Estimation of uncertainties of regression ACSPO SST from statistical structure of matchups

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Objective

- **GDS2 format for L2 SST requires every pixel to be supplied with Single Sensor Error Statistics (SSES) – bias and SD.**
- **GHRSST-XV has reviewed existing SSES practices and recommended to "revisit SSES"**
- **The SSES algorithm has been redesigned for the v.2.40 of the Advanced Clear-Sky Processor for Oceans (ACSPO)**
- **The main objective of redesign was to enable efficient correction of SST biases from SSES information**
- **The presentation describes the concept and the performance of the ACSPO v.2.4 SSES algorithm**

Baseline Regression SST algorithm in ACSPO

Day:

$$T_S = a_0 + (a_1 + a_2 S_\vartheta) T_{11} + [a_3 + a_4 T_S^0 + a_5 S_\vartheta] (T_{11} - T_{12}) + a_6 S_\vartheta$$

Night:

$$T_S = b_0 + (b_1 + b_2 S_\vartheta) T_{3.7} + (b_3 + b_4 S_\vartheta) (T_{11} - T_{12}) + b_5 S_\vartheta$$

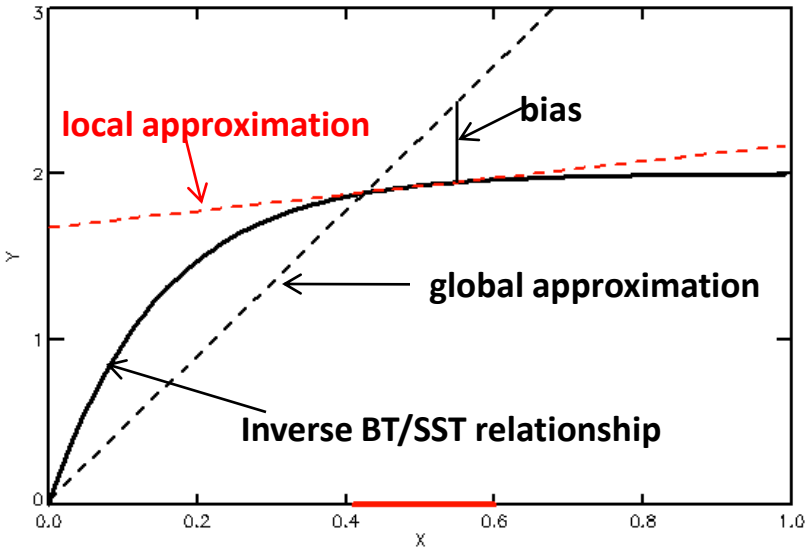
$T_{3.7}, T_{11}, T_{12}$	observed BTs
$S_\vartheta = 1/\cos(\vartheta)$	
ϑ	satellite view zenith angle (VZA)
T_S^0	first guess SST (in °C)
a's and b's	regression coefficients

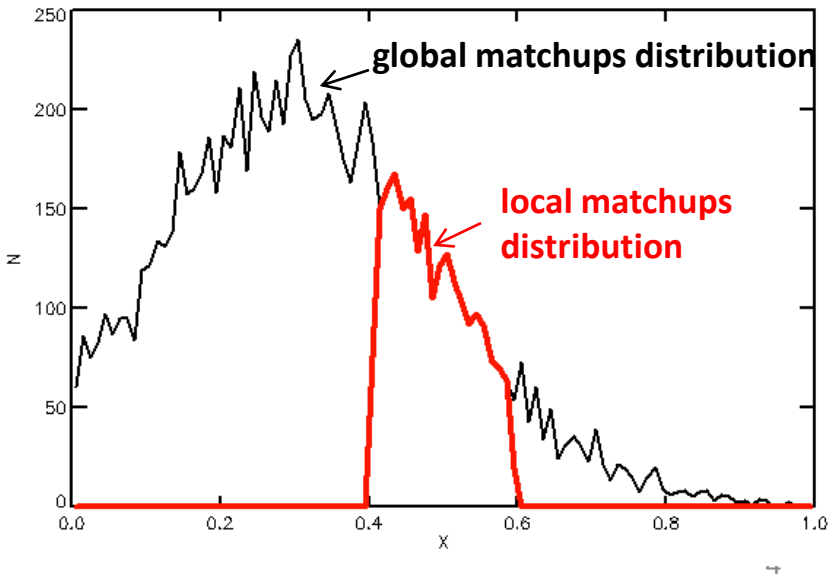
- **Regression equations use EUMETSAT OSI-SAF formulations**
- **A single set of coefficients is derived from global dataset of matchups (MDS) and used globally**
- **In this presentation, this SST will be called Single Regression SST (SR SST)**

The concept of ACSPO SSES

- Biases in SR SST result from inaccurate approximation of the inverse relationship between satellite BTs and SST with a single regression equation
- The biases can be reduced by replacing a single regression equation with a set of local regression approximations

- The ACSPO SSES algorithm:
  - Generates an auxiliary SST from a set of local regressions. This will be called <u>Piecewise Regression SST (PWR SST)</u>
  - Estimates SST bias as difference between SR SST and PWR SST
  - Estimates SSES SD from local differences between SR SST and in situ SST





Segmentation of the SST retrieval domain.
1. Metric in the space of regressors

- **General form of regression equation:** $T_s=\langle T_{in\ situ}\rangle + \mathbf{c}^T(\mathbf{R}-\langle\mathbf{R}\rangle)$

  c *vector of coefficients,* <*> *notifies averaging over MDS*
  R *vector of regressors* <**R**> *average of* **R** *over the MDS*
  $T_{in\ situ}$ *in situ SST*

- **SR SST error:** $\delta T_s= \boldsymbol{\delta}\mathbf{c}^T(\mathbf{R}-\langle\mathbf{R}\rangle)$

- **SR SST error depends on R-<R>;**
- **It is best to be analyzed in the space of regressors (R-space) as a function of R-<R>**

- **<u>Gaussian approximation of the empirical PDF of regressors:</u>**

$$P(\mathbf{R})= [(2\pi)^N det(D)]^{-0.5} exp[-\rho(\mathbf{R})^2],$$

- ρ(**R**) **is <u>Fisher distance (FD)</u>**:

$$\rho= [(\mathbf{R}-\langle\mathbf{R}\rangle)^T D^{-1}(\mathbf{R}-\langle\mathbf{R}\rangle)]^{1/2}$$

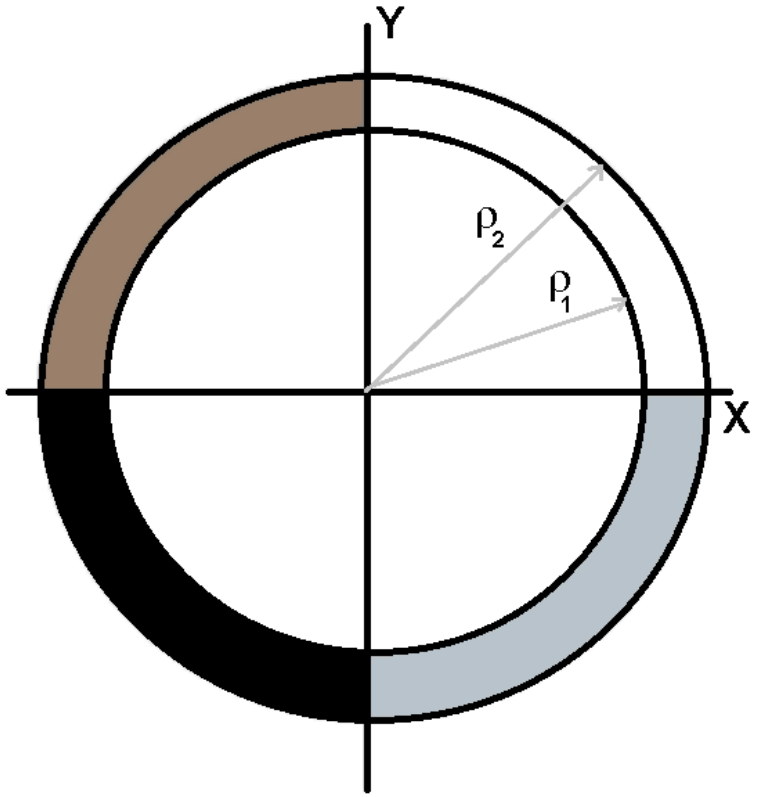
D *covariance matrix of regressors in the MDS,* $D=\langle(\mathbf{R}-\langle\mathbf{R}\rangle)(\mathbf{R}-\langle\mathbf{R}\rangle)^T\rangle$

Parameterization of SSES in terms of ρ takes the following advantages:
- **ρ^2 has a χ^2 – distribution; matchups are concentrated within a limited range of ρ values**
  - The analysis can be restricted with a compact area in R-space
- **SD of SST wrt in situ SST is a monotonic function of ρ**

Segmentation of the SST retrieval domain
2. Accounting for SSES anisotropy

•SSES dependencies may be anisotropic in R-space. For example, if <X> corresponds to some intermediate atmospheric absorption than SSES dependencies will be different in the directions of decreasing and increasing absorption

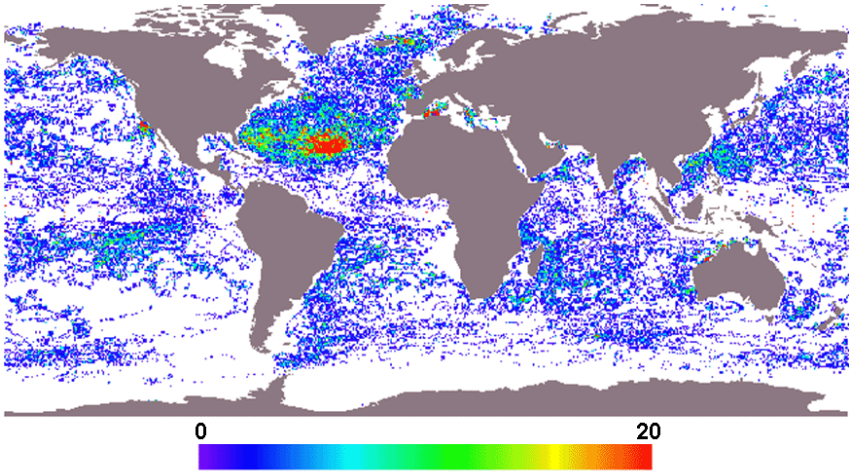
- **We introduce an orthogonal basis in the R-space with the origin at <X>**
- **Segmentation in terms of ρ is independent within each quadrant of this basis**
- **Local regression coefficients are calculated within each segment and store them in LUT**
- **During processing, SR SST and PWR SST are produced and estimate bias as SR SST – PWR SST**
- **Estimate SD from SR SST-in situ SST within each segment**

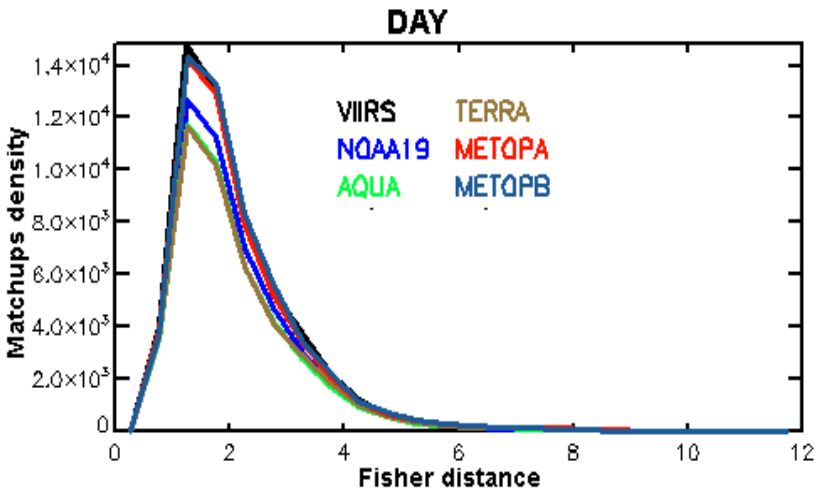


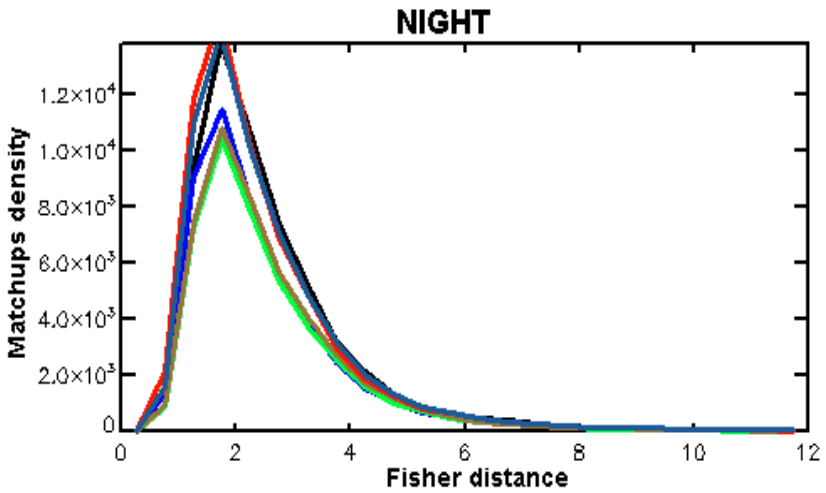
Validation with matchups

- Matchups covered the time period 15 May 2013 – 8 Aug 2014
- Data from S-NPP VIIRS, Aqua/Terra MODIS and Metop-A/Metop-B/NOAA-19 AVHRR were processed with ACSPO and matched with buoys

Matchups density (VIIRS)



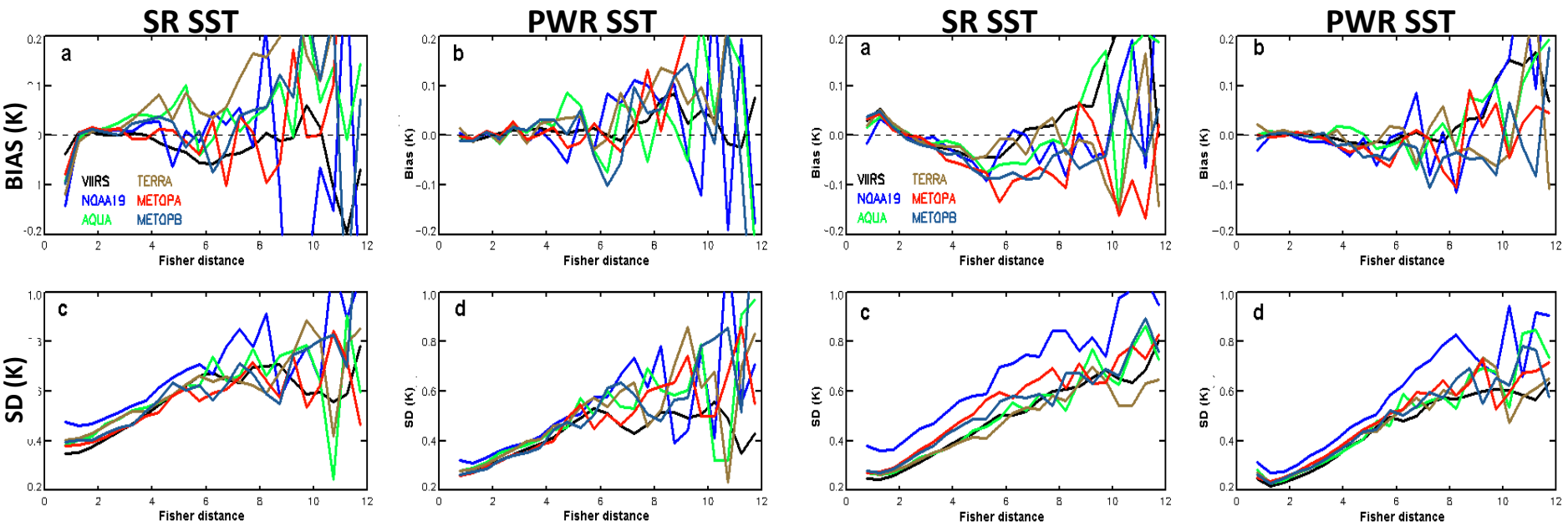




- The matchups are concentrated within a limited range of Fisher distances, ~0.5<ρ<~8

Bias and SD wrt *in situ* SST as functions of Fisher distance

Day | **Night**



- Statistics are stable for ~1 < ρ < ~6
- SDs monotonically increase with ρ
- Compared with SR SST, PWR SST flattens out biases and reduces SDs

Daytime global bias and SD wrt *in situ* SST

SST	Statistics	S-NPP VIIRS	Aqua MODIS	Terra MODIS	Metop-A AVHRR	Metop-B AVHRR	NOAA-19 AVHRR
SR SST	Bias	0.	0.	0.	0.	0.	0.
	SD	**0.41**	**0.45**	**0.46**	**0.43**	**0.44**	**0.50**
PWR SST	Bias	0.	0.	0.	0.	0.	0.
	SD	**0.31**	**0.33**	**0.32**	**0.31**	**0.30**	**0.34**
CMC*	Bias	-0.19	-0.20	-0.06	-0.01	-0.01	-0.21
	SD	**0.34**	**0.34**	**0.31**	**0.30**	**0.30**	**0.35**

***CMC is Canadian Met Centre L4 SST**

- **PWR SST reduces SD from 0.41 - 0.50 K to 0.30 – 0.34 K**
- **PWR SST brings SDs close to ones for L4 CMC but without daytime biases caused by diurnal warming**

Nighttime global bias and SD of fitting *in situ* SST

SST	Statistics	S-NPP VIIRS	Aqua MODIS	Terra MODIS	Metop-A AVHRR	Metop-B AVHRR	NOAA-19 AVHRR
SR SST	Bias	0.	0.	0.	0.	0.	0.
	SD	**0.33**	**0.35**	**0.38**	**0.38**	**0.38**	**0.46**
PWR SST	Bias	0.	0.	0.	0.	0.	0.
	SD	**0.25**	**0.26**	**0.26**	**0.27**	**0.27**	**0.29**
CMC*	Bias	0.01	0.02	-0.04	-0.07	-0.07	0.03
	SD	**0.27**	**0.28**	**0.29**	**0.29**	**0.29**	**0.29**

***CMC is Canadian Met Centre L4 SST (CMC)**

- **PWR SST reduces SD from 0.33 - 0.46 K to 0.25 – 0.29 K**
- **PWR SST makes SDs close to (or smaller than) ones for L4 CMC**

Stability of daytime PWR SST

- Training MDS: Summer 2013
- Validation MDS: Summer 2013 and Summer 2014

SST	Statistics	S-NPP VIIRS	Aqua MODIS	Terra MODIS	Metop-A AVHRR	Metop-B AVHRR	NOAA-19 AVHRR
Validation MDS: Summer 2013							
SR SST	Bias	0	0	0	0	0	0
	SD	0.43	0.47	0.47	0.45	0.46	0.53
PWR SST	Bias	0	0	0	0	0	0
	SD	0.32	0.34	0.33	0.33	0.32	0.36
Validation MDS: Summer 2014							
SR SST	Bias	-0.02	-0.03	-0.04	-0.02	-0.01	-0.02
	SD	0.43	0.47	0.47	0.45	0.46	0.54
PWR SST	Bias	-0.01	-0.02	-0.02	-0.02	-0.01	-0.01
	SD	0.33	0.36	0.35	0.34	0.33	0.38

- The difference in PWR SST SDs for Summer 2013 and Summer 2014 is much less than the difference in SDs for PWR SST and SR SST
- PWR SST is stable in time and fits *in situ* SST more precisely than SR SST

Stability of nighttime PWR SST

- Training MDS: Summer 2013
- Validation MDS: Summer 2013 and Summer 2014 MDS

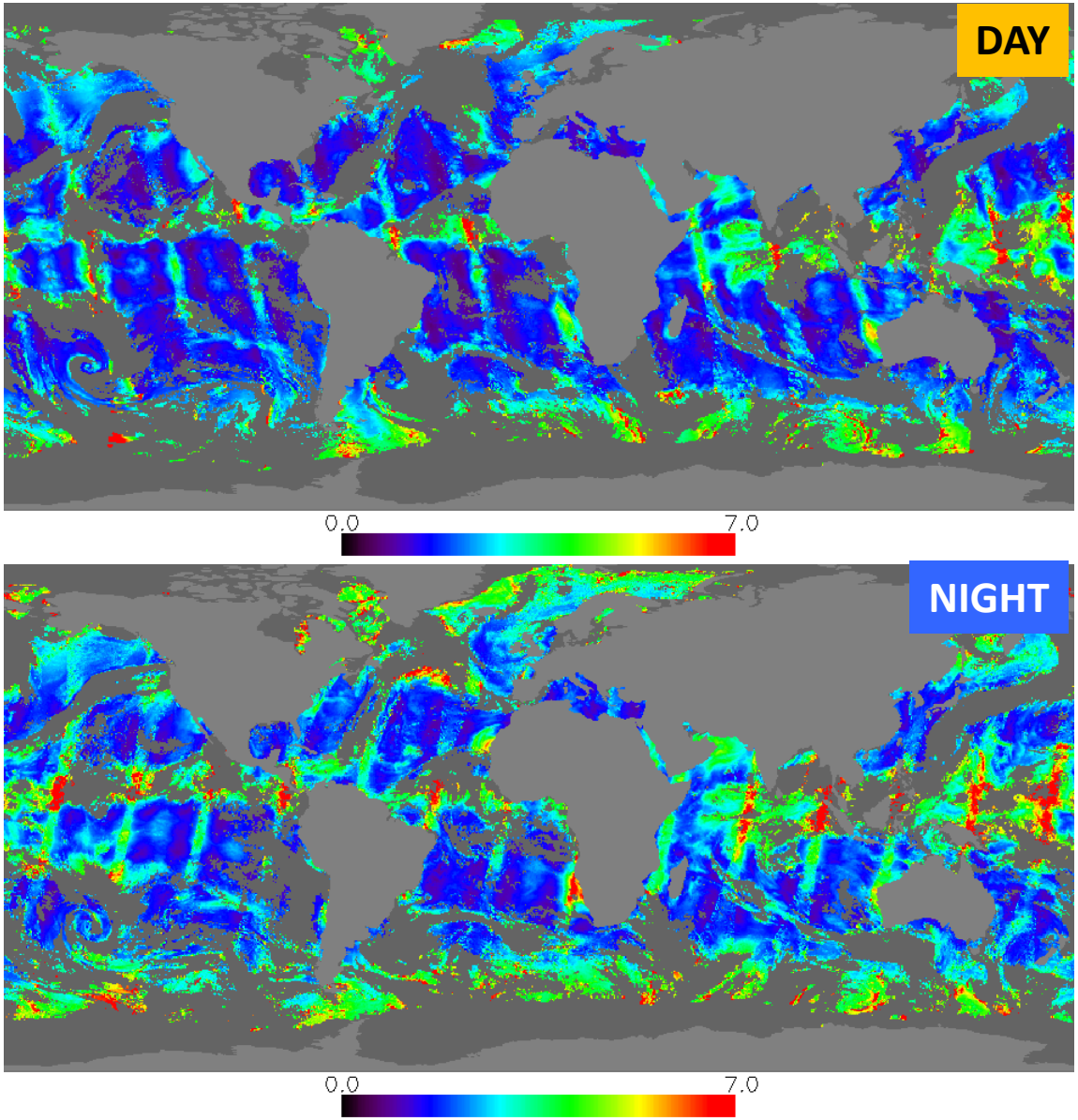
SST	Statistics	S-NPP VIIRS	Aqua MODIS	Terra MODIS	Metop-A AVHRR	Metop-B AVHRR	NOAA-19 AVHRR
Validation MDS: Summer 2013							
SR SST	Bias	0.	0.	0.	0.	0.	0.
	SD	0.34	0.35	0.35	0.39	0.38	0.48
PWR SST	Bias	0.	-0.	0.	0.0	0.	0.
	SD	0.26	0.27	0.27	0.29	0.28	0.29
Validation MDS: Summer 2014							
SR SST	Bias	0.	0.	0.	0.01	-0.01	-0.01
	SD	0.34	0.35	0.35	0.39	0.38	0.48
PWR SST	Bias	0.	-0.01	-0.01	-0.01	-0.01	-0.01
	SD	0.27	0.27	0.27	0.29	0.28	0.33

- The difference in PWR SST SDs for Summer 2013 and Summer 2014 is small and much less than the difference between SDs for PWR SSTs and SR SSTs
- PWR SST is stable in time and fits *in situ* SST more precisely than SR SST

Fisher distance (VIIRS, 4 November 2014)

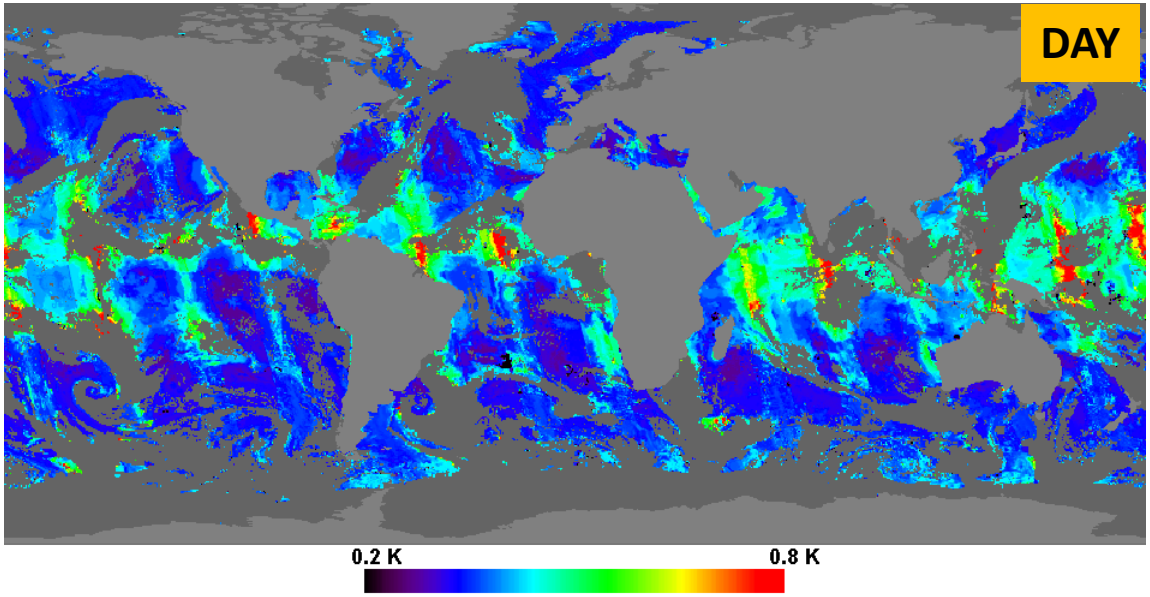
- The SSES algorithm was implemented within ACSPO
- Results of processing of one day of VIIRS data are presented

- Fisher distance characterizes how well a given set of regressors is represented in the training MDS
- Elevated ρ indicate underrepresented situations
- The underrepresented situations take place mostly in high latitudes, tropics and at swath edges

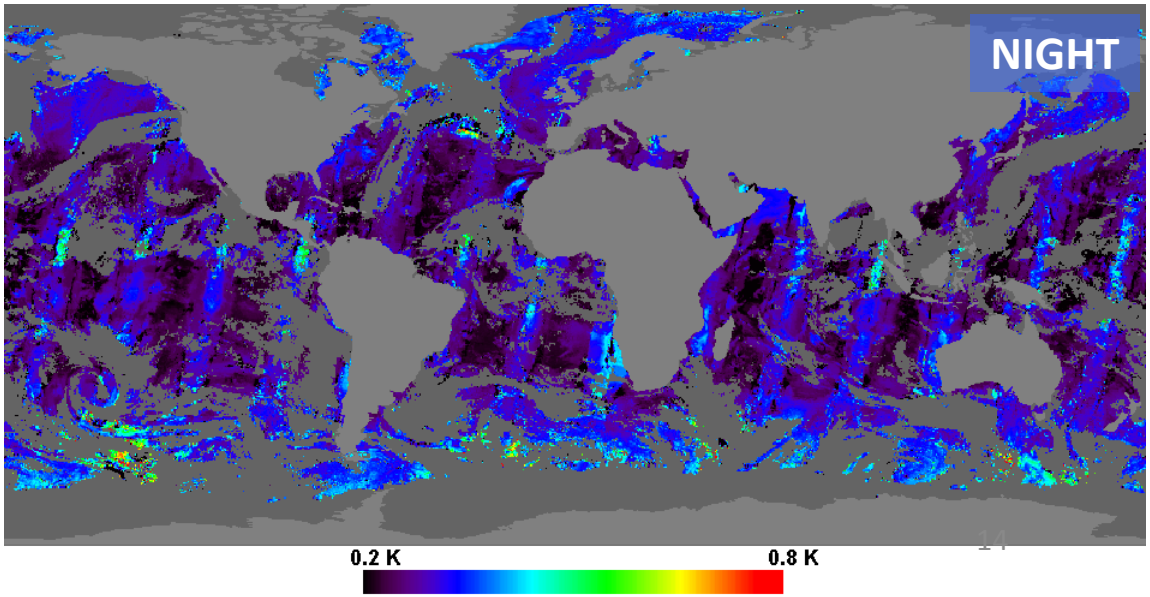


SSES SDs for SR SST (VIIRS, 11.04.2014)

- Daytime SSES SD is correlated with Fisher distance;
- SD is larger in the tropics, at high latitudes and at large view zenith angles

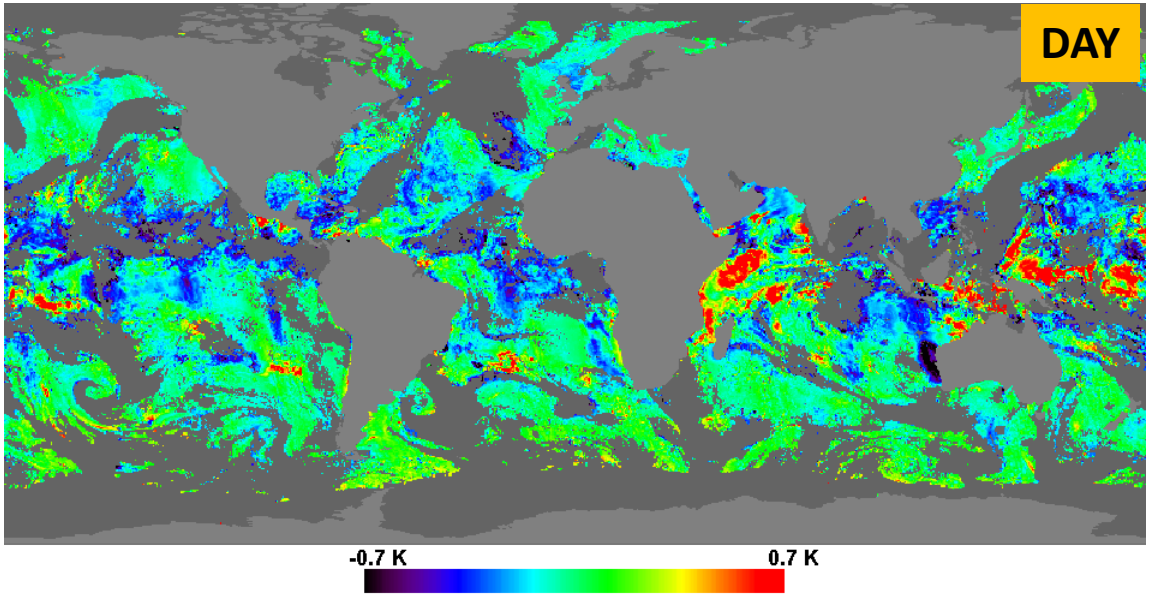


- At night, SSES SDs are lower but correlation with Fisher distance is still noticeable

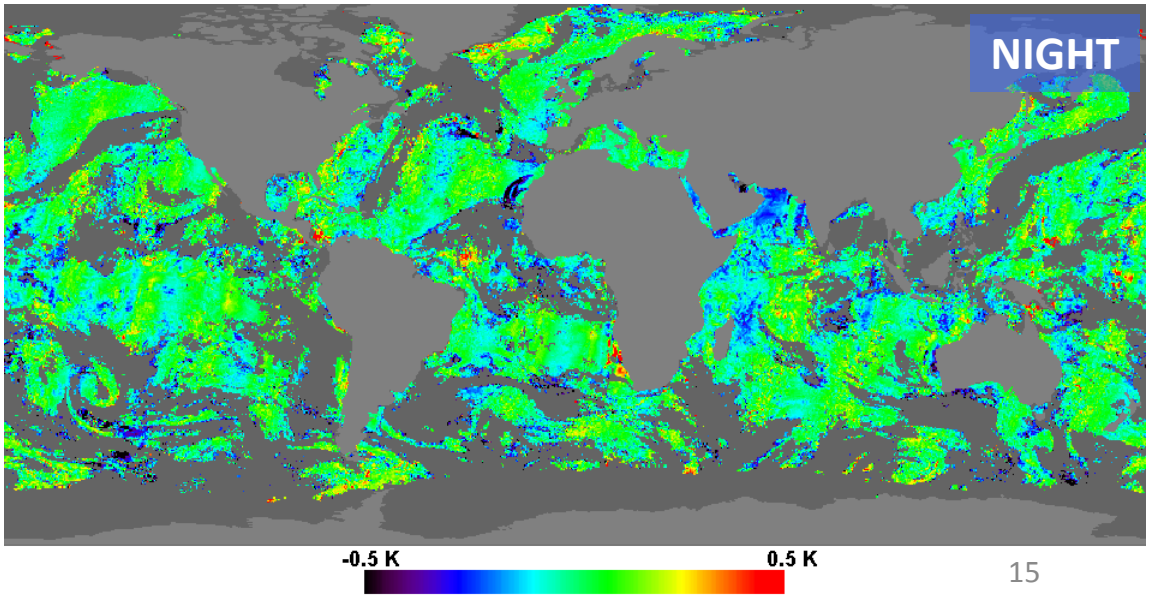


SSES bias = SR SST – PWR SST (VIIRS, 11.04.2014)

- Positive daytime biases respond to diurnal surface warming
- Negative daytime biases are associated with residual cloud, large water vapor contents, and large view zenith angles

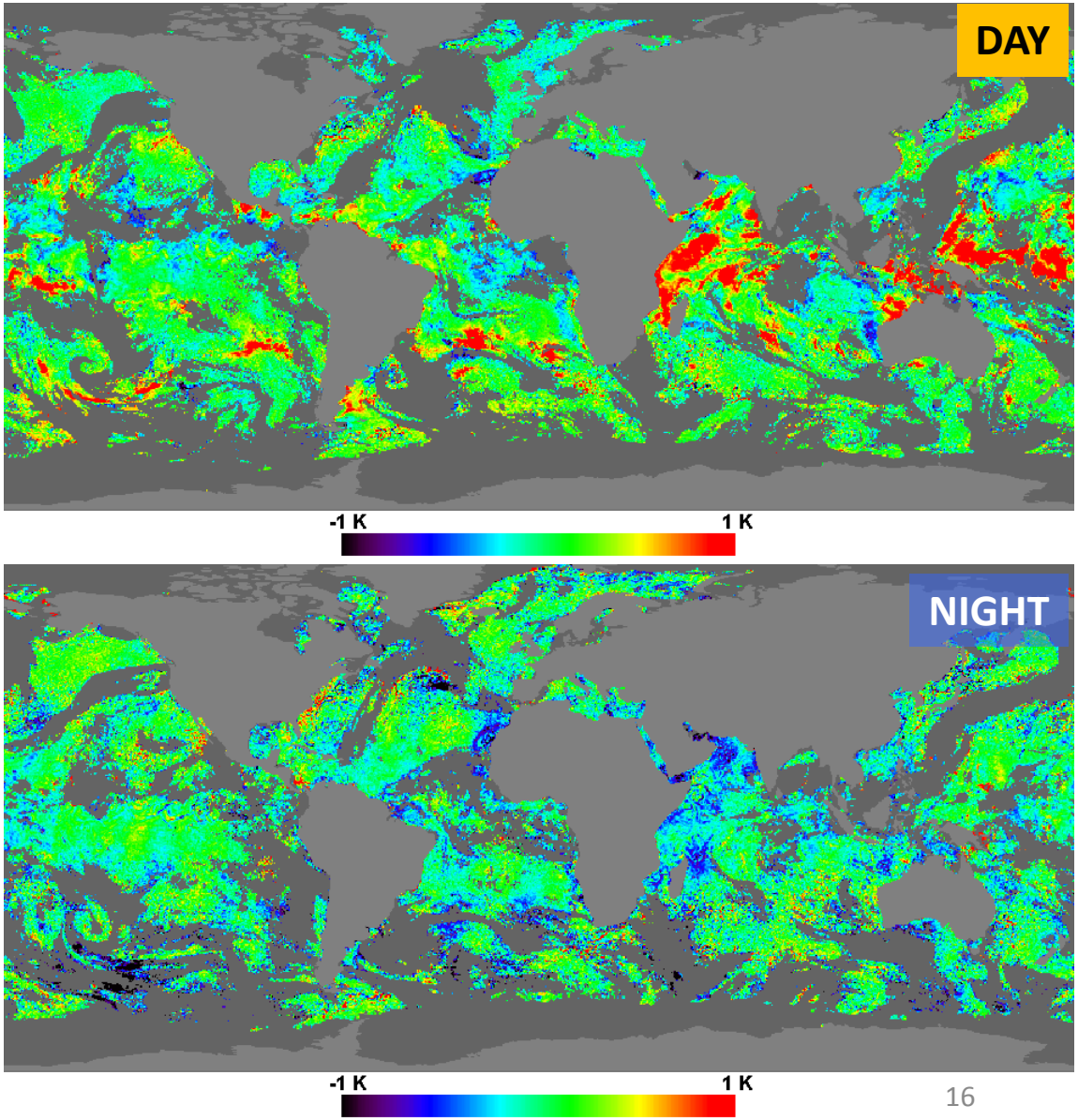


- At night, SSES biases depend on VZAs and respond to cloud leakages



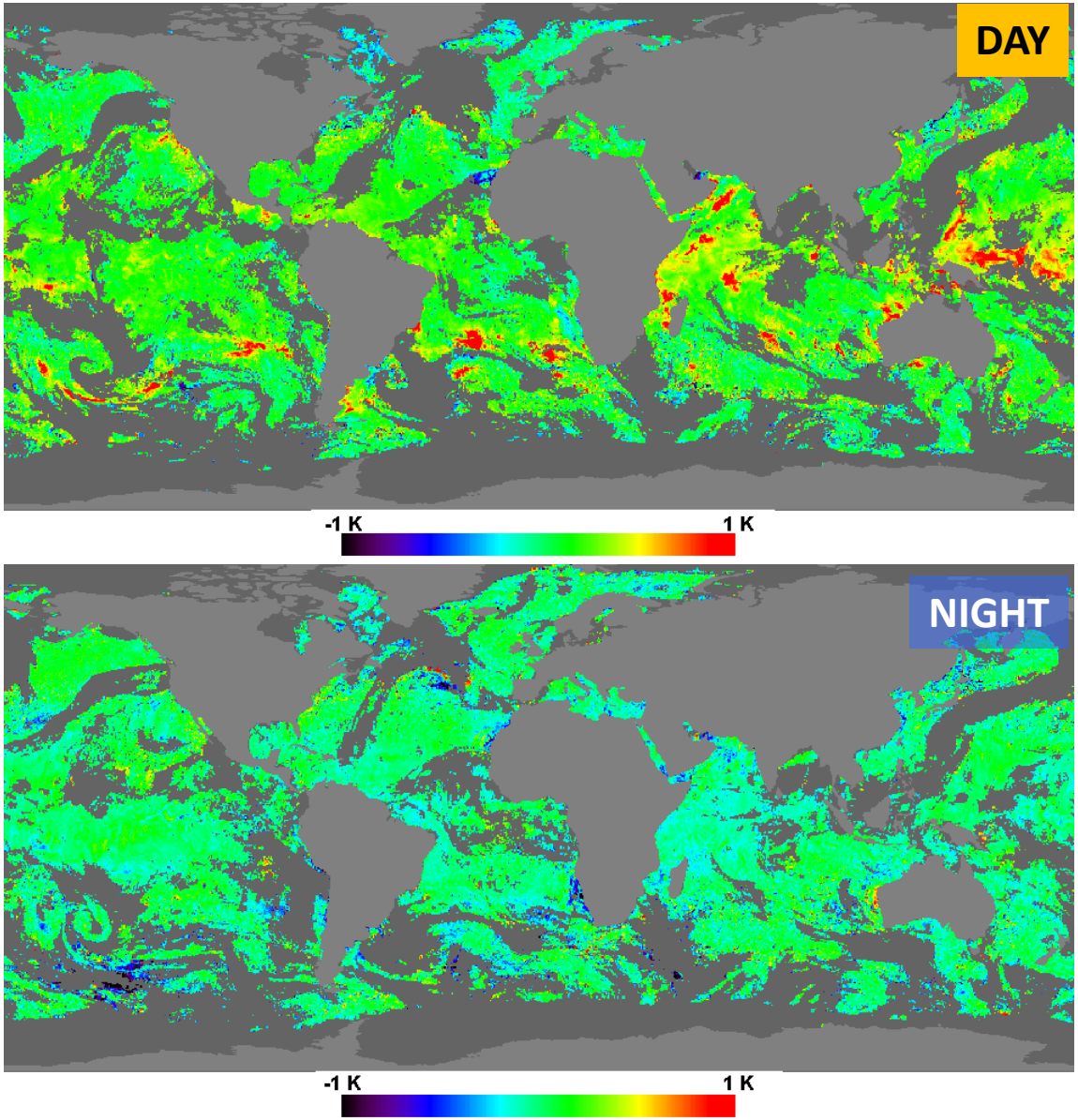
SR SST – CMC (VIIRS, 11.04.2014)

SR SST - CMC is consistent with SSES biases



PWR SST – CMC (VIIRS, 11.04.2014)

PWR SST – CMC is much smoother than SR SST - CMC



Global bias and SD of SR SST – CMC and PWR SST – CMC (VIIRS, 4 Nov 2014)

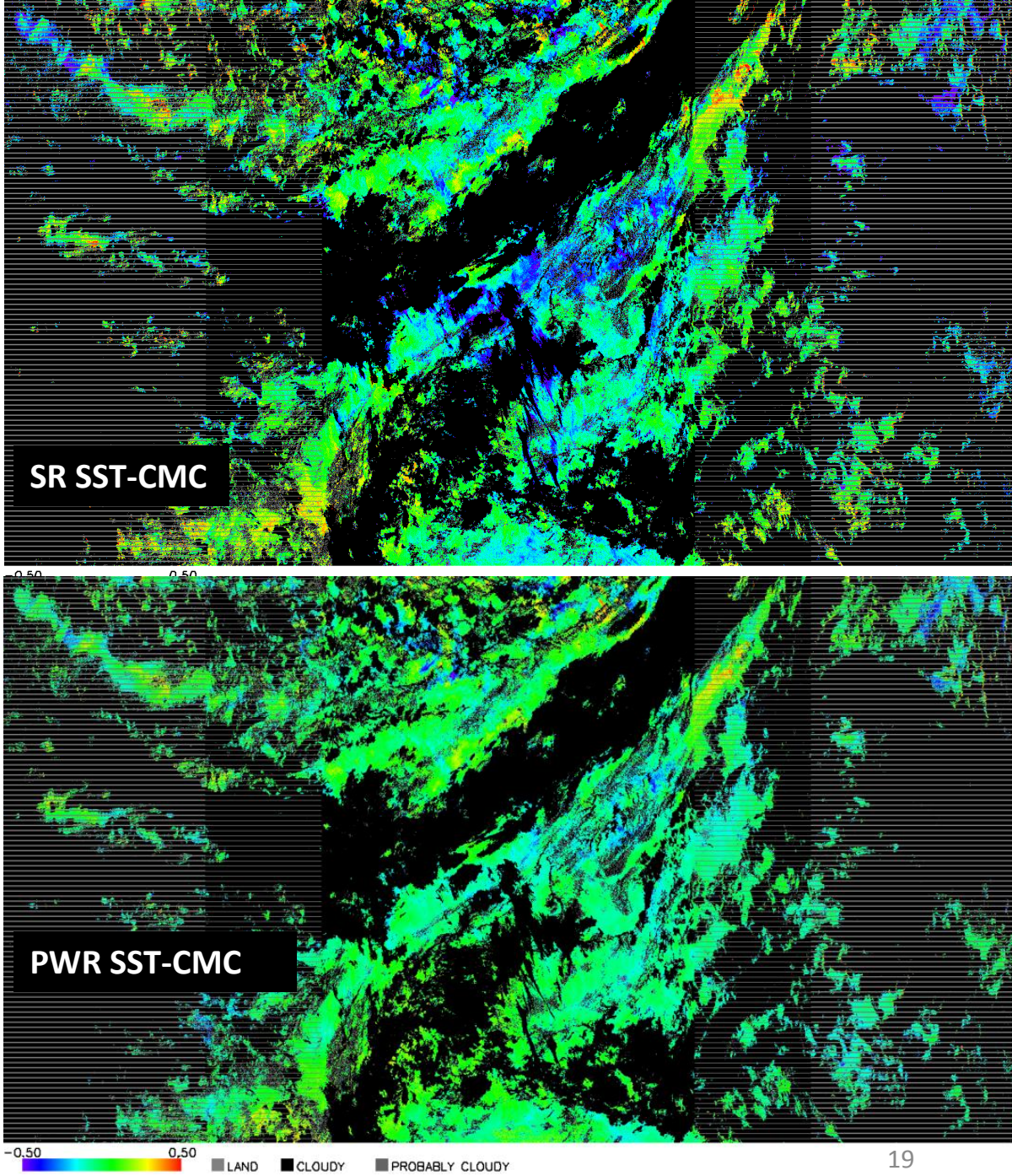
SST	Statistics	S-NPP VIIRS	Aqua MODIS	Terra MODIS	Metop-A AVHRR	Metop-B AVHRR	NOAA-19 AVHRR
Day							
SR SST	Bias	0.25	0.35	0.16	0.06	0.03	0.24
	SD	0.53	0.61	0.52	0.42	0.43	0.60
PWR SST	Bias	0.24	0.28	0.11	0.04	0.02	0.25
	SD	0.36	0.37	0.29	0.24	0.23	0.35
Night							
SR SST	Bias	0.	-0.01	0.06	0.05	0.04	-0.08
	SD	0.32	0.37	0.32	0.33	0.34	0.41
PWR SST	Bias	-0.01	-0.04	0.04	0.06	0.05	-0.04
	SD	0.25	0.25	0.24	0.23	0.23	0.22

- Daytime global SD reduces from 0.42 – 0.61 K to 0.23-0.37 K
- Nighttime SD reduces from 0.32-0.41 K to 0.23-0.25 K

Nighttime bias correction (Pacific ocean, VIIRS, 10.30.2014)

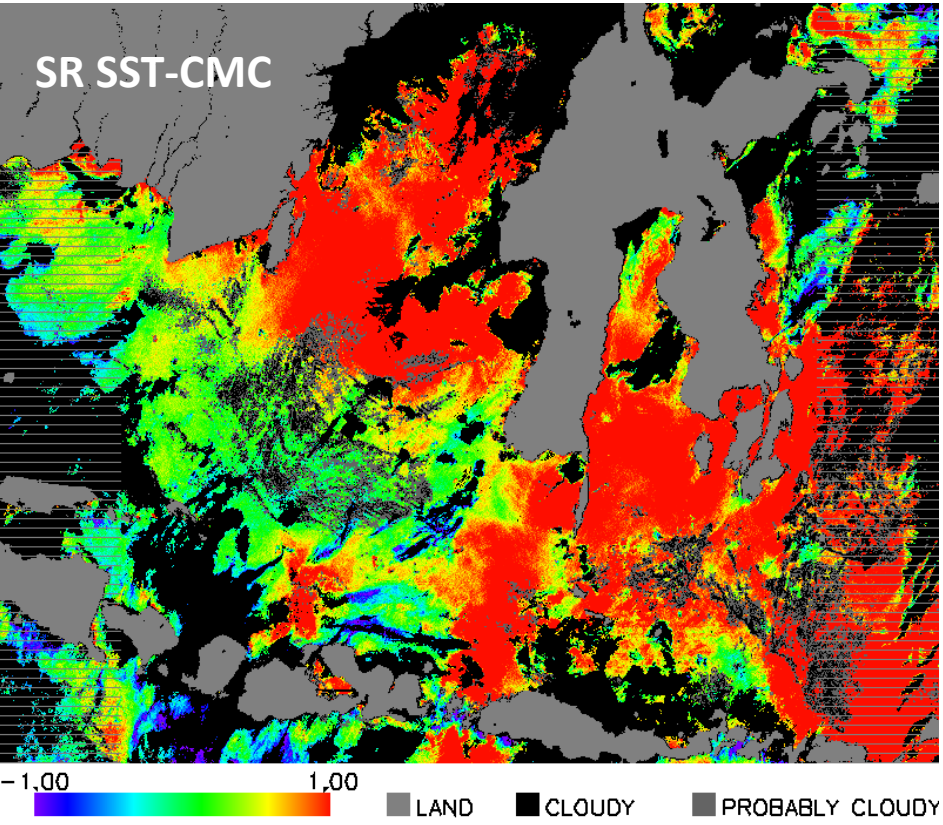
SSES bias correction minimizes

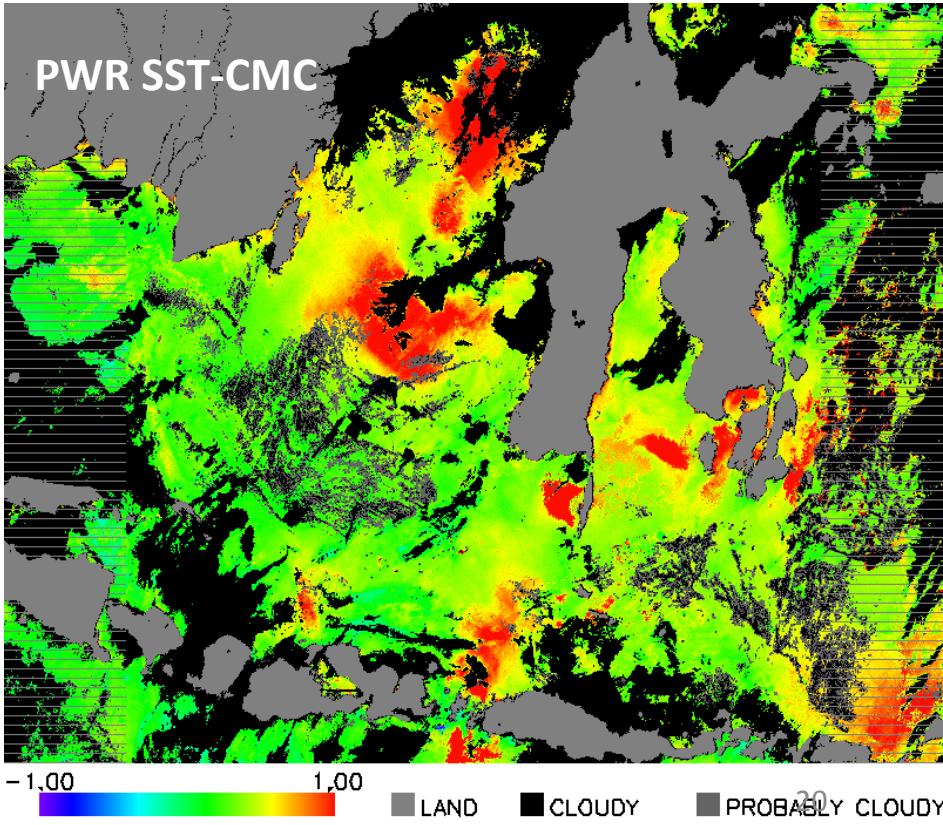
- **Dependencies on VZA (cold biases at small and large VZAs, and warm biases at intermediate VZA from 40^o to 50^o)**
- **Cloud leakages**



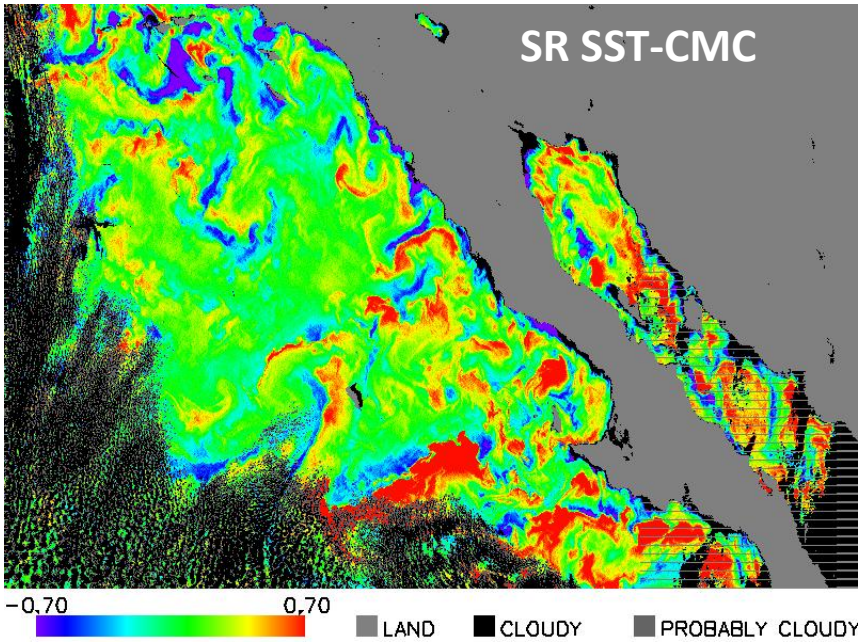
Daytime bias correction (VIIRS, Java sea, 11.04.2014)

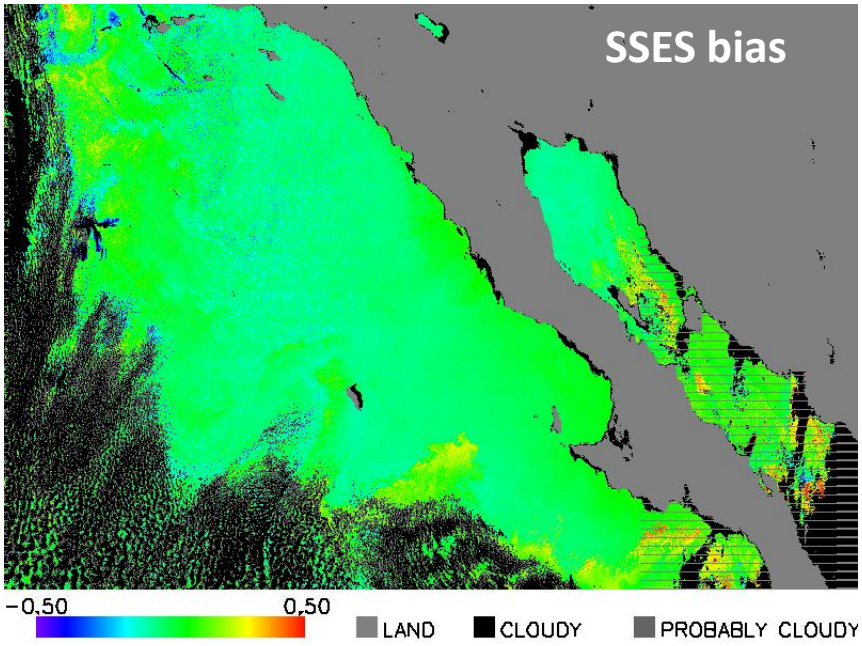
SSES bias correction suppresses diurnal surface warming and cloud leakages

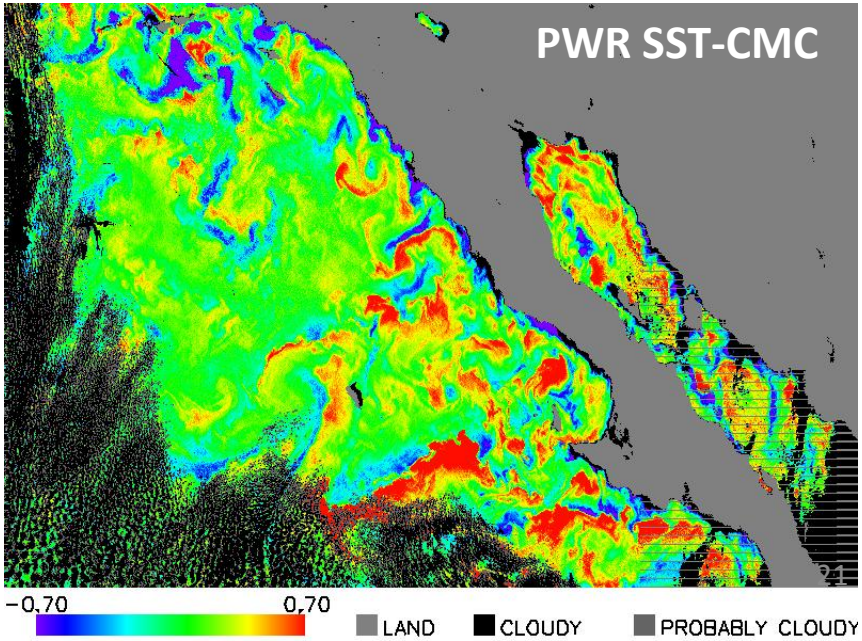




Nighttime bias correction (Pacific ocean, VIIRS, 11.04.2014)







In this case, SSES bias correction preserves true SST variations

Summary

- **The renovated ACSPO SSES algorithm:**
  - **Produces an auxiliary Piecewise Regression SST (PWR SST)**
  - **Estimates biases in SR SST as difference between SR SST and PWR SST**
- **The SSES by-product, PWR SST:**
  - **Fits *in situ* SST much more precisely than regular SR SST does**
  - **Brings precision to the level of L4 SST, but without creating daytime biases**
  - **May be considered an improved satellite estimate of "bulk" SST**

Future work

- **The new SSES will go operational with the upcoming v. 2.40 of ACSPO**
- **Pending testing on longer time series, PWR SST may be designated as a new ACSPO "bulk SST" product, in addition to the current ACSPO "sub-skin" SST**
- **Producers of "foundation L4 SST" are expected to benefit from the ACSPO "bulk SST" because it is already very close to their products**