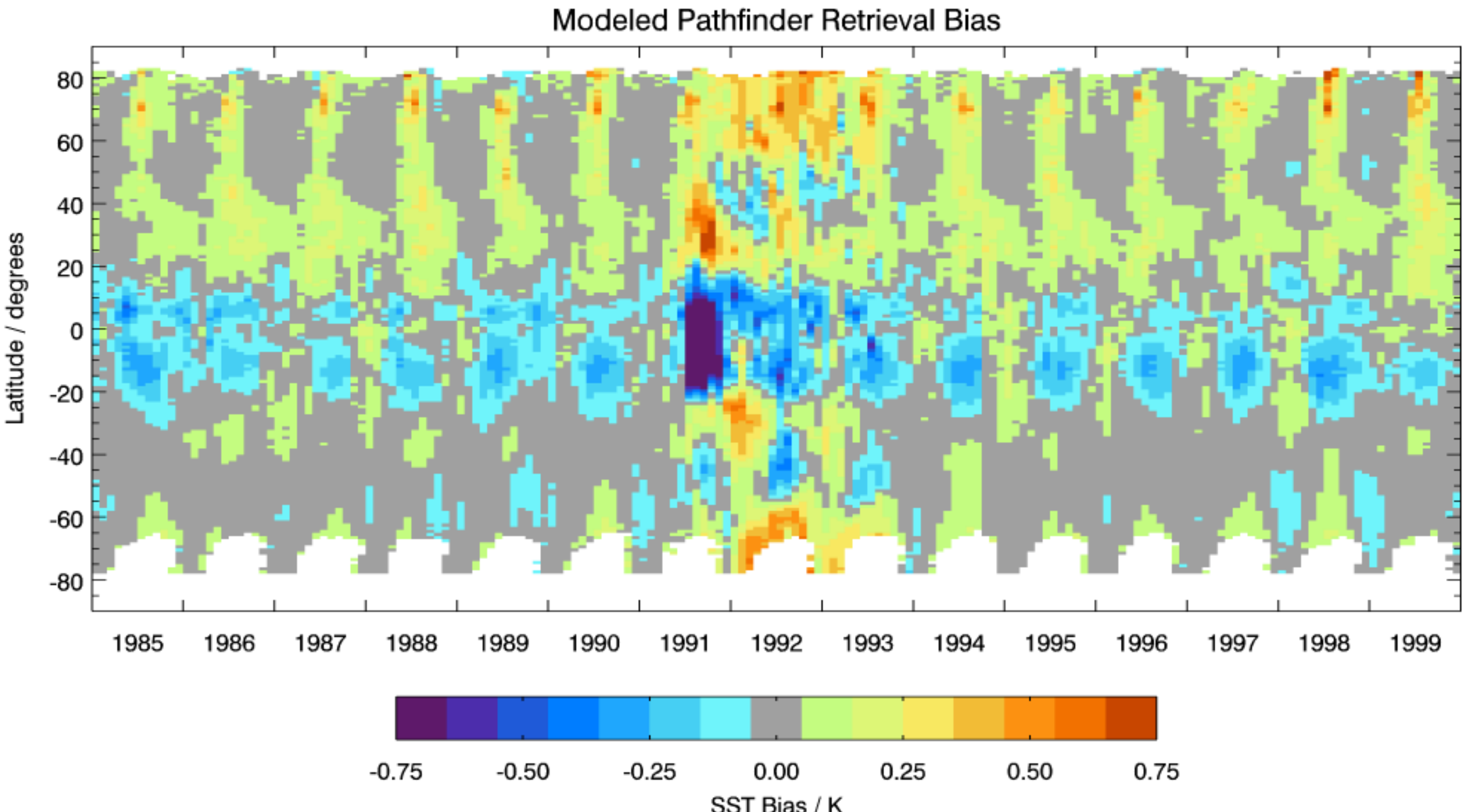
What happens when we include volcanic aerosol?

Simulated Pathfinder Retrieval Errors



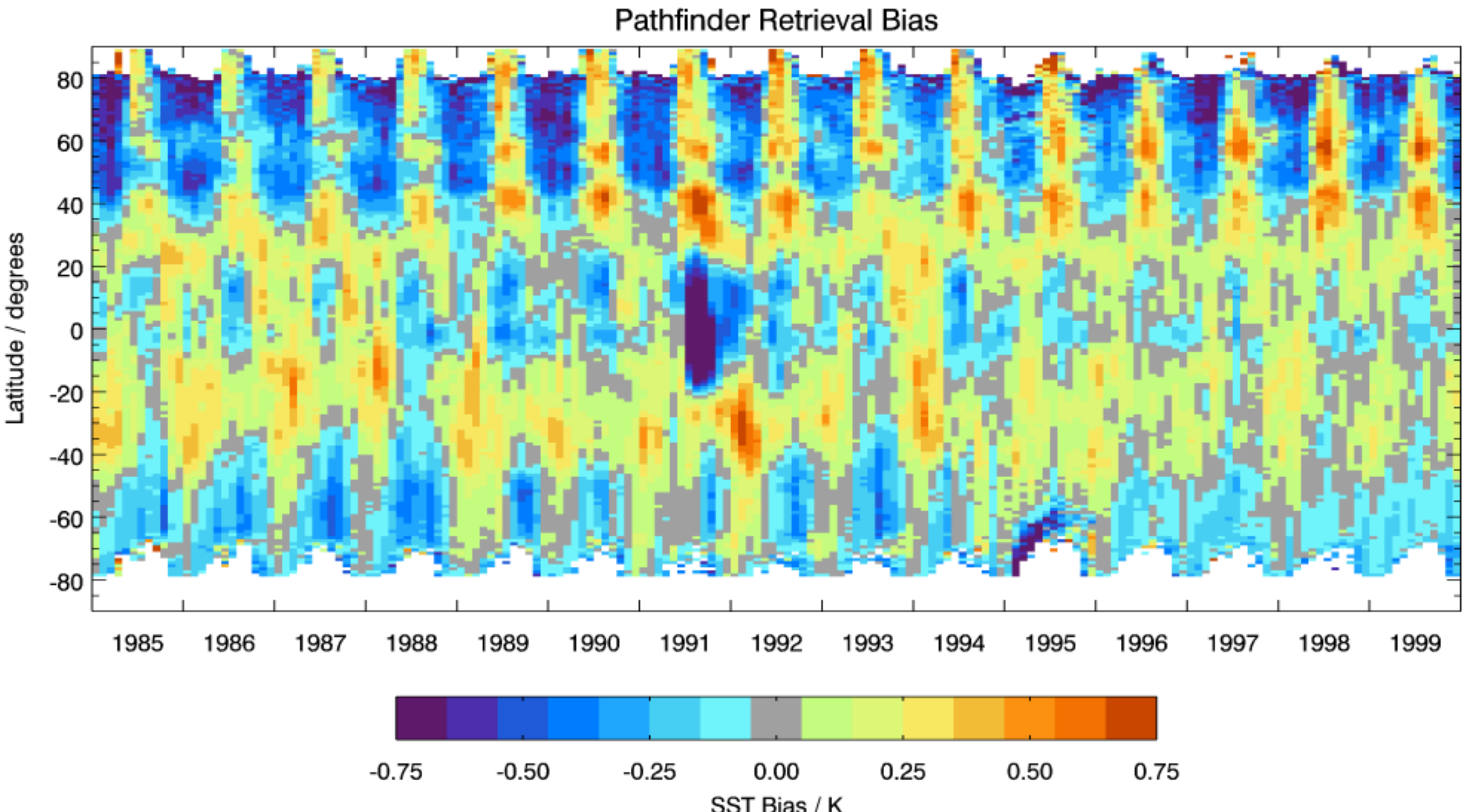
N.B. Bias is ***Pathfinder SST – ERA-40 SST***

Include Pinatubo in RTM radiances



- Negative bias is reduced, but positive biases are propagated N & S
- Split-window based algorithm has **no skill** in compensating for aerosol

Pathfinder V5 – Daily OI ¼ °



- Common features w.r.t. biases induced by Pinatubo aerosol
- Actual seasonal variability is greater than predicted by modeling

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:**

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

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

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

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

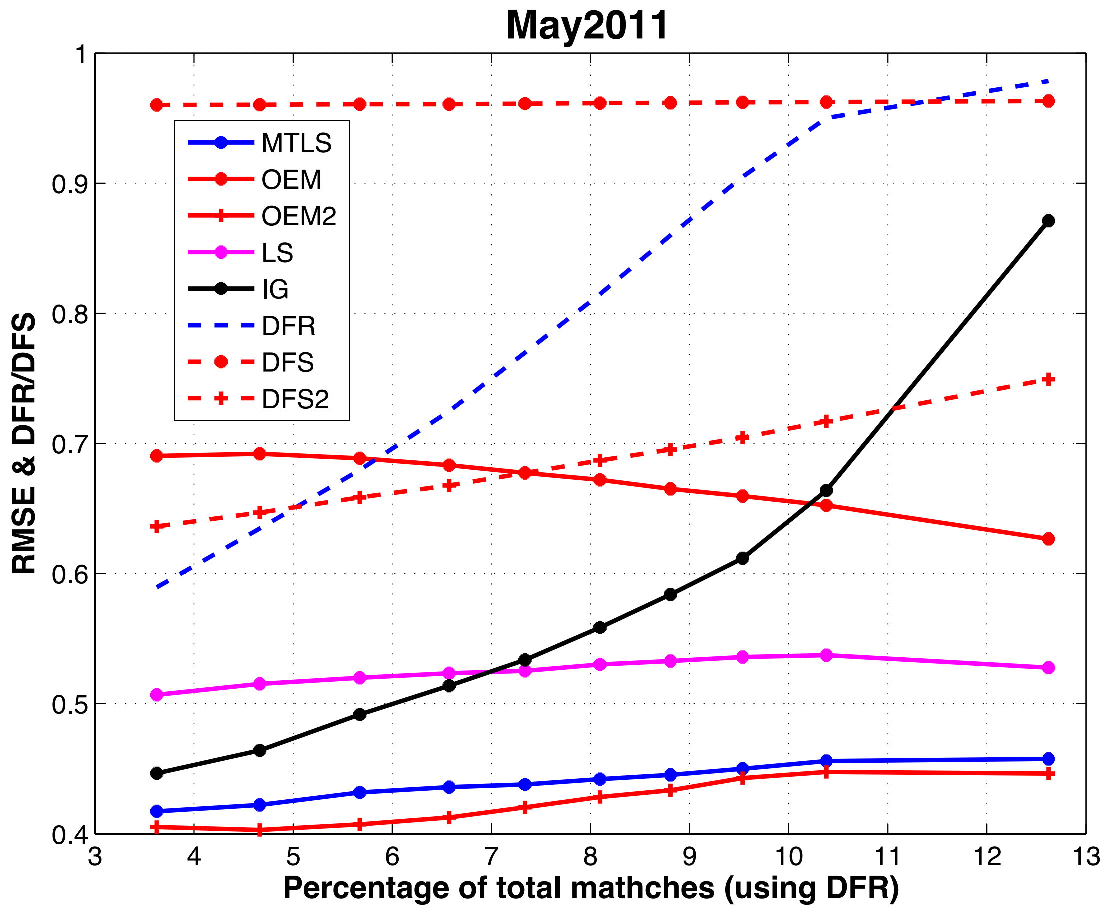
(σ^2_{end} = lowest singular value of $[K\ \Delta y]$)

Total Error

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

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

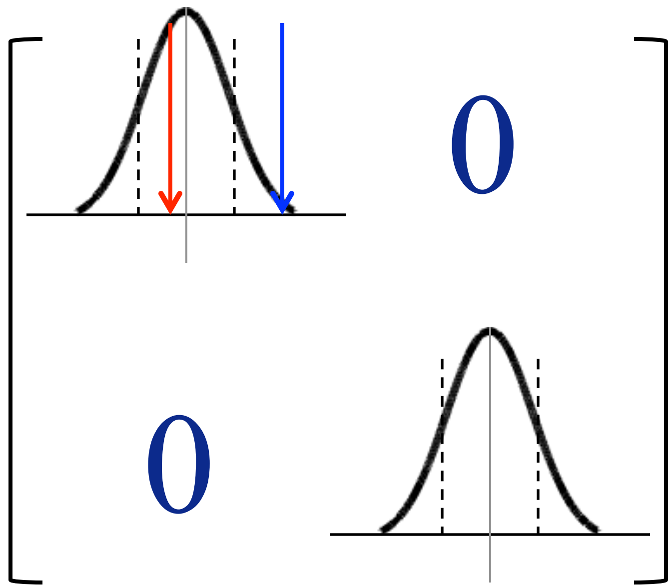
DFS/DFR and Retrieval error



- 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

"Optimized" OE

- $[S_e]$, S_a =

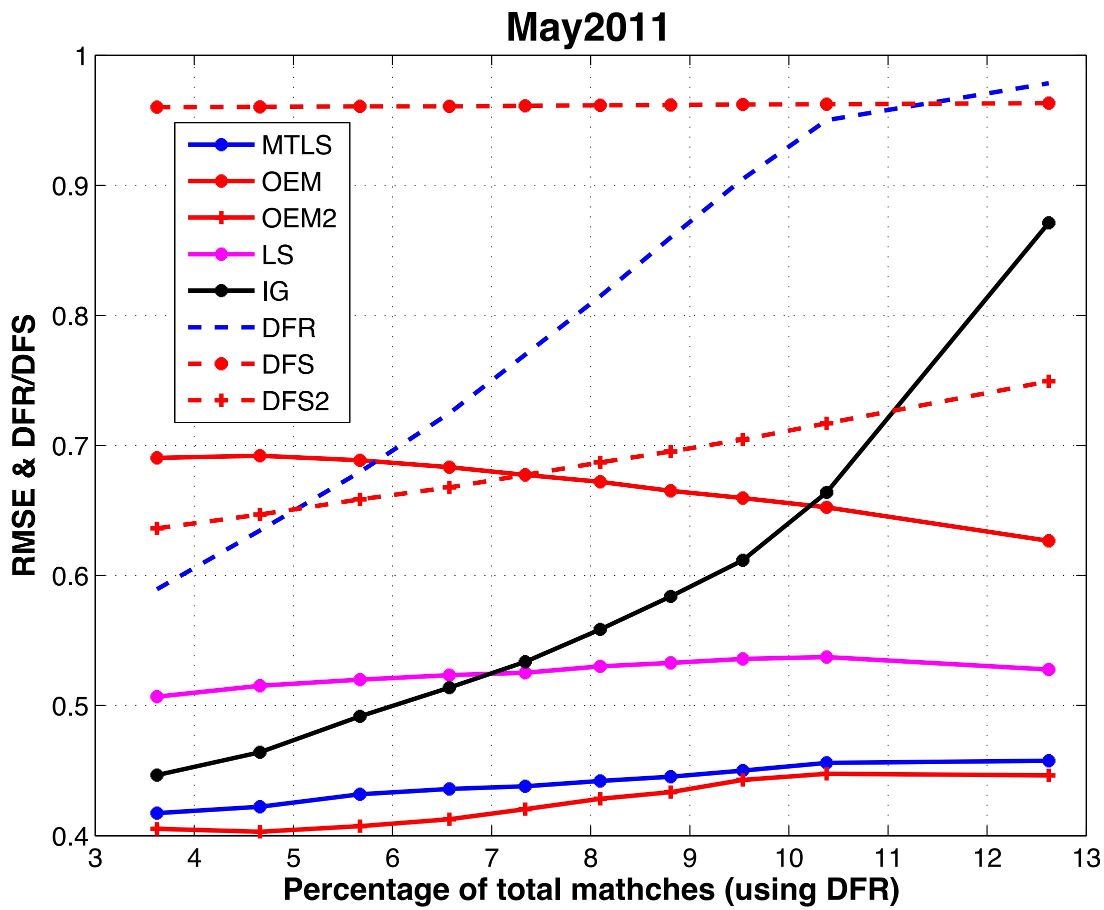


σ^2 is an overestimate…

…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

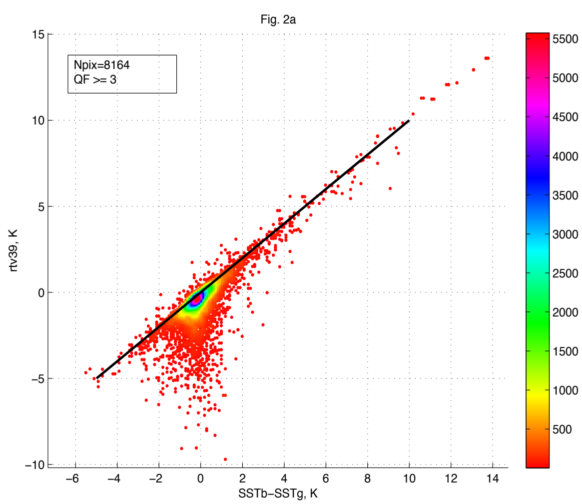
DFS/DFR and Retrieval error

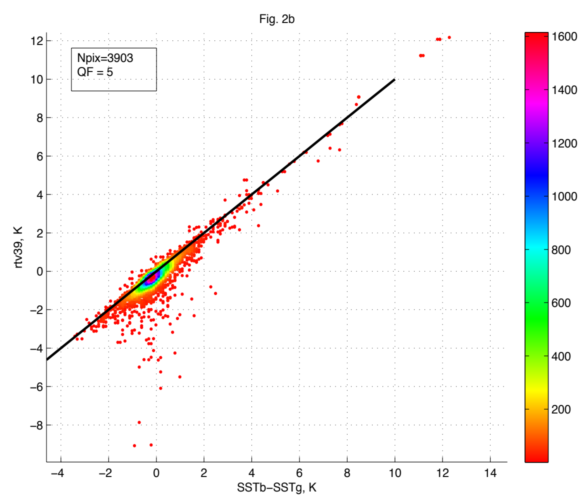


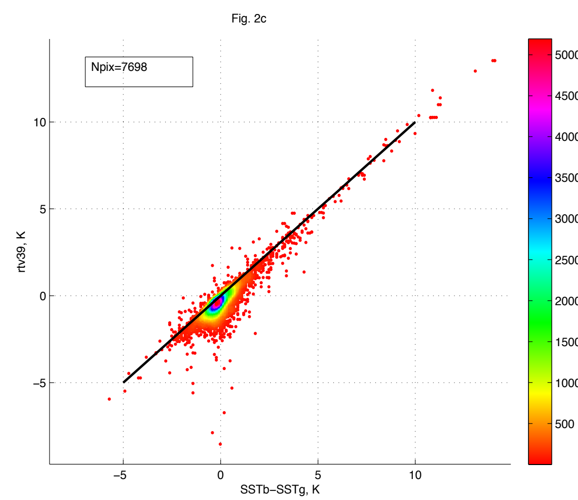
- ❑ Retrieval error of OEM higher than LS
- ❑ More than 75% OEM retrievals are degraded w.r.t. *a priori* error
- ❑ DFR of MTLS is high when *a priori* error is high
- ❑ The retrieval error of OEM is good when *a priori* SST is perfectly known, but DFS of OEM is much lower than for MTLS

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**

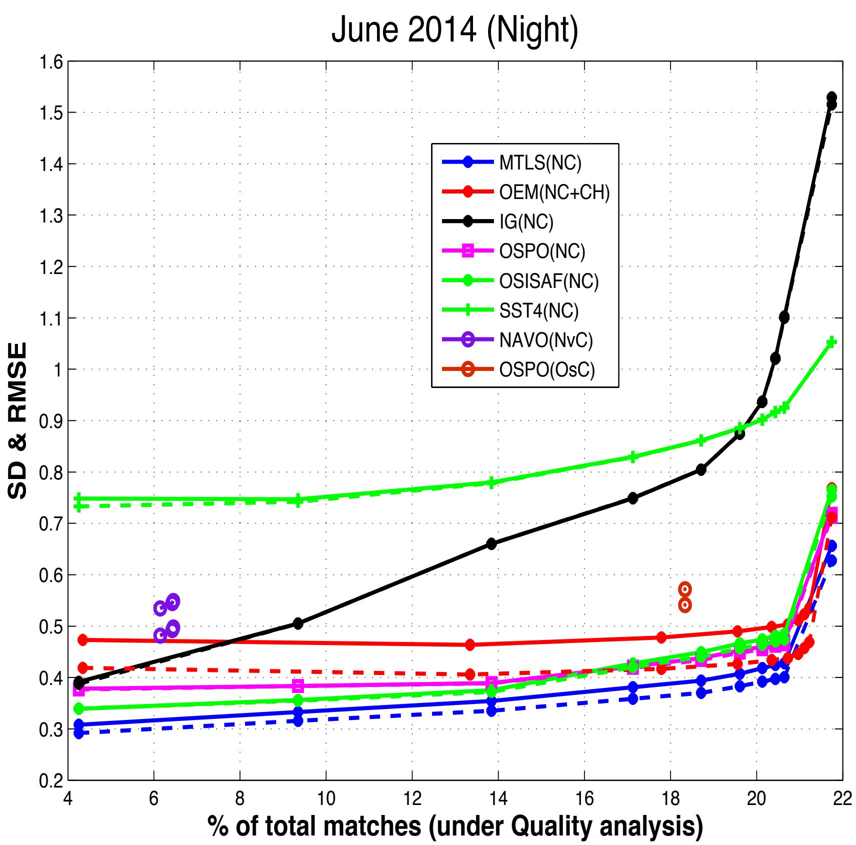


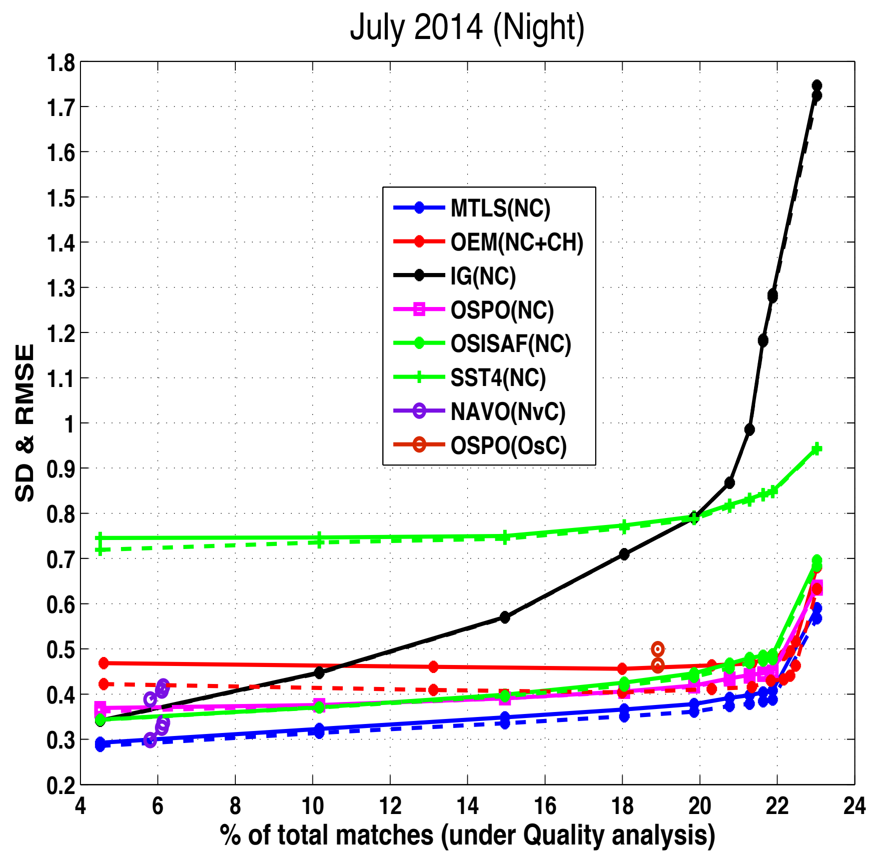




- **Almost as many as GHRSST QL3+, but with greatly reduced leakage**

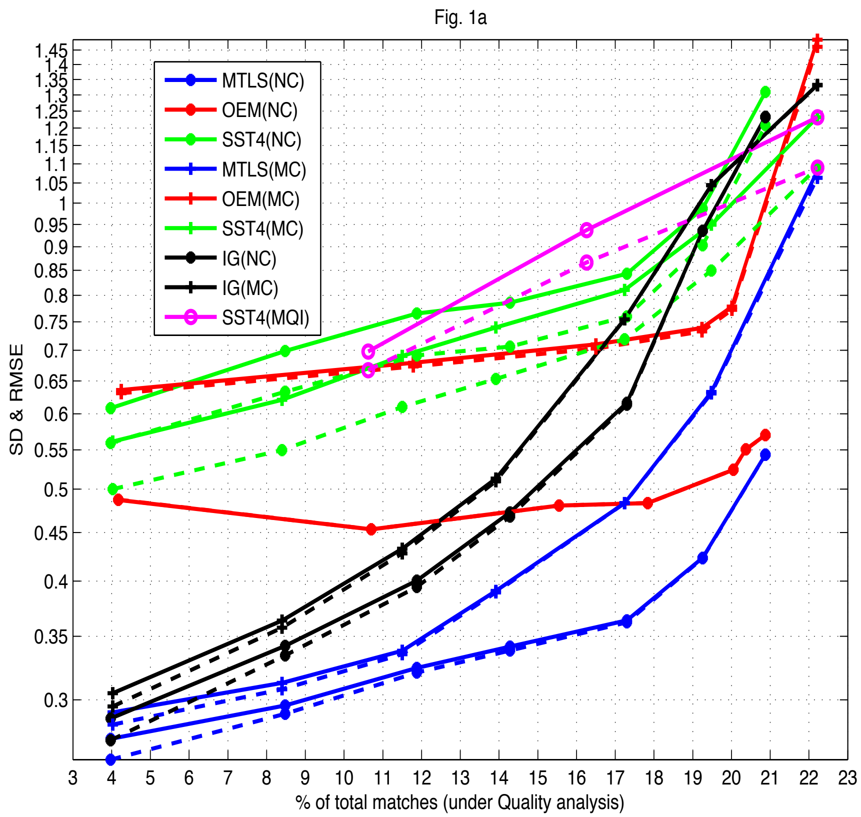
VIIRS Initial Results

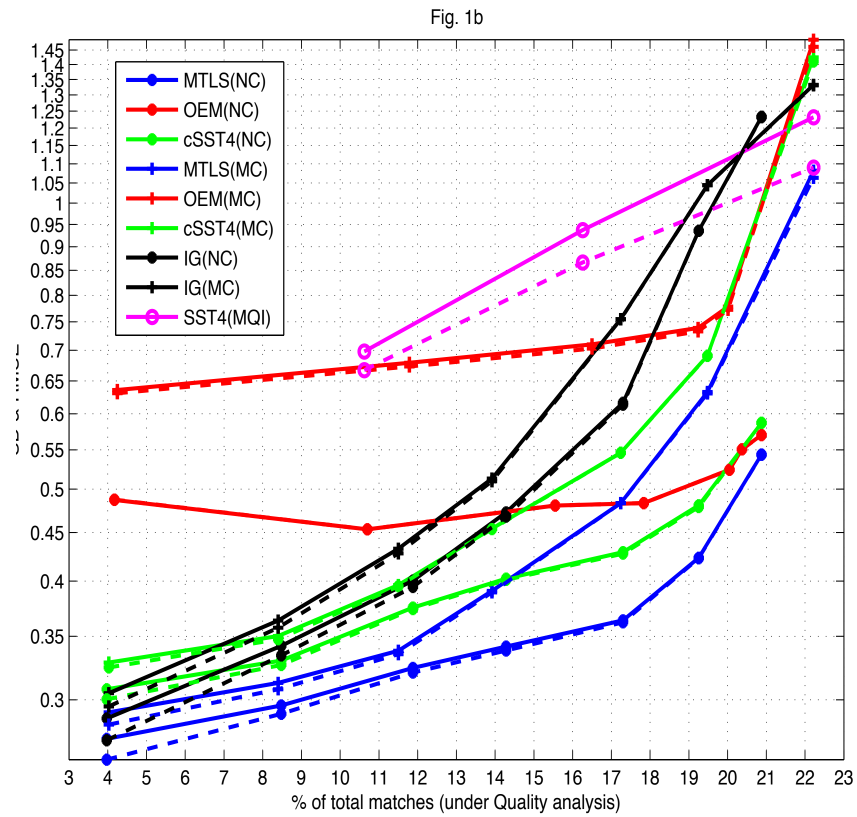




- **Data are ordered according to MTLS error**
  - Reliable guide for regression as well as MTLS
  - Trend of initial guess error is expected

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**

Things to consider

- **It seems "obvious" that a sensitivity of 1 is desirable**
  - *E.g.* if there is diurnal warming of 5 K, it will be observed in the data, and strong upwellings will be accurately observed, *etc*.
- **However, there is a penalty to be paid**
  - Ill-conditioned problem ➔ noise propagates from measurement space to parameter space
  - Compromise is usually struck (*e.g.* minimum least squares result for training data in a regression algorithm)
- **Regression algorithms may have sensitivity <1 for large regions**
  - *E.g.* daytime algorithms in the tropics (diurnal warming!)
  - Causes bias if local atmospheric conditions are different from the ensemble mean for the training data

Things to consider cont'd

- **Physical retrieval methods locally linearizes the retrieval**
  - Ameliorate regional bias issues
- **Physical retrievals still ill-conditioned**
  - Least-Squares generally considered to have unacceptable noise
- **Optimal Estimation can have sensitivity ~1**
  - Requires somewhat inflated SST error covariance
  - Leads to relatively poor noise performance
  - Using "true" SST error greatly improves retrieval accuracy
  - However, SST sensitivity is substantially reduced
- **MTLS algorithm adjusts its sensitivity**
  - Sensitivity <1 when initial guess is close to truth
  - Sensitivity ➔ 1 when initial guess is far from truth
  - Retrieval accuracy approaches "optimized" OEM
  - May still be an issue for fine structure

Summary

- **MTLS seems applicable to VIIRS**
  - Well-calibrated instrument, with reliable fast RTM available
  - Error calculation useful quality indicator
- **MODIS offers even more possibilities**
  - "Sounding" channels permit inclusion of basic profile shape information in the state vector
  - **See Prabhat's presentation at the Oceans Breakout**
- **Cloud detection can be aided by RTM**
  - "Single-channel" retrieval consistency, MTLS error calculation
- **Options for improvement**
  - Close to validation limit for conventional *in situ*
  - 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

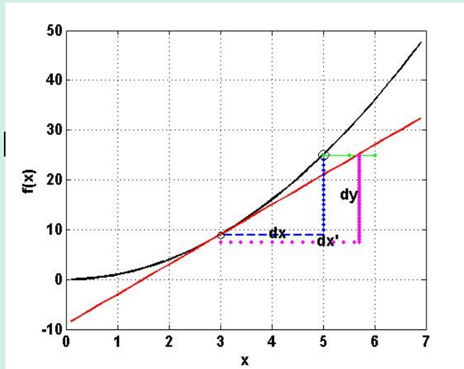
Deterministic & Stochastic

Determinitic	Stochastic/Probabilistic

MTLS/RTLS/Tikhonov: Single pixel

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

measurement error



Lengendre (1805) Least Squares:

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

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

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

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

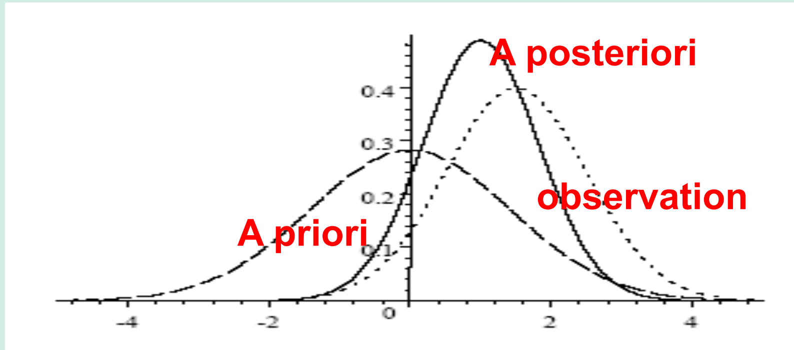
MTLS: $[\mathbf{u}\ \sigma\ \mathbf{v}] = [\mathbf{K}\quad d\mathbf{Y}_\delta];\quad \mathbf{R} = \mathbf{I}$

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

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

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

OEM: A set of measurement



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

Low confidence for pixel retrieval

Chi-Square test:

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

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

Regression: A set of measurement

Historical heritage in SST retrieval using Window channels.

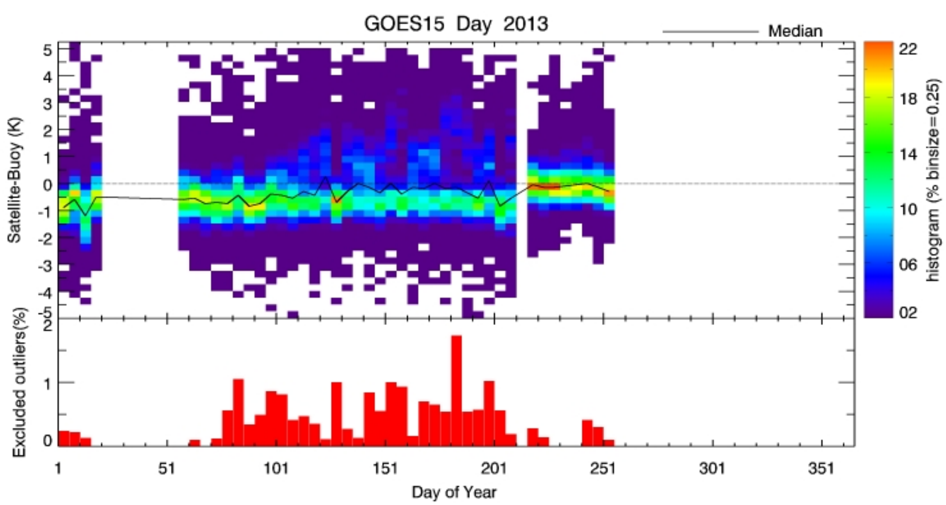
Coefficient Vector/matrix**: C** $X_{reg} = \mathbf{C}\ \mathbf{Y}_\delta$

Main concerns: Correlation & Causation

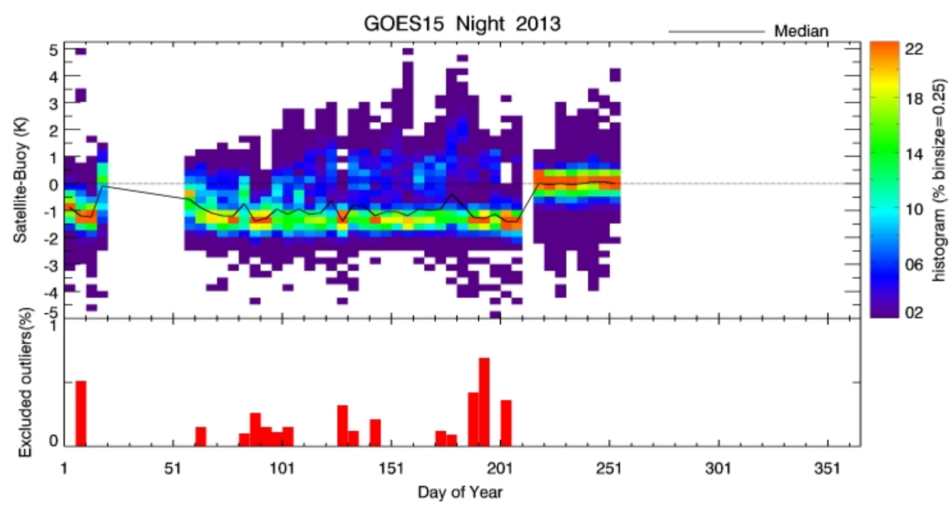
Recent update to Geo-SST

- **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?

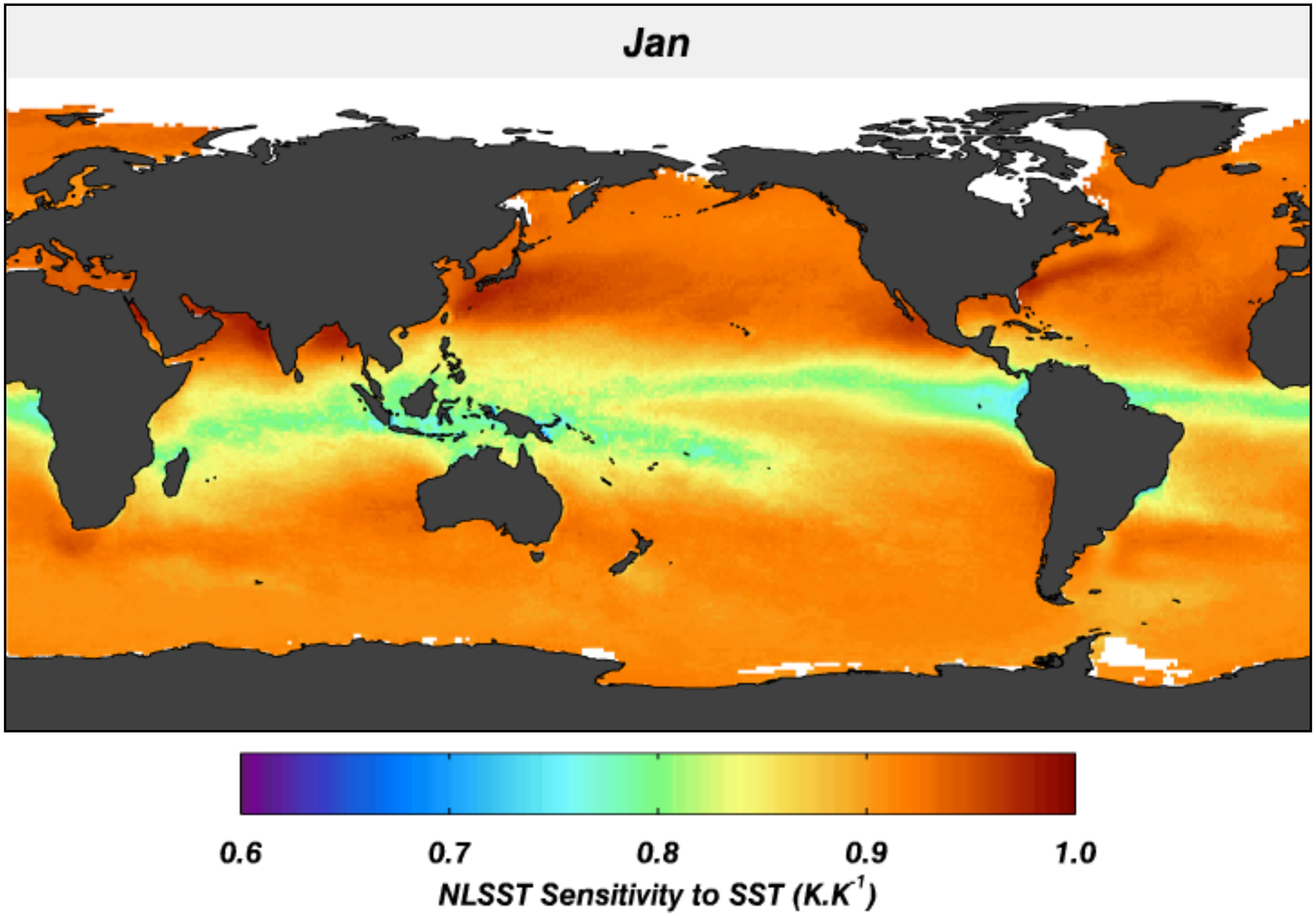
- If SST changes by 1 K, does retrieved SST change by 1 K?
- CRTM provides tangent-linear derivatives $\partial T_{11} / \partial SST_{\mathrm{true}}$ $\partial T_{12} / \partial SST_{\mathrm{true}}$

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

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

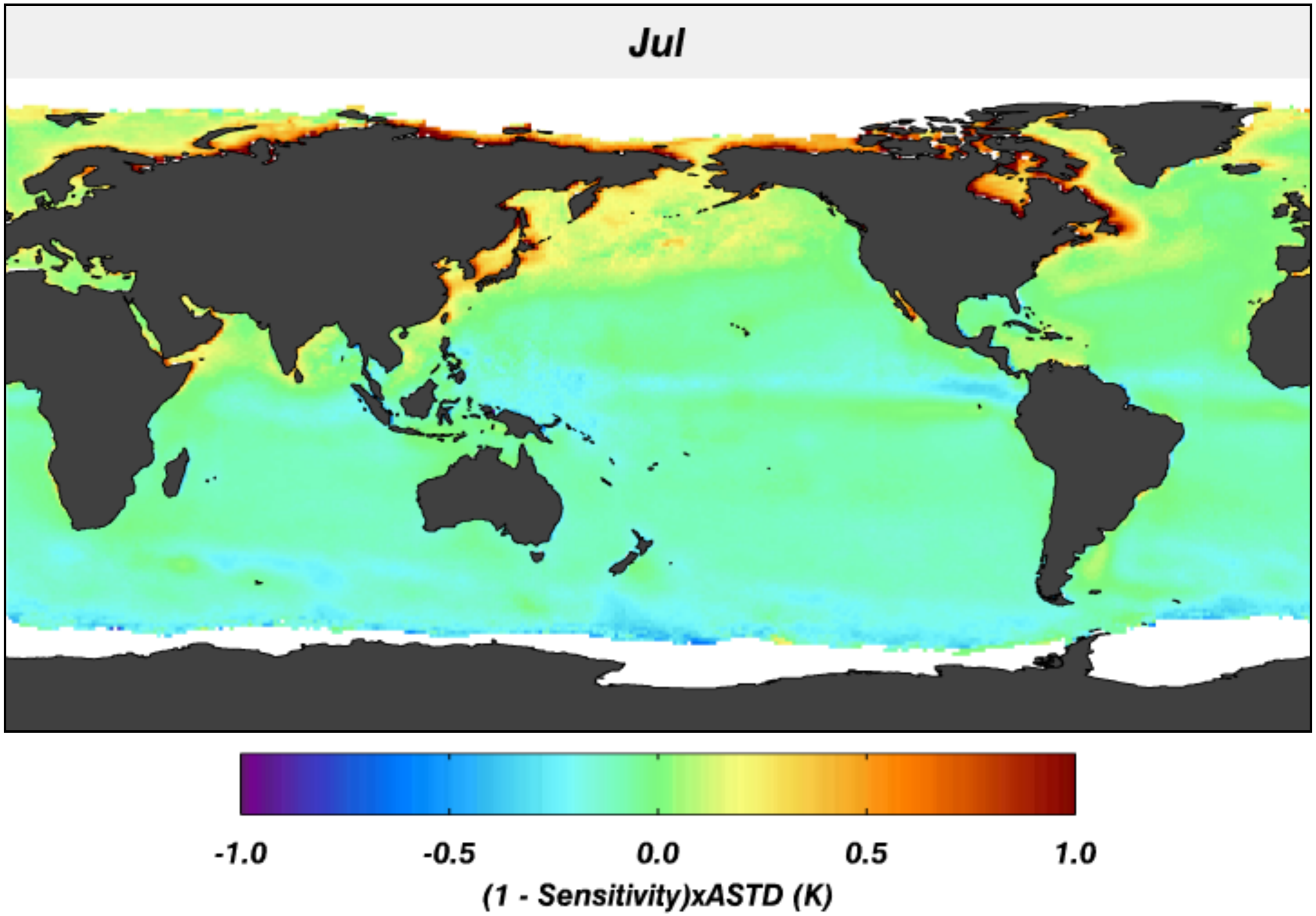
Merchant, C.J., A.R. Harris, H. Roquet and P. Le Borgne, Retrieval characteristics of non-linear sea surface temperature from the Advanced Very High Resolution Radiometer, Geophys. Res. Lett., **36**, L17604, 2009

Sensitivity to true SST

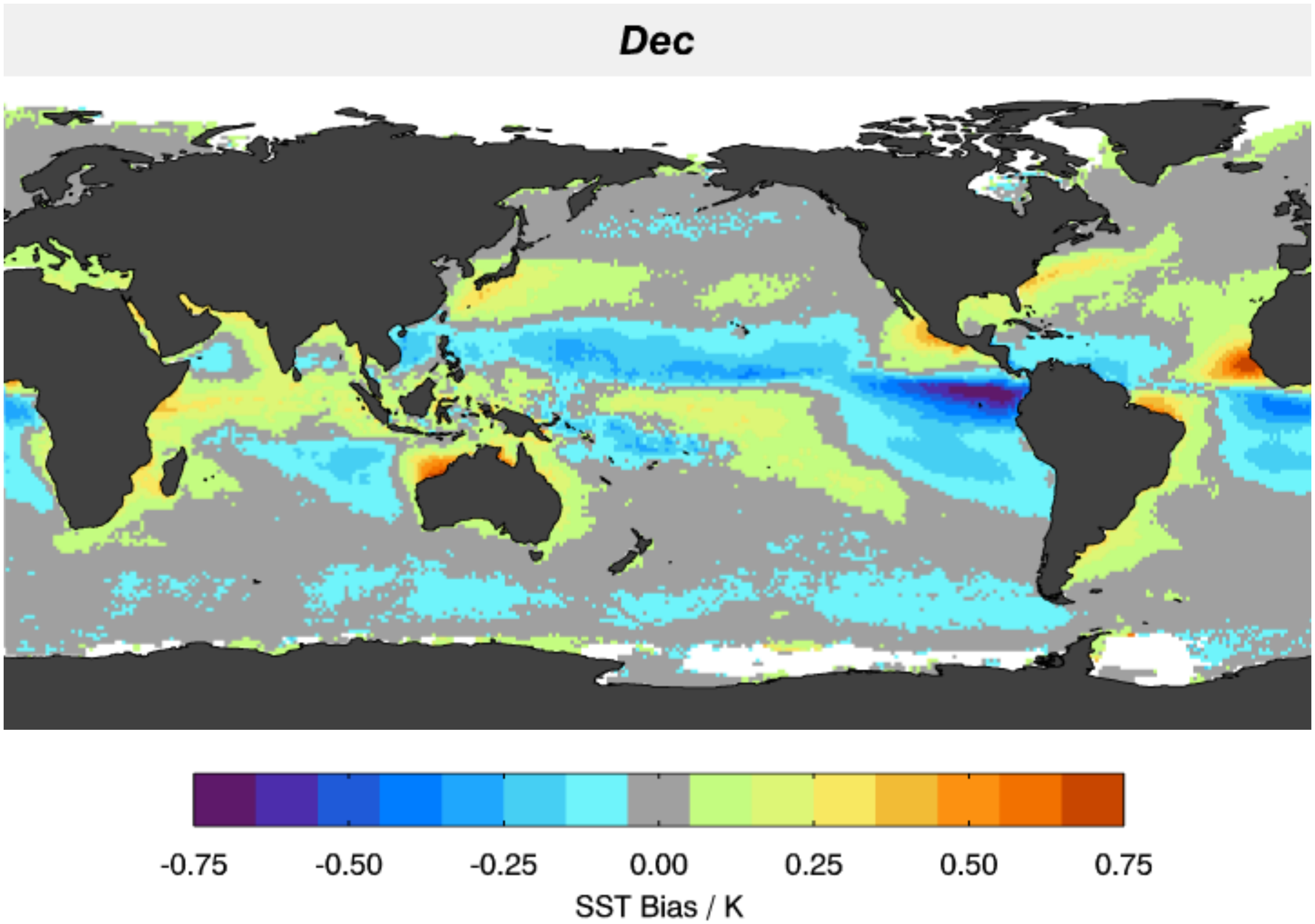


Sensitivity often <1 and changes with season

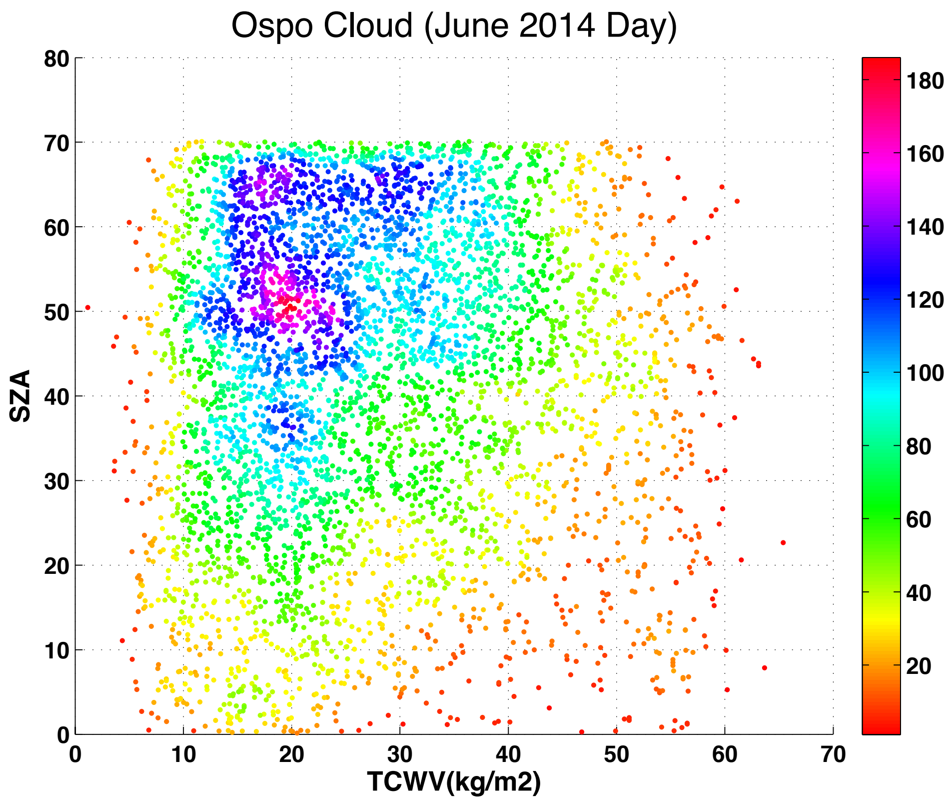
Sensitivity to true SST
Air – Sea Temperature Difference

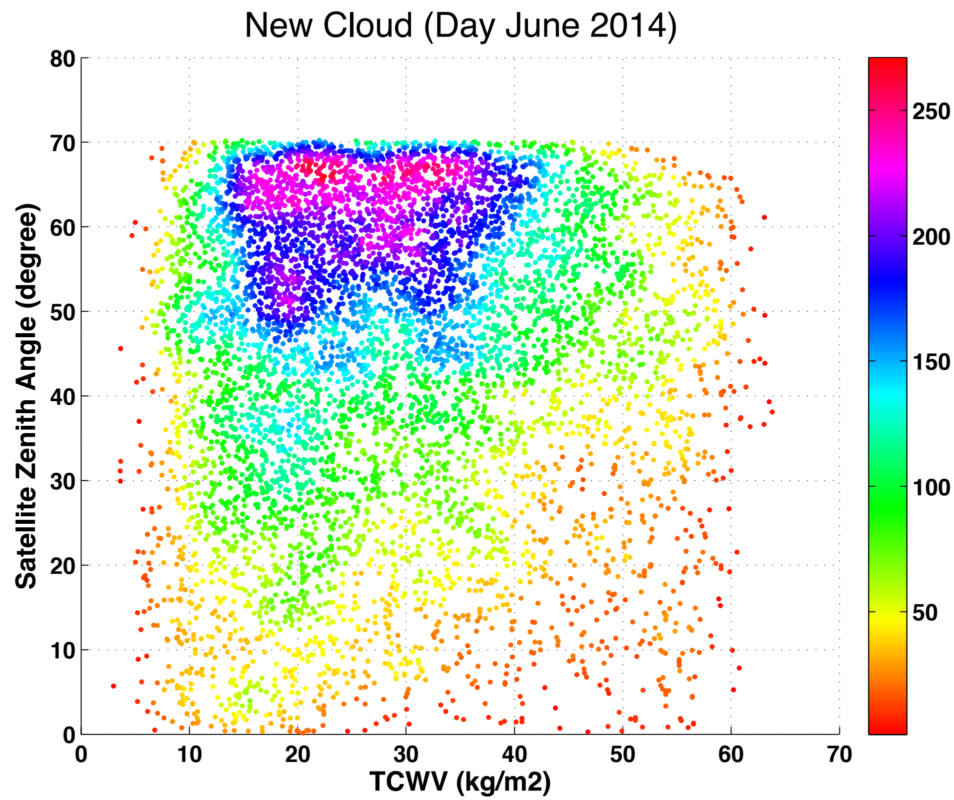


Seasonal Geographic Distribution of Bias



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).