Sea Surface Temperature algorithm refinement and validation though ship-based infrared spectroradiometry

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What is SST?

- The infrared emission from the ocean originates from the uppermost <1mm of the ocean – the skin layer.
- The atmosphere is in contact with the top of the skin layer.
- Ocean-to-atmosphere heat flow through the skin layer is by molecular conduction: this causes, and results from, a temperature gradient through the skin layer.
- Conventional measurements of SST are from submerged thermometers – a “bulk” temperature.
- $T_{\text{depth}}$ below the influence of diurnal heating is the “foundation” temperature.

Marine-Atmospheric Emission Radiance Interferometer

The M-AERI is a Michelson-Morley Fourier-transform infrared (FTIR) interferometric spectroradiometer. These were first developed in the 1880’s to make accurate measurements of the speed of light. Here we use it to make very accurate measurements of the sea-surface temperature, air temperature and profiles of atmospheric temperature and humidity. We also measure surface emissivity and the temperature profile through the skin layer, which is related to the flow of heat from the ocean to the atmosphere.
Michelson interferometer

Schematic representation of a Michelson interferometer. The median ray is shown by the solid line, and the extremes of the collimated beam are shown by the broken lines.
The innards.....

Oscillating yoke

Beam splitter

Corner cube reflectors

HeNe laser
Marine - Atmospheric Emitted Radiance Interferometer. M-AERI

- Oscillating yoke provides a robust infrared radiometer for shipboard deployments.
- Visible laser used for wavelength calibration.
- Two blackbodies used for radiometric calibration.
M-AERI cruises for MODIS, AATSR & AVHRR validation

ISAR cruises for MODIS, AATSR & AVHRR validation
Measuring skin SST from ships

\[
R_{\text{water}}(\lambda, \theta) = \varepsilon(\lambda, \theta)B(\lambda, T_{\text{skin}}) \\
+ (1 - \varepsilon(\lambda, \theta))R_{\text{sky}}(\lambda, \theta) \\
+ R_h(\lambda, \theta)
\]

\[
T_{\text{skin}} = B^{-1}\left\{R_{\text{water}}(\lambda, \theta) - [1 - \varepsilon(\lambda, \theta)]R_{\text{sky}}(\lambda, \theta) \\
- R_h(\lambda, \theta)\right\}/\varepsilon(\lambda, \theta)
\]

- Scan-mirror mechanism for directing the field of view at complementary angles.
- Excellent calibration for ambient temperature radiances.
- Moderately good calibration at low radiances.
Sea surface emissivity ($\varepsilon$)

- Conventional wisdom gave decreasing $\varepsilon$ with increasing wind.
- Not confirmed by at-sea hyperspectral measurements
- Improved modeling confirms at-sea measurements.


Internal Calibration
NIST water-bath black-body calibration target

Traceability to NIST TXR
M-AERI, ISAR…. measurements

Satellite-derived SSTs

Laboratory calibration

Matchup analysis of collocated measurements

CDR of SST

NIST Traceable error statistics

NIST-designed water-bath blackbody calibrator

NIST-traceable thermometers

NIST TXR for radiometric characterization
Next-generation ship-based FTIR spectroradiometer

M-AERI Mk-2 undergoing tests at RSMAS.
Mk1 & Mk2
Sky emission measurements

Measurements taken in Quebec City, February 24, 2011.
Comparison with LBLRTM simulations
Comparison with Arctic M-AERI measurements

M-AERI spectrum from I/B Oden

M-AERI Mk 2 spectrum from Quebec

M-AERI & M-AERI Mk 2 spectra

M-AERI Mk 2 & LBLRTM simulated spectra
M-AERI Cruise opportunities

• Continue with *Explorer of the Seas*
• Two additional RCCL cruise liners
• NOAA Ship *Ronald H Brown* – Pirata moorings; July – August 2011
• R/V *Kilo Moana* – Samoa to Hawaii; November 2011
• Cunard *Queen Victoria*, Long Beach to Hawaii; February 2012 (tbc)
• VIIRS validation ????
Ron Brown cruise 2011
Equation Discovery using Genetic Algorithms

- Darwinian principles are applied to algorithms that “mutate” between successive generations.
- The algorithms are applied to large data bases of related physical variables to find robust relationships between them. Only the “fittest” algorithms survive to influence the next generation of algorithms.
- Here we apply the technique to the MODIS matchup-data bases.
- The survival criterion is the size of the RMSE of the SST retrievals when compared to buoy data.
Successive generations of algorithms

The formulae are represented by tree structures; the “recombination” operator exchanges random subtrees in the parents. Here the parent formulae \((y^x + z)/\log(z)\) and \((x + \sin(y))/zy\) give rise to children formulae \((\sin(y) + z)/\log(z)\) and \((x + y^x)/zy\). The affected subtrees are indicated by dashed lines.

Subsets of the data set can be defined in any of the available parameter spaces.

(From Wickramaratna, K., M. Kubat, and P. Minnett, 2008: Discovering numeric laws, a case study: CO\textsubscript{2} fugacity in the ocean. *Intelligent Data Analysis*, 12, 379-391.)
Fittest Algorithm

The “fittest” algorithm takes the form:

\[
SST = c_0 + c_1 T_{11} + c_2 (T_{11} - T_{12}) T_4 + \frac{c_3 (T_{11} - T_{12})}{\cos(1.13 \times \theta_s)} + c_4 \times \cos(1.0078 \times \theta_a - 0.7099)
\]

where:
- \(T_i\) is the brightness temperature at \(\lambda = i \, \text{\textmu m}\)
- \(\theta_s\) is the satellite zenith angle
- \(\theta_a\) is the angle on the mirror (a feature of the MODIS paddle-wheel mirror design)

Which looks similar to the NLSST:

Non-Linear SST (NLSST)

\[
NLSST = b_0 + b_1 T_{11} + b_2 T_{sfc} + (T_{11} - T_{12}) + b_3 (T_{11} - T_{12}) \times (\sec(\theta) - 1.0)
\]
Variants of the new algorithms

* Terra SST4:

\[ SST = c_0 + c_1 T_{4.0} + c_2 (T_{3.9} - T_{4.0}) T_{3.9} + \frac{c_3 (T_{3.9} - T_{4.0})}{\cos(1.13 \times \theta_a)} + c_4 \times \cos(1.0078 \times \theta_a - 0.7099) \]

* Terra SSTnight, SSTday, SST:

\[ SST = c_0 + c_1 T_{11} + c_2 (T_{11} - T_{12}) + \frac{c_3 (T_{11} - T_{12})}{\cos(1.13 \times \theta_a)} + c_4 \times \cos(1.0078 \times \theta_a - 0.7099) \]

* Terra newSSTnight:

\[ SST = c_0 + c_1 T_{3.9} + c_2 (T_{3.9} - T_{4.0}) T_{3.9} + \frac{c_3 (T_{3.9} - T_{4.0})}{\cos(1.13 \times \theta_a)} + c_4 \times \cos(1.0078 \times \theta_a - 0.7099) \]

* Aqua SST4:

\[ SST = c_0 + c_1 T_{3.9} + c_2 (T_{3.9} - T_{4.0}) T_{3.9} + \frac{c_3 (T_{3.9} - T_{4.0})}{\cos(1.13 \times \theta_a)} + c_4 \times \cos(1.0078 \times \theta_a - 0.7099) \]

* Aqua SSTnight, SSTday, SST:

\[ SST = c_0 + c_1 T_{11} + c_2 (T_{11} - T_{12}) + \frac{c_3 (T_{11} - T_{12})}{\cos(1.13 \times \theta_a)} + c_4 \times \cos(1.0078 \times \theta_a - 0.7099) \]

* Aqua newSSTnight:

\[ SST = c_0 + c_1 T_{3.8} + c_2 (T_{11} - T_{12}) T_{3.9} + \frac{c_3 (T_{11} - T_{12})}{\cos(1.13 \times \theta_a)} + c_4 \times \cos(1.0078 \times \theta_a - 0.7099) \]

Coefficients are different for each equation

Note: No $T_{sfc}$
Preliminary Results

- The new algorithms with regions give smaller errors than NLSST or SST\(_4\)
- \(T_{sfc}\) term no longer required
- Night-time 4\(\mu\)m SSTs give smallest errors
- Aqua SSTs are more accurate than Terra SSTs
- Regression-tree induced in one year can be applied to other years without major increase in uncertainties
- SVM results do not out-perform GA+Regression Tree algorithms
Next steps

• Can some regions be merged without unacceptable increase in uncertainties?
• 180°W should not necessarily always be a boundary of all adjacent regions.
• Iterate back to GA for regions – different formulations may be more appropriate in different regions.
• Allow scan-angle term to vary with different channel sets.
• Introduce “regions” that are not simply geographical.
• Suggestions?
Modeling Diurnal Warming and Cooling

- Prior models generally failed to raise temperatures sufficiently quickly, were not sufficiently responsive to changes in the wind speed, and retained too much heat into the evening and the night.
- New diurnal model that links the advantages of bulk models (speed) with the vertical resolution provided by turbulent closure models.
- Profiles of Surface Heating (POSH) model:

Diurnal Heating in Shallow Water
(Xiaofang Zhu)

• How does the presence of the sea floor influence diurnal heating and cooling?

• Can a 1-D model be used in a hydro-dynamically complex situation to simulate the diurnal signals?

• Are satellite skin SSTs a good representation of the $T_{\text{depth}}$ at the surface of coral reefs, for example?
Surface measurements include light (three band UV and PAR measurements), wind, air temperature, pressure, humidity and precipitation.

Underwater measurements include light and temperature (CTD) measurements at nominal 1m and 3m depth

Station water depths: about 6 meters

Data resolution

Nearby tidal station

http://ecoforecast.coral.noaa.gov/
Diurnal temperature signals
Little Cayman Coral Reef Temperatures

Internally recording thermometers added to the ICON pylon to resolve vertical temperature structure.

Significant differences are measured:
The Australian Great Barrier Reef.

This map shows the reef surveys that were conducted in response to the bleaching events. The red colors indicate where the bleaching was observed to be severe while the green shows low levels of bleaching. From http://www.reelfutures.org/topics/toolbox/webmaps.cfm#

Automatic weather stations will provide measurements of surface forcing for the model. E.g. at Davies Reef ~100km NE of Townsville, North Queensland. (http://www3.aims.gov.au/pages/facilities/weather-stations/weather-stations-images.html)
Temperature loggers on the GBR

- Data are obtained from in-situ data loggers deployed on the reef.
- Temperatures every 30 minutes and are exchanged and downloaded approximately every 12 months by divers.
- Temperature loggers on the reef-flat are generally placed just below Lowest Astronomical Tide level.
- Reef-slope (or where specified as Upper reef-slope) generally refers to depths 5 - 9 m while
- Deep reef-slope refers to depths of ~20 m.
Diurnal heating signal on the GBR

Example of the large diurnal heating during the 2006 bleaching event in the Keppel Islands (Great Barrier Reef). In situ temperatures were measured at 6m depth during the peak of the bleaching that killed 35% of coral in this area.
Future

• Continue MODIS (VIIRS?) validation cruises, including M-AERI Mk2
• Continue research into CDR generation
• Continue improving atmospheric correction algorithms
• Continue research into upper ocean thermal structure (skin effect, diurnal heating....)
Thank you for your attention.

Questions?

_Aqua MODIS SST_
MODIS SST atmospheric correction algorithms

The form of the daytime and night-time algorithm for measurements in the long wave atmospheric window is:

\[
SST = c_1 + c_2 \cdot T_{11} + c_3 \cdot (T_{11}-T_{12}) \cdot T_{sfc} + c_4 \cdot (\sec(\theta)-1) \cdot (T_{11}-T_{12})
\]

where \( T_n \) are brightness temperatures measured in the channels at \( n \) \( \mu \)m wavelength, \( T_{sfc} \) is a ‘climatological’ estimate of the SST in the area, and \( \theta \) is the satellite zenith angle. This is based on the Non-Linear SST algorithm.


The MODIS night-time algorithm, using two bands in the 4\( \mu \)m atmospheric window is:

\[
SST4 = c_1 + c_2 \cdot T_{3.9} + c_3 \cdot (T_{3.9}-T_{4.0}) + c_4 \cdot (\sec(\theta)-1)
\]

Note, the coefficients in each expression are different. They can be derived in three ways:

– empirically by regression against SST values derived from another validated satellite instrument
– empirically by regression against SST values derived surface measurements from ships and buoys
– theoretically by numerical simulations of the infrared radiative transfer through the atmosphere.
Genetic Mutation of Equations

• The initial population of formulae is created by a generator of random algebraic expressions from a predefined set of variables and operators. For example, the following operators can be used: {+, -, /, ×, √, exp, cos, sin, log}. To the random formulae thus obtained, we can include “seeds” based on published formulae, such as those already in use.

• In the recombination step, the system randomly selects two parent formulae, chooses a random subtree in each of them, and swaps these subtrees.

• The mutation of variables introduces the opportunity to introduce different variables into the formula. In the tree that defines a formula, the variable in a randomly selected leaf is replaced with another variable.
GA-based equation discovery

*initial state:* randomly generated formulas plus manually created “seed” formulas

1. Randomly selected mating partners exchange genetic information by the recombination operator.
2. 20% randomly selected individuals are subjected to mutation of variables; 20% randomly selected individuals are subjected to mutation of operators; and all individuals are subjected to mutation of coefficients.
3. All individuals are subjected to mutation of inter-region borders.
4. The fitness of each individual (children as well as parents) is calculated as the formula’s error on the training data. The top 50% are retained, and the remaining formulas are discarded.
5. Unless a termination criterion is satisfied, return to step 1.
Mirror effects: two-sided paddle wheel has a multi-layer coating that renders the reflectivity in the infrared a function of wavelength, angle of incidence and mirror side.
Regression tree

• Regions identified by the regression tree algorithm
• The tree is constructed using
  – input variables: latitude and longitude
  – output variable: *Error in retrieved SST*
• Algorithm recursively splits regions to minimize variance within them
• The obtained tree is pruned to the smallest tree within one standard error of the minimum-cost subtree, provided a declared minimum number of points is exceeded in each region
• Linear regression is applied separately to each resulting region (different coefficients result)
Mean SST retrieval error. Aqua MODIS 4um SST. Night - 1st Quarter. 2007
Regression tree performance

• Terra 2004 SSTday
  NLSST (no regions) – RMSE: 0.581
  New formula (no regions) – RMSE: 0.615
  New formula (with regions) – RMSE: 0.568

• Terra 2004 SST4 (night)
  SST4 (no regions) – RMSE: 0.528
  New formula (no regions) – RMSE: 0.480
  New formula (with regions) – RMSE: 0.456
Support Vector Machines (SVM)

- Best accuracy observed when data set is large (lower accuracy when splitting into regions)
  - Terra 2004 SSTday –
    - RMSE (no region): 0.513, RMSE (with regions): 0.557

- Problems:
  - Computational costs
  - Black-box approach