A methodology for calibration of hyperspectral and multispectral satellite data in coastal areas

Authors: Giuliana Pennucci[(1)], Giulietta Fargion[(2)], Alberto Alvarez[(1)], Charles Trees[(1)] and Robert Arnone [(3)]

(1) NATO Research Centre, Viale San Bartolomeo 400, La Spezia, Italy.
(2) San Diego State University, San Diego, CA, USA.
(3) NRL, Stennis Space Center, MS, USA.

ABSTRACT

The objective of this work is to determine the location(s) in any given oceanic area during different temporal periods where *in situ* sampling for Calibration/Validation (Cal/Val) provides the best capability to retrieve accurate radiometric and derived product data (lowest uncertainties). We present a method to merge satellite imagery with *in situ* measurements, to determine the best *in situ* sampling strategy suitable for satellite Cal/Val and to evaluate the present *in situ* locations through uncertainty indices.

This analysis is required to determine if the present *in situ* sites are adequate for assessing uncertainty and where additional sites and ship programs should be located to improve Calibration/Validation (Cal/Val) procedures.

Our methodology uses satellite acquisitions to build a covariance matrix encoding the spatial-temporal variability of the area of interest. The covariance matrix is used in a Bayesian framework to merge satellite and *in situ* data providing a product with lower uncertainty. The best *in situ* location for Cal/Val is then identified by using a design principle (A-optimum design) that looks for minimizing the estimated variance of the merged products.

Satellite products investigated in this study include Ocean Color water leaving radiance, chlorophyll, and inherent and apparent optical properties (retrieved from MODIS and VIIRS). *In situ* measurements are obtained from systems operated on fixed deployment platforms (e.g., sites of the Ocean Color component of the AErosol RObotic NETwork-AERONET-OC), moorings (e.g, Marine Optical Buoy-MOBY), ships or autonomous vehicles (such as Autonomous Underwater Vehicles and/or Gliders).

Keywords: *remote sensing, calibration, validation, radiances, statistical analysis, merging, optimum design*

1. INTRODUCTION

State-of-art satellite ocean color missions require the indirect calibration of the space sensor (vicarious calibration) and the following validation of derived data products (processes commonly denoted as Cal/Val)[1]. These post launch activities, should complement extended the pre-launch sensor characterization and on-orbit stability monitoring constituting the background for any successive action[2]. The ocean color community has recognized that ground-based measurements are an essential element for Cal/Val activities. During the last two decades, Cal/Val activities benefitted of advances in the parameterization of radiative transfer processes (e.g., in-water radiance distribution), development of in situ measurement protocols and processing schemes, design of new field instruments (e.g., hyperspectral), and the quantification measurement uncertainties[3].This study provides a further through the identification of location(s) in various geographic regions where in situ measurements support of Cal/Val activities provides the lowest uncertainties as a function of annual periods.

Merging of remote sensing data with *in situ* measurements is a viable way to increase the quality of satellite-derived products. Conventionally, covariance analysis is applied to oceanographic and meteorological data sets to decompose space- and time-distributed data into modes ranked by their temporal variance, while optimum sampling analysis is applied to find an adequate amount and allocation of *in situ* data to improve satellite quality by reducing their uncertainties. To address our goal (i.e., minimize uncertainty to do Cal/Val activities), we needed to draw on methodologies from different fields and we introduce:

- techniques to evaluate the covariance from time-series of satellite imagery;
- methodology to merge satellite and *in situ* measurements; and

- methodology to generate uncertainty maps and uncertainty indices from the available time series images and historical information.

We then implement these methodologies on several optical data sets. In particular, we focus on satellite MODIS time-series water leaving radiances and several optical *in situ* platforms, such as Marine Optical Buoy (MOBY) and the Ocean Color component AErosol RObotic NETwork (AERONET-OC).

2. DISTRIBUTED SENSOR SYSTEM DESCRIPTION

2.1 Satellite sensors

The daily satellite images used in this study were collected from the Moderate Advanced Very High Resolution Radiometer (MODIS) on the NASA AQUA platform, and from the Visible Infrared Spectrometer (VIIRS) on the NASA NPOESS Preparatory Project (NPP) satellite launched on October 28th, 2011. Satellite images were processed at the US Naval Research Laboratory (Stennis Space Center) with APS-4 software (extension to the NASA L2gen) and archived at NATO NURC. All satellites images were corrected for distortion and registered to a map using the Lambert Projection[6]. The ground resolution is 1 km for MODIS sensor and 0.75 km for VIIRS sensor. The available images have been processed to select a set of clear areas (cloud coverage <10%) in a box of about 30 by 30 km^2 around the areas of interest (i.e., *in situ* measurement sites). This procedure has led to the construction of time-series that could subsequently be used to perform historical analyses.

2.2 *In situ* data

The term Cal/Val refers to vicarious calibration of the space sensor and the validation of satellite derived products through the use of in situ measurements[3]. Presently, the ocean color community collects in situ measurements of various quality, and therefore these data are ranked for different use from highest quality to lowest, in (a) vicarious calibration, (b) validation, (c) algorithm development, (d) general research and (e) monitoring. *In situ* data collected for vicarious calibration should exhibit the minimum measurement uncertainties and additionally refer to sites characterized by low natural variability (oceanic and atmospheric) in view of minimizing the effects of environmental perturbations[3].

For the development of this study, we focused on two *in situ* data sets: those from the Ocean Color component of AErosol RObotic NETwork (AERONET-OC) [4], established to support satellite ocean color validation activities through standardized measurements performed at multiple sites generally located in coastal regions; and those from the Marine Optical Buoy (MOBY), a unique site established to support the vicarious calibration of satellite ocean color sensors with measurements of very high accuracy. These sites produce a large number of optical parameters (such as the water leaving radiance, nLw), which can be used to evaluate the statistical uncertainty for Calibration and Validation procedures. More specifically,

- AERONET (http://aeronet.gsfc.nasa.gov/) is an optical, ground-based aerosol monitoring network and data archive supported by NASA's Earth Observing System and expanded by federation with many non-NASA institutions. The network hardware consists of identical, automatic, sun-sky scanning spectral radiometers owned by national agencies and universities. Data from this collaboration provides globally distributed, near-real time observations of aerosol spectral optical depths, aerosol size distributions, and precipitable water in diverse aerosol regimes. The network imposes standardization of instruments, calibration, processing and distribution. The AERONET-OC sub-network provides the additional capability of measuring the radiance emerging from the sea (i.e., water-leaving radiance) with modified sun-photometers (SeaPRISM) installed on offshore platforms like lighthouses, and oceanographic and oil towers. NASA manages the network infrastructure (instrument calibration, data collection, processing and distribution within AERONET); the Joint Research Center, European Commission (JRC) has the scientific responsibility for the processing algorithms and performing quality assurance of data products[5]; and PIs are responsible for establishing and maintaining the sites. Data products include the normalized water leaving radiance and aerosol optical thickness at the nominal center-wavelengths of 412, 443, 488, 531, 551, 665 and 870 nm. Near-real time data products are accessible at the AERONET web site. For this study, we used quality-assured, Level 2 data available at the end of each deployment period (generally lasting 6-12 months) after post-deployment calibration of SeaPRISM. Uncertainty estimates are thoroughly documented and discussed[4].
- Since late 1996, MOBY has been the primary basis for the on-orbit vicarious calibrations of many missions (OCTS, SeaWiFS, GLI, POLDER, MODIS, MERIS, VIIRS). System characteristics, characterization efforts, and uncertainty budget have been duly presented in literature[6,7]. MOBY is a 14-meter long buoy system developed and instrumented to measure upwelling radiance and down-welling irradiance at the sea surface and at three subsurface depths. Subsurface light is transmitted by fiber optics to the MOBY spectrograph for continuous energy measurements at sub-nanometer resolution from 340 nm (ultraviolet) to 950 nm (near-infrared) wavelengths. Standard meteorological

observations are collected concurrently with the wavelength measurements, and supplemental oceanographic measurements, such as natural phytoplankton fluorescence, are also collected. MOBY transmits the collected data to Marine Optical Characterization Experiment (MOCE) Team members on a daily basis. These data are then processed and made available to SeaWiFS and MODIS Ocean Science Team members. These data are available for download from http://data.moby.mlml.calstate.edu.

3. THEORETICAL APPROACH

Satellite time-series data can be used to build a covariance matrix describing the spatial-temporal variability of the area of interest. *In situ* observational resources can then be adaptively distributed following the covariance-oriented criterion from the time-series to assign the best value for *in situ* field at grid points using a regular grid coincident with the centers of the satellite pixels. The best *in situ* sampling locations can be found using an optimum design procedure, such as an 'A-optimum' design.

3.1 Covariance

Consider an oceanographic field $\psi(x, y, t)$ measured from satellite at a given time and known observation error, a generic satellite time-series can be represented as:

$$\psi_{ijk} = \psi(x_i, y_j, t_k) \quad \mathrm{i = 1...N_x,\ j = 1...N_y,\ k = 1...N} \qquad (1),$$

The result of Equation (1) is a three-dimensional grid that depends on the longitude (*x*), the latitude (*y*) and the time (*t*). This grid of data can be reshaped as a two-dimensional grid of M rows by N columns:

$$T_{MN} \equiv T(M, N) \qquad (2),$$

where M (=N_x x N_y) represents the number of spatially distributed points (the product of *x* by *y*) while N represents the number of points over time (*t*). Using this representation, the covariance matrix (C) can be evaluated by multiplying T by its transpose or vice versa, depending on the size of the working dimensions (space and time)[8]. Because the data that we have retrieved from satellite observations are much more densely in space than in time (N<M), the covariance matrix has been evaluated implementing the following equation:

$$C_{NN} = (T_{MN})' \cdot T_{MN} = T_{NM} \cdot T_{MN} \qquad (3),$$

from which results a matrix of N rows by N columns. It is important to note that each element of the C matrix represents the correlation between two columns of T. In other words, it represents the time correlation between two satellite pixels. Moreover, the preliminary results from our simulations and real data have shown that C is also dependent on the sensor noise (satellite). For this reason, we have investigated a methodology to remove the sensor noise dependence (supposing that it is known *a priori*), making C independent of that noise. To achieve this, C is decomposed into two orthogonal matrixes following Equation 4:

$$C \cdot V = V \cdot D \qquad (4),$$

where *V* and *D* are the eigenvalues and the eigenvectors of C, respectively; in particular, D is the canonical form of C (a diagonal matrix with C's eigenvalues on the main diagonal), while V is the modal matrix (its columns are the eigenvectors of C). These characteristics make it possible to remove the sensor noise (σ^2_{sat}) by using the eigenvalues of C. Therefore the matrix D can be modified as follows:

$$D = \frac{1}{|K|}(D - \sigma^2_{sat} \cdot K) \qquad (5),$$

where *k is* a vector that contains ones at locations of positive eigenvalues. Finally, replacing the negative eigenvalues with zeros, the new covariance matrix can be evaluated using the formula:

$$C = V \cdot D \cdot V' \qquad (6).$$

3.1 Merging procedure

Merging remote sensing data with *in situ* measurements is a standard procedure that aims at increasing the accuracy of satellite-derived products. The idea is to study the spatial-temporal variability of satellite data and to distribute the *in situ* measurements over the image following the covariance criterion. Therefore, once the covariance C has been obtained from Equation (6), a new field, resulting the merging of *in situ* and satellite data, is determined by maximizing the probability distribution:

$$P(\psi_K) \propto \exp[-(\psi_{obs} - H\psi_k)^T \textstyle\sum_{obs}^{-1}(\psi_{obs} - H\psi_K) - (\psi_K - \overline{\psi})^T C^{-1}(\psi_K - \overline{\psi})] \qquad (7),$$

where ψ_K represents the estimated pixel value, ψ_{obs} is the observation vector, H is the observation matrix and Σ_{obs} is the observation error matrix. The first term in the exponential represents the likelihood density while the second product of the matrices represents the *a priori* probability. The merging procedure is performed maximizing the *a posteriori* probability distribution, and therefore, the best estimation is represented by the field ψ :

$$\psi_{merged} = \arg\min_{\psi}\left((\psi_{obs} - H\psi_k)^T \Sigma_{obs}^{-1}(\psi_{obs} - H\psi_k) - (\psi_k - \overline{\psi})^T C_\varepsilon^{-1}(\psi_k - \overline{\psi})\right) \qquad (8).$$

The solution of Equation (8) represents the merged image. It is important to point out that the merging technique can be applied to *in situ* measurements that pass the following criteria:

- *In situ* and satellite acquisitions have to be almost coincident (in this study they are kept for the analysis if performed within 1 hour);
- *In situ* acquisitions have to be taken under low wind conditions (less than 12 m/s) and with solar zenith angle lower than 70 degrees; and
- The satellite area has to have cloud coverage <10%. It is important to note that the covariance analysis is directly dependent on cloud size and position, in the sense that the introduction of clouds causes a loss of information and decreases the correlation length (as expected). More details can be found in literature[9].

3.2 Optimum design

Sampling strategies of *in situ* observational resources driven by a design principle called A-optimality could substantially improve the accuracy of the final blended products. The scope of A-optimal designs is to minimize the spatial average variance of the estimated field with respect the sample locations. This approach can be used to identify the best locations for *in situ* sampling for Cal/Val. This optimal criterion will select locations in regions with low uncertainty and large spatial representation. Like other standard variance-oriented criteria in optimal experimental design, a covariance model must be known *a priori*. Satellite information could be employed to build a covariance matrix encoding the spatial-temporal variability of the area of interest. *In situ* measurements could then be adaptively distributed following the variance-oriented criterion, to assign the best values of the *in situ* observed fields at points of a regular grid coincident with the centers of satellite pixels. This procedure would ensure the optimality of merged products for limited *in situ* observational resources. The implementation of this technique was initially performed using a Genetic Algorithm (GA) that mimics the process of natural evolution. This algorithm iteratively searches for the best *in situ* position which minimizes the variance of the retrieved solutions. The optimization problem was also investigated using a Simulated Annealing (SA) strategy that is a generic probabilistic metaheuristic for the global optimization problem of locating a good approximation to the global optimum of a given function in a large search space. The retrieved optimization results from GA and from SA were comparable, but SA results are achieved much faster; therefore the SA method is here used.

3.3 Uncertainty Index (UI)

The approach presented above is adequate when there is the possibility to plan the *in situ* sampling. However, we also need to determine if the current, geographically fixed *in situ* sites (such as MOBY and AERONET-OC) are adequate for assessing the uncertainty. For this purpose, we have defined an Uncertainty Index (UI) that is independent of the geographic position and on the size of the considered area. In particular, we have defined an index that relates the goodness of the measurements in a user-defined location in relation to a reference site. The idea is to define a parameter that is independent of the size of the study area in order to provide an absolute value that can be used for several areas. This index is defined as a complex number:

$$UI = g + js \qquad (9),$$

UI takes into account:

- The goodness of the measurements in respect to the reference site – g (for example g = 2 means that the performance of the new position is lower of a factor 2);
- The area of influence of the retrieved result (s).

In order to have an absolute reference to relate the goodness of the study measurements, an *in situ* reference has to be defined. On the basis of our covariance-oriented analysis, we have decided to use MOBY (Hawaii) as reference because of its expected ideal performance due to the homogeneity of the area and the major effort put in system characterization and calibration. Using MOBY as normalization reference, equation (9) can be re-written as:

$$UI = \frac{Var_{insitu}}{Var_{Moby}} + j\frac{Area_{insitu}}{Area_{Moby}} \qquad (10),$$

where

- $Var_{insitu} \equiv Cov(i,i)$ is the value of the covariance matrix corresponding to the *in situ* pixel position (i, i),
- $\frac{Var_{insitu}}{Var_{Moby}}$ is the ratio of variance retrieved from the covariance matrix of the *in situ* source of interest (for example,

AERONET-OC), and the covariance matrix of the reference *in situ* (MOBY). The value of the matrix is an index that represents the correlation of the pixel *i* with the surrounding pixels in the area. The ratio provides a value that takes into account the *goodness* with respect to the reference site; for example if $\frac{Var_{Aeronet}}{Var_{Moby}} = 2$, the estimated variance of AERONET-OC is two times higher than MOBY.

- $\frac{Area_{insitu}}{Area_{Moby}}$ is the ratio retrieved from the evaluation of the area with a higher correlation. This area is defined using a

threshold that depends on the correlation of the pixels of interest: $Threshold = \frac{Cov(i,i)}{2}$.

In the following table we have listed the MOBY results (covariance and area) that have been used to retrieve the UI of the *in situ* region of interest.

MOBY	COV	Area
Jan	0.9532	1321
Feb	0.9668	1040
Mar	0.9771	914
Apr	0.9144	1426
May	0.9787	480
Jun	0.7215	782
Jul	0.7862	701
Aug	0.9450	1180
Sep	0.9951	1222
Oct	0.988	631
Nov	0.9270	751
Dec	0.9453	382

Table 1: MOBY reference table.

4. DATA PROCESSING RESULTS

The focus of the analysis presented here is the evaluation of the covariance field in MODIS images to study the performance of AERONET-OC and MOBY. The idea is to distribute the *in situ* observational resources following the variance-oriented criterion, to assign the best values of the *in situ* observed fields at points of a regular grid coincident with the centers of satellite pixels. This procedure ensures the optimality of merged products for limited *in situ* acquisitions. In the following two paragraphs, we present the results of an historical characterization from the implementation of the procedures described above using MODIS time-series images.

4.1 AAOT results

The objective of this study was to monitor the temporal and spatial variation of satellite imagery in the area of the Acqua Alta Oceanographic Tower (AAOT) site and to determine the best location(s) (i.e., those exhibiting the lowest variability) for *in situ* sampling. The site, established to support validation activities in coastal moderately optically complex waters, is located at 8 nautical miles from the coast can be characterized by high seasonal and spatial variability. This makes the site more suitable to support validation activities with a range of water types and bio-optical regimes, rather than vicarious calibration. For the purpose of the current investigation we have downloaded and processed daily MODIS imagery from January 2005 to December 2009, for a total of 2135 images. The 438 images with <10% cloud coverage were processed (and archived) and the box area defined by the 900 km^2 area (30 km by 30 km) around the AAOT site was extracted (fixed for the convenience of computation and analysis). Each monthly time series was arranged into a two-dimensional array T(x, t), where *x* and *t* are the spatial and temporal indices. Because the data retrieved from MODIS are much more dense in space than in time ($x >> t$), the covariance matrix was evaluated by implementing equation 10 for each month. To represent the monthly statistic analysis we focused our attention on the normalized water leaving radiance (nLw) at 547 nm and have evaluated the mean of each time series and also defined a "Historical Covariance Map" that represents the pixel standard deviation for the considered time-series, as showed in Figure 1. Using this technique, it is possible to produce twelve monthly Historical Covariance Maps that have been used to perform uncertainty analysis without satellite acquisitions but taking into account the "statistical behavior" of the environmental. Figure 2 shows the results for the month of January.

This approach can be used to identify the best locations of *in situ* sampling for the selected area around the AAOT site and to define where *in situ* data should be collected in order to have the best results for Cal/Val purposes, as shown in Figure 3. As presented in Figure 4, these results show that the "best" locations are about 8.5 km to the southwest of the actual AAOT site in agreement with an increased distance from the coast.

4.2 Hawaii MOBY results

The second objective was to monitor the temporal and spatial variation of Hawaii area surrounding the MOBY location and to determine the best location(s) with lowest variability for *in situ* sampling. Similar to the AAOT region, for this location we downloaded and processed daily MODIS imagery from January 2005 to December 2007, for a total of 1325 images. The 233 images with cloud coverage <10% were processed and archived, and we focused our analysis on the 30 by 30 km box around the MOBY site. As before, each monthly time series was arranged into a two-dimensional array T(x, t), where x and t are the spatial and temporal indices, and the covariance matrix was evaluated by implementing equation 10 for each month.

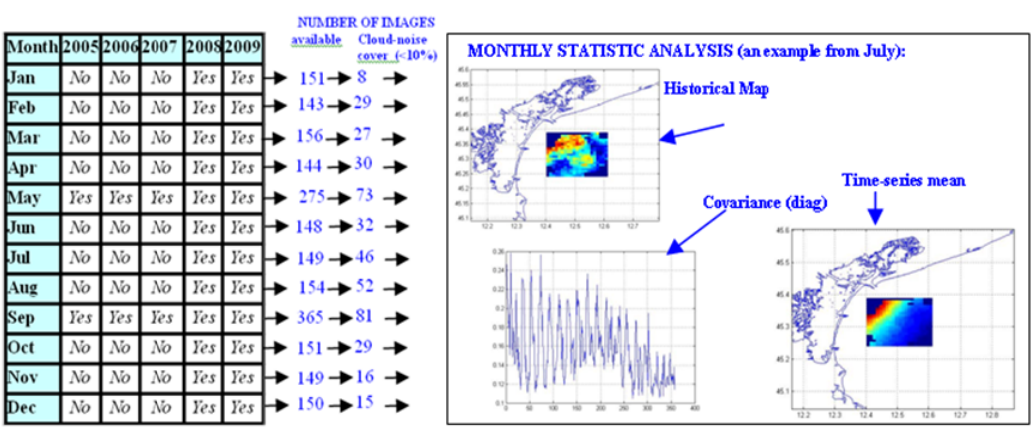

Figure 1: Processing chain applied for the statistical analysis of the MODIS time series images for the AAOT site.

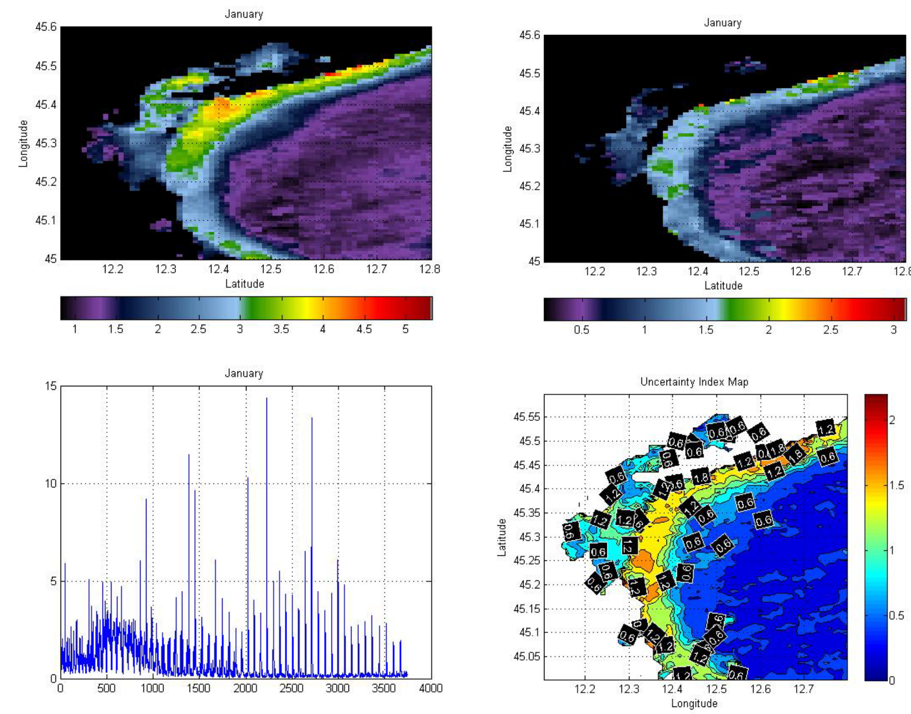

Figure 2: Statistical analysis for the month of January. (a) Historical Map, (b) Time series mean, (c) Covariance (diagonal) (c) Uncertainty Map.

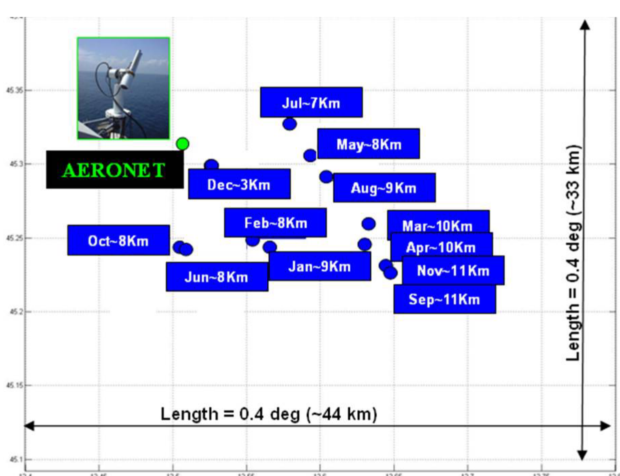

Figure 3: Historical results for the region around the AAOT site.

AAOT	UI index
Jan	0.7576+j0.1528
Feb	0.9742+j0.4338
Mar	0.9800+j0.4200
Apr	1.0539+j0.2824
May	0.9877+j0.4333
Jun	1.2895+j0.7200
Jul	1.2388+j0.5669
Aug	1.0172+j0.4414
Sep	1.0100+j0.2700
Oct	0.9786+j0.7862
Nov	1.0673+0.6794
Dec	1.0247+j0.2907

Table 2: Uncertainty Index table for the region around the AAOT site.

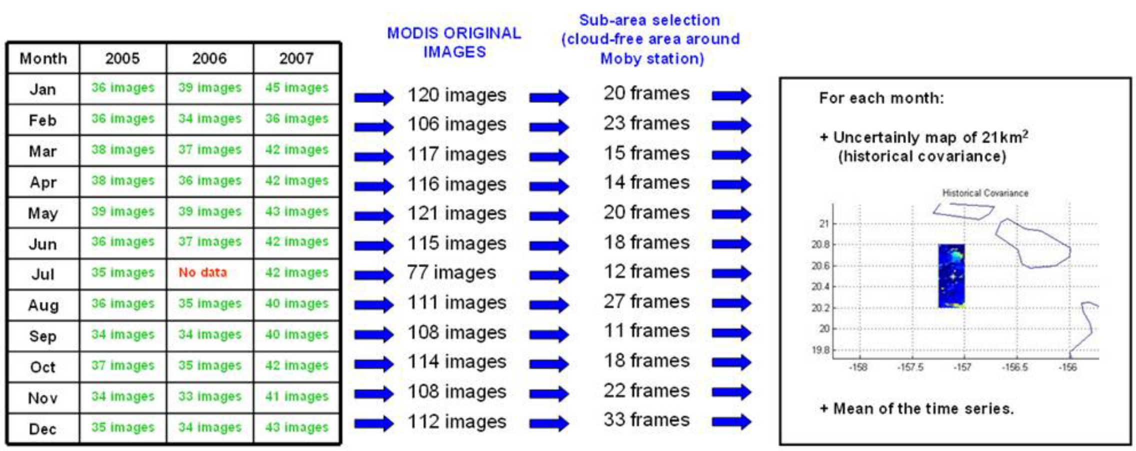

Figure 4: Processing chain applied for the statistical analysis of the MODIS time series images for the MOBY site.

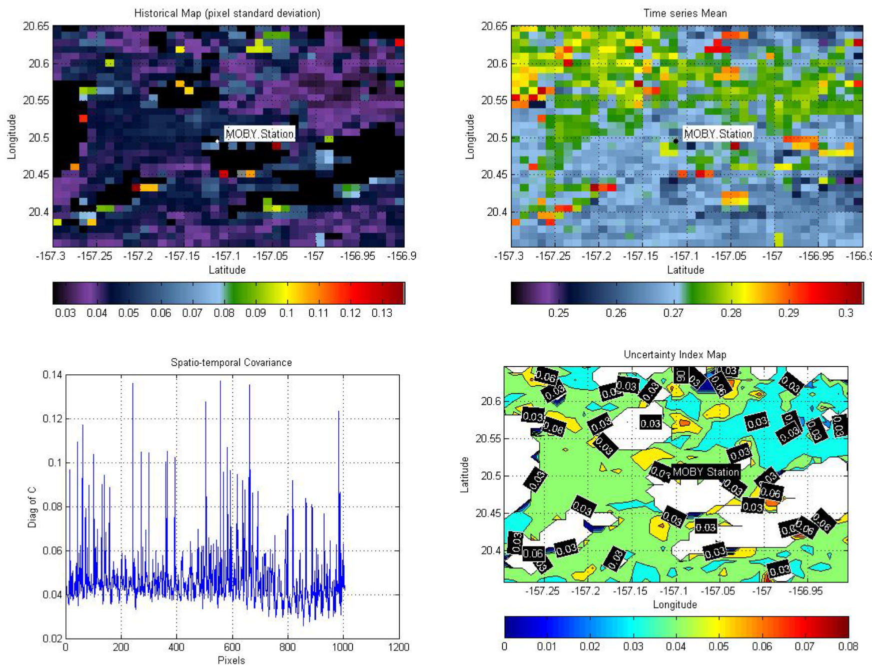

Figure 5: Statistical analysis for the month of January. (a) Historical Map, (b) Time series mean, (c) Covariance (diagonal) (c) Uncertainty Map

As for the region around the AAOT site, we produced twelve monthly Historical Covariance Maps that have been used to calibrate *in situ* data without satellite acquisitions but taking into account the "statistical behavior" of the satellite. Figure 6 shows the results from the identification of the best locations of *in situ* sampling using our A-optimum design methodology.

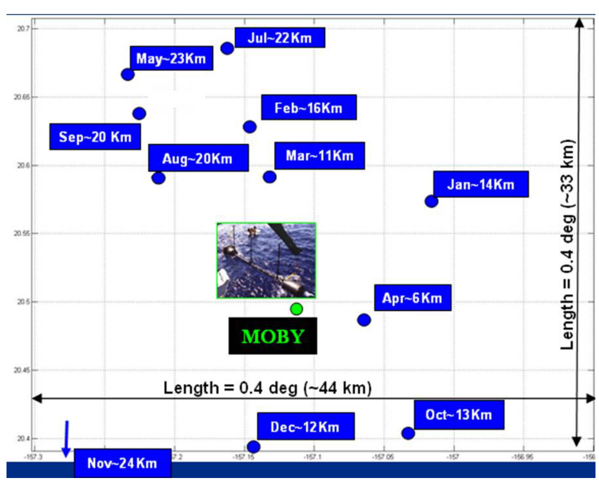

Figure 6: Historical results for the region around MOBY.

Compared with the AAOT AERONET-OC, the "best" results for the MOBY area Hawaii are farther (~15 km) from the actual MOBY site, but are more regularly spaced around the station in agreement with the open ocean character of the region.

5. Conclusion

We have presented methodologies to perform product retrieval uncertainties in order to estimate optimal *in situ* sampling strategies. In particular, we have studied a procedure for merging satellite data with *in situ* measurements to decrease satellite uncertainties. This methodology can be used to define optimum locations where *in situ* data should be collected to support Cal/Val activities. Satellite ocean color products include water leaving radiance, chlorophyll, and inherent and apparent properties. *In situ* measurements can be obtained from moorings (MOBY), ships, autonomous vehicles (such as Autonomous Underwater Vehicles and/or Gliders) or grounded platforms (AERONET-OC).

We have evaluated the capabilities of two existing *in situ* measurement sites in support of satellite ocean color Cal/Val activities. In particular, we have applied our method to MODIS time-series images surrounding the AAOT AERONET-OC site in the northern Adriatic Sea and those surrounding MOBY site in Hawaii. The covariance matrix of the available time-series was used in a Bayesian framework to estimate the best *in situ* location for vicarious calibration (requiring low variability) using a Simulated Annealing Algorithm and the resulting Historical Maps have been used to analyze those areas. As expected, results show that the open ocean MOBY site is located in a more homogeneous area in comparison to the coastal AAOT site, and therefore provides higher performance. This fully supports the use of MOBY as a reference for future analysis aiming at producing of an Uncertainty Index (UI) that is independent of geographic position and on the size of the considered area. Our methodologies will be used to support the Cal/Val effort for the Visible Infrared Spectrometer Sensor (VIIRS).

Acknowledgements

We greatly appreciate the support we have received from our sponsors from the JPSS Program Office, NOAA and to NRL. Appreciation is extended to the NASA AERONET team for the continuous effort in supporting the Ocean color sub-network. Giuseppe Zibordi is acknowledged for the effort in maintaining the AAOT site and comments on the early version of the manuscript. MOBY data was contributed by Stephanie Flora. Further, we would like to thank the MOBY Team for producing such as outstanding data set. This work was also supported by the Naval Research Laboratory basic research effort in Satellite Processing, and specifically through the contributions of Adam Lawson.

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