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Long-term evaluation of three satellite ocean color algorithms for identifying harmful algal blooms (*Karenia brevis*) along the west coast of Florida: A matchup assessment

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Abstract

We present a simple algorithm to identify *Karenia brevis* blooms in the Gulf of Mexico along the west coast of Florida in satellite imagery. It is based on an empirical analysis of collocated matchups of satellite and *in situ* measurements. The results of this *Empirical Approach* is compared to those of a *Bio-optical Technique* – taken from the published literature – and the *Operational Method* currently implemented by the NOAA Harmful Algal Bloom Forecasting System for *K. brevis* blooms. These three algorithms are evaluated using a multi-year MODIS data set (from July, 2002 to October, 2006) and a long-term *in situ* database. Matchup pairs, consisting of remotely-sensed ocean color parameters and near-coincident field measurements of *K. brevis* concentration, are used to assess the accuracy of the algorithms. Fair evaluation of the algorithms was only possible in the central west Florida shelf (i.e. between 25.75°N and 28.25°N) during the boreal Summer and Fall months (i.e. July to December) due to the availability of valid cloud-free matchups. Even though the predictive values of the three algorithms are similar, the statistical measure of success in red tide identification (defined as cell counts in excess of 1.5×10^4 cells L^{-1}) varied considerably (sensitivity—*Empirical*: 86%; *Bio-optical*: 77%; *Operational*: 26%), as did their effectiveness in identifying non-bloom cases (specificity—*Empirical*: 53%; *Bio-optical*: 65%; *Operational*: 84%). As the *Operational Method* had an elevated frequency of false-negative cases (i.e. presented low accuracy in detecting known red tides), and because of the considerable overlap between the optical characteristics of the red tide and non-bloom population, only the other two algorithms underwent a procedure for further inspecting possible detection improvements. Both optimized versions of the *Empirical* and *Bio-optical* algorithms performed similarly, being equally specific and sensitive (~70% for both) and showing low levels of uncertainties (i.e. few cases of false-negatives and false-positives: ~30%)—improved positive predictive values (~60%) were also observed along with good negative predictive values (~80%).

Keywords

Algorithm development; Chlorophyll; Detection; Gulf of Mexico (west Florida shelf); Harmful algal bloom (HAB); Florida Red Tide (*Karenia brevis*); Ocean color (MODIS); Satellite remote sensing; Water-leaving radiance

1. Introduction

Considerable social and human consequences associated with harmful algal blooms (HABs; or “red tides”) have been impacting local food supply and economies throughout history (Mitchell, 2003). Chronic HABs have long caused numerous negative ecological impacts in the Gulf of Mexico (Magaña et al., 2003), especially along the west coast of Florida (Fig. 1). In this region, the toxic marine dinoflagellate, *Karenia brevis*, blooms throughout the year but is mostly observed during the boreal Summer and Fall months (locally referred to as “Florida Red Tide”). It is responsible for water discoloration and fish kills that litter shorelines with tons of dead fish, contributing to the impairment and detrimental degradation of the coastal aesthetics (Van Dolah, 2000).

Besides the localized negative economic impacts that are associated with *K. brevis* blooms (Larkin & Adams, 2007), this organism produces a suite of neurotoxic brevetoxins that bioaccumulate in the food web as they pass to higher trophic levels (Tester et al., 2000). Scavenging seabirds have been found ill, moribund, and are susceptible to death during Florida Red Tide events (Forrester et al., 1977). Widespread die-offs of marine mammals such as manatees and dolphins have been associated with *K. brevis* blooms (Trainer & Baden, 1999).

In addition to environmental damage, blooms of *K. brevis* can also adversely affect public health and welfare in two distinct ways: (1) by ingesting brevetoxin-contaminated shellfish consumers have the risk of acquiring neurotoxic shellfish poisoning (NSP), a temporary but unpleasant illness characterized by gastrointestinal and neurological problems (Poli et al., 2000); and (2) ashore, the inhalation of the odorless aerosolized brevetoxin in the sea spray may cause burning of the eyes, induce coughing, sneezing and potentially causing an acute, but fortunately reversible, upper respiratory syndrome (Fleming et al., 2007). Hazardous consequences may also arise by direct contact with brevetoxin, but there have been too few cases to establish the consequences (Kusek et al., 1999). No human fatalities have yet been directly attributed to brevetoxins, but levels of brevetoxin during *K. brevis* blooms can reach levels potentially fatal to humans (Baden et al., 1984; Landsberg, 2002).

An effective and consistent way to accurately identify HABs using space-borne measurements is highly desirable, and an automated surveillance system could provide an economically viable system for documenting the location, magnitude and transport of *K. brevis* blooms (Babin et al., 2005). Indeed, remotely-sensed ocean color efforts have long contributed to the better understanding of the origin, maintenance, and termination mechanisms of the Florida Red Tide (e.g. Mueller, 1979). The ability to track, document and monitor HABs, besides helping to ameliorate local economic impacts, could bring tremendous societal benefits not only to resource and environmental managers, but also to medical health practitioners, the scientific community, coastal inhabitants, and to the tourism and aquaculture industries.

The overall purpose of the current investigation is to couple a remotely-sensed ocean color parameter library with near-coincident *in situ* measurements of the abundance of *K. brevis* to determine the long-term accuracy of three ocean-color algorithms for detecting the Florida

Red Tide. This matchup analysis, pairing satellite data with field observations, is used to test the performance of a new HAB-specific algorithm, entitled the *Empirical Approach* (Carvalho, 2008), and those of two other published algorithms: a *Bio-optical Technique* (Cannizzaro, 2004; Cannizzaro et al., 2008) and an *Operational Method* (Stumpf et al., 2003; Tomlinson et al., 2004, 2009).

Here we report for the first time the use of a multi-year data set (from July, 2002 to October, 2006) of measurements of the MODerate Resolution Imaging Spectroradiometer (MODIS; Esaias et al., 1998) to study *K. brevis* blooms along the west coast of Florida. Furthermore, by using the same *in situ* data set for the validation of the satellite indications, the accuracy of the *Empirical Approach* is compared to that of the *Bio-optical* and *Operational* algorithms.

This study is motivated, in part, by attempting to understand if an algorithm (i.e. *Empirical Approach*) based on variables closer to the satellite measurement and less close to the geophysical variables (i.e. primary optical variables; POVs) could be as effective in discriminating between the presence or the absence of *K. brevis* blooms, as those (i.e. *Bio-optical* and *Operational* algorithms) using more highly-derived parameters, as each step of the processing chain is likely to introduce, or amplify, uncertainties in the derived products.

2. HAB-specific algorithms

Throughout this paper the terms “non-bloom” and “non-blooming condition” are used to refer to the absence of the Florida Red Tide, thus accounting for lower concentrations of *K. brevis* cells. However, this could include different concentrations of chlorophyll (Chl): either high-Chl conditions (due to other non-*K. brevis* blooming organisms, such as diatoms) or low-Chl waters.

Details of the three HAB-specific algorithms applied to the satellite imagery are given below.

2.1. Operational method

The high Chl content of *K. brevis* blooms has been suggested to provide means to use satellite Chl anomalies for identifying the Florida Red Tide (Stumpf, 2001; Thomas, 2000). The National Oceanic and Atmospheric Administration's HAB Forecasting System (NOAA-HAB-FS) has implemented a monitoring strategy that exploits the concept of satellite Chl-anomalies (Stumpf et al., 2003; Tomlinson et al., 2004, 2009). Routinely, Chl-anomaly bulletins are issued indicating the possible occurrence of *K. brevis* blooms in the Gulf of Mexico (<http://tidesandcurrents.noaa.gov/hab/>) using data from the Sea-viewing Wide Field-of-view Sensor (SeaWiFS; McClain et al., 2004). In the current manuscript, this algorithm is referred to as the *Operational Method*.

This algorithm takes into account the difference (i.e. anomaly) between the current satellite Chl image and a background field derived as the running mean of the 60 previous days. At least 10 pixels per bin are required. To avoid mean biases in the presence of slowly changing blooms, a 14-day window is left unused between the analyzed image and those contributing to the generation of the mean. The resolution used for the spatial binning process for generating the Chl mean is 1 km. In the NOAA-HAB-FS implementation of the *Operational Method*, Chl retrievals are calculated using a regional algorithm (referred to here as Stumpf00; Stumpf et al., 2000).

Characteristics of the NOAA-HAB-FS application of the *Operational Method* include the requirement of analyst interpretations and the use of ancillary attributes (Fisher et al., 2005).

Environmental conditions in the form of the information of past and forecast wind, along with wind transport models, are also aggregated to the knowledge of pre-existing blooms identified by water sampling monitoring. These are combined with the information of bloom size, patchiness and other auxiliary rules for the skill assessment of this algorithm (Stumpf et al., 2009). In the course of the investigation presented here, however, aspects of forecast skill are not explored, as our intention is focus on the automated identification of HABs in satellite data using a matchup analysis, as described in Section 3.3.

In the *Operational Method*, satellite-measured Chl anomalies of 1 mg m^{-3} could correspond to a potential increase of $10 \times 10^4 K. brevis$ cells L^{-1} ; demarcating the cause of major fish kills (Steidinger et al., 1998). Thus, an alert indicating possible *K. brevis* blooms containing $\geq 10 \times 10^4$ cells L^{-1} arise whenever Chl anomalies are $\geq 1 \text{ mg m}^{-3}$. However, this cell count limit is nearly two orders of magnitude greater than regulatory guideline for shellfish bed closure (i.e. 0.5×10^4 cells L^{-1} ; FDA, 2005).

2.2. Bio-optical technique

Since Chl is present in all marine microalgae, methods to optically detect HABs and distinguish them from non-toxic species should use unique spectral features associated with these HABs (Garver et al., 1994). Assuming *K. brevis* experience lower grazing rates due to their toxins, distinguishable optical characteristics in the water column may occur, e.g. reduced levels of detritus (Lester et al., 2008; Schofield et al., 2006). Using this assumption, Cannizzaro (2004) and Cannizzaro et al. (2008) developed a classification scheme for detecting *K. brevis*. We refer to this algorithm as the *Bio-optical Technique*.

Using a shipboard radiometric bio-optical data set, a drop in remote-sensing reflectance ($R_{rs}(\lambda)$) for a given wavelength (λ) was noted in Chl-rich waters containing high concentrations of *K. brevis* cells, compared with $R_{rs}(\lambda)$ of areas with lower *K. brevis* concentrations. Variations in the particulate backscatter ($b_{bp}(\lambda)$) were observed to cause this $R_{rs}(\lambda)$ change, rather than changes attributed to absorption. Thus, this algorithm detects *K. brevis* blooms based on the simultaneous occurrence of two criteria. First, the measured particulate backscatter at $\lambda=551 \text{ nm}$ ($b_{bpSAT}(551)$) must be lower than the particulate backscatter calculated at $\lambda=550 \text{ nm}$ ($b_{bpMOREL}(550)$; p. 10,760 in Morel (1988)). Second, the measured Chl value has to be $\geq 1.5 \text{ mg m}^{-3}$. Cases not meeting these two criteria are classified as HAB-negative. This technique is independent of an analyst and can be applied to single satellite images meaning the construction of background fields is not necessary.

An updated variation of the *Bio-optical Technique* criteria has been proposed in an informal report (Carder, 2007). This includes: (1) lowering the Chl limits to 1.0 mg m^{-3} ; (2) using an additional fluorescence line-height (FLH) threshold; and (3) modifying the Morel (1988) function. However, our evaluation of this technique strictly followed the same criteria as those published by Cannizzaro et al. (2008) to detect HABs—i.e. $b_{bpSAT}(551) < b_{bpMOREL}(550)$ and $\text{Chl} \geq 1.5 \text{ mg m}^{-3}$. Conversely, a subsequent adjustment of the Morel (1988) threshold slope line is considered below, being further detailed in Section 3.5.

Originally, the *Bio-optical Technique* was only applied to a field-verified *K. brevis* bloom at the end of August 2001 using data from a single SeaWiFS image (Cannizzaro et al., 2008) for which the satellite retrievals were calculated using a semi-analytical ocean color algorithm (referred to here as Carder99; Carder et al., 1999). In that study, a cell count of 1.0×10^4 cells L^{-1} , that is one order of magnitude more sensitive than that of the *Operational Method*, was used to define a detectable *K. brevis* bloom, and *in situ* data were taken within a relaxed temporal window of a few days of the satellite overpass, justified because blooms could last more than a day or two in the same site (Shanley & Vargo, 1993).

2.3. Empirical approach

In a study directed towards replicating the original results of the *Bio-optical Technique*, in differentiating the presence or absence of a particular Florida Red Tide event using the same single SeaWiFS image (August 30, 2001) as published by Cannizzaro et al. (2008), Carvalho et al. (2007) and Carvalho (2008) confirmed that similar *K. brevis* detection could also be achieved using a MODIS image. The previous day (August 29, 2001) had to be used as there were no useful MODIS measurements on the same day as the SeaWiFS analysis. MODIS-Terra measurements were used because the case study period predated the launch of Aqua satellite. An additional purpose of that multi-sensor investigation was the development of an alternative HAB-specific algorithm entitled the *Empirical Approach* (Carvalho et al., 2007). The *Empirical Approach* produced equivalent spatially-coherent outcomes to those of the *Bio-optical Technique* using both SeaWiFS and MODIS imagery—please refer to Figures 7.1 and 7.2 in Carvalho (2008).

In the course of developing the *Empirical Approach* using a pair of satellite images from SeaWiFS and MODIS-Terra from 2001 (Carvalho et al., 2007), the use of a precursor of $b_{bp}(\lambda)$ in the ocean color processing chain (i.e. the water-leaving radiance; $L_w(\lambda)$) was explored—please refer to Figures 7.3 and 7.4 in Carvalho (2008). This was motivated, in part, by the fact that inherent optical properties (IOPs) of the seawater are satellite products derived from variables more directly measured by ocean color sensors (Carder et al., 1999). In that study, and in the results reported here, we found the use of $L_w(\lambda)$ rather than its normalized form, $nL_w(\lambda)$, was effective in identifying HABs using the *Empirical Approach*. This can be explained by the limited geographical and seasonal ranges in which the algorithm could be tested (see below), as well as the consequent narrow range of solar zenith angles and atmospheric variability.

Although the use of a POV, i.e. $L_w(\lambda)$, removes the algorithm from variables directly related to HABs, it avoids possible inaccuracies introduced by the calculation of more highly-derived variables; $b_{bp}(\lambda)$ is subject to greater uncertainties as it is derived from $L_w(\lambda)$ retrievals (IOCCG, 2006). Even though simple linear functions are used to derive $b_{bp}(\lambda)$ from POVs, errors are introduced as the coefficients or estimated geophysical variables used in the derivation are also prone to uncertainties (Carder et al., 1999; Gordon et al., 1988).

As the maximum effective penetration depth (EPD) for Case-2 waters occurs around $\lambda \sim 600$ nm and total absorption in the vicinity of this wavelength is somewhat low, the *Empirical Approach* uses the nearest band currently available from satellite ocean color sensors, i.e. λ centered at ~ 550 nm (Gordon & McCluney, 1975; Pope & Fry, 1997; Sackmann & Perry, 2006); 555 nm for SeaWiFS and 551 nm for MODIS. The *Empirical Approach* differentiates waters with *K. brevis* blooms from non-blooming conditions based on measurements of $L_w(551)$ as a function of Chl; both derived from satellite data.

In the original application of the *Empirical Approach* (Carvalho et al., 2007; section 7.1 in Carvalho, 2008), standard global blue-green ratio algorithms (i.e. OC4 for SeaWiFS, and OC3M for MODIS; O'Reilly et al., 2000) were used to estimate Chl concentrations, and validation was done using *in situ* data (FWRI, 2002) with the same temporal window that was used to validate the original development of the *Bio-optical Technique* (Cannizzaro et al., 2008). Accordingly, the same reference cell count limit, i.e., 1.0×10^4 cells L^{-1} , defined detectable HABs in the outcomes of the *Empirical Approach*.

In the *Empirical Approach*, a pixel is classified as HAB-positive if the magnitude of the satellite-measured $L_w(551)$ is lower than the related magnitude of the total scatter calculated at $\lambda=550$ nm ($b_{MOREL}(550)$; derived with equation 18 from Morel (1988))—as a function of Chl. HAB-negative cases are those cases not meeting this condition. Thus, by exploring Chl

and a POV in conjunction with a specific Morel (1988) threshold slope line, the *Empirical Approach* moves away from the *Bio-optical Technique* that uses Chl and an IOP with another Morel (1988) threshold slope line. Neither the *Empirical Approach*, nor the *Bio-optical Technique* requires an analyst and can be applied to single satellite images without the need for building background fields.

3. Methods

3.1. Satellite imagery

A total of 1665 level-1A MODIS-Aqua scenes (Collection 4) containing the area of interest (25°N–30°N and 81°W–87°W; Fig. 1) from July, 2002 to mid October, 2006 and with native ocean color band resolution (i.e. 1 km² at the nadir point), were downloaded from the NASA Ocean Color Website (<http://oceancolor.gsfc.nasa.gov/cgi/browse.pl?sen=am>). Images were processed using the NASA-provided software package SeaDAS version 5.0.3 (<http://oceancolor.gsfc.nasa.gov/seadas>). All level-1A files were radiometrically calibrated and geometrically corrected to produce independent level-2 products using MSL12,4 version 5.2.3.

Each level-2 file included a large geophysical parameter library, listed in Appendix A. In our evaluation of the *Empirical*, *Bio-optical* and *Operational* algorithms, Chl concentrations have been retrieved in the same manner using the OC3M; $b_{bp}(\lambda)$ was calculated using Carder99. Default masks were applied (i.e. cloud, land, and observed total radiance very high or saturated [hi-lt]) and only the best quality data were used. Pixels having satellite zenith angles >60° were excluded because of atmospheric correction inconsistencies experienced in the ocean color data set for high viewing angles (Bailey & Werdell, 2006). A series of quality control tests was applied, to guarantee that most sources of errors were eliminated, and is discussed in Section 3.3.

3.2. Field measurements

The Florida Fish and Wildlife Conservation Commission's Fish and Wildlife Research Institute maintains a database of the genus *Karenia* consisting of both historical cell concentration observations and current state *K. brevis* monitoring data (Haverkamp et al., 2004). The Florida HAB Historical Database (henceforth FWRI-database) was used to confirm the identification of the Florida Red Tide in the satellite measurements. All individual entries of this data set contain four common attributes: (1) *Karenia* abundances (in cells L⁻¹); (2) sampling date; (3) sampling depth; and (4) site location (latitude and longitude).

Some extra ancillary data (e.g. Chl, temperature, salinity, nutrients and the presence of other phytoplanktonic species) are also available, but not consistently. Since this database was compiled from observations collected over time by a variety of institutions, agencies and individuals, it lacks standardization, e.g. sampling collection methods and counting procedures. Whereas some monitoring programs had routine site revisits, the majority of the contributions to this database was in response to events, and had no established sampling stations; consequently, sampling depth and location were not constant. Most stations did not include appropriate information for validating satellite ocean color data in near-shore areas (e.g. sampling time and water column depth), nor other HAB-relevant aspects (e.g. water stratification and quantitative bloom patchiness size).

Even though the FWRI-database contains data extending over 50 years from 1956, our comparisons are limited to part of the MODIS-Aqua mission: from 2002 to 2006. Congenerics of *K. brevis*, such as *Karenia papilionacea*, *Karenia mikimotoi*, and *Karenia selliformis*, are known to occur throughout the Gulf of Mexico, but *K. brevis* has been

reported to be the most abundant species and is recognized for its toxic effects, besides being the species on which all monitoring and regulatory decisions are based (FDA, 2005; Heil & Steidinger, 2009). Hence, the current analysis only considers *K. brevis* samples.

The FWRI-database was divided into two sub-groups: “red tides” and “non-blooms”. The term “bloom” is somewhat arbitrary and *K. brevis* impacts are observed at very low cell concentrations, e.g. closure of shellfish beds occurs when cells exceed 0.5×10^4 cells L^{-1} due to NSP threats (FDA, 2005). However, this concentration of cells is generally below the level that can be detected with confidence with currently available ocean color sensors. Here, the long-term accuracies of the *Empirical*, *Bio-optical* and *Operational* algorithms are determined using a binary classification based on whether water samples contain more than or less than 1.5×10^4 cells L^{-1} of *K. brevis* to differentiate between detectable cases of red tides and non-blooms. This cell count limit is a compromise between the low level of cells that would actually be a good value to identify HABs (e.g. 0.5×10^4 cells L^{-1}), but which cannot be attained with the current generation of ocean color sensors, and that which can be actually achieved (e.g. 1.5×10^4 cells L^{-1}).

Other studies have asserted that the lower level for detecting the Florida Red Tide using satellite measurements is 10×10^4 cells L^{-1} (Tester et al., 1998). To facilitate comparisons with the original basis of the *Operational Method*, we also conducted an evaluation of this algorithm using this much higher cell count classification limit of 10×10^4 cells L^{-1} that is officially implemented by the NOAA-HAB-FS.

3.3. Matchup analysis and data quality control

A matchup analysis compares data acquired from space with collocated field measurements of what is actually present in the water (e.g. Bailey & Wang, 2001). Our matchup pairs consist of remotely-sensed ocean color parameters and near-coincident field measurements of the abundance of *K. brevis*. These matchups, spanning more than four years, are used to assess the accuracies of the *Empirical*, *Bio-optical* and *Operational* algorithms.

A major concern during matchup analyses is to create confidence of the *in situ* satellite pairs. Therefore, specific stringent automated tests – detailed below – have been carefully designed to identify and discard possibly flawed data.

The matchup pairs were characterized based on temporal and spatial attributes. For the temporal scale, we considered all *in situ* observations within the same day of each satellite image. This has been rendered necessary by the frequent lack of the sampling time in the FWRI-database that precluded any screening based on a shorter time interval between satellite overpasses and the field sampling. The spatial scale is defined by extracting single pixel values at the location of the *in situ* data point. MODIS images have geolocation accuracy of ~150 m at satellite nadir (Wolfe et al., 2002). Because the NOAA-HAB-FS implementation of the *Operational Method* requires the generation of a Chl reference field, matchups for this algorithm are performed on mapped binned images, rather than on unprojected granules as used for the *Empirical* and *Bio-optical* algorithms.

A “buffer zone” around the Florida coast was introduced to exclude pixels prone to errors resulting from shallow regions influenced by terrigenous sediment load, so all *in situ* stations within distances of half pixel (i.e. 500 m) from the coastline have been discarded. This also avoids pixels contaminated by radiances from the land being included in the analysis.

The Earth TOPOgraphy database at two-minute gridded resolution (ETOPO2—http://www.ngdc.noaa.gov/mgg/gdas/gd_designagrid.html#) was used to determine local

bathymetry, as water column depths were not given in the FWRI-database. But because the distance between each ETOPO2 point is ~4 km, this caused some near shore stations to be excluded when the corresponding ETOPO2 value contained altitude rather than depth. To prevent possible contamination of the satellite measurement signal by bottom reflectance (Lee et al., 1998, 1999) any *in situ* sample collected within 2 m of the ETOPO2 bottom depth was removed.

Two “bottom reflection thresholds” were tested to determine whether data from shallow regions could be retained. First, a shallow water mask was applied to restrict matchups to waters deeper than 10 m, after Subramaniam et al. (2002). Because the most severe human impacts caused by red tides occur near shore, an alternative threshold was tested and retained matchups where the local ETOPO2 bathymetry was deeper than the calculated apparent optical depth (AOD; Bailey & Werdell, 2006) plus 2 m (Figure 6.3 of Carvalho (2008)). The use of AOD avoids possible EPD uncertainties in the calculation of the downwelling diffuse attenuation coefficient (K_{490}), and the value of 2 m should provide a conservative error margin for the use of the ETOPO2 bathymetry.

Typically, the range of satellite zenith angles is limited to reduce uncertainties in the satellite retrievals caused by long atmospheric path lengths. However, small angles also restrict spatial coverage and reduce the number of valid matchups available. To explore the consequences of expanding the acceptable range of satellite zenith angles, we carried out an analysis considering the impacts of two “satellite zenith angle thresholds”: (1) restricted to 45° as recommended by Ding and Gordon (1994); and (2) relaxed up to 60° (Wang, 2002).

Ensuring that all *in situ* samples are within the penetration depth of the remotely-sensed signal, matchups were only considered if the distance from the sea surface to the depth of the *in situ* sample was shallower than the calculated EPD (Bailey & Werdell, 2006) minus 2 m (Figure 6.3 of Carvalho (2008)). The value of 2 m used in this “light penetration mask” should ensure that the *in situ* samples were shallow enough to contribute to the satellite-measured signal.

For the validation of classification algorithms it is important to have only the best quality data to give unambiguous results; this is particularly important in automated analyses. Consequently, the entire geophysical parameter library (Appendix A) was filtered to constrain the working data set to the best possible quality. Undetected cloud contamination poses a significant risk of introducing errors; since the infrared measurements from which sea-surface temperature (SST) is derived are very sensitive to cloud contamination, a test rejected matchups with SST < 15 °C, given that water temperature on the west Florida shelf rarely drops below this level, even during upwelling events (<http://tidesandcurrents.noaa.gov/>). The acceptable range for satellite-retrieved Chl was defined between 0 and 100 mg m⁻³. In addition, pixels having negative FLH (Gower & Borstad, 2004) were eliminated; these are caused by very low Chl concentrations (Letelier & Abbott, 1996) and were not retained because *K. brevis* blooms are unlikely to be found. Only satellite pixel values of $0 < K_{490} < 1$ were accepted for computing EPDs and AODs. Matchup pairs were only considered valid if IOP retrievals had positive physical values in all of the first six bands, and values of zero for the last three bands (Appendix A). Pixels with negative primary optical variable values (i.e. $L_w(\lambda)$, $nL_w(\lambda)$ and $R_{rs}(\lambda)$) in any of the nine bands were filtered out.

Recognizing the geographical and seasonal distributions of valid cloud-free matchup pairs were not uniform, we performed a spatiotemporal investigation to determine the locations and periods with adequate data availability. Firstly, the entire west coast of Florida was analyzed, and then the coast was divided into three regions: (1) North-FL—north of

28.25°N, near Tampa Bay; (2) South-FL—south of 25.75°N, near Cape Romano; and (3) the central west Florida shelf (CWFS) in between these latitudes (Fig. 1). Secondly, a year-round investigation was done, and then the data were divided into two seasons: (1) when *K. brevis* is most likely to bloom (i.e. boreal Summer–Fall months: July to December); and (2) when the occurrences of these HABs are less frequent (i.e. boreal Winter–Spring months: January to June).

3.4. Statistical concepts

To assess and compare the accuracy of the algorithms, the success rate of identifying HABs and non-blooms is evaluated using basic statistical measures (Congalton, 1991; Mangnussón & Mourão, 2004). An error matrix (Table 1a) presents the frequencies of successful and unsuccessful detection of *K. brevis* blooms and non-blooming conditions. This contingency table expresses the number of *a priori* known red tide samples correctly, and incorrectly, detected (A and B), and the number of *a priori* known non-bloom samples incorrectly, and correctly, identified (C and D). These four relevant quantities (i.e. A, B, C and D) are used to calculate the prevalence of red tide (i.e. the observed frequency of red tide expressed as the ratio between the red tide samples and the total population of outcomes; $[A + B] / [A + B + C + D]$) and the “odds” of red tide (i.e. the probability of red tide with respect to the non-bloom samples; $[A + B] / [C + D]$). An ideal data set should have equal sample numbers of red tides and non-blooms ($[A + B] = [C + D]$), giving rise to a prevalence of 50%, and “odds” equal to one.

The overall accuracy provides details about the total success rate of the algorithms at identifying correct field conditions ($[A + D] / [A + B + C + D]$; Table 1a). However, when used alone this quantity could hide the real performance of the algorithm. Thus, other detailed statistical aspects should be invoked and reviewed together to fully understand and to better extract useful information about the true ability of the algorithms to detect red tides. Hence, for an algorithm to achieve detection excellence, it must have simultaneously good characteristics in two distinct sets of statistical measures.

The foremost set of requirement (Table 1b) is that an algorithm should accurately identify known red tide and non-bloom samples by having good sensitivity (Sens; $A / [A + B]$); also referred to as producer's accuracy; Congalton, 1991) and specificity (Spec; $D / [C + D]$). Besides being aware of these metrics, by knowing the uncertainties of the algorithm, i.e. false-negatives (Fneg; $B / [A + B]$) and false-positives (Fpos; $C / [C + D]$), end users (e.g. resource managers, a scientist studying HABs, or the general public) can judge whether a particular algorithm is providing useful information on which to base appropriate decisions.

Accordingly, another set of attributes (Table 1c) should also be used to gain user confidence: most indications of HAB-positive should be represented by red tide samples (i.e. positive predictive value; posPV; $A / [A + C]$); also referred to as user's accuracy; Congalton, 1991) and those of HAB-negative by non-bloom samples (i.e. negative predictive value; negPV; $D / [B + D]$). These metrics along with the uncertainties of the algorithm (i.e. their inverse; IposPV ($C / [A + C]$) and InegPV ($B / [B + D]$), respectively) can assist end users to make a better decision of which algorithm to trust.

An assessment of an algorithm's accuracy is found incomplete if one of these two set of statistical measures is addressed but not the other. Both of these aspects should have moderate-to-high confidence for the algorithm to be deemed successful, accurate and, most importantly, useful.

3.5. Algorithm optimization

An optimization procedure was developed to achieve best practical levels of sensitivity and specificity along with simultaneous low numbers of false conditions. Here we focused on the threshold slope lines used in the algorithms to distinguish HAB-positive and HAB-negative cases. These were multiplied, in steps of 0.01, by a factor varying from 0.33 to 3.0, and the successful identification rates at each step were estimated. The multiplier producing high sensitivity along with high specificity was used as the new “best” threshold slope line. Subsequently, the two sets of statistical measures (Section 3.4) were computed again to measure the accuracies of the “optimized versions of the algorithms”.

4. Results

4.1. Availability of valid cloud-free matchups

The distribution of the ~76000 entries of the *in situ* FWRI-database (1956–2006) revealed an increasing sampling effort for the Florida Red Tide during the decade up to 2006. This pattern was particularly striking in the last 2 years of this period and was reflected in the final number of red tide valid matchups—Figures 7.5 and 7.8 in Carvalho (2008). As the current investigation is restricted to the MODIS-Aqua mission, from 2002 to 2006, a total of 21015 *in situ* observations were available to begin the analysis.

Major data elimination occurred under any of three conditions: (1) *in situ* cell counts did not correspond to *K. brevis* samples; (2) bathymetry was uncertain due to the use of the relatively coarse ETOPO2 data set; and (3) *in situ* samples were collected too close to the shoreline, i.e. within the buffer zone (see above). Of the 21015 *in situ* observations, only 7929 samples passed these tests (Table 2 [a1 and a2]). In a second set of tests, ~78% ($n = 6146/7929$; Table 2 [a3]) of these observations were retained as they fell within the MODIS swaths on the same day; therefore forming the workable subset used in the matchup analysis. At this stage, almost half of the initial 1665 MODIS-Aqua scenes ($n = 744$) had at least one *in situ* sample on the same day within the swath range.

The validity of the thresholds used in two widely-applied tests was examined to assess whether the exclusion of matchups that fail these tests is necessary (Section 3.3). These tests were used to evaluate the presence of bottom reflection and the range of usable satellite zenith angles. The analysis produced no reasons for rejecting data with either shallow water depths or large satellite zenith angles. That means data with depths shallower than 10 m and large satellite zenith angles (θ ; $45^\circ < \theta < 60^\circ$) could be included without introducing undesired artifacts.

A third set of tests revealed that most of the matchups were unusable based on the light penetration mask and the geophysical parameter filtering. Cloud cover played an important role in this data removal. In the end, only a small fraction of the workable subset within the FWRI-database (~13%; $n = 778/6146$; Table 2 [b1]) was accepted as final, having valid matchup pairs. The 778 samples used to assess the accuracy of the algorithms were divided in 274 red tide and 531 non-bloom samples (Table 2 [b2 and b3]), where the cell count classification based on 1.5×10^4 *K. brevis* cells L^{-1} defines red tide ($\geq$) and non-bloom ($<$) samples.

Most valid matchups came from the CWFS (~68%; Table 2 [c1]) and were comprised of ~1/3 red tides samples (Table 2 [c2]) and of ~2/3 non-blooms cases (Table 2 [c3]). Moreover, the CWFS valid matchups were predominantly from the Summer–Fall months (~70%; $n = 371/529$; Table 2 [d1]). Of the 175 MODIS-Aqua scenes that are used here over the CWFS, 107 are from the Summer and Fall months corresponding to the temporal pattern of the *in situ* sampling: the majority of the red tide cases throughout this region was from

this period (~80%; $n = 145/182$; Table 2 [d2]), as was the majority of non-bloom samples (~65%; $n = 226/347$; Table 2 [d3]). The higher incidence of red tide in the CWFS Summer–Fall is in accordance with the published literature (e.g. Walsh & Steidinger, 2001). This pattern is also found when using the official cell count limit implemented by the NOAA–HAB-FS, i.e. 10×10^4 *K. brevis* cells L^{-1} .

Since the *Operational Method* requires the calculation of a Chl anomaly, with a minimum number of 10 pixels per bin, a further ~100 potential matchups were rejected, thus leaving only 680 observations sampled year-round along the entire west coast of Florida to be used with this algorithm (Table 3). This imposition also caused the final number of matchups used to test the *Operational Method* during the CWFS Summer–Fall to be smaller ($n = 328$).

4.2. Spatio-temporal investigation

Fig. 2 illustrates the performances of the algorithms with data sampled year-round along the entire west coast of Florida; the sampling sub-groups (i.e. red tides and non-blooms) are displayed separately. The detection results shown in these scatter-plots are expressed as percentages of correct identifications divided by the subgroup population.

Along the entire west coast of Florida the three algorithms had good detection success in identifying non-bloom samples: 73% and 82% for the *Empirical* and the *Bio-optical* algorithms, respectively; and 85% for both cell count limits of the *Operational Method* (Fig. 2b, d, f, h). However, their success at identifying red tides was quite different, ranging from moderate to low: 61% for the *Empirical*; 53% for the *Biooptical*; and only ~35% for both cell count limits of the *Operational* (Fig. 2a, c, e, g).

During the Winter–Spring, high non-bloom detection rates were observed for the three algorithms (>90%), but the small number of valid red tide valid matchups ($n = 44$; Table 3) may have resulted in low red tide detection accuracies (10–20%; data not shown). In the Summer–Fall, the three algorithms correctly detected 60–80% of the non-bloom cases, and the red tide detection rates of the *Empirical* and *Bio-optical* algorithms (both with ~65%; data not shown) were slightly improved during this period as compared to those observed with the data collected year-round (Fig. 2). The *Operational Method* flagged ~35% of the red tides at both of the cell count limits.

Table 3 shows the geographical and seasonal data availability. Besides having a very small number (<44) of red tide valid matchups, most regions and periods had far more cases of non-bloom than red tide cases; thus producing low prevalence and odds of red tide. This makes the statistical testing unbalanced and the results not convincing. The exception is in the CWFS during the Summer and Fall months, where a large number of valid red tide matchups was observed ($n = 145$; Table 2 [d2]). Thus, since small sample sizes could compromise conclusions about the red tide detection accuracy, the rest of our analysis (i.e. statistical assessment and optimization procedure) is only applied to CWFS Summer–Fall data set—using the cell count classification limit of 1.5×10^4 cells L^{-1} , unless otherwise stated.

4.3. Statistical assessment

Data sampled along the CWFS during the Summer and Fall months has been used for the final assessment of the accuracy of the algorithms (dashed lines in Fig. 3). To facilitate the visualization of these scatter-plots the detection results (i.e. frequency and percentages) of the initial version of the algorithms are presented separately (Table 4c, e, f). This information is used to construct Table 5 that provides and compares the results of the two sets of detailed statistical measures.

The population of valid matchups of the *Operational Method* ($n = 328$) was not the same as the other two algorithms ($n = 371$); neither were the number of red tide ($n = 130$; $n = 145$) and non-bloom ($n = 198$; $n = 226$) samples (Table 3). However, the prevalence of red tides and “odds” of red tides of the three algorithms were about the same ($\sim 39\%$ and $\sim 65\%$), so were the overall accuracies: $[243/371] \sim 65\%$, $[258/371] \sim 70\%$, and $[201/328] \sim 61\%$ for the *Empirical*, *Biooptical*, and *Operational* algorithms (Table 5a, d, g).

Considering the 1st set of statistical measures (Table 5b, e, h), the *Empirical Approach* exhibited the best sensitivity (86% ; $n = 124/145$) and with it a desirable low rate of false-negative cases (14% ; $n = 24/145$). On the other hand, this algorithm was the least accurate in correctly flagging non-bloom samples, i.e. specificity of 53% ($n = 119/226$) that accounted for 47% ($n = 107/226$) of false-positives cases. The *Bio-optical Technique* sensitivity was 77% ($n = 111/145$) while its specificity was 65% ($n = 147/226$). It had 23% of false-negative ($n = 34/145$) and 35% ($n = 79/226$) of false-positive cases. The *Operational Method* had the lower success in identifying red tides (26% ; $n = 34/130$), along with an undesirable high rate of false-negatives (74% ; $n = 96/130$). However, the outcome of the detection of non-bloom cases was reverse and this algorithm had the best specificity (84% ; $n = 167/198$) with a low number of false-positive cases (16% ; $n = 31/198$).

In the scatter-plots of the *Empirical* and *Bio-optical* algorithms, the circles in Figs. 2a, c and 3a, c highlight that most failures in the red tide detection (i.e. false-negative cases) came from regions and periods other than the CWFS Summer–Fall. Also depicted in Figs. 2a–d and 3a–d is the fact that the majority the correct indications on the satellite measurements (i.e. HAB-positive and HAB-negative) were indeed on the CWFS Summer–Fall.

The 2nd set of statistical measures (i.e. the four predictive values) of the matchup pairs sampled along the CWFS during the Summer and Fall months are presented in Table 5c, f, i. The positive predictive values ($\sim 55\%$) – and its inverse ($\sim 45\%$) – of all three algorithms were similar, while the negative predictive values (and its inverse) varied from $\sim 63\%$ ($\sim 37\%$) for the *Operational Method* to $\sim 80\%$ ($\sim 20\%$) for the *Empirical* and *Bio-optical* algorithms.

4.4. Optimized outcomes

Because of the considerable overlap in the optical characteristics of the red tide and non-bloom populations observed in the outputs of the *Operational Method* (Figs. 2e–h and 3e–h), the optimization procedure was only performed on the *Empirical Approach* and *Biooptical Technique* (Fig. 4). This procedure does not changes the prevalence of red tides or the “odds” of red tides (Table 5a, d), as the red tide and non-bloom classification is pre-defined by the cell count limit of 1.5×10^4 cells L^{-1} in the *in situ* data (Section 3.4).

Higher multiplicative factors caused both algorithms to have a large number of red tide samples correctly identified (i.e. good sensitivity), but the accuracy of detecting non-bloom cases was very degraded, thus causing many false-positive cases (Fig. 4). With the highest multiplicative factor (3.0), the *Empirical Approach* flagged 100% of the red tides cases, but just 10% of non-bloom cases were correctly detected. The same pattern was observed for the *Bio-optical Technique* where up to 86% of the red tides were correctly flagged, and only 43% of the non-bloom cases being correctly detected—maximum factor in Fig. 3a–d and Table 4a.

Both algorithms had higher percentages of correct identification of non-bloom cases (i.e. good specificity) when the multiplicative factor was set low, but these factors worsen the percentage of correct identification of red tide, thus causing many false-negatives (Fig. 4). With the lowest multiplicative factor (0.33), both *Empirical* and *Biooptical* algorithms

successfully detected >90% of non-blooms but only 5.5% of the red tide samples—minimum factor in Fig. 3a–d and Table 4b.

The optimized detection threshold function was generated with similar factors: 0.82 for the *Empirical Approach*, and 0.87 for the *Biooptical Technique* (Fig. 4: vertical solid line). Multiplying the original Morel (1988) threshold slope lines by these factors defines the best threshold separating HAB-positive from HAB-negative cases (Fig. 3a–d: solid lines). This step created a better balance in the sense of having algorithms that are as sensitive as specific (Table 4d), thus changing the 1st set of statistical measures: both algorithms correctly classified most red tides and non-bloom cases similarly (~70%), having low (~30%) false conditions (Table 6b, e).

Optimization caused the number of samples flagged as HAB-positive and HAB-negative cases to change, resulting in a slight improvement in the overall accuracy (Table 6a, d). The 2nd set of statistical measures also changed (Table 6c, f). Even though there was a slight drop in the good negative predictive values (~80%), improvements were achieved in the positive predictive values (~60%). The uncertainties were: InegPV ~20% and IposPV ~40%.

4.5. Examples of imagery

Fig. 5 shows MODIS-Aqua measurements along the west coast of Florida during boreal Summer and Fall months: August 24, 2005 (1st column) and September 29, 2005 (2nd column); November 09, 2005 (3rd column). The 1st row (A-panels) illustrates the $L_w(551)$, the 3rd row (C-panels) shows Chl concentration derived with OC3M, and the 5th row (E-panels) presents the derived $b_{bp}(551)$ using Carder99.

The results of applying the *Empirical Approach* (B-panels) and the *Bio-optical Technique* (D-panels) are shown in Fig. 5 between the pair of images depicting the variables used in the algorithms (Section 2). The red areas in these maps represent those pixels which were identified as being HAB-positive following the optimization procedure (see above); the green areas are HAB-negative and the white represent cloud or no-data.

The outcomes of the application of the *Empirical* and *Bio-optical* algorithms shown in the in these examples (i.e. Fig. 5b, d) are quite similar; results that are in accordance with initial expectations of Carvalho et al. (2007) and Carvalho (2008). But, examination of images does not provide us with any means of knowing which, if either, algorithm is producing a meaningful and useful outcome. To provide a quantitative estimate of the accuracy of the algorithms, comparisons with independent *in situ* measurements are required (Section 3.3). Furthermore, a rigorous statistical analysis is required to establish the required metrics of performance (Section 3.4). The study of matchups between satellite data and collocated *in situ* measurements of *K brevis*, as the one presented here, has the objective of obtaining convincing estimates of the ability of algorithms applied to distinguish between presence or absence of HABs.

Some HAB-positive regions (i.e. the red areas) appear near the Florida Panhandle, Florida Keys, and also on the east coast of Florida (Fig. 5). Referring to the results of the spatio-temporal investigation (Section 4.2) the algorithms are domain specific and should be limited to the CWFS (i.e. between 25.75°N and 28.25°N). Thus, the outcomes beyond this region are not necessarily trustworthy.

5. Discussion

5.1. Valid matchup considerations

Because the quality of the validation data set is critical for assessing the accuracies of the algorithms, the steps of the automated matchup analysis are discussed in this section. The numerous data exclusion criteria, intended to eliminate possible sources of errors, introduced more confidence in our findings. On the other hand, even though we were very careful in designing our stringent quality control tests, it is still possible that bad data might have been accepted. In fact, some biases are commonly present in automated matchup analyses, especially when long-term data records are used. The occurrence of unusual environmental conditions, e.g. extreme weather events such as an intense rainy season bringing greater riverine input, enriched with colored organic dissolved matter (CDOM) to coastal regions, can create inaccuracies in the interpretation of the satellite ocean color signal, and the incorporation of such data may add errors to the analysis. Likewise, as some stations of the FRWI-database were sampled at multiple depths at the same site, more than one *in situ* sample might have passed the quality control imposed by the light penetration mask in some locations. If some of these coincident observations consisted of different cell counts (i.e. lying above and below 1.5×10^4 cells of *K. brevis* L⁻¹), some uncertainties may have been incorporated.

The half pixel (i.e. 500 m) buffer zone applied around the Florida coast may still lead to the use of few inappropriate satellite observations since satellite imagery is subject to geolocation inaccuracies (Patt, 2002), even though these are much smaller than one pixel for MODIS (Wolfe et al., 2002). As the MODIS scan lines are roughly perpendicular to the Florida coast, distances of three pixels (i.e. ~3 km) from coastlines or bright targets (e.g. clouds or sun glint) could perhaps help to eradicate residual along-scan effects from near field scattering (Franz et al., 2005).

Matchup analyses usually suffer from a low number of available data. Wider matchup acceptance windows, both temporal and spatial, may overcome this limitation (Bailey et al., 2000). We accepted *in situ* satellite pairs within the same day, which is not too critical given the relative slow e-folding time of *K. brevis* growth rates compared to other phytoplankton species (Shanley & Vargo, 1993). However, near-surface currents could have added noise in circumstances with localized algal concentration variability (Denman et al., 1977). Similarly, sub-pixel variability likely results in some uncertainties in the validation process, as point *in situ* measurements might not always be representative of the areal averaging implicit in the spatially integrated signal sensed by the satellite field-of-view (Mahadevan & Campbell, 2002). Since a pixel-by-pixel analysis can limit the final number of matchup pairs, multi-pixel areas centered on the field measurements (e.g. 3×3 , 5×5 or 7×7 pixels) are commonly used to increase the number of samples by accepting cloud-free pixels adjacent to the collocated cloudy matchup pair. Conversely, multi-pixel areas can add other uncertainties in the presence of horizontal gradients.

Even though our number of final valid matchups appears small when compared to the initial *in situ* FWRI-database population – [778/6146] ~13% in the west coast of Florida, and [371/3420] ~11% in the CWFS Summer–Fall – these matchups refer to a fully quality-assured data set. On the other hand, it is important to note that in our analysis, the accuracy of the *Empirical*, *Bio-optical* and *Operational* algorithms has been determined with a large number of samples compared to other ocean color studies in the published literature. Here, around 195 samples year⁻¹ were available off the west coast of Florida; in the CWFS in the Summer and Fall months we had around 95 samples year⁻¹ (Table 2 [b1 and d1]). To validate SeaWiFS Chl in Massachusetts Bay, Hyde et al. (2007) used ~60 samples year⁻¹; in

the Mediterranean Sea, Volpe et al. (2007) used ~ 50 samples year^{-1} ; and Otero and Siegel (2004) had only about 45 samples year^{-1} in the Santa Barbara Channel.

Some complications may occur when using satellite ocean color imagery in shallow water, e.g. the presence of in-water constituents that vary independently of phytoplankton (IOCCG, 2000). This can skew the estimation of absorbing aerosols and the subsequent atmospheric corrections, decreasing the derived $L_w(\lambda)$ signal at the top of the atmosphere (Morel & Bélanger, 2006). Applications of standard global blue-to-green band-ratio algorithm (e.g. OC3M; O'Reilly et al., 2000) may overestimate Chl concentrations in certain coastal waters (Ruddick et al., 2000). Therefore, the use of different Chl retrieval algorithms (e.g. Stumpf00, Carder99 or OC3M) may lead to slightly different results. Similarly, challenges to validating HAB detection algorithms are inherent in the nature of the field measurements. As we only focused on *K. brevis*, other investigations conducted in a similar fashion as here but, accounting for the occurrence of the entire genus *Karenia* may produce somewhat different results.

5.2. Performance of the HAB-specific algorithms

We have used, for the first time, a long-term data set of MODIS-Aqua measurements (2002 to 2006) to identify optical characteristics – in terms of $L_w(551)$ and $b_{bp}(551)$, as a function of Chl – related with blooms of *K. brevis* containing $\geq 1.5 \times 10^4$ cells L^{-1} (Figs. 2 and 3). Even though the FWRI-database was not compiled for the purpose of validating satellite-based algorithms (Haverkamp et al., 2004), these *in situ* measurements provided a very valuable resource to study the identification of *K. brevis* using an automated matchup analysis (i.e. independent of the intervention of analysts) and establishing the accuracy of the three different HAB-specific algorithms (Tables 5 and 6).

The overall detection capabilities of the *Empirical* and *Bio-optical* algorithms are promising when analyzing the samples collected year-round along the west coast of Florida; conversely, this was not so for the *Operational Method*, as shown in Fig. 2. The data distribution had geographical constraints: relatively few red tide samples were valid matchups in the South-FL and North-FL regions (Table 3), and so our conclusions here are limited to the CWFS (Fig. 1). Also, as the data density did not permit a study of the time-dependent signal throughout the year, or from year to year, our conclusions are seasonally restricted to the Summer and Fall months (Table 3). Thus, our results are domain specific and solely related to the CWFS in Summer–Fall (Fig. 3; Table 5), using the cell count of 1.5×10^4 cells L^{-1} .

Even though Carvalho (2008) has shown comparability between the performances of the *Empirical* and *Bio-optical* algorithms in differentiating between the presence or absence of the Florida Red Tide, in a particular field-verified event at the end of August 2001 using data from SeaWiFS and MODIS-Terra, the research reported here evaluates the accuracies of these two algorithms in a more comprehensive fashion using a multi-year MODIS-Aqua data set (from 2002 to 2006). The initial version of the *Empirical Approach* did not perform as satisfactorily as the initial version of the *Bio-optical Technique* in terms of the 1st statistical measures (Table 5d–f), but the optimization process improved the performance of both. Our results have demonstrated that the long-term performance of the *Bio-optical Technique* is indeed in accordance with early expectations of Cannizzaro et al. (2008).

Our findings regarding the *Bio-optical Technique* differ from those presented by Hu et al. (2008), who concluded that this technique was not effective at detecting HABs. Reasons for this disparity may include: (1) the conclusions of Hu et al. (2008) were based on SeaWiFS imagery from 1997 to 2002; (2) the matchups pairs produced in Hu et al. (2008) were conducted with a 3×3 pixel-box, rather than the single pixels used here; (3) the stringent

quality control tests with rigorous data exclusion performed in our study retained only the best available data; (4) our red tide detection analysis was constrained to the CWFS area (Fig. 1); (5) our application of the *Bio-optical Technique* replicated Cannizzaro et al. (2008) scheme using the $b_{bp}^{MOREL}(550)$ function from Morel (1988), whereas Hu et al. (2008) used a different approach using a threshold ratio between $b_{bp}(555)$ and Chl; and (6) we used Carder99 to estimate $b_{bp}(\lambda)$ following suggestions of the original development of the *Biooptical Technique* (Cannizzaro et al., 2008) whereas Hu et al. (2008) derived $b_{bp}(\lambda)$ using Lee et al. (1999). Tomlinson et al. (2009) used visual means for the validation of a selection of SeaWiFS images (from 1998 to 2005, with *a priori* known blooms of *K. brevis* [$n = 34$] and non-blooms [$n = 18$]), their conclusions on the performance of the *Bio-optical Technique* are in general agreement with our findings.

When comparing the statistical results of the *Empirical Approach* with the *Operational Method*, both algorithms perform inversely in terms of the detection of known red tide and non-bloom cases. At one conceptual extreme, it is expected that an algorithm flagging the majority of the ocean as HAB-positive would correctly identify nearly all red tide samples, but would cause many false-positive cases (e.g. maximum factor in Fig. 3a–d and Table 4a). This was in fact the tendency of the initial version of the *Empirical Approach* (original factor in Fig. 3a, b; Tables 4c and 5b), which was the best algorithm at flagging red tides samples (86%; excellent sensitivity) but not as accurate in identifying non-bloom cases (53%; modest specificity). At the other extreme, a conceptual algorithm classifying most of the ocean as non-bloom would have high specificity but an excess of undesirable false-negatives cases (e.g. minimum factor in Fig. 3a–d and Table 4b). Indeed, the *Operational Method* (Fig. 3e, f; Tables 4e and 5h) was the most effective in identifying non-bloom cases (84%; excellent specificity) but less effective at detecting red tides samples (26%; weak sensitivity); the same pattern observed while using the NOAA-HAB-FS cell count limit of 10×10^4 cells L^{-1} (Fig. 3g, h; Table 4f).

From Bayes' theorem, it should be expected that false-positives as opposed to false-negatives occur more frequently in lower prevalence populations (Sokal & Rohlf, 1995). This was indeed observed for the initial versions of the *Empirical* and *Bio-optical* algorithms that had fewer false-negatives than false-positives cases, but was not found for the *Operational Method*. This divergent performance could be related to the sole use of anomaly fields of Chl in the *Operational* algorithm. As the Chl content is not solely related to the presence of any specific HAB species, since all microalgal species contain Chl pigments (Garver et al., 1994), caution should be exercised given that any major bloom-forming photosynthetic group can give rise to such a Chl anomaly. Also, if blooms persist long enough to robustly contribute to the reference Chl mean signal, this may prevent the correct identification of a particular HAB event (Tomlinson et al., 2004). Another plausible reason for the poorer performance of the *Operational Method* in detecting known red tide samples (Table 5g–i and Figs. 2e–h and 3e–h) is the fact that in the NOAA-HAB-FS implementation additional ancillary information (Section 2.1) is incorporated along with a series of rules for including the interpretation of analysts (Stumpf et al., 2009), while our investigation completed a matchup analysis with the purpose of being automated, based on the stringent quality control tests (Section 3.3).

The findings of our analysis of the *Operational Method* suggest it was not able to automatically separate red tide and non-bloom samples with certainty, regardless of cell count limit used. This is depicted in Fig. 3e–h and by the statistics shown in Tables 4e, f and 5g–i. Tomlinson et al. (2009) also reported on the performance of the *Operational Method*, and even when involving visual validation of 52 selected SeaWiFS scenes (from 1998 to 2005), their results are consistent with our findings. Accordingly, in an analogous multi-year

in situ satellite pairing, using SeaWiFS data (from 1997 to 2002), Hu et al. (2008) reported the success of this method only at detecting “new” blooms having $\geq 10 \times 10^4$ cells L^{-1} .

According to some metrics (e.g. overall accuracy) the initial versions of the three algorithms exhibited similar, moderate levels of success (Table 5a, d, g). Nonetheless, the detection excellence in terms of sensitivity and specificity, as well as the level of false conditions, varied considerably (Table 5b, e, h). This confirms that the exclusive use of overall accuracy could mislead end users by not being a fair representation of the real performance of the algorithms. However, this metric could be satisfactorily utilized (Table 6a, d) once specificity and sensitivity values present similar magnitudes, e.g. as observed in the optimized versions of the *Empirical* and *Bio-optical* algorithms (Table 6b, e).

After the optimization procedure, the number of samples flagged as HAB-positive and HAB-negative of the *Empirical* and *Bio-optical* algorithms changed (Table 6a, d). As a result, the accuracies of the 1st set of statistical measures also changed (Table 6b, e). While more non-bloom samples were correctly identified (lowering the false-positive cases), slightly fewer red tides were correctly detected (increasing the number of false-negatives). In spite of the changes in the number of samples correctly detected, both algorithms end up being equally specific and sensitive (~70%) at identifying *K. brevis* blooms and non-blooming conditions.

Besides creating balanced algorithms that performed satisfactorily and similarly at correctly detecting known HABs and non-blooming conditions (Table 4d), the 2nd set of statistical measures of the optimized algorithms (Table 6c, f) showed improved capability in the sense of having more red tide samples correctly flagged as HAB-positive (i.e. better positive predictive values; ~60%) compared to before optimization. However, slightly fewer non-bloom samples were correctly identified as HAB-negative, but the negative predictive values of both *Empirical* and *Bio-optical* algorithms are still high (~80%).

The long-term evaluation of the accuracy of the HAB-specific algorithms provides a range of perspectives for end users who might have different priorities and objectives. For example, if there is interest in promoting improved seafood safety regulations, thus being more protective of human health, the best option could be the initial version of the *Empirical Approach* that detected most of the known red tides and caused the smaller number of false-negative cases (Table 5a, b). But, given a need to avoid significant localized negative economic impacts, a user could opt for using the *Operational Method* that produced fewer false-positive cases, being the best algorithm to correctly detect non-bloom cases (Table 5g, h). Therefore, end users have the choice of which algorithm to select.

However, if decision makers have to cover a wide range of mitigation action plans, such as possible human health problems at the same time as reducing local economic consequences, the choice should be either one of the optimized versions of the two algorithms (i.e. *Empirical*: Table 6a, b and *Bio-optical*: Table 6d, e), as both showed simultaneously good capabilities to detect red tides and non-blooms (~70%) along with few false-negatives and -positives cases (~30%). Besides this good balance in correctly detecting known cases, the optimized versions of these two algorithms also showed improved positive predictive values (i.e. better correct indications of HAB-positive) along with good negative predictive values (Table 6c, f). The characteristics of the 2nd set of statistical measures are useful in locating sites where possible events of the Florida Red Tide might be present and where there likelihood of facing one is lower. This can assist in better direction in field monitoring surveys, optimizing the efficient use of scarce resources.

Although the performances of the *Empirical Approach* and the *Bio-optical Technique* are similar, it is evident that the cases of red tides and non-blooms samples correctly identified

by these two algorithms are not identical (Table 4a–d). Even though the *Empirical Approach* does not use a Chl threshold criterion as does the *Bio-optical Technique* (i.e. $\text{Chl} \geq 1.5 \text{ mg m}^{-3}$; graphically represented by the vertical dashed line in Fig. 3c, d), a careful examination of the scatter-plots in Fig. 3a to c, and those in Fig. 3b to d, indicates that a number of samples with high-Chl concentrations are not correctly identified by this algorithm but are correctly detected by the other, and vice-versa. This is explicable by the fact that the two algorithms are based on different combinations of variables, i.e. they are attempting to discriminate red tides and non-blooming conditions on two different plane surfaces in multi-dimensional parameter space. While it is true that $b_{\text{bp}}(551)$ derived using Carder99 ($b_{\text{bp}}(551) = [2.058 * R_{\text{rs}}(551)] - 0.00182$), is related to $L_{\text{w}}(551)$, there are increased uncertainties inherent in using $b_{\text{bp}}(551)$ as this expression is a simple linearization of a complex set of processes, and the coefficients in the linear relationship (i.e. slope and offset) are themselves subject to uncertainties. Furthermore, the threshold slope lines used to discriminate between red tide and non-bloom conditions are not the same in the two algorithms. This suggests that sequential, or parallel, application of the *Empirical* and *Bio-optical* algorithms could provide end users with additional information on which to base decisions (Carvalho et al., 2010).

Independently, Tomlinson et al. (2009) emphasize that improvements in detecting the Florida Red Tide using satellite measurements can occur if different methods are combined. Using SeaWiFS imagery, they found that better results could be achieved if an ensemble of different methods were to be applied together: they suggest the *Operational Method*, an adapted version of the *Bio-optical Technique* using a different threshold ratio between $b_{\text{bp}}(551)$ and $b_{\text{bp}}^{\text{MOREL}}(551)$, and a spectral shape function of nL_{w} at $\lambda \sim 490 \text{ nm}$. In addition, Tomlinson et al. (2009) explored the use of FLH but found its success in identifying the Florida Red Tide to be inconclusive as a restricted number of images were available ($n < 10$). Other researchers investigating the use of FLH to detect *K. brevis* blooms, such as Hu et al. (2005), have found promising correlation with *in situ* Chl concentration and identified a particular field-verified HAB event during 2004 along the southwest Florida coast using MODIS FLH measurements. We also explored the use of FLH using our final quality-controlled matchup data set but found it not to be amongst the best variables, as listed in Appendix A, suited for *K. brevis* detection.

An advantage of using either the *Empirical Approach* or the *Bio-optical Technique* over the *Operational Method* to detect the Florida Red Tide lies in the use of additional variables, i.e. $L_{\text{w}}(551)$ and $b_{\text{bp}}(551)$, as well as Chl. As a consequence, the combined use of the *Empirical* and *Bio-optical* algorithms in an automated surveillance system could become an attractive option for locating *K. brevis* blooms (Carvalho et al., 2010).

6. Concluding remarks

For the first time the identification of the Florida Red Tide (defined as cell counts of *K. brevis* $\geq 1.5 \times 10^4 \text{ cells L}^{-1}$) was accomplished using MODIS-Aqua data ($n = 744$ satellite scenes) over >4 years, from July, 2002 to October, 2006. Near-coincident *K. brevis* abundances ($n = 6146$ field observations) were used for optimizing the algorithms and for validation. Stringent quality control tests (Section 3.3), removed sources of potential contamination from the matchup data set and guaranteed that only the best available data were used as final valid cloud-free matchup pairs ($n = 778$ matchups collected year-round along the entire west coast of Florida). These matchups supported the long-term evaluation of the performance of the *Empirical Approach* (Carvalho, 2008) and the comparison to that of the *Bio-optical Technique* (Cannizzaro, 2004; Cannizzaro et al., 2008) and the *Operational Method* (Stumpf et al., 2003; Tomlinson et al., 2004, 2009). The detection success in identifying non-bloom samples was similarly good for all algorithms: >70% (Fig.

2b, d, f, h). But, the correct identification of red tide samples was quite different: 61%, 53%, and ~35% for the *Empirical*, *Bio-optical* and *Operational* algorithms, respectively (Fig. 2a, c, e, g).

Largely because of the distribution of the available *in situ* data (Section 4.2), the best results were domain specific being limited to the central west Florida shelf (CWFS) during the boreal Summer and Fall months ($n = 371$ matchups; Fig. 3 and Table 5). These were derived from 107 MODIS-Aqua scenes. Despite the fact that the three algorithms derived similar predictive values (Table 5c, f, i), the *Operational Method* was not as effective as the other two algorithms in distinguishing known cases of red tides from non-blooms (Table 5b, e, h). None of the algorithms is perfect and this could be due to the incomplete information provided by satellite sensors, the existing uncertainties in the satellite and *in situ* measurements, and the overlap observed in the optical characteristics of situations containing more or less than 1.5×10^4 cells of *K. brevis* per L^{-1} .

The *Empirical Approach* and *Bio-optical Technique* were optimized and produced more balanced detection rates (Fig. 4) having higher sensitivity simultaneously with higher specificity (~70% for both) together with low levels of uncertainties (i.e. fewer cases of false-negatives and false-positives: ~30%) and improved positive predictive values (~60%) along with good negative predictive values (~80%)—Table 6. Hence, by incorporating the outcomes of these optimized algorithms in mitigation action plans, several societal groups can be assisted—e.g. beachgoers, coastal inhabitants, medical health practitioners, the scientific community, resource and environmental managers, and to the tourism and aquaculture industries. Even though both optimized versions of the *Empirical Approach* and *Bio-optical Technique* have reached simultaneously good detection levels, there remains scope for improving the detection of the Florida Red Tide using satellite measurements such as the sequential scheme application of these two algorithms (Carvalho et al., 2010); or other innovative approaches.

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Fig. 1. ETOPO2 bathymetry from the west coast of Florida (units in meters). Horizontal lines indicate sub-regions limits (28.25°N and 25.75°N): North-FL, South-FL and central west Florida shelf (CWFS).

Fig. 2.

Detection results of the whole data set, i.e. year-round valid matchups sampled along the entire west coast of Florida. Red tides (redT; “□”; left panels) and non-blooms (nonB; “×”; right panels) are $\geq$ or $< 1.5 \times 10^4$ *K. brevis* cells L⁻¹, respectively. Shaded area indicates HAB-positive algorithm classification. (a, b) *Empirical Approach* (dashed line: theoretical total backscatter at $\lambda = 550$ nm calculated using Morel (1988) models). (c, d) *Bio-optical Technique* (vertical dashed line: 1.5 mg m^{-3} of chlorophyll; and inclined dashed line: theoretical particulate backscatter at $\lambda = 550$ nm calculated using Morel (1988) models). (e, f) *Operational Method* (dashed line: chlorophyll anomalies of 1 mg m^{-3}). (g, h) *Operational Method* (same as e, f but using the official cell count limit of 10×10^4 *K. brevis* cells L⁻¹

implemented by the NOAA-HAB-FS). The circles in panels a and c indicate the failure in the red tide detection (i.e. false-negatives).

Fig. 3.

Final valid matchups of the central west Florida shelf (CWFS) sampled during the Summer and Fall months. Red tides (redT; “□”; left panels) and non-blooms (nonB; “×”; right panels) are $\geq$ or $< 1.5 \times 10^4$ *K. brevis* cells L^{-1} , respectively. (a, b) *Empirical Approach*. (c, d) *Bio-optical Technique*. (e, f) *Operational Method*. The official cell count limit of 10×10^4 *K. brevis* cells L^{-1} implemented by the NOAA-HAB-FS in used in the *Operational Method* is shown in g and h. Dashed lines indicate the original threshold lines (multiplying factor of 1.00; same as in Fig. 2)—the shaded area indicates HAB-positive algorithm classification with this factor. The upper and lower dotted lines indicate the threshold lines multiplied by the maximum (3.00) and minimum (0.33) factors, respectively (Section 3.5). The solid lines

are the product of the optimized multiplying factors: 0.82 for the *Empirical Approach* and 0.87 for the *Bio-optical Technique* (See Fig. 4). Table 4 presents the detection results of red tides and non-blooms for each factor. The circles on panels a and c are equivalent to those in Fig. 2a, c—thus confirming that most of the failure in the red tide detection (i.e. false-negatives) did not come the CWFS Summer–Fall.

Fig. 4.

Optimized procedure of the *Empirical Approach* (left panel) and *Bio-optical Technique* (right panel). Frequency of correct identification (Y-axis) in the central west Florida shelf (CWFS) during the Summer and Fall months as a function of the threshold slope lines (Morel, 1988) multiplied, in steps of 0.01, by a factor varying from 0.33 to 3.00 (X-axis). The vertical dashed lines represent the original thresholds (multiplying factor of 1.00)—the percentages of correct identification of the “initial” versions of the algorithm are shown. The vertical solid lines represent the optimized factors (0.82 for the *Empirical Approach* and 0.87 for the *Bio-optical Technique*). The crossing of the two segment-lines identifies the higher, and simultaneous, red tide (redT) and non-bloom (nonB) detection (~70%). See Fig. 3a–d for the scatter-plots referent to these results and Table 4 for the detection frequency of the different factors.

Fig. 5.

Examples of MODIS-Aqua imagery along the west coast of Florida during boreal Summer and Fall: August 24, 2005 (Column-1); September 29, 2005 (Column-2); November 9, 2005 (Column-3). Top panels (A's) illustrate the water-leaving radiance ($L_w(551)$). Middle panels (C's) show chlorophyll (Chl) concentration derived with OC3M. Bottom panels (E's) present the derived particulate backscatter ($b_{bp}(551)$; Carder et al., 1999). In the spatial distributions of the outcomes from the *Empirical Approach* (B's) and *Bio-optical Technique* (D's) the presence of the Florida Red Tide is shown in red (i.e. HAB-positive) and its absence in green (i.e. HAB-negative). White indicates missing data, most often caused by cloud cover.

Table 1

Error matrix (a) expressed in terms of *a priori* known red tides (RT; correctly flagged as HAB-positive [A; in red] and incorrectly flagged as HAB-negative [B]), and *a priori* known non-blooms (NB; incorrectly flagged as HAB-positive [C] and correctly flagged as HAB-negative [D; in green]). For ideal algorithms $B = C = 0$. Also shown: overall accuracy, prevalence and “odds” of RT, and the two sets of detailed statistical measures ($b^{\dagger}$, $c^{\ddagger}$) used to evaluate the accuracy of the algorithms. See Section 3.4 for further details.

a) Detection frequency

Algorithm version		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	A	B	A+B
	False (NB)	C	D	C+D
Sum		A+C	B+D	Total
Overall accuracy=[A+D]/[A+B+C+D]				
Prevalence of RT=[A+B]/[A+B+C+D]				
“Odds” of RT=[A+B]/[C+D]				

b) 1st set of statistical measures †

Algorithm version		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	A/[A+B] Sens	B/[A+B] Fneg	A+B
	False (NB)	C/[C+D] Fpos	D/[C+D] Spec	C+D

c) 2nd set of statistical measures ‡

Algorithm version		Algorithm outcome	
		True (RT)	False (NB)
<i>In situ</i> cell count	True (RT)	A/[A+C] posPV	B/[B+D] InegPV
	False (NB)	C/[A+C] IposPV	D/[B+D] negPV
Sum		A+C	B+D

† Based on the “*in situ* cell count” (rows). Red indicates known HABs (A + B) while green indicates known non-blooms (C + D), such that: sensitivity (Sens; A/[A + B]), false-negatives (Fneg; B/[A + B]), false-positives (Fpos; C/[C + D]), and specificity (Spec; D/[C + D]).

‡ Based on the “algorithm output” (columns). Red indicates flagged as HAB-positive (A + C) while green indicates identified as HAB-negative (B + D), such that: positive predictive value (posPV; A/[A + C]), inverse of the positive predictive value (IposPV; C/[A + C]), inverse of the negative predictive value (InegPV; B/[B + D]), and negative predictive value (negPV; D/[B + D]).

Table 2

Data frequency. Shaded areas indicate the number of all samples through the phases of the matchup analysis, thus illustrating the decrease in data availability—see Section 4.1 for details deeming different data elimination filtering. The cell count limit of 1.5×10^4 *K. brevis* cells L^{-1} defines red tide ($\geq$) and non-blooms ($<$) samples; color coded in red and green, respectively.

	Total number of samples within the Florida HAB Historical Database	MODIS mission (from 2002 to 2006)	All samples	
			21015	
a1				
a2		After filtering: 1st data elimination	Considering <i>K. brevis</i> samples, ETOPO2 and the buffer zone.	7929 (a2/a1) ~38%
a3		After filtering: 2nd data elimination	Workable subset within MODIS swaths	6146 (a3/a2) ~78%
b1	Valid cloud-free match-ups sampled year-round along the entire west coast of Florida.		All samples	778 (b1/a3) ~13%
b2		After filtering: 3rd data elimination	Red Tide	247 (b2/b1) ~32%
b3			Non-bloom	531 (b3/b1) ~68%
c1	Final valid match-ups of the central west Florida shelf (CWFS)		All samples	529 (c1/b1) ~68%
c2		Sampled year-round	Red Tide	182 (c2/c1) ~34%
c3			Non-bloom	347 (c3/c1) ~66%
d1	Sampled during the Summer and Fall months		All samples	371 (d1/c1) ~70%
d2			Red Tide	145 (d2/c2) ~80%
d3			Non-bloom	226 (d3/c3) ~65%

Final number of valid cloud-free matchups of the *Empirical Approach* and *Bio-optical Technique* presented by region (i.e., North-FL, South-FL and central west Florida shelf) and period (i.e., Winter–Spring (WS) and Summer–Fall (SF)); after stringent quality control tests of Section 3.4. The presence (red tide; $\geq$; in red) and absence (non-bloom; $<$; in green) of *K. brevis* is based on the cell count limit of 1.5×10^4 cells L^{-1} . As the *Operational Method* requires additional processing steps (i.e. a Chl anomaly calculation imposing a minimum number of pixels per bin; Section 2.1) the total number of valid matchup pair used for this algorithm is smaller and indicated († and ‡).

Table 3

		(n = 778)				(n = 84)				(n = 165)				(n = 529)			
		Entire west coast of Florida				North-FL				South-FL				CWFS			
Sub-group	Year-round	WS	SF	WS	SF	WS	SF	WS	SF	WS	SF	WS	SF	WS	SF	WS	SF
Red tide	247	44	203	0	22	7	36	37	145								
Non-bloom	531	195	336	14	48	60	62	121	226								
All samples	778 [†]	239	539	14	70	67	98	158	371 [‡]								

[†] [223, 497, 680] and [‡] [130, 198, 328].

Table 4

Detection results of the valid matchups of the central west Florida shelf during the Summer and Fall months (2002 to 2006) during the optimization procedure (Section 3.5). Different multiplying factors used in the optimization procedure are shown: maximum (a), minimum (b), original (c; gray shading) and optimized (d; bold). For the *Operational Method* (e, f) only the original factor is shown but with different cell count limits (as indicated). Dotted, dashed and solid lines are the same as in scatter-plots of Fig. 3. Percentages are expressed as the number of samples correctly identified in each sub-group (n), based on the cell count limit of 1.5×10^4 *K. brevis* cells L^{-1} (a color code indicates red tides and non-blooms), divided by the sub-group population (pop)—thus indicating sensitivity and specificity. See Table 5 for the complete detection frequency of the two sets of detailed statistical measures of the “initial” versions of the algorithms.

<i>Empirical Approach</i> (Total = 371)		Red tides (pop = 145)		Non-blooms (pop = 226)	
Multiplying Factor		n	Sensitivity	n	Specificity
a) Maximum	3.00	 145	100%	23	10%
b) Minimum	0.33	 8	5.5%	218	97%
c) Original	1.00	----- 124	86%	119	53%
d) Optimized	0.82	— 102	70%	152	67%
<i>Bio-optical Technique</i> (Total = 371)		Red tides (pop = 145)		Non-blooms (pop = 226)	
Multiplying Factor		n	Sebsitivity	n	Specificity
a) Maximum	3.00	 125	86%	97	43%
b) Minimum	0.33	 8	5.5%	209	93%
c) Original	1.00	----- 111	77%	147	65%
d) Optimized	0.87	— 104	72%	162	72%
<i>Operational Method</i> (Total = 328)		Red tides (pop = 130, 85)		Non-blooms (pop = 198, 243)	
Cell count limit		(n/pop)	Sensitivity	(n/pop)	Specificity
e) 1.5×10^4 Cells L^{-1}	-----	(34/130)	26%	(167/198)	84%
f) 10×10^4 cells L^{-1}	-----	(28/85)	30%	(206/243)	85%

Table 5

Detection frequency for the “initial” versions of the *Empirical Approach* (a), *Bio-optical Technique* (d), and *Operational Method* (g) along the central west Florida shelf during Summer and Fall months (from 2002 to 2006). Presence (RT) and absence (NB) of *K. brevis*, respectively $\geq$ and $< 1.5 \times 10^4$ cells L^{-1} . Overall accuracy, prevalence and “odds” of RT are also shown along with the two sets of detailed statistical measures (1st set: panels b,e,h; and 2nd set: panels c, f, i). Refer to Table 1 for detailed information about how to calculate these metrics and color-coding.

a) Detection frequency

<i>Empirical Approach</i>		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	124	21	145
	False (NB)	107	119	226
Sum		231	140	371
Overall accuracy = (243/371) ~65%				
Prevalence of RT = (145/371) ~39%				
“Odds” of RT = (145/226) ~64%				

b) 1st set of statistical measures

<i>Empirical Approach</i>		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	80% Sens	14% Fneg	100%
	False (NB)	47% Fpos	53% Spec	100 %

c) 2nd set of statistical measures

<i>Empirical Approach</i>		Algorithm outcome	
		True (RT)	False (NB)
<i>In situ</i> cell count	True (RT)	54% posPV	15% InegPV
	False (NB)	46% IposPV	85% negPV
Sum		100%	100%

d) Detection frequency

<i>Bio-optical Technique</i>		Algorithm outcome		Sum
		True (RT)	False (RT)	
<i>In situ</i> cell count	True (RT)	111	34	145
	False (NB)	79	147	226
Sum		190	181	371
Overall accuracy = (258/371) ~70%				
Prevalence of RT = (145/371) ~39%				
“Odds” of RT = (145/226) ~64%				

e) 1st set of statistical measures

<i>Bio-optical Technique</i>		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	77% Sens	23% Fneg	100%
	False (NB)	35% Fpos	65% Spec	100%

f) 2nd set of statistical measures

<i>Bio-optical Technique</i>		Algorithm outcome	
		True (RT)	False (NB)
<i>In situ</i> cell count	True (RT)	59% posPV	19% InegPV
	False (NB)	41% IposPV	81% negPV
Sum		100%	100%

g) Detection frequency

<i>Operational Method</i>		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	34	96	130
	False (NB)	31	167	198
Sum		65	263	328
Overall accuracy = (201/328) ~61%				
Prevalence of RT = (130/328) ~40%				
“Odds” of RT = (130/198) ~66%				

h) 1st set of statistical measures

<i>Operational Method</i>		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	26% Sens	74% Fneg	100%
	False (NB)	16% Fpos	84% Spec	100%

i) 2nd set of statistical measures

<i>Operational Method</i>		Algorithm outcome	
		True (RT)	False (NB)
<i>In situ</i> cell count	True (RT)	52% posPV	37% InegPV
	False (NB)	48% IposPV	63% negPV
Sum		100%	100%

Table 6

Detection frequency for the “optimized” versions of the Empirical Approach (a) and Bio-optical Technique (d) along the central west Florida shelf during Summer and Fall months (from 2002 to 2006). Presence (RT) and absence (NB) of *K. brevis*, respectively $\geq$ and $< 1.5 \times 10^4$ cells L^{-1} . Overall accuracy and the two sets of detailed statistical measures (panels b,e for 1st set, and panels c,f for 2nd set) are shown. See Section 3.4 and Table 1 for additional information.

a) Detection frequency

Optimized Empirical A.		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	102	43	145
	False (NB)	74	152	226
Sum		176	195	371
Overall accuracy = (254/371) ~68%				

b) 1st set of statistical measures

Optimized Empirical A.		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	70% Sens	30% Fneg	100%
	False (NB)	33% Fpos	67% Spec	100%

c) 2nd set of statistical measures

Optimized Empirical A.		Algorithm outcome	
		True (RT)	False (NB)
<i>In situ</i> cell count	True (RT)	58% posPV	22% InegPV
	False (NB)	42% IposPV	78% negPV
Sum		100%	100%

d) Detection frequency

Optimized Bio-optical T.		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	104	41	145
	False (NB)	64	162	226
Sum		168	203	371

d) Detection frequency

Optimized <i>Bio-optical T.</i>	Algorithm outcome		Sum
	True (RT)	False (NB)	
	Overall accuracy = (266/371) ~72%		

e) 1st set of statistical measures

Optimized <i>Bio-optical T.</i>		Algorithm outcome		Sum
		True (RT)	False (NB)	
<i>In situ</i> cell count	True (RT)	72% Sens	28% Fneg	100%
	False (NB)	28% Fpos	72% Spec	100%

f) 2nd set of statistical measures

Optimized <i>Bio-optical T.</i>		Algorithm outcome	
		True (RT)	False (NB)
<i>In situ</i> cell count	True (RT)	62% posPV	20% InegPV
	False (NB)	38% IposPV	80% negPV
Sum		100%	100%

Appendix A

MODIS-Aqua geophysical parameter library used during the quality control tests (Section 3.3) to assure that inappropriate information was not retained in the matchup analysis. The best variables for identifying the HABs using the *Bio-optical*, *Empirical* and *Operational* algorithms are indicated with gray shading (Section 2).

Variables	
$b_{bp}(\lambda)$	Particulate backscatter
$b(\lambda)$	Total scatter
$a_{ph}(\lambda)$	Absorption due to phytoplankton
$a_{dg}(\lambda)$	Absorption due to detritus and CDOM
$a(\lambda)$	Total absorption
The above inherent optical properties (IOPs) were retrieved as in Carder et al. (1999).	
$L_w(\lambda)$	Water-leaving radiance
$nL_w(\lambda)$	Normalized water-leaving radiance
$R_{rs}(\lambda)$	Remote-sensing reflectance
$kd(\lambda)$	Downwelling diffuse attenuation
All quantities above were processed in the following nine MODIS ocean-color bands centered at ($\lambda = \text{nm}$): 412, 443, 488, 531, 551, 667, 678, 748, and 869.	
Chl	Chlorophyll (OC3M; O'Reilly et al., 2000)
K_{490}	Downwelling diffuse attenuation coefficient
FLH	Fluorescence line-height
SST	Sea-surface temperature
Θ	Satellite zenith angle