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1	Shallow water bathymetry with multi-spectral satellite ocean color
2	sensors: leveraging temporal variation in image data
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21 Abstract

22 Polar-orbiting ocean color satellites such as Landsat-8, Suomi National Polar-orbiting 23 Partnership (SNPP), and Sentinel-3 offer valuable image data for the derivation of water 24 bathymetry in optically shallow environments. Because of the multi-spectral limitation, however, 25 it is challenging to derive bathymetry over global shallow waters without reliable mechanistic algorithms. In this contribution, we present and test a physics-based algorithm for improved 26 27 retrieval of bathymetry with multi-spectral sensors. The algorithm leverages the temporal variation 28 of water-column optical properties in two satellite measurements. By incorporating two remote 29 sensing reflectance spectra in an optimization procedure, it enhances the spectral constraining 30 condition for the optimization, thus leading to improved retrieval accuracy. This scheme was first 31 evaluated using synthetic multi-spectral data. It is shown that the new approach can provide 32 accurate estimation of water depths over 0-30 m range with three types of benthic substrates 33 (corals, seagrass, and sand) and for a wide range of water column optical properties. Based on the 34 degree of improvement, Landsat-8 appears to be benefited the most, followed by SNPP, and then 35 Sentinel-3. The application of the new approach is demonstrated with satellite images over shallow 36 waters (0-30 m) dominated with coral reefs, seagrass, and sand, respectively. This proof-of-37 concept study confirms the promise of multi-spectral satellite sensors for accurate water depth 38 retrieval by accounting for the temporal characteristics in multiple measurements, suggesting a 39 path forward for the derivation of bathymetry from the existing satellites over global shallow 40 waters.

⁴¹ Keywords: shallow water; bathymetry; spectral optimization; remote sensing reflectance;

⁴² temporal variation; Landsat-8; SNPP; Sentinel-3.

44 **1. Introduction**

45 Shallow water bathymetry is a basic geophysical parameter of coastal environments. Accurate 46 determination of bathymetry is pivotal for coastal utilization, including navigation, tourism, 47 resource management, and engineering. It is also important for many ecosystem-related studies, 48 such as benthic diversity and class identification, carbon cycling, and water quality. For almost 50 49 years, the derivation of shallow water bathymetry characteristic of various spatial resolutions has 50 been a hot spot for the ocean remote sensing community.

51 Advanced methods exist for measuring the bathymetry in shallow environments. Active sensing 52 instruments, such as multi-beam sonar and LiDAR, are widely used for shallow water exploration. 53 Provided necessary support, they allow for accurate bathymetric retrieval over targeted areas 54 (Goodman et al., 2013; McIntyre et al., 2006; Tuell et al., 2005; Wang and Philpot, 2007). Satellite 55 ocean color remote sensing is a passive yet powerful alternative for deriving depth. In optically 56 shallow waters, where the contribution of bottom reflection is non-negligible, the emerging light 57 spectra carry important information on the water depth, bottom albedo, and water column inherent 58 optical properties (IOPs) (Lyzenga, 1978). As such, the remote sensing reflectance $(R_{rs}(\lambda))$ has 59 long been utilized to derive bathymetry maps over optically shallow environments (Brando et al., 60 2009; Hedley et al., 2016; Klonowski et al., 2007; Kutser et al., 2020; Lee et al., 1999).

There are two main categories of algorithms available for satellite remote sensing of shallow water: empirical approaches and physics-based approaches. The empirical approaches are established upon the statistical relationships between known depth data and $R_{rs}(\lambda)$ measurements at one or several bands (e.g., Stumpf et al., 2003). They are relatively straightforward to implement with either multi-spectral or hyper-spectral satellite images (Caballero and Stumpf, 2019; Liu et al., 2019; McIntyre et al., 2006; Pacheco et al., 2015). In view of the variation of benthic substrates 67 and water IOPs in shallow environments, empirical approaches face hurdles toward global 68 application. Their performance is often dependent on the similarity between data used for 69 algorithm development and those for applications (Dekker et al., 2011). Physics-based or semi-70 analytical approaches refer to those formulated out of radiative transfer theory (e.g., Lee et al., 71 1999; Lyzenga et al., 2006; Philpot, 1989). In principle, this type of approach does not need in situ 72 data for model tuning and thus has the potential to be employed for global waters. A caveat is that 73 the shallow water radiative transfer equation is complex to solve, more so than deep waters. 74 According to earlier studies (Lee et al., 1998; Lee et al., 1999), the shallow water properties can 75 be well determined from hyper-spectral $R_{rs}(\lambda)$ data with a spectral optimization algorithm (SOA). 76 The SOA proves to be an effective procedure in estimating the water depth and has been 77 extensively evaluated and continuously refined (Brando et al., 2009; Dekker et al., 2011; Fearns et al., 2011; Giardino et al., 2012; Goodman et al., 2008; Klonowski et al., 2007). The SOA, 78 79 however, is susceptible to an increase of uncertainty when the band numbers available to the $R_{rs}(\lambda)$ 80 data are significantly reduced, as is the case with multi-spectral sensors (Lee and Carder, 2002; 81 Werdell and Roesler, 2003).

82 The current polar-orbiting ocean color satellites are generally considered multi-spectral sensors. 83 A non-exhaustive list of multi-spectral satellites includes the fine-spatial resolution (typically less 84 than a few meters) satellites such as WorldView-2 (five visible bands) and RapidEye (three visible 85 bands), the fine-moderate-spatial resolution (~10-30 m) satellites such as Landsat-8 and Sentinel-86 2 (four visible bands), and the moderate-spatial resolution (\sim 300–1000 m) satellites such as Aqua 87 (seven visible bands) and Sentinel-3 (ten visible bands). The multi-spectral satellite $R_{rs}(\lambda)$ data of 88 different spatial resolutions are increasingly tested for the water depth retrieval in many shallow 89 regions (Caballero and Stumpf, 2019; Cahalane et al., 2019; Li et al., 2019; Stumpf et al., 2003). 90 Despite the ever-increasing amounts of ocean color images, the small number of bands available 91 to the $R_{rs}(\lambda)$ data has largely limited the applicability of existing physics-based algorithms such as 92 the SOA for shallow water depth retrieval (Barnes et al., 2018; Lee et al., 2010). A gap clearly 93 exists between the need for shallow water bathymetry of fine- to moderate-spatial resolution and 94 the available multi-spectral algorithms useful for the water depth retrieval over global coastal areas.

95 In this study, we develop and test an optimization approach for improved derivation of 96 bathymetry from multi-spectral ocean color data over global shallow waters. This new approach 97 takes advantage of the temporal variation in the satellite-derived $R_{rs}(\lambda)$ data. The assumption made 98 here is that the temporal variation in two satellite $R_{rs}(\lambda)$ images over a short enough time period is 99 caused by variation in the IOPs, while the bottom albedo (magnitude and shape) and depth remain 100 the same. As such, our optimization algorithm requires two satellite multi-spectral $R_{rs}(\lambda)$ spectra 101 acquired at the same location as input. Distinct from earlier studies, the two $R_{rs}(\lambda)$ spectra are 102 processed simultaneously in the optimization procedure.

103 Our analysis is focused on three satellite ocean color sensors. With more information given in 104 Table 1, the Landsat-8 Operational Land Imagers (L8/OLI) has four visible bands, including a blue 105 band at 443 nm that was nonexistent on its predecessors (Loveland and Irons, 2016). The Visible 106 Infrared Imaging Radiometer Suite (VIIRS) onboard SNPP has six visible bands, including one 107 aggregated from an imaging band at 638 nm (Wang and Jiang, 2018). The Sentinel-3A Ocean and 108 Land Colour Instrument (S3A/OLCI) has ten visible bands, with a purple band at 400 nm. The 109 model performance is assessed with both synthesized and satellite $R_{rs}(\lambda)$ data. Our results show 110 that the new algorithm can estimate the water depth with improved accuracy, a result of leveraging 111 the temporal variation of the $R_{rs}(\lambda)$ data over the same shallow water pixels.

113 **2. Two-spectrum optimization algorithm**

114 The two-spectrum optimization algorithm, or 2-SOA, works with two multi-spectral remote sensing reflectance spectra, $R_{rs}^{obs}(\lambda, t_1)$ and $R_{rs}^{obs}(\lambda, t_2)$, observed at the same location but at two 115 116 different times, t_1 and t_2 , respectively. The difference between t_1 and t_2 is short enough that the 117 bottom albedo and water depth (after tidal correction) are assumed unchanged. The 2-SOA algorithm first models each of the two reflectances, $R_{rs}^{mod}(\lambda, t_1)$ and $R_{rs}^{mod}(\lambda, t_2)$, as a function of 118 119 water depth, bottom albedo, and water IOPs. It then evokes spectral optimization to reach an 120 optimal solution for the water depth by searching for the minimum between the two observed and 121 two modeled reflectance spectra. The workflow of the 2-SOA approach for shallow water ocean color inversion of $R_{rs}^{obs}(\lambda, t_1)$ and $R_{rs}^{obs}(\lambda, t_2)$ is illustrated in Figure 1. In the following two 122 123 subsections, we describe the optical modeling process and spectral optimization, respectively.

124

125 **2.1 Shallow water optical modeling**

We adopt the forward optical models of the hyper-spectral optimization processing exemplar (HOPE) (Lee et al., 1998; Lee et al., 1999) to describe the water-column inherent optical properties and bottom albedo. First, the phytoplankton absorption coefficient $(a_{ph}(\lambda))$ is modeled by an empirical function (Lee et al., 1998)

130
$$a_{ph}(\lambda) = \left[a_0(\lambda) + a_1(\lambda) \ln a_{ph}(443)\right] a_{ph}(443)$$
(1)

131 where $a_0(\lambda)$ and $a_1(\lambda)$ are wavelength-specific constants initially given from 400 nm to 800 nm for 132 every 10 nm. In this analysis, $a_0(\lambda)$ and $a_1(\lambda)$ are interpolated onto the specific bands of interests. 133 The light absorption of colored dissolved organic matter (CDOM) and detritus (collectively, CDM) 134 are treated together due to the similarity of their spectral behavior, denoted as $a_{dg}(\lambda)$, with

135
$$a_{dg}(\lambda) = a_{dg}(443) \exp\left[-S_{dg} \times (\lambda - 443)\right]$$
(2)

where S_{dg} refers to the spectral slope for $a_{dg}(\lambda)$ in the visible domain and is assumed to be a constant equal to 0.015 nm⁻¹, following Lee et al. (1998). The particle backscattering coefficient ($b_{bp}(\lambda)$) is characterized by a power function,

139
$$b_{bp}(\lambda) = b_{bp}(443) \left[\frac{443}{\lambda}\right]^{\eta}$$
(3)

140 where the parameter η is estimated from the spectral ratio of $R_{rs}(\lambda)$ at 443 nm and ~550 nm bands, 141 following Lee et al. (2002). Thus, the total absorption and backscattering coefficients can be 142 expressed as

143
$$a(\lambda) = a_{ph}(\lambda) + a_{dg}(\lambda) + a_{w}(\lambda)$$
(4)

144
$$b_{h}(\lambda) = b_{hn}(\lambda) + b_{hw}(\lambda)$$
(5)

where $a_w(\lambda)$ and $b_{bw}(\lambda)$ refer to the absorption and backscattering coefficients of pure seawater, respectively, and are determined as constants following Lee et al. (2015) and Zhang et al. (2009), respectively. The bottom spectrum, $\rho(\lambda)$, is quantified by a normalized bottom albedo spectrum at ~550 nm, $\rho_n(\lambda)$, and a scaling factor, *B*,

$$\rho(\lambda) = B \cdot \rho_n(\lambda) \tag{6}$$

150 The $\rho_n(\lambda)$ spectrum is assumed to follow the shape of sandy substrate and adopted from Lee et al. 151 (1999). Figure 2 illustrates the spectral feature for this bottom reflectance spectrum.

With the above-modeled spectral optical properties, the remote sensing reflectance just below the water surface $(r_{rs}(\lambda))$ is approximated following the shallow water model of Lee et al. (1999), as

155

$$r_{rs}(\lambda) \approx r_{rs}^{dp}(\lambda) \cdot \left\{ 1 - \exp\left[-\left(\frac{1}{\cos\theta_{w}} + \frac{D_{0}\left(1 + D_{1} \cdot u(\lambda)\right)^{0.5}}{\cos\theta_{a}}\right) \cdot k(\lambda) \cdot H \right] \right\} + \frac{\rho(\lambda)}{\pi} \exp\left[-\left(\frac{1}{\cos\theta_{w}} + \frac{D_{0}\left(1 + D_{1} \cdot u(\lambda)\right)^{0.5}}{\cos\theta_{a}}\right) \cdot k(\lambda) \cdot H \right]$$
(7)

As shown in Eq. (7), $r_{rs}(\lambda)$ is the sum of the contribution from the water column and the contribution from the bottom reflection. Specifically, $r_{rs}^{dp}(\lambda)$ refers to the reflectance just below the water surface in optically deep waters; the parameter θ_a is the solar-zenith angle and θ_w is the subsurface solar-zenith angle; $k(\lambda)$ is an IOP, with $k(\lambda) = a(\lambda) + b_b(\lambda)$; *H* is the water depth to be solved; and the values of D_0 , D_1 , D_0^+ , and D_1^+ are adopted from Lee et al. (1999),

161
$$D_0 = 1.03, D_1 = 2.4$$

 $D_0 = 1.04, D_1 = 5.4$ (8)

162 According to Monte Carlo simulations (Gordon et al., 1988), $r_{rs}^{dp}(\lambda)$ can be estimated by a quadratic 163 function of $u(\lambda)$, as

164
$$r_{rs}^{dp}(\lambda) = g_0 u(\lambda) + g_1 [u(\lambda)]^2$$
(9)

where $u(\lambda)$ is the ratio of the backscattering to absorption coefficients, with $u(\lambda) = b_b(\lambda)/[a(\lambda) + b_b(\lambda)]$, and two model constants g_0 and g_1 were adopted from Lee et al. (2002), with $g_0 = 0.089$ sr⁻¹ and $g_1 = 0.125$ sr⁻¹. We note that the formulation of Eq. (7) provides an explicit description of various contributions to $r_{rs}(\lambda)$ omitting inelastic scattering (Raman scattering and fluorescence) (e.g. Lee and Carder, 2004), which does not make a strong contribution to optically shallow waters. Lastly, $r_{rs}(\lambda)$ is propagated through the water surface to obtain a $R_{rs}(\lambda)$ spectrum (Lee et al., 1999),

172
$$R_{r_s}(\lambda) = \frac{0.5r_{r_s}(\lambda)}{1 - 1.5r_{r_s}(\lambda)}$$
(10)

173 Note that an updated version of Eq. (10) is also available (Lee et al., 2002). The present analysis 174 still uses Eq. (10) to ensure consistency and comparability with earlier studies. Up to this step, 175 each $R_{rs}(\lambda)$ spectrum can be characterized by five unknowns: $a_{ph}(443)$, $a_{dg}(443)$, $b_{bp}(443)$, B and 176 H, i.e.,

177
$$R_{rs}(\lambda) = \operatorname{Fun}[P, G, X, B, H]$$
(11)

where the parameters *P*, *G*, and *X* refer to $a_{ph}(443)$, $a_{dg}(443)$, and $b_{bp}(443)$, respectively, for simplicity.

180

181 **2.2 Spectral optimization**

182 The standard HOPE algorithm solves Eq. (11) through a cost function which quantifies the least 183 square residual error (*err*) between $R_{rs}^{mod}(\lambda)$ and $R_{rs}^{obs}(\lambda)$,

184
$$err = \frac{\left[\sum \left(R_{rs}^{mod}(\lambda_{i}) - R_{rs}^{obs}(\lambda_{i})\right)^{2}\right]^{1/2}}{\sum R_{rs}^{obs}(\lambda_{i})}$$
(12)

Such a cost function is commonly found in ocean color inversions (Dekker et al., 2011; Lee et al.,
1999; Roesler and Perry, 1995; Werdell and Roesler, 2003). For convenience, this optimization
procedure using one input spectrum will be hereafter called one-spectrum optimization approach,
or 1-SOA for short.

The 2-SOA approach considers two independent input spectra obtained at different times. There is no strict requirement for the scale of the time difference. Nevertheless, these two spectra should be measured within a reasonably short period of time, which can be in the order of days or weeks, depending on the availability of utilizable image data. It is important to emphasize that the corresponding bottom albedo and water depth at two observation times should remain (approximately) unchanged, while the water inherent optical properties, including P, G, and X in Eq. (11), can vary. This requirement can be met under most conceivable situations, as abrupt changes of the bottom albedo and water depth are likely caused by extreme events such as hurricanes. The tides can also alter the water levels, which can be corrected (Garcia et al., 2014a). The impact of tidal levels is further discussed later in Section 6.

199 With two input spectra $(R_{rs}^{obs}(\lambda, t_1) \text{ and } R_{rs}^{obs}(\lambda, t_2))$, two new remote sensing reflectance spectra 200 can be modeled in the manner analogous to Eq. (11), as

201
$$\begin{cases} R_{rs}^{mod}(\lambda, t_1) = \operatorname{Fun}[P_1, G_1, X_1, B, H] \\ R_{rs}^{mod}(\lambda, t_2) = \operatorname{Fun}[P_2, G_2, X_2, B, H] \end{cases}$$
(13)

Note that, in Eq. (13), each modeled reflectance spectrum is characteristic of a unique set of P, G, and X parameters (denoted with subscripts "1" and "2", respectively), but of common bottom albedo and water depth. As a result, Eq. (13) has a total of eight unknowns: P_1 , G_1 , X_1 , P_2 , G_2 , X_2 , B, and H. To solve Eq. (13) in an optimization procedure, we quantify the difference between the two sets of modeled- and measured-spectra with the cost function given below,

207
$$err = \frac{\left[\sum \left(R_{r_s}^{mod}(\lambda_i, t_1) - R_{r_s}^{obs}(\lambda_i, t_1)\right)^2 + \sum \left(R_{r_s}^{mod}(\lambda_i, t_2) - R_{r_s}^{obs}(\lambda_i, t_2)\right)^2\right]^{1/2}}{\sum R_{r_s}^{obs}(\lambda_i, t_1) + \sum R_{r_s}^{obs}(\lambda_i, t_2)}$$
(14)

We use the MATLAB built-in optimization solver called *fmincon* to search for the minimum for Eq. (14). This routine employs the interior-point algorithm and allows the bound constraints to be applied to each variable. The optimization options include the maximum iterations of 2000 and tolerance of 10^{-5} . The constraints and initial values for the optimization procedure are given in Table 2. We note that the cost function of Eq. (14) and the standard function of Eq. (12) are essentially the same in the manner that they quantify the minimum. The difference rests on the innovative involvement of two collocated input $R_{rs}(\lambda)$ spectra in the optimization of Eq. (14).

215

216 **3. Evaluation data**

217 **3.1 Synthetic multi-spectral** $R_{rs}(\lambda)$ data

218 The forward models in Eqs. (1)–(10) are used to synthesize a hyper-spectral data set (400–700 219 nm, for every five nanometers) over shallow waters. The synthetic data mimic real-world optical 220 properties without associated measurement and human errors, and hence provide a straightforward 221 measure to evaluate the algorithm performance (e.g., Barnes et al., 2018; Carder et al., 2005; 222 Garcia et al., 2018; Manessa et al., 2018). The data used here represent a wide range of water 223 depths, IOP combinations, and multiple benthic classes (Table 3). Briefly, the water depths were varied from 0.5 m to 29.5 m with a step of one meter, resulting in 30 depth levels to be assessed. 224 225 For IOPs, both $a_{ph}(443)$ and $a_{dg}(443)$ were varied from 0.01 to 0.19 m⁻¹ with a step of 0.03 m⁻¹. 226 According to analyses of field measurements, the CDM spectral slopes in "clear" waters vary over 227 a relatively narrow range (within $\pm 10\%$ of a median value) across various geomorphic zones (Russell et al., 2019). Therefore, the present study assumed a constant spectral slope with S_{dg} = 228 0.015 nm⁻¹. Particle backscattering, b_{bp} (443), was varied between 0.001 m⁻¹ and 0.019 m⁻¹ with 229 230 an increment of 0.004 m⁻¹. The spectral slope for $b_{bp}(\lambda)$ was varied from -0.5 to 2.5 with a step of 231 0.5. The solar-zenith angle was assumed to be $\theta_a = 30^\circ$. There are many hyper-spectral bottom spectra measured over various benthic substrates (Hochberg et al., 2003). The inclusion of every 232 233 spectra in the present simulation would require significant computing capability. Instead, we 234 obtained the median spectra for brown coral, seagrass, and sand from Hochberg et al. (2003) to 235 represent the bottom reflectance spectra for three substrates. As shown in Figure 2, the spectral 236 shape of the sandy substrate is flatter and relatively featureless, while the seagrass spectrum has a 237 broad peak between 500-650 nm and the coral spectrum contains three peaks with a local 238 maximum in the yellow and red domain. Three levels of bottom albedo B were considered for each 239 benthic substrate, with the largest B values assigned to the sandy substrate (Table 3). Finally, for 240 each benthic substrate, a total of 216,090 combinations of water depths (N = 30), bottom albedo 241 (N = 3), and IOPs (N = 2401) were constructed. We acknowledge that realistic benthic spectra are 242 more likely to be mixtures of different species rather than a "pure" type, especially considering the 243 spatial resolution of L8/OLI, SNPP/VIIRS, and S3A/OLCI. Simulation of such mixtures is 244 however beyond the focus of current study.

245 For each level of simulated water depths and substrates, we randomly chose 400 simulated $R_{rs}(\lambda)$ 246 spectra at each depth level and for each bottom albedo to form the first set of "collocated" spectra, $R_{rs}^{obs}(\lambda, t_1)$. Repeating this process led to the second data set, namely, $R_{rs}^{obs}(\lambda, t_2)$. The resulting 247 collocated $R_{rs}^{obs}(\lambda, t_1)$ and $R_{rs}^{obs}(\lambda, t_2)$ data represent 36,000 pairs of simulations (400 × 30 H × 3 248 249 B) with respect to each bottom type. Further, the paired $R_{rs}(\lambda)$ data were spectrally subsampled 250 according to the band settings of L8/OLI, SNPP/VIIRS, and S3A/OLCI. For L8/OLI, we adopted 251 four visible bands of 443, 482, 565, and 665 nm for our analysis. For SNPP/VIIRS, six visible 252 bands of 410, 443, 486, 551, 638, and 671 nm were used. For S3A/OLCI, nine visible bands of 400, 413, 443, 490, 510, 560, 620, 665, and 674 nm were considered. OLCI also has a red band 253 254 centered at 681 nm, which is omitted in our scheme, given that $R_{rs}(681)$ is subject to the 255 chlorophyll-a fluorescence effect (Gordon, 1979) and the spectral optical models discussed in 256 Section 2.1 do not account for the fluorescence effect.

258 **3.2 Satellite images**

259 We acquired two L8/OLI Level-1 images from the USGS Earth Explorer (Table 1). The 260 observation times for the two images are 16 days apart, which is the revisit period of Landsat-8. 261 According to the NOAA tidal data (https://tidesandcurrents.noaa.gov), both images were captured 262 during the low-tide periods, with the estimated tidal difference within 0.33 meters. The images 263 were processed to Level-2 products with the SeaWiFS Data Analysis System (SeaDAS) (Franz et 264 al., 2015). SeaDAS implements the atmospheric correction developed out of the work of Gordon 265 and Wang (1994). In the analysis, the near-infrared (NIR) and shortwave infrared (SWIR) band 266 combination (865 and 2201 nm) was adopted for the determination of aerosol types, which has 267 been validated for shallow water applications (Wei et al., 2018). An iterative procedure was 268 employed to further correct for the estimated aerosol contributions at the NIR bands (Bailey et al., 269 2010).

270 The S3A/OLCI and SNPP/VIIRS images were obtained from the NOAA ocean color data 271 archive (http://coastwatch.noaa.gov) (Table 1). In the Florida Keys, the two Sentinel-3A images 272 were captured around 15:30 UTC, with the estimated tide levels at ~0.3 meters; the tidal difference 273 between the two images is very small. In the Bahamas, the water level differences between two observation times for two collated images were < 0.3 m. We processed the Level-1 images with 274 275 the Multi-Sensor Level-1 to Level-2 (MSL12) procedure (Wang et al., 2013). MSL12 is based on 276 the NASA SeaDAS 6.4 with modifications and improvements. It can switch among the NIR-, 277 SWIR-, and NIR-SWIR-based atmospheric correction algorithms for open ocean, coastal, and 278 inland waters applications (Wang, 2007; Wang and Shi, 2007; Wang et al., 2009). For 279 SNPP/VIIRS images, a combination of NIR-SWIR bands was used in the current analysis to determine the aerosol types from an aerosol look-up table generated from 12 aerosol models (Wang,
2007). For S3A/OLCI, two NIR bands (779 nm and 865 nm) were chosen for the determination of
aerosol types (Gordon and Wang, 1994). The image processing was accomplished with the ocean
color data processing system (OCDAPS) at the NOAA Center for Satellite Applications and
Research (STAR).

In addition to the above specifics, we kept the default model settings for image processing. The residual glint correction was performed with the standard approach (Wang and Bailey, 2001). The standard Level-2 quality flags, including cloud, high sunglint, straylight, high sensor- and solarzenith angles, etc., were applied (Mikelsons et al., 2020). Finally, the processed Level-2 images were re-projected onto the Geographic Lat/Lon (WGS 84) Coordinate Reference System (CRS), following the equidistant cylindrical projection. The re-projected images were then collocated using the nearest neighbor resampling procedure.

292

3.3 Metrics for performance evaluation

294 To evaluate the algorithm performance in estimating water depth, we calculated the bias $(\bar{\epsilon})$ as

295
$$\overline{\varepsilon} = \operatorname{median}\left\{ (M - T) / T \right\} \times 100\% \tag{15}$$

where *M* and *T* refer to the estimated and known values, respectively. Correspondingly, we derived the absolute percentage difference ($|\overline{\epsilon}|$) as,

298
$$|\overline{\varepsilon}| = \operatorname{median}\left\{ \left| (M - T) / T \right| \right\} \times 100\%$$
 (16)

The root-mean-square difference (RMSD) was also computed to assess the model uncertainty,with

$$RMSD = \sqrt{\text{median}\left\{ \left(M - T \right)^2 \right\}}$$
(17)

301

4. Assessment results of the synthetic data

304 Implementation of the 2-SOA approach with the synthetic data allows insight into the algorithm 305 performance. Along with 2-SOA, we also present the results from the 1-SOA algorithm for which 306 only one $R_{rs}(\lambda)$ spectrum was used. Such comparisons highlight the performance of 2-SOA and 307 the degree of improvement relative to the standard optimization approach.

308 First, the overall statistical results over the full range of depths (0–30 m) are given in Table 4. 309 It is evident that the 2-SOA approach can estimate water depths with substantially smaller errors 310 $(\overline{\varepsilon}, \overline{\varepsilon}, \text{ and RMSD})$ than the 1-SOA approach where one multi-spectral $R_{rs}(\lambda)$ spectrum is used as 311 the input. Among three simulated satellite sensors, L8/OLI has benefited to the largest degree from 312 the 2-SOA approach, mostly because it has the fewest number of wavelengths available for spectral 313 optimization. In contrast, the water depth retrievals for S3A/OLCI have experienced the smallest 314 degree of improvement, because the OLCI has the largest number of bands. The degree of 315 improvement for SNPP/VIIRS remains relatively moderate among three satellites.

Distinctive performance of the 2-SOA algorithm is also revealed in accordance with the benthic substrates, after comparing the statistical results in Table 4. This is expected as 2-SOA assumed a fixed spectrum for the bottom albedo, which is different from the simulated benthic reflectance spectra (recall Figure 2). For the three benthic substrates, the 2-SOA approach yielded the highest degree of improvement for depth retrievals in coral reefs and seagrass environments. The retrievals for sandy environments have also benefited to a relatively smaller extent from the use of two $R_{rs}(\lambda)$ spectra for optimization. This can partially be explained by the very different amplitudes of the bottom albedos. Specifically, sand is usually much brighter and spectrally flatter than coral and
seagrass substrates (recall Figure 2 and Table 3) (also see Hochberg et al., 2003). As a result, the
subsequent water depth retrievals over sandy substrates tend to be more accurate than the other
two bottom types.

327 We further examined the model performance with respect to its dependence on water depths 328 under investigation. In Figure 3, the absolute percentage errors for the model-estimated depths are 329 plotted as a function of known water depths. For SNPP/VIIRS and S3A/OLCI, the largest errors 330 in retrieved depths are always found in waters where the bottom is shallower than five meters, 331 partially as a result of the small values of water depths themselves. The model errors are generally 332 constrained within ~20% if the waters are deeper than five meters. For L8/OLI, the errors for 333 estimated depths generally increase with the decrease of water depths from about 10 m. For water 334 depths less than three meters, the errors can be in the order of hundreds of percent, particularly 335 over simulated coral and seagrass substrates (Figure 3a and Figure 3d). Besides the small values 336 of water depths themselves, the markedly large errors in waters of less than five meters (Figure 3a, 337 Figure 3d, and Figure 3g) are likely caused by the fact that L8/OLI does not have an additional 338 deep blue band around 412 nm. In waters of 5–30 m, the algorithm appears to perform well with 339 L8/OLI, with acceptably small errors ($\sim 20\% - 30\%$).

The comparisons in Figure 3 illustrate the performance of the 2-SOA algorithm in improving the water depth retrieval over a wide range of depths. With L8/OLI data, the performance of 2-SOA exceeds 1-SOA at almost every level of depth discussed in this context. The most noticeable improvement for L8/OLI lies in the waters of ~0.5–15 m deep. The degree of improvement, or the absolute difference of the model errors, can be greater than 100% (Figure 3d and Figure 3g). For SNPP/VIIRS and S3A/OLCI, the 2-SOA approach outperforms 1-SOA over the depth range of 5–

346 20 m. In coral and seagrass substrates, the degree of improvement is about 20% (Figure 3b-Figure 347 3c, and Figure 3e–Figure 3f); it remains relatively small for sandy bottoms (Figure 3h–Figure 3i). 348 Since the synthetic data are composed of a wide range of water depths and IOPs, certain 349 combinations of $a(\lambda)$, $b_b(\lambda)$, and H may favor an extremely large water-column attenuating 350 component in Eq. (7), leading to negligible contributions from bottom reflectance. We calculated 351 the ratio of the bottom contribution to the total remote sensing reflectance for each simulation, following $r_{rs}^{b}\% = r_{rs}^{b}(\lambda_{ref})/r_{rs}(\lambda_{ref}) \times 100\%$, where $r_{rs}^{b}(\lambda_{ref})$ is the bottom contribution term in Eq. (7) 352 at a reference wavelength (λ_{ref} = 561, 551, and 560 nm for L8/OLI, SNPP/VIIRS, and S3A/OLCI, 353 354 respectively). In Figure 4, the absolute percentage errors for model-estimated depths are plotted against ten levels of bottom contribution ratios from 0-10% to 90%-100%. As 2-SOA used two 355 synthetic $R_{rs}(\lambda)$ spectra, we chose the maximum $r_{rs}^{b}(\lambda_{ref})$ values as the representative bottom ratio 356 357 for the two spectra. It can be found that the errors of the derived depths vary with the bottom ratio 358 in a pattern approximately opposite to the model error-depth relationship demonstrated in Figure 359 3. This is expected and, to a large extent, related to the fact that the bottom reflection tends to 360 contribute more to $R_{rs}(\lambda)$ in shallower environments, in which environments, however, accurate 361 estimation of water depths from 2-SOA (and 1-SOA) is usually more challenging.

362

363 5. Assessment results of satellite ocean color images

364 5.1 Hawaiian coral reefs

The Olowalu Reef (20.79°N–20.81°N, 156.63°W–156.59°W) at the southwest coast of Maui, Hawaii (Figure 5b and Figure 5c) is selected for algorithm evaluation. Located on the leeward side of northeasterly winds and large swells, it represents the largest fringing reef in the main

368 Hawaiian Islands. This study area covers about three-square kilometers and thus is more suitable 369 for the L8/OLI footprint than the other two sensors. In Figure 6a, the bathymetry map (0–30 m) 370 for this unique reef system is derived from two L8/OLI images using the 2-SOA approach. For 371 comparison, we obtained in situ water depth data from the Scanning Hydrographic Operational 372 Airborne LiDAR survey (SHOALS) (http://www.soest.hawaii.edu/coasts/data/maui/shoals.html). 373 In Figure 6b, the LiDAR data are spatially averaged over pixels within 30 m from the L8/OLI 374 coordinates. First, the satellite- and LiDAR-derived bathymetry maps exhibit almost identical 375 spatial distribution pattern over the range of 0–30 m, which decreases from the coastline towards 376 offshore waters. Figure 6c compares the water depths from L8 and LiDAR in a scatterplot, 377 superimposed with the data density (in colors and contours). Quantitatively, the L8/OLI and LiDAR bathymetry data are consistent with each other except for differences ($|\overline{\epsilon}| = 27\%$, $\overline{\epsilon} = 21\%$, 378 379 RMSD = 5.3 m, and N = 4036). The majority of the data points are distributed closely to the 1:1 line, with a Type-II linear regression equation of Y = 0.96X + 3.21, and $R^2 = 0.70$. To further 380 381 validate the L8-derived depths, we extracted the water depth data along the longitudinal lines of 382 36°37'W, 36°36.5'W, 36°36'W, and 36°35.5'W, respectively. In Figure 7, the similarity of the 383 water depth profiles from L8 and LiDAR is clearly illustrated. Each pair of depth profiles are found with large coefficients of correlation ($R^2 = 0.68 - 0.90$), close-to-unity linear regression coefficients, 384 and acceptably small differences ($|\overline{\epsilon}| = 20\% - 36\%$, $\overline{\epsilon} = -7.6\% - 35\%$, RMSD = 3.1–6.4 m). 385

The outliers and biases in the L8-generated water depths in Figure 6 and Figure 7 are worth further discussion. In waters of less than five meters, tens of L8-generated depths are found overestimated. These outliers are in part due to the algorithm itself as its performance with four Landsat-8 bands can be somewhat impeded when the water depths are shallow than five meters (e.g., Figure 3). Besides, dozens of L8-derived data points in relatively deep environments (> 10 391 m) are present around five meters, apparently underestimated in comparison to the LiDAR map. 392 These underestimated data points coincidently aligned themselves with the initial guess for water 393 depth during spectral optimization, suggesting a possible origin. Despite the deviations from the 394 LiDAR data, these outliers only account for a relatively small percentage (< 2%) of the data points, 395 and hence exert limited impact on the consistency between two sets of depth data. It is important 396 to emphasize that the errors of derived depths could be partially due to the complexity of the 397 substrates and uncertainties in the satellite data. The heterogeneous substrates, including the 398 presence of sand channels, independent of coral colonies, or variable morphologies, and the 399 difference in the instruments' footprints, can contribute to the observed uncertainty. In addition, 400 the tide levels (< 0.3 m) at the observation times of L8 images may be partially responsible for the 401 observed positive biases in Figure 6 and Figure 7. Lastly, the disparity between the L8/OLI and 402 LiDAR water depth derivations is, to a certain degree, attributable to the propagation of the 403 uncertainty of the satellite $R_{rs}(\lambda)$ data (e.g., Garcia et al., 2014b; Goodman et al., 2008).

404

405 **5.2 Florida Keys seagrass environments**

406 The second shallow environment is located in the east of the Florida Keys National Marine 407 Sanctuary (Figure 5d). It covers part of the Florida Bay and the Hawk Channel in the Reef Tract 408 (24.94°N-25.05°N, 80.33°W-80.632°W). This shallow water is characteristic of extensive 409 seagrass beds as well as some typical coral barrier reefs. The study area is large enough (the surface 410 area is about $3.5 \times 6 \text{ km}^2$) to derive and evaluate the water depths from S3A/OLCI images. Note 411 that LiDAR measurements are scarcely available in this region. Instead, the rasterized bathymetry 412 map from the NOAA coastal relief model (CRM) (NGDC, 2001) was acquired for the validation 413 of retrieved water depth from S3A/OLCI. Figure 8a and Figure 8b are the bathymetry maps (0-30 m) derived from S3A/OLCI and CRM, respectively. The S3A- and CRM-derived bathymetry
maps are highly comparable to each other. With the majority of the water depths less than ~10 m,
the bathymetry in this area gradually increases from the Florida Bay towards the barrier reefs. It
also appears that the two bathymetry maps do not sufficiently differentiate land/water pixels in the
Florida Bay (northwest to the land shown in Figure 5d), which can be corrected in the future with
higher-resolution land masks.

420 The S3A-derived water depths are quantitatively compared with the CRM data in Figure 8c. To 421 accommodate their different spatial resolutions (~300 m vs. 90 m), the CRM data were averaged 422 over a box of 3×3 pixels centered at the S3A/OLCI coordinates. As the scatterplot shows, two sets 423 of depth data agree with each other very well, with $\overline{\epsilon} = 16\%$, $\overline{\epsilon} = -3.5\%$, and RMSD = 2.5 m. 424 There exist some data points showing relatively large deviations from the 1:1 line. In the Florida 425 Bay, for instance, a dozen of satellite-derived water depth data are biased high. Two main factors 426 might explain the overestimation in this shallower portion of waters. The first one is related to the 427 possible contamination of S3A/OLCI $R_{rs}(\lambda)$ data; within the S3A/OLCI footprint, narrow sandbars, 428 shoals, and small islands are mixed with surrounding waters, partially impacting the $R_{rs}(\lambda)$ data 429 and subsequent water depth retrievals. Second, it might be a result of the problematic CRM data 430 themselves. After all, the CRM data were generated by spatial interpolation based on many 431 historical low-tide hydrographic data. The instantaneous tide levels are low (< 0.3 m) (Table 1), 432 the impact of which on the comparison is expected to be small. In the relatively deeper waters (> 433 10 m), the S3A data appear biased low relative to the CRM data. This underestimation is likely 434 related to the bottom heterogeneity around the \sim 15–30 m isobaths, where the CRM data have 435 undergone spatial gridding, extrapolation, and other arbitrary operations, resulting in possibly 436 unrealistic data.

438 **5.3 The Bahamas**

The Bahamas Bank is a massive shallow body of water in the southern Bahamas (22.5°N-439 25.5°N, 79.5°W–75.75°W) (Figure 5e). The vast shallow area (about 300×300 km²) is dominated 440 441 by sandy substrate, with seagrass distributed primarily along the perimeters of the Great Bahamas 442 Bank and the southern bank (Dierssen and Zimmerman, 2003). The extensive flats of the Bahamas 443 are not currently included in the NOAA CRM products. As an alternative, we extracted about 444 1,200 water depth points from a digital navigation chart – Explorer Charts near the Bahamas, for 445 validation. Figure 9a and Figure 9c show the highly comparable bathymetry maps obtained from 446 the SNPP/VIIRS images and the S3A/OLCI images, respectively. Note that these maps only show 447 the results at pixels for $R_{rs}(443)/R_{rs}(486) \le 1$ and $R_{rs}(\sim 745) \ge 0$. Some pixels in the southeastern 448 portion of the shallow area are masked out due to clouds. In the vicinity of Andros Island (24.43°N, 449 77.95°W), the water depths are largely confined within five meters. Relatively deep waters (around 450 10 m) are generally found in the middle and southern parts of the bank, similar to the presentation 451 of Lee et al. (2010). In Figure 9b and Figure 9d, the satellite-generated water depths are compared 452 with the depth data extracted from the digital navigation chart. In general, satellite-derived water 453 depths appear to be biased high, with $\overline{|\varepsilon|} = \sim 40\%$. This can be largely explained by the fact that the 454 in situ water depth data represent the approximate level of the mean low water springs (MLWS). 455 The satellite-derived depths in our analysis are not corrected for the tide differences either, which 456 are less than half meters at each satellite overpass (Table 1). Dozens of water depths in the 457 northwest edge of the bank are underestimated by satellite data, probably due to the bottom 458 heterogeneity. These underestimated points render the linear regressions deviating to a large 459 degree from the 1:1 line.

460 Figure 9e is a cross-comparison of the bathymetry data derived from SNPP/VIIRS and 461 S3A/OLCI. The S3A/OLCI depths are averaged over 3×3 pixels to compensate for the difference 462 in two sensors' spatial resolution. As expected, the two sets of water depth estimates are found 463 tightly distributed around the 1:1 line. The differences between two data sets are negligibly small, 464 with $|\overline{\epsilon}| = 9.3\%$, $\overline{\epsilon} = -7.3\%$, and RMSD = 1.3 m. We note that the SNPP/VIIRS and S3A/OLCI 465 images were acquired on exactly the same two days, except that the overpass time was slightly 466 different, with SNPP/VIIRS in the early afternoon and S3A/OLCI in the late morning (Table 1). 467 This time discrepancy resulted in different water levels due to the tides, which are, however, negligibly small (and the tide level in this region is usually less than a meter). The consistency 468 469 between the SNPP/VIIRS and S3A/OLCI depths echoes the assessment results of the synthetic 470 data in Figure 3, where the depths derived with 2-SOA are highly comparable for these two 471 satellites.

472

473 **6. Discussion**

474 The spectral optimization approach uses typically $R_{rs}(\lambda)$ to estimate multiple shallow water 475 properties including water depth (Dekker et al., 2011; Doerffer and Fisher, 1994; Lee et al., 1998; 476 Lee et al., 1999; Philpot, 1989). This approach is sensitive to the number and position of 477 wavelengths included in $R_{rs}(\lambda)$. In general, a hyper-spectral $R_{rs}(\lambda)$ usually generates much more 478 accurate water depth retrievals than an $R_{rs}(\lambda)$ spectrum with 3–7 bands (Lee and Carder, 2002). 479 The 2-SOA approach takes advantage of the temporal characteristics of water and bottom 480 properties such that it can mitigate the limitation imposed by the few wavelengths to eventually 481 obtain better-constrained retrievals from multi-spectral ocean color observations. Two questions 482 specific to the 2-SOA algorithm are worth further discussion: temporal variation and algorithm483 limitation.

484

485 **6.1 Temporal variation of satellite** $R_{rs}(\lambda)$

486 Our analyses demonstrated that 2-SOA could estimate accurate bathymetry by including two 487 reflectance spectra in one optimization procedure (Figure 3 and Table 4). The number of spectra 488 involved in the optimization is the fundamental distinction from the standard approach or 1-SOA. It is also obvious that, if $R_{rs}^{obs}(\lambda, t_1)$ and $R_{rs}^{obs}(\lambda, t_2)$ are the same, the two-spectrum optimization 489 490 of Eq. (14) will revert to the one-spectrum optimizaiton of Eq. (12). Should such a situation occur, 491 one would expect equivalent performance for 2-SOA and 1-SOA. Thus, it is important to 492 understand that the temporal variation of $R_{rs}(\lambda)$ in shallow environments, specifically, of their 493 absolute spectral values, are caused at least to a large degree by the variation of water IOPs. With 494 the collocated satellite images (Table 1), we assessed the relative percentage difference for satellite-measured $R_{rs}(443)$ values in shallow waters as $\varepsilon = \left[R_{rs}^{obs}(t_1) - R_{rs}^{obs}(t_2) \right] / R_{rs}^{obs}(t_2) \times 100\%$. As 495 496 shown in Figure 10, the values of $R_{rs}(443)$ in two images are found to vary significantly (far 497 exceeding $\pm 25\%$) over the vast majority of the shallow waters (0–30 m), supporting the application of 2-SOA. Such temporal variation can be explained by the fact that the shallow waters are liable 498 499 to the action of wind stress and current advection, and favor a dynamic environment with variable 500 water absorption and backscattering coefficients (Russell et al., 2019).

501 It is acknowledged that, even with high revisit frequency, two consecutive satellite images will 502 capture image data impacted with different tide phases. In this study, the variation of water level 503 difference due to the tidal influence is usually within half meters, which are small in comparison

504 to the uncertainties of some in situ water depth data. Still, the tide-induced water level difference 505 (ΔH) on two images could result in different $R_{rs}(\lambda)$ spectra. This is expected as the water column 506 contributes to the light attenuation in accordance with the radiance transfer. To understand the role 507 of the tide, we carried out a sensitivity analysis for the $R_{rs}(\lambda)$ spectra based on the model given in 508 Eq. (7). It is assumed that H is the water depth for the first image and $H + \Delta H$ for the second image. 509 We randomly sampled the water IOPs and bottom albedo from the synthetic data for each of the 510 three benthic substrates. As shown in Figure 11, a tide difference between -0.4 m and 0.4 m barely 511 impacts $R_{rs}(443)$ for waters deeper than five meters, irrespective of the bottom types. For waters 512 shallower than five meters, however, ΔH does exert non-negligible influence on R_{rs} (443). The 513 maximum differences are usually present in the shallowest waters; the median absolute percentage 514 errors are less than 20%. Compared with the results given in Figure 10, the influence of the tides 515 on the remote sensing reflectance appears small.

516 There is limited knowledge of the temporal change of the bottom albedo. A recent satellite 517 analysis reported possible seasonal fluctuations of the bottom albedo (Barnes et al., 2018). This 518 time scale (i.e., seasonal) is long enough that it will not be a problem for obtaining required images 519 from an ocean color satellite. Another study reported rapid wind-driven shifting of unattached 520 benthic macroalgae within half months in the lower Exumas, Bahamas (Dierssen et al., 2009). 521 Furthermore, some benthic substrates and henceforth bottom albedo can also be impacted by 522 extreme weather or long-term climate change (Hoegh-Guldberg, 1999). Such episodic variations in the bottom albedo, if neglected, will cause some errors in water depth retrievals for all 523 524 algorithms. From an operational perspective, however, these events are less likely to be a 525 ubiquitous matter.

527 **6.2** Limitation and uncertainty

528 The processing routines of satellite ocean color measurements flag or mask optically shallow 529 pixels (OSP) based on bathymetry. A typical example is the coastal zone (COASTZ) Level-2 530 quality control flag (12_flag) developed by NASA. With that flag, the areas shallower than 30 m 531 can be identified as OSP in the ocean color images; a recent update is available from McKinna and 532 Werdell (2018). That approach does not specifically determine whether a pixel is optically shallow, 533 which dictates the range of applicability of the shallow water algorithms including 2-SOA. In the 534 current analysis, we briefly discussed the contribution of bottom reflection to $R_{rs}(\lambda)$ and its 535 potential influence on the algorithm performance. However, it is not clear if a threshold for the 536 bottom ratio can be established to separate optically shallow and deep waters. Such a threshold, if 537 exists, will vary with the bottom types and water's optical properties.

538 Adoption of a fixed bottom spectrum in the algorithm is common for shallow water remote 539 sensing (Barnes et al., 2018; Goodman et al., 2008; Lee et al., 2010). The reason for this practice 540 lies in the difficulty of determining it from the input $R_{rs}(\lambda)$ spectra. In a recent study, Garcia et al. 541 (2018) demonstrated that the benthic classification based on hyper-spectral $R_{rs}(\lambda)$ data is a very 542 complex problem. The three simulated bottom substrates are specifically intentioned in this study. 543 Despite the uncertainties brought about by the mismatch between them and the bottom spectrum 544 adopted by 2-SOA, our assessments are more realistic than those assuming an exactly known 545 bottom spectrum. Other methods do exist for tackling the bottom spectra, such as the blending of 546 a few pre-fixed bottom spectra (McKinna et al., 2015). A potential problem incurred therein is the 547 addition of at least one new unknown quantity to the optical models/relationships of Eq. (11) and 548 Eq. (13), which might undermine the application of ocean color sensors with too few wavelengths, 549 such as L8/OLI.

550 The 2-SOA approach estimates bathymetry and other properties simultaneously, including the 551 bottom albedo. After comparing each quantity, we found that the bottom albedo retrievals can also 552 be substantially improved by the 2-SOA approach. In Table 5, the statistical results for estimated 553 bottom albedo at ~555 nm are presented along with those from 1-SOA. The model performance, 554 as demonstrated for B, is very similar to the above observations for water depth retrievals. Yet, the 555 magnitudes of the uncertainties, especially for $\overline{\epsilon}$ and $\overline{\epsilon}$, are close to 100% even for the 2-SOA 556 approach, partly due to the very small values adopted for *B* (Table 3). Dependence on water depth 557 is observable for model-derived bottom albedo as well (results not presented). We note that, as the 558 current approach takes a fixed bottom spectrum, it is not clear how to appropriately interpret the 559 resulted bottom albedo.

560 The spectral optimization approach relies on the accuracy of the absolute values of $R_{rs}(\lambda)$. It is 561 certain that satellite $R_{rs}(\lambda)$ measurements are subject to errors as a result of insufficient calibration 562 and/or atmospheric correction over shallow waters. Recent validation effort has provided 563 preliminary evidence for the $R_{rs}(\lambda)$ errors in shallow waters (Wei et al., 2018). Errors in $R_{rs}(\lambda)$ data 564 can propagate to the subsequent retrieval of water bathymetry (Garcia et al., 2014b). This makes 565 it challenging to compare the satellite-derived bathymetry with field-derived bathymetry. At 566 present, there is a lack of an effective approach to identify the data quality of the satellite $R_{rs}(\lambda)$ 567 spectra in optically shallow environments.

568

569 7. Conclusions

570 Polar-orbiting ocean color satellites image global waters with spectral, spatial and temporal 571 information, providing a great data resource for remote sensing of important shallow water properties. In this study, we presented a novel algorithm that makes use of the temporal variation in satellite $R_{rs}(\lambda)$ data. As the water depth and bottom albedo approximately remain the same at two acquisition times, the temporal variation of $R_{rs}(\lambda)$ is mostly a result of the variation of the water inherent optical properties. As such, our algorithm employs two multi-spectral $R_{rs}(\lambda)$ spectra in one optimization process to obtain better-constrained estimation for water depth. To our knowledge, this study represents the first effort that has considered the temporal variation in the satellite image data for semi-analytical bathymetry retrieval.

579 We evaluated the two-spectrum optimization algorithm with the synthesized data, with a focus 580 on Landsat-8, SNPP, and Sentinel-3A satellites. The analyses show that the new algorithm can 581 substantially improve the estimation of water depths over coral reef, seagrass, and sand substrates. 582 The most pronounced performance improvement is found with Landsat-8 since it has the smallest 583 number of visible bands. Although the SNPP and Sentinel-3A satellites have different band 584 settings, our analyses show much improved yet comparable water depth retrieval using the new 585 algorithm. This study provides a proof of concept that the temporal variation in multi-spectral 586 satellite ocean color data can be leveraged for accurate water depth retrievals with a physics-based 587 scheme. We acknowledge that there is room for further algorithm improvement. In particular, the 588 retrievals in waters shallower than five meters need to be improved, and more accurate modeling 589 of benthic substrates is still needed. Nevertheless, the new approach has shown to be applicable to 590 Landsat-8, SNPP, and Sentinel-3A and probably many other multi-spectral ocean color satellites 591 for reliable bathymetry derivation.

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- 601

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761Table 1. Instrument specifications, observation time, data access and processing for762three ocean color satellites (Landsat-8, SNPP, and Sentinel-3A). The online NOAA763tidal data (https://tidesandcurrents.noaa.gov) were used to estimate the tidal difference764for the two collocated satellite images. The tidal data for images of Hawaii, Florida765Keys, and the Bahamas shallow waters were specific to the local harbor data of766Lahaina (20°53' N, 156°41' W), Key Largo (25°17.4' N, 80°20.3' W), and North Cat767Cay (25°33' N, 79°17' W), respectively.

	Landsat-8	SNPP	Sentinel-3A		
Instrument	OLI	VIIRS	OLCI		
Spatial resolution (m)	30	750	300		
Visible bands (nm)	443, 482, 561, 655	410, 443, 486, 551, 638, 671	400, 413, 443, 490, 510, 560, 620, 665, 674, 681 [†]		
Data access	USGS	NOAA	NOAA		
Processing software	L2GEN	MSL12	MSL12		
tmospheric correction	NIR-SWIR	NIR-SWIR	NIR		
Images at t ₁ and t ₂ (Hawaii)	2017-03-15, 063/048 2017-03-31, 063/048	-	-		
Images at t ₁ and t ₂ (Florida Keys)	-	-	2018-01-13 15:33 UTC 2017-12-29 15:21 UTC		
Images at t ₁ and t ₂ (Bahamas)	-	2019-01-30 18:46 UTC 2019-02-04 18:53 UTC	2019-01-30 15:29 UTC 2019-02-04 14:59 UTC		
Tide difference at <i>t</i> ₁ and <i>t</i> ₂ (m)	< 0.3	< 0.3	< 0.3		
Tide levels at t_1 and t_2 (m)	< 0.3	< 0.3	< 0.5		
' The 681 nm band i	s excluded from the cu	rent analysis			

776 Table 2. Spectral constraints and initial values used by the spectral optimization 777 procedure of the two-spectrum optimization approach (2-SOA). The initial values for P, G, and X are generally adopted from Lee et al. (1999). Note that the wavelengths 778 779 used for the initial values are specific to the ocean color sensors. When the 550 nm or 670 nm band is not available, an alternative band closest to 550 or 670 nm bands will 780 781 be used.

	Lower boundary	Upper boundary	Initial values [†]
$P_1 (m^{-1})$	0.005	0.35	$0.072 \times [R_{r_s}^{obs}(443,t_1)/R_{r_s}^{obs}(550,t_1)]^{-1.62}$
$G_1 (m^{-1})$	0.001	0.6	$0.072 \times [R_{rs}^{obs}(443,t_1)/R_{rs}^{obs}(550,t_1)]^{-1.62}$
$X_1 (m^{-1})$	0.0001	0.08	$30 \times a_w(670) \times R_{rs}^{obs}(670, t_1)$
$P_2 (m^{-1})$	0.005	0.35	$0.072 \times [R_{rs}^{obs}(443, t_2) / R_{rs}^{obs}(550, t_2)]^{-1.62}$
$G_2 (m^{-1})$	0.001	0.6	$0.072 \times [R_{rs}^{obs}(443, t_2) / R_{rs}^{obs}(550, t_2)]^{-1.62}$
$X_2 (m^{-1})$	0.0001	0.08	$30 \times a_w(670) \times R_{rs}^{obs}(670, t_2)$
В	0.001	0.8	0.5
<i>H</i> (m)	0.1	30.5	5

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Table 3. Values of water column inherent optical properties (P, G, X, η , and S_{dg}), water 784 785 depth (*H*), solar-zenith angle (θ_a), and bottom albedo (*B*) used for modeling the remote 786 sensing reflectance data. Three bottom types (coral, seagrass, and sand) are considered.

Quantities	Values (intervals)	Number of levels
Р	0.01-0.19 (0.03)	7
G	0.01-0.19 (0.03)	7
X	0.001-0.019 (0.004)	7
Н	0.5–29.5 (1.0)	30
η	-0.5-2.5 (0.5)	7
S_{dg}	0.015	1
$ heta_a$	30°	1
B: coral	0.005, 0.05, 0.1	3
B: seagrass	0.01, 0.035, 0.08	3
B: sand	0.1, 0.25, 0.6	3

787

Table 4. Retrieval accuracy of water depth (*H*) derived from the synthetic data with
three ocean color satellites (L8/OLI, SNPP/VIIRS, and S3A/OLCI). The results from
both the two-spectrum optimization approach (2-SOA) and the standard approach (1SOA) are provided for comparison of their performance.

		L8/OLI			S	SNPP/VIIRS			S3A/OLCI		
	-	coral	seagrass	sand	coral	coral seagrass		coral	seagrass	sand	
	3	42%	43%	21%	22%	31%	13%	22%	26%	10%	
1-SOA	$\overline{3}$	14%	13%	7%	6%	18%	2%	5%	14%	3%	
	RMSD ⁺	9.3	9.5	6.0	8.8	9.1	4.6	8.3	8.5	4.1	
	3	26%	28%	15%	14%	19%	11%	14%	16%	10%	
2-SOA	\overline{a}	1%	1%	3%	4%	9%	0%	1%	5%	2%	
	RMSD	8.3	8.7	5.2	7.7	8.2	4.0	7.2	7.8	3.9	

[†] RMSD is represented in units of meters.

Table 5. Same as Table 4 but for the bottom albedo (*B*) at a reference wavelength.

		L8/OLI				SNPP/VIIRS				S3A/OLCI		
		coral seagrass sand			с	coral seagrass		sand	coral	seagrass	sand	
	3	203%	167%	50%	1	87%	263%	24%	145%	139%	19%	
1-SOA	$\overline{3}$	203%	167%	8%	1	87%	263%	10%	145%	139%	7%	
	RMSD ⁺	0.18	0.17	0.21	().21	0.23	0.18	0.19	0.17	0.16	
	3	87%	83%	31%	9	91%	132%	18%	74%	80%	16%	
2-SOA	$\overline{3}$	67%	41%	6%	8	38%	132%	8%	63%	65%	7%	
	RMSD	0.21	0.21	0.21	().19	0.23	0.17	0.18	0.19	0.16	

[†] RMSD is given as dimensionless value.



Figure 1. Schematic workflow of the two-spectrum optimization approach (2-SOA) for semi-analytically deriving water depths from two multi-spectral satellite images. Definitions of all quantities: -satellite-observed remote sensing reflectance; -modeled remote sensing reflectance; P-phytoplankton absorption coefficient at ~443 nm; G-CDM absorption coefficient at ~443 nm; X-particle backscattering coefficient at ~443 nm; B-normalized bottom albedo at ~550 nm; H-water depth; err-least square residual error. The subscripts 1 and 2 refer to the quantities observed, modeled, or derived from two collocated images accessed at observation time t_1 and t_2 , respectively.



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- 815



817 Figure 2. Normalized bottom albedo spectra $(\rho_n(\lambda))$ for coral, seagrass, and sand 818 substrates used for the synthesis of $R_{rs}(\lambda)$ spectra, which were derived from Hochberg 819 et al. (2003). The black curve indicates the bottom albedo spectrum adopted by 2-SOA, 820 which is available from Lee et al. (1999).

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Figure 3. Dependence of the absolute percentage errors ($\overline{|\epsilon|}$) for the water depth retrieval on the range of known water depths. The two-spectrum optimization approach (2-SOA) and the standard approach (1-SOA) are compared in these illustrations. Each subplot represents a particular bottom type and a specific ocean color sensor combination. Each row indicates the results from different satellites (L8/OLI, SNPP/VIIRS, and S3A/OLCI), while each column refers to the results for different bottom types (coral, seagrass, and sand).



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Figure 4. Dependence of the accuracy (specifically, absolute percentage error) of the water depth retrieval on the contribution of bottom reflection. The bottom ratio, or the ratio of bottom reflection contributed to the remote sensing reflectance, is calculated and used as the reference in the x-axis. Each subplot represents a particular bottom type and a specific ocean color sensor combination. Each row indicates the results from different satellites (L8/OLI, SNPP/VIIRS, and S3A/OLCI), while each column refers to the results for different substrates (coral, seagrass, and sand).





Figure 5. (a) Locations of selected study areas; (b) location of the study area in Hawaii; (c) a true-color image of the coral reefs in Maui, Hawaii; (d) a true-color image of the Florida Keys; and (e) a true-color image of the Bahamas (highlighted in dashed line).



Figure 6. (a) Bathymetry map (in meters) in the reef system of Hawaii derived from the L8/OLI images with the two-spectrum optimization approach (2-SOA). (b) Bathymetry map derived from LiDAR measurements. (c) Scatterplot for the water depths derived from L8/OLI and LiDAR (with colors and contours indicating the data density), where the LiDAR matchup data were determined from the nearest pixels. The red solid line in (c) is the linear regression for L8/OLI- and LiDAR-derived water depths: Y = 0.96X + 3.21, $R^2 = 0.70$.



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Figure 7. Comparison of the water depth retrievals from the L8/OLI images with the two-spectrum optimization approach (2-SOA) and the LiDAR sensing technique along with four pre-selected meridional transect lines, $-36^{\circ}37'W$, $-36^{\circ}36.5'W$, $-36^{\circ}36'W$, and $-36^{\circ}35.5'W$, respectively. The x-axis is given in the number of pixels (40 pixels are equivalent to a horizontal distance of about 1200 m). The equations of the form of H_{L8} = A×H_{lidar} + M in each subplot refer to the Type-II linear fit between the water depths derived from L8/OLI and LiDAR.



865Figure 8. (a) Bathymetry map (in meters) for the seagrass environment of Florida Keys866derived from the S3A/OLCI images with the two-spectrum optimization approach. (b)867Bathymetry map (in meters) derived from the NOAA CRM model. (c) Scatterplot for868the water depth retrievals from S3A/OLCI and CRM (with the colors and contours869indicating the data density), where the CRM matchup data were averaged over 3×3870pixels. The red solid line in (c) is the linear regression for L8/OLI- and LiDAR-derived871water depths: Y = 0.57X + 1.72, R² = 0.75.



Figure 9. (a) The bathymetric map (in meters) in the Bahamas derived from 873 SNPP/VIIRS images (the black dots indicate the sites with available navigation depth 874 data). (b) Validation of SNPP/VIIRS-derived depths with the water depth data from 875 the nautical chart (with colors and contours indicating the data density). (c) The 876 bathymetry map derived from S3A/OLCI images using 2-SOA (the black dots indicate 877 the sites with available depth data). (d) Validation of S3A-derived depths with the 878 water depth data extracted from the nautical chart. (e) Scatterplot for the water depth 879 880 retrievals from SNPP/VIIRS and S3A/OLCI; for the latter, the water depths were averaged over 3×3 pixels. 881



883 Figure 10. Relative difference (ε) of $R_{rs}(443)$ values in two collocated satellite images 884 in three different benthic environments: (a) coral reefs, (b) seagrass, and (c) sand. The 885 relative difference is derived as $\varepsilon = \left[\frac{R_{rs}^{obs}(t_1) - R_{rs}^{obs}(t_2)}{R_{rs}^{obs}(t_2)} \right] / \frac{R_{rs}^{obs}(t_2)}{R_{rs}^{obs}(t_2)}$. The detailed 886 information on the L8/OLI, S3A/OLCI, and SNPP/VIIRS images is given in Table 1.



889 Figure 11. Influence of the water level difference induced by tides (ΔH) on $R_{rs}(443)$ in 890 shallow waters (0–30 m). The simulations considered various inherent optical 891 properties and bottom albedo randomly sampled from the synthetic data for each 892 bottom types; the total number of simulations is 28479. Eight levels of ΔH are 893 considered, which vary from -0.4 m to 0.4 m, with a step of 0.1 m.