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Satellite remote sensing of harmful algal blooms: A new multialgorithm method for detecting the Florida Red Tide (Karenia

<u>brevis</u>)

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Abstract

In a continuing effort to develop suitable methods for the surveillance of Harmful Algal Blooms (HABs) of Karenia brevis using satellite radiometers, a new multi-algorithm method was developed to explore whether improvements in the remote sensing detection of the Florida Red Tide was possible. A Hybrid Scheme was introduced that sequentially applies the optimized versions of two pre-existing satellite-based algorithms: an Empirical Approach (using water-leaving radiance as a function of chlorophyll concentration) and a Bio-optical Technique (using particulate backscatter along with chlorophyll concentration). The long-term evaluation of the new multi-algorithm method was performed using a multi-year MODIS dataset (2002 to 2006; during the boreal Summer-Fall periods – July to December) along the Central West Florida Shelf between 25.75°N and 28.25°N. Algorithm validation was done with in situ measurements of the abundances of K. brevis; cell counts $\geq 1.5 \times 10^4$ cells l⁻¹ defined a detectable HAB. Encouraging statistical results were derived when either or both algorithms correctly flagged known samples. The majority of the valid match-ups were correctly identified (~80% of both HABs and non-blooming conditions) and few false negatives or false positives were produced (~20% of each). Additionally, most of the HAB-positive identifications in the satellite data were indeed HAB samples (positive predictive value: ~70%) and those classified as HAB-negative were almost all non-bloom cases (negative predictive value: ~86%). These results demonstrate an excellent detection capability, on average ~10% more accurate than the individual algorithms used separately. Thus, the new Hybrid Scheme could become a powerful tool for environmental monitoring of K. brevis blooms, with valuable consequences including leading to the more rapid and efficient use of ships to make in situ measurements of HABs.

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Keywords

Algorithm development; Central West Florida Shelf (Gulf of Mexico); Detection; Harmful Algal Bloom (HAB); Hybrid Scheme; Florida Red Tide (<u>Karenia brevis</u>); Ocean color (MODIS-Aqua); Satellite remote sensing

1. Introduction

A host of negative impacts can result when algal concentrations exceed background levels particularly when the algal species are capable of producing toxic substances, often know as "harmful algal blooms" (HABs) or as "red tides" (Smayda 1997a;1997b). Due to the apparent worldwide increase of HABs over recent years, the study of the possible effects of certain HABs on human health has spurred public attention from the media and society at large (e.g., Fleming and Laws, 2006;Schrope, 2008).

The West coast of Florida (Figure 1) often experiences severe HABs caused by the toxic dinoflagellate, <u>Karenia brevis</u>, which produces potent neurotoxins called brevetoxins (Steidinger, 2009). Human health can be effected during <u>K. brevis</u> blooms if brevetoxin-contaminated shellfish are consumed and/or the aerosolized toxin is inhaled (Kirkpatrick et at., 2004;Fleming et al., 2007). When present, blooms of <u>K. brevis</u> may also poison sea life, such as seabirds, fish and marine mammals (Landsberg, 2002;Shumway et al., 2003). Serious localized economic losses have also been linked with the "Florida Red Tide" (Hoagland et al., 2009). Because of the recurring and undesirable consequences caused by <u>K. brevis</u> blooms, monitoring of water quality for the occurrence of HABs is a continuing and pressing need in this region, and thereby a fundamental requirement for mitigation efforts and sustainable resource management (Dyble et al., 2008;Heil and Steidinger, 2009).

Improved capabilities for monitoring HABs with high temporal and spatial resolution have long been desired (McCluney, 1974; Murphy et al., 1975). Indeed, there is a widespread interest in the ability to locate and forecast HABs in the world's coastal areas (e.g., Sacau-Cuadrado et al., 2003; Olascoaga et al., 2008). Early warning systems using autonomous underwater vehicles, prototypes of sentinel instruments, real-time monitoring, and other approaches such as moorings, profiling floaters, drifting buoys, and sophisticated numerical modeling have all added high-quality contributions to traditional environmental research and monitoring efforts (e.g., Lee et al., 2005; Robbins et al., 2006). However, most <u>in situ</u> monitoring programs are affected by spatial and temporal biases due to sparse non-uniform coverage. Thus, many questions regarding the origin and development mechanisms of the Florida Red Tide (and other HABs elsewhere) remain unanswered (Tester et al., 1993, Walsh and Steidinger, 2001, Brand and Compton, 2007).

Since their inception, satellites carrying ocean color instruments proved to be a valuable complementary tool for synoptically monitoring trends of oceanographic features associated with <u>K. brevis</u> blooms (e.g., Haddad, 1982). Throughout the last decade, an analyst-dependent HAB Forecasting System (http://tidesandcurrents.noaa.gov/hab) has been used by the National Oceanic and Atmospheric Administration (NOAA) to detect potential blooms of <u>K. brevis</u> in the Gulf of Mexico using data of the Sea-viewing Wide Field-of-view Sensor (SeaWiFS; McClain et al., 2004). In short, the conceptual basis of this "Operational Method" lies in using satellite-measured chlorophyll (Chl) anomalies computed relative to the average of the previous two months (with a window of two weeks to the start of the mean calculation); an anomaly of 1 mg m⁻³ indicates a likely increase of 10×10^4 cells l⁻¹ in the concentration of <u>K. brevis</u> (Stumpf et al., 2003; Tomlinson et al., 2004; 2009).

More recently, two other satellite-based algorithms have also shown promise at the remote detection of K. brevis blooms. Both are applied to single images, therefore avoiding the use to construct a reference field. The Empirical Approach, introduced by Carvalho (2008) and Carvalho et al. (2010), identifies HABs when the magnitude of the satellite-measured water leaving radiance ($L_{wSAT}(\lambda \sim 550)$) is lower than the value of modeled total scatter (b_{MOREL} (550); Morel, 1988), as a function of satellite-measured Chl. The Bio-optical Technique, developed by Cannizzaro (2004) and Cannizzaro et al. (2008), employs a similar approach but uses two independent criteria that should occur simultaneously for indicating a pixel as HAB-positive: the satellite-measured Chl value must be high (≥ 1.5 mg m⁻³) at the same time as the value of a more highly-derived satellite product, i.e., the particulate backscatter $(b_{bpSAT}(\lambda \sim 550))$, should be less than the calculated value for this product using Morel (1988) model (b_{bpMOREL}(550)). In both algorithms, pixels not satisfying these conditions were classified as HAB-negative cases. A similar cell count threshold was used to define a detectable HAB in the identifications of the Empirical and Bio-optical algorithms: $\geq 1.5 \times 10^4$ and $\geq 1.0 \times 10^4$ cells l⁻¹, respectively; samples containing fewer cells than these thresholds were classified as non-bloom cases.

These two algorithms were based on the same reference wavelength, i.e., λ ~550nm. While the Bio-optical Technique was developed with a shipboard optical dataset but tested originally with one SeaWiFS image, which has λ =555nm as its closed band (Cannizzaro et al, 2008), the Empirical Approach was developed using data from MODIS (MODerate Resolution Imaging Spectroradiometer; Esaias et al., 1998) where the closest band is centered at λ =551nm. At these wavelengths, total absorption is small and b_{bp}(λ ~550) is the major attenuation facto allowing factor allowing one to estimate b_{bp}(λ ~550) from L_w(λ ~550) measurements (Pope and Fry, 1997; IOCCG, 2006).

In a preliminary investigation, Carvalho (2008) demonstrated that the Empirical Approach was able to produce spatially-coherent outcomes comparable to the HAB detection produced in the original Bio-optical Technique application of Cannizzaro et al. (2008) – a field-verified bloom of <u>K. brevis</u> at the end of August 2001 was successfully identified in a multi-sensor case of study using both algorithms applied to data of both SeaWiFS and MODIS. The application of the Bio-optical Technique to a long-time series of SeaWiFS data did not produce persuasive results (Hu et al., 2008), but this technique has subsequently been successfully applied to MODIS data in conjunction with data from three ~5-day cruises in 2005 and 2006 (Cannizzaro et al., 2009). In the study of Carvalho et al. (2010), an analysis of the Bio-optical Technique was carried out using a nearly five-year MODIS dataset from 2002 to 2006; results suggested that this technique could perform well provided the satellite dataset was carefully quality controlled and considering data distribution with seasonal and latitudinal restrictions.

Carvalho et al. (2010) also completed a long-term comparative investigation of the performances of the Empirical Approach, the Bio-optical Technique and the Operational Method. With an automated pixel-based match-up analysis that used the same <u>in situ</u> dataset for validation of the three algorithms, the Operational Method did not identify distinct populations of HABs and non-blooms as effectively as did the other two algorithms using MODIS data. When cell counts were plotted against the optical parameters used in the algorithms, the two populations produced by the Operational Method overlapped significantly (refer to Figures 7.10 through 7.18 in Carvalho (2008)). The Empirical and Bio-optical algorithms could be optimized by varying the appropriate threshold values – this was done with geographical and seasonal restrictions – and this resulted in modified versions which had improved performance in differentiating HABs from non-blooming conditions – summarized in Table 1 [panels X-XII]. The user was left with a choice of using one or the other of the optimized algorithms.

There is still scope for improving HAB detection with satellite measurements, and the objective of the current study was to determine whether the sequential application of the optimized versions of the Empirical Approach and the Bio-optical Technique would lead to improvements in identifying the optical characteristics related with the Florida Red Tide. The combination of these two algorithms has not been attempted previously, and represents a new approach to the problem. Thus, by exploiting the detection capabilities of the Empirical and the Bio-optical algorithms, a new method to detect \underline{K} . brevis blooms using satellite measurements was explored.

2. Methods

In the current study, the methodology used to establish the long-term detection capabilities of the optimized versions of the Empirical Approach and the Bio-optical Technique was followed (Carvalho et al., 2010). This involved performing an analysis with the same rigorous quality control to produce the "valid cloud-free match-ups" between satellite and <u>in situ</u> measurements (Figure 2). Shipboard and satellite measurements were matched in space (i.e., the pixel containing the <u>in situ</u> measurement) and time (i.e., <u>in situ</u> data within the same day of the satellite overpass). The rationale behind using only satellite measurements from the pixel containing the position at which the sample was taken avoids uncertainties from the use of larger areas including neighboring pixels to the field location, while the use of this time-acceptance window was justified by the slow growth rate of <u>K. brevis</u> cells (i.e., between 0.05 to 0.5 doublings day⁻¹; Shanley and Vargo, 1993). As the optimal accuracies of the Empirical and Biooptical algorithms were temporally and spatially constrained (Carvalho et al., 2010), the data selected for the current investigation were taken only during the boreal Summer-Fall periods (i.e., July to December) along the region of the Central West Florida Shelf (CWFS; south of 28.25°N close to Tampa Bay and north of 25.75°N near Cape Romano; Figure 1).

A comprehensive <u>in situ</u> database containing historical and current <u>K. brevis</u> monitoring data (Haverkamp et al., 2004) was used to validate the outcome of the new multi-algorithm method; the Florida Fish and Wildlife Conservation Commission's Fish and Wildlife Research Institute provided this database. As this database has been previously used for validating the long-term performance of the Empirical, Bio-optical and Operational algorithms (Carvalho et al., 2010), the same cell count threshold was used to evaluate the accuracy of the new multialgorithm. A binary classification sorted the database for the presence of Florida Red Tide (i.e., "red tide"; samples containing $\geq 1.5 \times 10^4$ cells of <u>K. brevis</u> l⁻¹) and for the absence of HABs (i.e., "non-blooming" conditions; samples with $< 1.5 \times 10^4$ cells of <u>K. brevis</u> l⁻¹).

The satellite imagery used was obtained from the Ocean Color Website (http://oceancolor.gsfc.nasa.gov/cgi/browse.pl?sen=am) for the period of July 2002 to mid October 2006. All level-1A MODIS-Aqua scenes (L1A files), covering the region of interest (Figure 1), were processed to level 2 (L2 files) with SeaDAS version 5.0.3 using default settings of the MSL12,4 version 5.2.3 (http://oceancolor.gsfc.nasa.gov/seadas). A large library of geophysical parameters derived from the satellite data was generated: total scatter($b(\lambda)$); particulate backscatter ($b_{bp}(\lambda)$); total absorption ($a(\lambda)$); absorption due to detritus and colored organic dissolved matter together $(a_{dg}(\lambda))$; and absorption due to phytoplankton $(a_{ph}(\lambda))$; these inherent optical properties (IOPs) of sea-water were derived with the Carder semi-analytical algorithm (Carder et al., 1999). This library also included: water-leaving radiance $(L_w(\lambda))$; normalized water-leaving radiance $(nL_w(\lambda))$; remote-sensing reflectance $(R_{rs}(\lambda))$; and were produced in 9 bands centered at $\lambda \sim 412, 443, 488, 531, 551, 667, 678, 748$ and 869nm. In addition, Chl (derived with the global OC3M band-ratio algorithm; O'Reilly et al., 2000); downwelling diffuse attenuation coefficient (K490); fluorescence line-height (FLH); seasurface temperature (SST); and satellite zenith angle (θ) were included. Figure 2 shows the flowchart illustrating the processes to obtain the pairs of valid match-ups to determine the

3. Statistical assessment

The ability to differentiate between HABs and non-blooming conditions, i.e., the satellitedetection effectiveness, was evaluated using basic statistical metrics (Congalton, 1991; Sokal and Rohlf, 1995; Mangnusson and Mourão, 2004), as described below. Following Carvalho et al. (2010), these measures were also used in the current study to evaluate the accuracy of the new multi-algorithm method; and in a comparison with the accuracies of the individual optimized versions of the Empirical Approach and the Bio-optical Technique. Error matrices (Table 1 [panel I-III]) give details of some applicable quantities used in the process of evaluating the accuracies of the algorithms derived from the numbers of: <u>a priori</u> known red tide samples correctly flagged as HAB-positive (designated as A); <u>a priori</u> known red tide samples incorrectly flagged as HAB-negative (B); <u>a priori</u> known non-bloom samples incorrectly flagged as HAB-positive (C); and <u>a priori</u> known non-bloom samples correctly flagged as HAB-negative (D) – see Table 2.

A standard and widely-used metric to assess the accuracy of classification algorithms is the overall accuracy, i.e., total of successful identifications divided by the total population ([A+D]/[A+B+C+D]; Table 2). However, the user can be misled if this metric is used alone; thus other basic metrics should be considered collectively. To help to understand these metrics they were divided in two groups; as shown in Table 1 [panels II and III].

The first set of metrics evaluated how many <u>in situ</u> samples, among the <u>a priori</u> known observed presence or absence of <u>K. brevis</u> blooms, were correctly identified by the algorithms, so as it gave the rate of failure in the detection (Table 1 [panel II]). Thus, four questions should be answered:

Question 1a. What portion of the red tide population was correctly flagged as HAB-positive (i.e., A/[A+B])? This is the sensitivity of the algorithm, also called as producer's accuracy (Congalton, 1991).

Question 1b. Among the red tide population, how many samples were not correctly detected by the algorithm (i.e., B/[A+B])? This is the fraction of false negatives.

Question 1c. Among the non-bloom population, how many samples were wrongly classified by the algorithm (i.e., C/[C+D])? This is the fraction of false positives.

Question 1d. What portion of the non-bloom population was correctly identified as HABnegative (i.e., D/[C+D])? This is the specificity of the algorithm.

The second set of metrics evaluated the accuracies of the algorithms (i.e., the predictive values; Table 1 [panel III]). These metrics are important as they represent the probability of the algorithm correctly identifying observed in situ conditions (i.e., the actual satellite identification based on the presence or absence of <u>K</u>. brevis blooms determined by microscopic analysis of the water samples). Hence, the answer to four other questions were sought:

Question 2a. What portion flagged as HAB-positive was represented by red tide samples (i.e., A/[A+C])? This is the positive predictive value, also known as user's accuracy (Congalton, 1991).

Question 2b. Among the cases flagged as HAB-positive, how many samples were in fact non-blooms (i.e., C/[A+C])? This is the inverse of the positive predictive value.

Question 2c. Among the cases identified as HAB-negative, how many samples were in fact red tides (i.e., B/[B+D])? This is the inverse of the negative predictive value.

Question 2d. What portion identified as HAB-negative was represented by non-bloom samples (i.e., D/[B+D])? This is the negative predictive value.

Predictive values are strongly dependent on the prevalence of red tides (i.e., the number of known red tide samples over the total population; [A+B]/[A+B+C+D]; Table 2). One should note that ideal algorithms should have both of the inverse, positive and negative of the predictive values equal to zero. Also, an ideal algorithm should have no cases of false negatives nor false positives.

4. The Hybrid Scheme

Despite the satisfactory performances of the optimized version of the Empirical Approach and the Bio-optical Technique (Table 1 [panels X-XII]), there were still some samples that were correctly identified by one algorithm, but not by the other; and vice-versa (Carvalho et al., 2010). Therefore, we hypothesized that HAB-detection improvements could be possible with the sequential application of the Empirical and Bio-optical algorithms into a single multi-algorithm method. Thus, we proposed a Hybrid Scheme dedicated to detect <u>K. brevis</u> blooms in the CWFS Summer-Fall using satellite ocean color imagery.

The new Hybrid Scheme was applied in two configurations; as depicted by the color-code in Figure 3a. In the 1st configuration of the Hybrid Scheme, a positive identification occurred when either or both algorithms correctly flagged known samples (Figure 3a: YELLOW +BLUE), while both algorithms had to fail simultaneously in detecting a known sample to establish false conditions (Figure 3a: WHITE). To determine the detection accuracy of the 2nd configuration of the Hybrid Scheme, both algorithms had to flag simultaneously known samples correctly for a positive identification (Figure 3a: BLUE), while false conditions occurred when either or both algorithms failed to classify a known sample correctly (Figure 3a: YELLOW+WHITE).

The two configurations of the Hybrid Scheme were compared to quantify whether improved detection of the <u>K</u>. brevis blooms could be achieved compared to the separate use of the Empirical Approach and the Bio-optical Technique, and if so, proposed as a potential remotesensing monitoring tool. The basic statistical assessments (as described by the eight questions of Section 3) were calculated individually at the two configurations of the Hybrid Scheme.

5. Results

Of the 371 <u>in situ</u> samples of the CWFS Summer-Fall that passed the match-up analysis quality control tests (Figure 2), 145 counted as red tides while the rest were non-bloom cases (n=226). The detection frequency observed by the identification of red tide and non-blooming conditions in the satellite data are shown in Figure 3 [b, c] for the individual optimized versions of the Empirical and Bio-optical algorithms, and in Table 2 for both configurations of the Hybrid Scheme. The answers to the first set of four questions (Section 3: 1a-1d) can be found in Table 1 [panels V, VIII, and XI], while the answers to the second set of four questions (Section 3: 2a-2d) can be found in Table 1 [panels VI, IX, and XII].

In terms of the observed incidence of red tide, established by the cell count threshold of 1.5×10^4 cells 1^{-1} , both configurations of the Hybrid Scheme had equal values: prevalence of red tides of ~39%; n=145/371 (Table 2). On the other hand, the results of the overall accuracy varied (Table 2), as this metric was determined by the total number of correct samples each configuration detected: the 1st configuration of the Hybrid Scheme had a good value (~79%; n=293/371), while the 2nd configuration had a moderate value (~62%; n=227/371). In comparison, the overall accuracies of the individual optimized versions of the Empirical and

Bio-optical algorithms were between these values (~70%; refer to Table 6 in Carvalho et al. (2010)).

The 1st configuration of the Hybrid Scheme had better detection rates than the 2nd configuration (Table 1). The sensitivity (80%; n=116/145) and specificity (78%; 177/226) observed for the 1st configuration were good, and were accompanied by low levels of false negatives (20%; n=29/145) and false positives (22%; n=49/226); as shown in Table 1 [panel V]. Poorer sensitivity (62%; 90/145) and specificity (61%; n=137/226) were observed at the 2nd configuration along with more cases of false negatives (38%; n=55/145) and false positives (39%; n=89/226); as shown in Table 1 [panel VIII]. The long-term detection accuracies of the individual optimized versions of the Empirical Approach and Bio-optical Technique, derived in Carvalho et al. (2010), are summarized in Table 1 [panel XI].

As can be seen in Table 2, of the total population (n=371), the 1st configuration of the Hybrid Scheme flagged 165 as HAB-positive ([A=116] plus [C=49]), while 206 samples were classified as HAB-negative ([B=29] plus [D=177]); Table 1 [panel IV]. In the case of the 2nd configuration, 179 samples were flagged as HAB-positive ([A=90] plus [C=89]), while 192 samples were classified as HAB-negative ([B=55] plus [D=137]); Table 1 [panel VII]. Thus, the derived positive predictive value of the 1st configuration of the Hybrid Scheme (Table 1 [panel VI]) was satisfactorily good (70%; n=116/165), so was the negative predictive value (86%; n=177/206). The excellent predictive values of the 1st configuration did not translate into the corresponding values of the 2nd configuration, which was less accurate (Table 1 [panel IX]). The predictive values of the individual optimized versions of the Empirical and Biooptical algorithms (Carvalho et al., 2010) are summarized in Table 1 [panel XII].

6. Discussion

The identification of HABs using satellite measurements and the establishment of the reliability of such retrievals are challenging tasks, largely because of the limited information in the satellite data, the problems of validating satellite ocean color retrievals in near-shore areas and the associated difficulties in finding a representative field dataset (Bailey and Wang, 2001; Werdell et al., 2003). Nevertheless, in this study, the use of the <u>in situ</u> database maintained by the Florida Fish and Wildlife Conservation Commission's Fish and Wildlife Research Institute successfully achieved the purpose of validating the detection of <u>K. brevis</u> blooms containing $\geq 1.5 \times 10^4$ cells l⁻¹ using MODIS measurements.

Although the relatively large native surface resolution of MODIS ocean color bands (of 1 km² at the nadir point) along with the fairly relaxed time-acceptance match-up window (in situ and satellite data within the same day) may have added some uncertainties to the analysis, the stringent exclusion criteria, which retained only pairs as free as possible of undesired artifacts, greatly improved the validity of our results (Figure 2). The final cloud-free match-ups (n=[371/3420] ~11%; comprising ~95 samples year⁻¹) served as a dataset for determining the long-term accuracy of the new Hybrid Scheme in the CWFS Summer-Fall. The number of red tide samples and the total population used in the current study ([n=145 and n=371; respectively]; Tables 1 and 2) was larger than those used in other related published studies to detect <u>K. brevis</u> blooms along the CWFS using satellite measurements – e.g., [n=42 and n=119; respectively] refer to Table 2 in Tomlinson et al. (2004); and [n=27 and n=90; respectively] refer to Table 3 in Cannizzaro et al. (2009).

The use of 2-by-2 tables to display the basic statistical results has been done to help the interpretation of the metrics used to establish the accuracy of the satellite-based algorithms (Table 1). Requiring the Empirical Approach and the Bio-optical Technique to flag correctly a sample at the same time (Figure 3a), the 2nd configuration of the Hybrid Scheme produced

modest detection results (i.e., sensitivity and specificity) with almost twice the number of false negatives and false positives than those of the 1st configuration (Table 1 [panels V and VIII]). This pattern was also observed in their predictive values (Table 1 [panels VI and IX]). Thus, after answering the eight questions of Section 3, the comparison of the HAB detection accuracies of both configurations of the Hybrid Scheme with the accuracies of the individual optimized version of the Empirical and the Bio-optical algorithms (Table 1 [panels X-XII]) revealed that the 1st configuration had better detection qualities (being in average ~10% superior; Table 1 [panels IV-VI]) while the 2nd configuration was not as accurate, being roughly ~10% worse (Table 1 [panels VII-IX]) than the individual algorithms used separately.

The strength of the Hybrid Scheme lies in the use of a multi-parameter approach (i.e., $L_w(\lambda \sim 550)$, $b_{bp}(\lambda \sim 550)$ and Chl), as the identification of <u>K. brevis</u> blooms was not solely derived from Chl retrievals. Therefore, the effectiveness of the 1st configuration of the Hybrid Scheme in correctly flagging red tide samples as HABs-positive was observed together with the ability to classify correctly as HAB-negative most of the non-blooming conditions, whether at low-Chl or at high-Chl concentrations dominated by other non-toxic algal species. Thus, the good detection accuracy of the 1st configuration suggests that the Hybrid Scheme could be an asset for reliable environmental monitoring. Indeed, it can be used to direct field-monitoring campaigns improving the timeliness of <u>in situ</u> sampling of HABs. This would assist scientists to investigate the Florida Red Tide in a more focused manner, thus generating better understanding of major issues related with the occurrence of HABs, e.g., the mechanisms that trigger, perpetuate and disperse blooms (Kusek et al., 1999; Smayda, 2007).

It is important to bear in mind that sensitivity and specificity are independent variables, as are false negatives and false positives; however, sensitivity is coupled with false negatives, and cases of false positives are the complements of specificity. From a resource manager's standpoint, an error in flagging a HAB (i.e., a false negative case) is not desirable given possible human and environmental health impacts (e.g., a failure in public protection may occur if shellfish beds are contaminated). The failure to identify correctly non-blooming conditions (i.e., false positive cases) is not financially acceptable since no HABs are present and erroneous announcements may have large localized economic consequences (e.g., loss of tourism). It can be argued under variations of the "Precautionary Principle" (Kriebel et al., 2001) that in the case of false positive errors, at least undesirable public health risks are avoided, which would be a more socially acceptable alternative to be integrated into decision-making management and strategies.

At the present time, the capabilities of the ocean color satellite sensors are not yet able to provide sufficient information for a confident identification of HABs species. Neither can the algorithms determine a decision for the closure of recreational and commercial shellfish beds based on remote sensing data alone as the reference threshold of 1.5×10^4 cell l⁻¹ is still above the guidelines used in monitoring and regulatory decisions (i.e., 0.5×10^4 cell l⁻¹; FDA, 2005). However, the reference level used in the current study to define detectable <u>K. brevis</u> bloom within the satellite measurements is more realistic and more sensitive than other values found in the published literature (e.g., 10×10^4 cells l^{×1} in Tester et al. (1998) – this is also the same threshold implemented in the Operational Method; Fisher et al., 2005).

On the other hand, as good monitoring capabilities were demonstrated in the current analysis, the uncertainties in detecting HABs with satellite imagery could indeed be reduced by using the Hybrid Scheme in the 1st configuration (where either or both algorithms correctly detecting a sample positively). Thus, resource managers or scientists studying HABs would have a better chance to be aware of, or to locate sites suspected of having the presence or absence of blooms of <u>K. brevis</u> based on the outcomes of the 1st configuration of the Hybrid Scheme. Similarly, beach-goers would have a more confidence in avoiding potentially contaminated areas. And,

as the new multi-algorithm method achieved potential for scientific and operational applications, the Hybrid Scheme could assist in accurately directing field monitoring, which would promote improved seafood safety action and reducing the risk of Neurotoxic Shellfish Poisoning (Watkins et al., 2008).

Even though <u>K. brevis</u> is believed to be mainly restricted to Gulf of Mexico waters, the genus <u>Karenia</u> can be found in different oceans and seas around the globe (Haywood et al., 2004; Steidinger et al., 2008). Therefore, the detection capabilities presented by the Hybrid Scheme could also be applicable, in principle, to other regions where blooms of <u>Karenia</u> species may impart the same optical characteristics to the water (Schofield et al., 1999).

7. Concluding remarks

The sequential application of the optimized versions of the Bio-optical Technique and the Empirical Approach (Carvalho et al., 2010) produced a new multi-algorithm method specifically dedicated to detect the Florida Red Tide using remote sensing measurements – this was the first-time application that this new method, referred to as Hybrid Scheme, has been reported. The validity of the Hybrid Scheme was verified with a comprehensive in situ database of <u>K. brevis</u> cell abundances along the Central West Florida Shelf during the Summer-Fall periods (i.e., July to December) using a multi-year MODIS-Aqua dataset (2002 to 2006).

With an automated analysis, the long-term performance of the Hybrid Scheme was evaluated in two configurations. Better detection accuracies for <u>K. brevis</u> blooms containing $\geq 1.5 \times 10^4$ cells 1⁻ were observed in the 1st configuration (i.e., equally good sensitivity and specificity (~80%) with simultaneously good predictive values (>70%); Tables 1 and 2; Figure 3). The 1st configuration of the Hybrid Scheme benefited from the strengths of the individual algorithms – when the Empirical Approach missed a red tide there was still a chance of the same sample being correctly flagged by the Bio-optical Technique, and vice-versa.

The application of the 1st configuration of the Hybrid Scheme could provide a valuable lowcost means of HAB surveillance. Resource managers would be able to inform the general public about the location of HABs as they occur, adding confidence to mitigation action and reducing local economic impacts. Moreover, the accurate detection of <u>K</u>. brevis blooms could assist researches in the early identification of HABs as well as helping to create more appropriate public guidance and medical health plans.

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Figure 1.

Florida Harmful Algal Bloom Historical Database (2002 to 2006; data provided by the Florida Fish and Wildlife Conservation Commission's Fish and Wildlife Research Institute; Haverkamp et al., 2004). "Identified <u>in situ</u> samples to be considered" (see Figure 2) illustrating the sampling location for <u>Karenia brevis</u>: red tides ($\geq 1.5 \times 10^{4}$ cells 1^{-1} ; " \square ") and non-blooms ($<1.5 \times 10^{4}$ cells 1^{-1} ; " \square "). The region of the Central West Florida Shelf (CWFS – south of 28.25°N close to Tampa Bay and north of 25.75°N near Cape Romano) is indicated.



Figure 2.

Flowchart representing the stringent quality control tests applied to all near-coincident satellite-<u>in situ</u> pairs; adapted from Carvalho (2008) and Carvalho et al. (2010). Steps to identify <u>in</u> <u>situ</u> samples to be considered (light gray); satellite processing to identify the geophysical parameter library (dark gray); level-by-level of the match-up analysis performed to derive the valid cloud-free match-ups (white); and data removed from the analysis (black). As the water column depth was not specified for the <u>in situ</u> sampling within the Florida HAB Historical Database provided by the Florida Fish and Wildlife Conservation Commission's Fish and Wildlife Research Institute (Haverkamp et al., 2004), the Earth TOPOgraphy database at twominute gridded resolution (ETOPO2 –

http://www.ngdc.noaa.gov/mgg/gdas/gd_designagrid.html#) was used. Refer to Figure 6.3 in Carvalho (2008) for graphical representation of effective penetration depth (EPD; Gordon and McCluney; 1975) and apparent optical depth (AOD; Bailey and Werdell, 2006). Inherent optical properties (IOPs) includes: $a(\lambda)$, $a_{ph}(\lambda)$, $a_{dg}(\lambda)$, $b(\lambda)$, $b_{bp}(\lambda)$. For additional and information see Section 2.



Figure 3.

Venn diagrams showing the structure of the two configurations of the Hybrid Scheme (Section 4), which is based on the detection frequency of the Empirical Approach and the Bio-optical Technique. a) The positive identifications of the 1st configuration are represented by YELLOW and BLUE (when either or both algorithms correctly flagged known samples), while the positive identifications of the 2nd configuration are represented only by the BLUE (both algorithms had to flag simultaneously known samples correctly). b, c) All valid match-ups (n=371=[145+226]) sampled along the Central West Florida Shelf during the Summer-Fall periods (2002 to 2006). b) Shown in RED are red tide samples (RT; $\ge 1.5 \times 10^4$ cells l⁻¹; n=145= [12+90+14+29]). c) Shown in GREEN are non-bloom samples (NB; <1.5×10⁴ cells l⁻¹; n=226=[25+137+15+49]). See Tables 1 and 2 for the detection frequency of the two configurations of the Hybrid Scheme.

Table 1

Detection frequency of the Hybrid Scheme along the Central West Florida Shelf during the Summer-Fall periods (2002 to 2006). Panels I-II: Error matrices (use Table 2 for assistance with A, B, C, and D); Panels IV-VI: 1st configuration of the Hybrid Scheme (when either or both algorithms needed to flag known samples correctly; see Figure 3); Panels VII-IX: 2nd configuration of the Hybrid Scheme (when both algorithms must have flagged simultaneously known samples correctly; see Figure 3); Panels X-XII: Individual versions of the Empirical Approach and the Bio-optimal Technique, respectively (* adapted from Table 6 in Carvalho et al. (2010)). Panels II, V, VIII, and XI take into account the rows of the table and are based on the number of a priori known in situ samples (i.e., "in situ cell count"), where the RED indicates red tide samples ($\geq 1.5 \times 10^4$ cells l⁻¹) and the GREEN indicates non-blooming conditions ($<1.5\times10^4$ cells l^{-1}); these panels answer the first set of questions (Section 3: 1a-1d): sensitivity (Sens; A/[A+B]; Question 1a), false negative (Fneg; B/[A+B]; Question 1b), false positive (Fpos; C/[C+D]; Question 1c), and specificity (Spec; D/[C+D]; Question 1d). Panels III, VI, IX, and XII take into account the columns and are based on the identifications in the satellite data (i.e., "algorithm outcome"), where the RED indicates samples flagged as HAB-positive and the GREEN indicates samples classified as HAB-negative; these panels answer the second set of questions (Section 3: 2a-2d): positive predictive value (posPV: A/[A+C]; Question 2a), inverse of the positive predictive value (IposPV: C/[A+C]; Question 2b), inverse of the negative predictive value (InegPV; B/[B+D]; Question 2c), negative predictive value (negPV; D/ [B+D]; Question 2d). For an ideal algorithm, B=C=0.

I) Detection frequency				II) 1 st set of questions (1a-1d)				III) 2 nd set of questions (2a-2d)			
1 st	st Algorithm		1 st	1 st Algorithm			1 st		Algorithm		
configuration	outc	outcome		configuration	outcome			configuration		outcome	
of the Hybrid	True	False	e	of the Hybrid	True	False	· · · · · ·	of the	Hybrid		False
Scheme	(RT)	(NB)	Sum	Scheme	(RT)	(NB)	Sum	Sch	neme	(RT)	(NB)
True	А	в	A+B	True	A/[A+B]	B/[A+B]	100%	unt "	True	A/[A+C]	B/[B+D
13 S (KI)		_		co co	Sens	rneg	1000/	sit	(RT)	posrv	megr v
E Faise	С	D	C+D		C/[C+D] 1 Fnos	D/[C+D] Spec	100%	In cell	(NB)	C/[A+C] InosPV	D/[B+D negPV
Sum	A+C	B+D	total	(ND)					Sum	100%	100%
				The state of the					d.e		
IV) Detection frequency				V) 1 set of qu	V) 1 st set of questions (1a-1d)				VI) 2 st set of questions (2a-2d)		
1^	Algorithm			1	rithm		1 ^m		Algorithm		
of the Uvbrid	oute	ome		of the Hybrid	outed	nile		config	uration Urbrid	oute	Jome
Scheme	True	False	Sum	Scheme	True	False	Sum	Sel	nyonu	True	False
Scheme	(RT)	(NB)		Scheme	(RT)	(NB)	1000/	30	m	(RT)	(NB)
a fi True	116	29	145	a fin Irue	80%	20%	100%	nut n	True	70%	14%
13 S (KI)				co (L)	Sens	r neg	1009/	sit	(KI) Falsa	posP v	Inegry
	49	177	226		2270 Enco	1870	100%	ll i	(NIP)	30%	80% nocDV
Sum	165	206	371	5 (NB)	rpos	spec			(IND) Sum	100%	100%
oun	100	200	0.11						0.000		10070
VII) Detection	frequenc	y		VIII) 1st set of	questions ((1a-1d)		IX) 2 ⁿ	d set of q	uestions (2	a-2d)
VII) Detection	frequenc Algo	y rithm		VIII) 1 st set of	questions (Algor	(1a-1d) ithm		IX) 2 ⁿ	^d set of q	uestions (2 Algo	a-2d) prithm
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2 nd configuration of the Hybrid	frequenc Algo outc True	y rithm come False	Sum	VIII) 1 st set of 2 nd configuration of the Hybrid	questions (Algor outco True	(1a-1d) ithm ome False		IX) 2 ⁿ config of the	^d set of qu 2 nd guration Hybrid	uestions (2 Algo outo True	a -2d) orithm come False
VII) Detection 2 nd configuration of the Hybrid Scheme	frequenc Algo outc True (RT)	y rithm come False (NB)	Sum	VIII) 1 st set of 2 nd configuration of the Hybrid Scheme	questions (Algor outco True (RT)	(1a-1d) ithm ome False (NB)	Sum	IX) 2 ⁿ config of the Sch	^d set of qu 2 nd guration Hybrid neme	uestions (2 Algo outo True (RT)	a-2d) orithm come False (NB)
VII) Detection 2 nd configuration of the Hybrid Scheme True	frequenc Algo outc True (RT) 90	y rithm come False (NB)	Sum	VIII) 1 st set of 2 nd configuration of the Hybrid Scheme True	questions (Algor outco True (RT) 62%	(1a-1d) ithm ome False (NB) 38%	Sum 100%	IX) 2 ⁿ config of the Sch	^d set of quant guration Hybrid neme True	uestions (2 Algo outo True (RT) 50%	rithm come False (NB) 29%
VII) Detection 2 nd configuration of the Hybrid Scheme True ting (RT)	frequenc Algo outc True (RT) 90	y rithm come False (NB) 55	Sum 145	VIII) 1 st set of 2 nd configuration of the Hybrid Scheme True (RT)	questions (Algor outco True (RT) 62% Sens	(1a-1d) ithm ome False (NB) 38% Fneg	Sum 100%	IX) 2 ⁿ config of the Sci	d set of quartion guration Hybrid neme True (RT)	Alge out True (RT) 50% posPV	rithm come False (NB) 29% InegPV
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VII) Detection 2 nd configuration of the Hybrid Scheme ¹ / ₂ ¹⁰ / ₂ ²⁰ / ₂ ¹ / ₂ ¹⁰ / ₂ ²⁰ / ₂ ¹ / ₂ ¹⁰ / ₂ ²⁰ / ₂ ¹ / ₂ ¹⁰ / ₂ ¹ / ₂ ¹⁰ / ₂ ¹ / ₂ ¹⁰ / ₂ <td>frequence Algo outc True (RT) 90 89 179 requency Algo outc True (RT)</td> <td>y rithm False (NB) 55 137 192 rithm come False (NB) (NB)</td> <td>Sum 145 226 371</td> <td>VIII) 1st set of quadratic 2nd 2nd configuration of the Hybrid Scheme Thrue (RT) False (NB) Xt) 1st set of quadration Individual optimized optimized algorithms* E</td> <td>questions (Algor outco True (RT) 62% Sens 39% Fpos estions (1: Algor outco True (RT) ~70%</td> <td>(1a-1d) ithm ome False (NB) 38% Fneg 61% Spec a-1d) ithm me False (NB) ~30%</td> <td>- Sum 100% 100%</td> <td>IX) 2" Config of the Scl miss uf algor XII) 2 Indi opti algor</td> <td>^d set of quartities yuration Hybrid heme (RT) False (NB) Sum nd set of c vidual mized ithms *</td> <td>estions (2 Algc outo True (RT) 50% posPV 50% IposPV 100% questions (Algc outo True (RT) ~60%</td> <td>a-2d) withm come False (NB) 29% InegPV 100% 2a-2d) withm come False (NB) ~20%</td>	frequence Algo outc True (RT) 90 89 179 requency Algo outc True (RT)	y rithm False (NB) 55 137 192 rithm come False (NB) (NB)	Sum 145 226 371	VIII) 1 st set of quadratic 2 nd 2 nd configuration of the Hybrid Scheme Thrue (RT) False (NB) Xt) 1 st set of quadration Individual optimized optimized algorithms* E	questions (Algor outco True (RT) 62% Sens 39% Fpos estions (1: Algor outco True (RT) ~70%	(1a-1d) ithm ome False (NB) 38% Fneg 61% Spec a-1d) ithm me False (NB) ~30%	- Sum 100% 100%	IX) 2" Config of the Scl miss uf algor XII) 2 Indi opti algor	^d set of quartities yuration Hybrid heme (RT) False (NB) Sum nd set of c vidual mized ithms *	estions (2 Algc outo True (RT) 50% posPV 50% IposPV 100% questions (Algc outo True (RT) ~60%	a-2d) withm come False (NB) 29% InegPV 100% 2a-2d) withm come False (NB) ~20%
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VII) Detection 2 ^{rdl} 2 ^{rdl} configuration of the Hybrid Scheme IIII IIIII Scheme IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	frequence Algo oute True (RT) 90 89 179 requency Algo oute True (RT) 102, 104 74, 64	y rithm some False (NB) 55 137 192 rithm some False (NB) 43,41 152,162	Sum 145 226 371 Sum 145 226	VIII) 1 st set of q 2 nd configuration of the Hybrid Scheme Image: Configuration Image: Configu	questions (Algor outco True (RT) 62% Sens 39% Fpos estions (H Algor outco True (RT) ~70% Sens ~30% Fpos	(la-ld) ithm ome False (NB) 38% Fneg 61% Spec a-1d) ithm ome False (NB) ~30% Fneg ~70% Spec	Sum 100% 100% Sum 100%	IX) 2 ⁿ configure of the sim coll count algor <i>XIII</i> 2 <i>Indi</i> opti algor	^d set of qu partition Hybrid neme (RT) False (NB) nd set of c vidual mized tithms * True (RT) False (RT) False vidual	estions (2 Algc out (RT) 50% posPV 50% IposPV 100% IposPV 100% Interference (RT) ~60% posPV ~40% IposPV	rithm come False (NB) 29% InegPV 71% 100% 2a-2d) rithm come False (NB) ~20% InegPV -80% negPV

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Table 2

Detection frequency of the Hybrid Scheme: 1^{st} configuration (Left) and 2^{nd} configuration (Right). The RED shows the incidence of red tides (n=[A+B]; samples containing $\geq 1.5 \times 10^4$ cells 1^{-1}), and the GREEN shows non-blooming conditions (n=[C+D]; samples containing $< 1.5 \times 10^4$ cells 1^{-1}). Use error matrices in Table 1 [panels I, IV, and VII] and Venn diagrams in Figure 3 to assist with the interpretation and for the use of A, B, C and D to access the accuracy of the Hybrid Scheme.

1 st configuration of the Hybrid Scheme		RED TIDE SAMPLES	2 nd configuration of the Hybrid Scheme			
	90	A priori known samples correctly flagged BY BOTH ALGORITHMS	90	A = 90		
A = 116	12	A priori known samples correctly flagged ONLY BY THE EMPIRICAL APPROACH	12			
	14	A priori known samples correctly flagged ONLY BY THE BIO-OPTICAL TECHNIQUE	14	B = 55		
B = 29	29	BOTH ALGORITHMS miss flagging samples	29			
A + B	145	Total red tide population	145	A + B		
C = 49	Scheme 49	BOTH ALGORITHMS miss flagging samples	49	oria Schem		
1 st configuration of		NON-BLOOM SAMPLES		2 nd configuration of		
C - 49	49		49	G 00		
D = 177	25	A priori known samples correctly flagged ONLY BY THE EMPIRICAL APPROACH	25	C = 89		
	15	A priori known samples correctly flagged ONLY BY THE BIO-OPTICAL TECHNIQUE	15			
	137	A priori known samples correctly flagged BY BOTH ALGORITHMS	137	D = 137		
C + D	226	Total non-bloom population	226	C + D		
1 st configuration of the Hybrid Scheme		STATISTICAL ASSESSMENT		2 nd configuration of the Hybrid Schem		
([116+29]/371)~39%		Prevalence of red tide = $([A+B]/[A+B+C+D])$	([90+55]/371)~39%			
([116+29]/37	·		([90+137]/371)~62%			

A = A priori known red tide samples correctly flagged as HAB-positive.

 $\mathbf{B} = A \ priori$ known red tide samples incorrectly flagged as HAB-negative

C = A priori known non-bloom samples incorrectly flagged as HAB-positive

D = A priori known non-bloom samples correctly flagged as HAB-negative