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# 1 Optical properties of Forel-Ule water types deduced from 15 years of 2 global satellite ocean color observations

- Jaime Pitarch<sup>1\*</sup>, Hendrik J. van der Woerd<sup>2</sup>, Robert J. W. Brewin<sup>3</sup>, Oliver Zielinski<sup>4,5</sup>
- <sup>1</sup>NIOZ Royal Netherlands Institute for Sea Research, Department of Coastal Systems, and
   Utrecht University, PO Box 59, 1790AB Den Burg, Texel, The Netherlands
- <sup>2</sup>Institute for Environmental Studies (IVM), Water & Climate Risk, VU University Amsterdam,
   De Boelelaan 1087, 1081HV Amsterdam, The Netherlands
- <sup>3</sup>National Centre for Earth Observation, Plymouth Marine Laboratory, Prospect Place, PL1 3DH
   Plymouth, United Kingdom
- <sup>4</sup>Center for Marine Sensors, Institute for Chemistry and Biology of the Marine Environment,
   Carl von Ossietzky University of Oldenburg, Schleusenstrasse 1, 26382 Wilhelmshaven, Germany
- <sup>5</sup>DFKI Research Group Marine Perception, Marie Curie Strasse 1, 26129 Oldenburg, Germany
- 13 <u>\*jaime.pitarch@nioz.nl</u>

## 14 Abstract

15 The Forel-Ule (FU) color comparator scale is the oldest set of optical water types (OWTs). This 16 scale was originally developed for visual comparison and generated an immense amount of data, 17 with hundreds of thousands of observations being gathered from the last 130 years. Since recently, 18 the FU scale is also applicable to remote sensing data. This has been possible thanks to an optical 19 characterization of the 21 FU colors in terms of the (x,y) CIE standards and new algorithms that 20 convert remote-sensing reflectances (Rrs) from satellite-borne ocean color sensors to FU. Rrs-derived 21 hue angle and FU have been recently applied with success in the assessment of color variability of 22 lakes and specific shelf areas, but an evaluation over global oceanic waters is still missing. By 23 clustering global climatological ESA-OC-CCI v2.0 R<sub>rs</sub> with the derived FU, we obtain a set of R<sub>rs</sub> to be 24 used as optical water types (OWTs). Diffuse attenuation coefficient, Secchi disk depth and chlorophyll 25 concentration are also associated to the FU classes. The angular distances of a given R<sub>rs</sub> to the two 26 nearest FU classes are proposed as simple and robust membership indexes, adding up to one. We 27 also evaluate the advantages and limitations of FU and the hue angle as monitoring tools over the 28 full marine range, from the most oligotrophic areas to the turbid and productive coastal zones. The 29 first 7 FU indexes cover 99 % of global surface waters. Unlike the hue angle, that resolves all spatio-30 temporal color variations, the FU scale is coarse as a monitoring tool for oligotrophic waters as all the 31 subtropical gyres saturate to FU=1, while the color of other seas varies across 2, 3 or even 4 FU classes. We illustrate the introduction of a new "zero" FU class that increases monitoring resolution 32 33 at the blue end of the color range. Finally, we show how optical diversity varies across the color 34 range and compare several sets of OWTs from a color perspective. Overall, we provide a valuable and 35 self-consistent dataset that enhances the usefulness of the FU scale by converting it to useful 36 information for the oceanographic community. This OWT scheme keeps the advantages of other 37 datasets, like being useful to study ocean color product quality and characterize the uncertainties, 38 but also allows to continue to monitor long-term change in optical diversity over the global ocean 39 color. Integration into the optical modules of ecosystem models can help verify past simulations that 40 predate the satellite age, through comparisons with in-situ FU data collected at the time.

## 41 **1. Introduction**

42 Classification of water masses into optical types has been an old practice in optical 43 oceanography and the quantity used for classification has varied with the available technology. The 44 first classification, the Forel-Ule scale (FU) (Forel 1890; Ule 1892), was developed as a visual color 45 comparator originally conceived for inland waters, although soon after it also started to be used in 46 sea water (Wernand et al. 2013b, and references therein). The FU scale is made of twenty-one colors 47 across a hue gradient, from blue to green, yellow and brown (Novoa et al. 2013). Currently, more 48 than 280000 observations over global marine areas are centralized by NOAA 49 (https://www.nodc.noaa.gov/OC5/WOD/secchi-data-format.html) and constitute the longest record of ocean color archive, extending up to thirteen decades into the past. FU derived climatological 50 51 maps show patterns consistent with our current understanding of the optics of the global oceans 52 (Boyce et al. 2012; Wernand et al. 2013b). FU observations correlate well with in-situ chlorophyll 53 until FU=10 (Boyce et al. 2012) and this principle was used to derive multi-decadal chlorophyll trends 54 from in-situ FU observations (Wernand et al. 2013b).

55 Morel and Prieur (1977) defined the famous classification case 1 and case 2 waters, in terms of 56 the relative amount of phytoplankton concentration and non-living material. This classification has 57 been interpreted by many as a distinction between water where all optically-active constituents 58 correlate to chlorophyll concentration and water where they do not (Lee and Hu 2006). In the last 59 years, the term "case 2" is being replaced by "optically complex", though keeping a similar 60 interpretation.

61 Jerlov (1976) categorized waters into five oceanic and five coastal types based on diffuse 62 attenuation coefficient (K<sub>d</sub>) spectra and provided maps of this classification from in-situ K<sub>d</sub> cruise 63 data. The popularity of the Jerlov's optical water types (OWTs) across disciplines was facilitated by their description in terms of light attenuation, a quantity with a clear meaning for all 64 65 oceanographers. Ecosystem modelers often parameterize light extinction by assuming a given Jerlov water type (Burchard et al. 1999; Cahill et al. 2008; Löptien et al. 2009). It is also widely used in the 66 67 field of underwater optical communications (Kaushal and Kaddoum 2016). Solonenko and Mobley 68 (2015) associated Jerlov's types to absorption and scattering coefficients in average marine waters 69 after bio-optical modeling.

70 Moore's original OWTs (Moore et al. 2001) are based on remote-sensing reflectance ( $R_{rs}$ ) and 71 have undergone modifications (Moore et al. 2009; Moore et al. 2012), being Jackson et al. (2017) the 72 last update (J17 from hereon). Mélin and Vantrepotte (2015) (M15 from hereon) generated their 73 OWTs from satellite R<sub>rs</sub> after removal of open oceanic waters, thus increasing the weight of optically 74 complex waters, although their dataset also included very clear waters, thus making their 75 classification arguably suitable for oceanic waters as well. Wei et al. (2016) developed a novel quality 76 assurance system for in-situ and satellite R<sub>rs</sub>. Its concept was that the quality of a given R<sub>rs</sub> needed to 77 be defined not only after a per-band matchup analysis, but also by assessing the spectral shape. 78 Therefore, they compiled in-situ R<sub>rs</sub> of a wide range of waters, from ultra-oligotrophic to eutrophic, 79 yellow, shallow and sediment-rich waters, and clustered them in classes (W16 from hereon).

Other than for algorithm blending, uncertainty assessment and quality control, OWTs are useful as indicators of seasonal and geographical variability, linked to physical and biological processes (Trochta et al. 2015). There have been other published OWTs over inland water for specific areas, but we do not include them in this short review as this work focuses on global oceanic waters.

OWTs classification can only be applied to satellite data if the quantity used to classify can be derived remotely. Benefits of this approach are many, as satellite data provide unique spatial coverage and temporal frequency. Wernand et al. (2013a) presented an algorithm to calculate FU from MERIS R<sub>rs</sub>. By using the hue angle as FU's continuous counterpart, FU can be derived using data from any satellite sensor where a hue angle algorithm is available (van der Woerd and Wernand

89 2015, 2018). Based on these cited works, hue angle and FU processors were developed for the ESA 90 SNAP software (http://step.esa.int/main/toolboxes/snap/). These algorithms have recently found 91 application to study color variability of a large amount of New Zealand lakes using five years of 92 Landsat 8 data (Lehmann et al. 2018), global inland waters using MODIS data for summer 2012 93 (Wang et al. 2018) and Mozambique and the Irish seas using twelve years of MODIS data (Jafar-Sidik et al. 2018). Dutkiewicz et al. (2019) incorporated an optical module to a global physics and 94 95 biogeochemistry model and were able to predict R<sub>rs</sub> changes during the 21<sup>st</sup> century, forced by a 96 predicted scenario of green-house gas emissions. They applied the hue algorithm to the predicted R<sub>rs</sub> 97 and found that the color of the oceans will change unevenly. They forecasted a bluer North Atlantic, 98 with a hue angle increase of ~  $10^{\circ}$  by 2100, whereas other zones displayed smaller hue angle 99 increases or decreases. Wang et al. (2019) presented a method to link combined Secchi disk depth 100 and Forel-Ule data to absorption and backscattering, with the motivation to bridge the gap between 101 historical and modern measurements in marine optics and build long time series, in a similar fashion 102 as previously done using chlorophyll as the target variable (Boyce et al. 2012).

103 In this article, we apply the FU and hue angle algorithms to ocean color data over global 104 marine waters, and study how seasonal variability of very diverse marine zones is resolved by them. 105 We also provide quantification of the optical diversity of marine waters and quantify the uncertainty 106 due to dimensionality reduction. We show that the FU scale can be interpreted as an OWTs set, by 107 clustering all marine R<sub>rs</sub> falling into a given FU and obtaining the mean value. If the same procedure is followed for the R<sub>rs</sub>-derived chlorophyll concentration (C<sub>a</sub>), as well as other IOPs and AOPs, a reliable 108 109 translation of the FU colors into modern optical variables is obtained, with major importance for the 110 interpretation of archived in-situ FU data, as well as for a rapid interpretation of marine R<sub>rs</sub> and FU 111 data in terms of other optical variables.

- 112 The aims of this work are to:
- Develop a historical, FU-class based method, to study optical diversity at global scale.
- Construct a global dataset of matched FU class data with standard variables used by the oceanographic community.
- Monitor global variability of selected marine zones with the hue angle.
- Provide a new framework for comparison of different OWT schemes.
- 118 The approach is significant, as unlike other OWT schemes, the FU scale can be used to:
- Continue to monitor long-term change in optical diversity over the global ocean color by
   stitching together in situ FU data collected over the past century with the satellite era.
- Bridge, in a consistent manner, satellite data from two different periods (e.g. 1970-80's CZCS and 1997-onward) using in situ FU data over the two periods.
- Verify past model simulations that predate the satellite era, through comparison with in situ FU
   data collected at the time by using an optical module within the ecosystem model.
- Facilitate the interpretation of FU color by the oceanographic community, useful for teaching
   and demonstrating the concepts of satellite ocean color at global scale, using a visual index.
- 127

## 128 **2. Materials and Methods**

### 129 **2.1. Satellite data**

The most suited source data to study the global seasonal variability are climatological reflectances derived from a long time series. The ESA-OC-CCI v2.0 R<sub>rs</sub> monthly climatological dataset at 0.25 degrees was downloaded from the ftp server at of the ESA-OC-CCI site. These files are monthly composites (1997-2013) of merged sensor (MERIS, MODIS, SeaWiFS) products, where R<sub>rs</sub> from MODIS and MERIS were band-shifted and bias-corrected to SeaWiFS bands and values. MODIS and SeaWiFS R<sub>rs</sub> products were derived from 4km resolution level-3 binned standard NASA products; MERIS was derived from a 4km level-3 binning of the output of the HYGEOS POLYMER algorithm.
 Downloadable NetCDF files include R<sub>rs</sub> available at the wavelengths 412, 443, 490, 510, 555 and 670
 nm as well as C<sub>a</sub>. Notably, the files include pixel-by-pixel bias estimates of all variables. This allows to
 obtain unbiased monthly estimates of each. Further information on the generated R<sub>rs</sub> and C<sub>a</sub>
 products can be retrieved in the Product User Guide (Grant et al. 2015).

From the unbiased  $R_{rs}$ , the absorption (a) and backscattering coefficient ( $b_b$ ) were retrieved using the QAA v6 algorithm (Lee et al. 2002) and the diffuse attenuation coefficient ( $K_d$ ) was derived from them (Lee et al. 2013). The Secchi disk depth was derived according to Lee et al. (2015). The derivations of the CIE (x,y) coordinates, the hue angle and the FU index are explained in the next section.

#### 146 **2.2. Reflectance conversion into color**

147 The FU scale was recently revisited, manufactured and optically characterized (Novoa et al. 148 2013). Derivation of the hue angle and the FU index from satellite data was recently presented as 149 well (van der Woerd and Wernand 2015, 2018; Wernand et al. 2013a). We provide here a complete 150 summary of the background needed in the article.

151 The calculations start with projecting a given spectrum ( $R_{rs}$  here) onto the CIE tristimulus space 152 (X,Y,Z) by weighting it with the three CIE standard observer color matching functions and integrating 153 over the full range  $\Lambda$ :

154 
$$X = \int_{\Lambda} R_{rs}(\lambda)\bar{x}(\lambda) \, d\lambda, Y = \int_{\Lambda} R_{rs}(\lambda)\bar{y}(\lambda) \, d\lambda, Z = \int_{\Lambda} R_{rs}(\lambda)\bar{z}(\lambda) \, d\lambda$$
(1)

155 These weighting functions are plotted in Fig. 1. Their sum,  $\bar{x} + \bar{y} + \bar{z}$ , is also plotted. This plot 156 illustrates the band range to which this algorithm is sensitive.





158 Fig. 1 The CIE standard observer color matching functions and the sum of all.

Equation (2) further reduces the dimensionality from three to two by normalizing the three quantities in eq. (1) by the sum of them. Information on the spectrum intensity or brightness is lost after this normalization. Therefore, a constant spectrum (white or gray) is projected onto ( $x_w,y_w$ )=(1/3,1/3). (Jackson et al. 2017). Here, division by (X+Y+Z) equals to a normalization by the sum of the three color matching functions,  $\bar{x} + \bar{y} + \bar{z}$ . Thus, two different R<sub>rs</sub> that differ by a constant factor would be projected onto the same (x,y) point.

165 
$$x = \frac{X}{X+Y+Z}, \ y = \frac{Y}{X+Y+Z}$$
 (2)



166

Fig. 2 The CIE 1931 color space in the (x,y) coordinates. The coordinates of the 21 FU colors after Novoa et al. (2013) are plotted as blue dots. The white point W lays on (1/3,1/3). An arbitrary spectrum is represented as point P, having polar coordinates ( $\alpha$ ,s) and laying between FU 3 and 4.

Fig. 2 illustrates a given  $R_{rs}$ , projected onto the (x,y) space as point P, following eqs. (1-2). The projection of a given  $R_{rs}$  onto the (x,y) coordinates is a great dimensionality reduction, but (x,y) still contain information on the spectrum shape. Points close to the white point W (lower s) have a broader spectral shape, and the closer they get to it, the more the definition of color loses its meaning. On the other hand, points far away from W have a higher saturation or purity, and they are spectrally narrower. Thus, saturation (s), and hue angle ( $\alpha$ ) can be separated by converting (x,y) to polar coordinates, setting the origin at W.

177 
$$\alpha = \arctan\left(\frac{y-y_w}{x-x_w}\right), \ s = \sqrt{(x-x_w)^2 + (y-y_w)^2}$$
 (3)

178 As every FU index has its relative (x,y) coordinates after Novoa et al. (2013), the FU of any 179 given spectrum is calculated as the nearest FU class in terms of the hue angle. As a matter of 180 nomenclature, we refer to "FU<sub>n</sub>" as the n-th FU index of any of the 21 classes, whereas we write 181 "FU=n" when a given spectrum is closest to FU<sub>n</sub> in terms of hue angle than to any other FU index.

In the practical implementation using satellite data, R<sub>rs</sub> is not a continuous spectrum but a set of discrete values as a result of the convolution with the sensor spectral response functions of each band. Van der Woerd and Wernand (2015) and van der Woerd and Wernand (2018) proposed a discretization of eq. (1) for the estimation of X,Y and Z. In particular, for a R<sub>rs</sub> at the SeaWiFS bands, the discrete integration leads the following linear combination of the bands:

187 
$$\binom{X}{Y} = \begin{pmatrix} 2.957 & 10.861 & 3.744 & 3.455 & 52.304 & 32.825 \\ 0.112 & 1.711 & 5.672 & 21.929 & 59.454 & 17.810 \\ 14.354 & 58.356 & 28.227 & 3.967 & 0.682 & 0.018 \end{pmatrix} R_{rs,sw}$$
(4)

where  $R_{rs,sw}$  is a column vector containing  $R_{rs}$  at the SeaWiFS bands. From eq. (4), the (x,y) coordinates and the hue angle can be obtained with eq. (2). Van der Woerd and Wernand (2015) and van der Woerd and Wernand (2018) showed that the discrete integration to estimate the hue angle contains an uncertainty that is only partially random, and has a rather predictable shape as a function of the estimated hue angle itself. This is a consequence of the generally smooth and 193 predictable R<sub>rs</sub> spectral shape across a wide range of natural waters. Therefore, they provided 194 uncertainty-fitted curves for the removal of this bias.



195

196 Fig. 3 Discretization errors  $\Delta x$  and  $\Delta y$  in the computation of the (x,y) coordinates as a function of x' 197 for the IOCCG synthetized dataset, and corresponding fitted curves  $c_x$  and  $c_y$  (Table 1).

198 Their approach provided unbiased hue and FU estimates, but left (x,y) biased. Since we consider (x,y) and also the saturation (s) important for our study, we decided to modify the method 199 200 and correct biases directly from (x,y). We used the same IOCCG synthetized dataset as van der Woerd and Wernand (2015) and van der Woerd and Wernand (2018) to perform this correction. 201 202 From every R<sub>rs</sub> in the dataset, the "exact" (x,y) coordinates were calculated using eqs. (1-2). Then, 203 every  $R_{rs}$  was convoluted with the SeaWiFS response functions centered at 412, 443, 490, 510, 555 and 670 nm, and from the spectra at the SeaWiFS bands, the "biased" (x',y') estimates were 204 205 calculated using eqs. (4 and 2). Fig. 3 shows the plotted errors  $\Delta x=x'-x$ ,  $\Delta y=y'-y$  as a function of x'. 206 Similarly to what reported by van der Woerd and Wernand (2015) and van der Woerd and Wernand (2018) for the hue angle, the errors  $\Delta x$  and  $\Delta y$  are largely systematic and therefore they can be 207 approximated by fitting functions. Here, we found that 6<sup>th</sup> grade polynomials provided good fits: 208  $c_x = \sum_{i=0}^{N} p_i h^i$ ,  $c_y = \sum_{i=0}^{N} q_i h^i$  (coefficients provided in Table 1), where N=6, h is the centered and 209 normalized x', based on the mean and standard deviation of the training dataset: h=(x'-m)/s, with 210 211 m=0.3017 and s=0.07398. Finally, biases are corrected as  $x_{cor}=x'-c_x$ ,  $y_{cor}=y'-c_y$ . For the remainder of 212 the article, we refer to the computed quantities  $(x_{cor}, y_{cor})$  as the exact (x, y).

213

Table 1 Coefficients of the polynomial fits to correct biases in (x,y), times 100.

I	0	1	2	3	4	5	6
100·p <sub>i</sub>	2.9653	-2.0032	-2.1461	0.034326	0.40886	0.091567	-0.03510
100·q <sub>i</sub>	-0.7786	-1.5604	1.2188	0.44135	-0.1067	-0.024582	-0.03253

214

From the original ESA-OC-CCI v2.0 climatological files, associated files were generated, that exported the original latitude, longitude and time variables and incorporated x, y, the hue angle and FU.These products have uncertainties though. Assuming an exact source  $R_{rs}$ , the discretization, after systematic biases compensation, leaves residual errors, which are  $\Delta x$ - $c_x$  and  $\Delta y$ -cy (Fig. 3). These errors are higher for green waters than for blue waters. This result can be interpreted as follows: the SeaWiFS bands are appropriate for capturing all relevant spectral features of blue waters, but for greener waters, some information is lost. Specifically, for x<0.25 (blue waters), the following uncertainties, quantified as the standard deviations for x, y and  $\alpha$  are obtained:  $\sigma_x=8.03\cdot10^{-4}$ ,  $\sigma_y=6.62\cdot10^{-4}$  and  $\sigma_{\alpha}=0.13^{\circ}$ . For x $\geq 0.25$ , one obtains  $\sigma_x=5.14\cdot10^{-3}$ ,  $\sigma_y=2.20\cdot10^{-3}$  and  $\sigma_{\alpha}=2.61^{\circ}$ . Even in this last case, uncertainties can be assumed very small compared to other sources of uncertainties in ocean color.

226 Such uncertainties must be added to the uncertainties of the R<sub>rs</sub> at sea level when these are derived from satellite measurements. Work in the framework of ESA-OC-CCI has provided 227 228 uncertainty maps related to R<sub>rs</sub> at each band, derived from comparison with in-situ observations. In brief, R<sub>rs</sub> uncertainties were calculated for matchups to an in-situ dataset and discriminated 229 230 according to Moore's OWTs (Moore et al. 2009). These uncertainties were then extended to the 231 global map by calculating the OWT membership for every pixel and assuming the uncertainty as the 232 weighted average of the uncertainties for all OWTs in the matchups, using the pixel's class 233 memberships as weights. Full details can be found at the Product User Guide (Grant et al. 2015).

234 ESA-OC-CCI provides maps of systematic biases and RMS differences. Biases were removed 235 from the data and subtracted from the RMS differences in the final uncertainty estimation. Resulting 236 standard deviation maps showed some seasonal variability, that was small compared to the 237 differences between bands. Geographically and seasonally averaged standard deviations for each R<sub>rs</sub> band are  $\sigma_{Rrs}$ =(0.0012631, 0.001063, 0.0007631, 0.00061579, 0.00051381, 0.0002132) sr<sup>-1</sup>. These 238 239 uncertainties were propagated to the (x,y) and  $\alpha$  estimations. We derived these variables and their 240 associated uncertainties from the IOCCG dataset but now adding random and normally distributed 241 errors with zero mean and  $\sigma_{Rrs}$  standard deviation to the re-sampled  $R_{rs}$  at the SeaWiFS bands, always 242 using the coefficients of Table 1. We repeated the procedure 1000 times and obtained the uncertainties for x<0.25:  $\sigma_x$ =0.011,  $\sigma_y$ =0.024 and  $\sigma_\alpha$ =6.44°. For x≥0.25, we obtained  $\sigma_x$ =0.026, 243  $\sigma_v$ =0.041 and  $\sigma_{\alpha}$ =18.38°. Thus, uncertainties in CCI R<sub>rs</sub> exceed in one or two orders of magnitude 244 uncertainties in the (x,y) and  $\alpha$  estimations from an exact discrete spectrum, but overall the total 245 246 uncertainties are low enough to obtain reliable estimates using CCI data, especially over blue waters. 247 There, uncertainties in the hue angle are about 3 % of its value, whereas for green waters, 248 uncertainties are about 20 %.

#### 249 2.3. Class membership

250 Optical water types have been proposed as tools for algorithm comparison and merging 251 (Jackson et al. 2017). In order to avoid discontinuous boundaries between classes, the class memberships have been suggested as weights for class-algorithm blending. Class memberships are 252 253 also useful for generating mapped product uncertainties. Uncertainties are estimated for every class 254 in a matchup dataset and are extrapolated to a given pixel by calculating the class memberships of it 255 and estimating the uncertainty as the weighted averaged of the calculated uncertainties per class, 256 using the class memberships as weights (Grant et al. 2015). However, the R<sub>rs</sub> of an OWT dataset are 257 not any orthogonal basis functions and correspondingly, the class membership coefficients of a given R<sub>rs</sub> are not any eigenvalues. This approach is therefore heuristic and may generate methodological 258 259 doubts, but still it may be applicable as a fit-for-purpose mechanism.







262 Unitarity is a desired property of any set of class membership coefficients. Additionally, for the 263 sake of an easier interpretation, coefficients shall be zero for classes that are far enough from a given 264 spectrum, and shall have non-zero values for a reduced number of classes. Here, we propose a class 265 membership coefficient set such that, given a R<sub>rs</sub>, its membership is non-zero only for the upper and 266 lower FU classes, being their values  $C_{U}$  and  $C_{L}$ , respectively, both memberships adding up to one and 267 being proportional to the distance in hue angle units. More specifically, for a given R<sub>rs</sub>, the hue angle 268 is calculated,  $\alpha_{R}$ . If  $\alpha_{L}$  and  $\alpha_{U}$  are the hue angles of the nearest lower and upper FU class, 269 respectively, then the membership value for each is, respectively:  $C_U = (\alpha_R - \alpha_L)/(\alpha_U - \alpha_L)$ ,  $C_L = (\alpha_U - \alpha_L)/(\alpha_L - \alpha_L)$  $\alpha_{\rm R}$ )/( $\alpha_{\rm U}$  -  $\alpha_{\rm L}$ ). If  $\alpha_{\rm R}$  is lower than the hue angle of FU<sub>1</sub> (or higher than FU<sub>21</sub>), then a membership equal 270 271 to one is assigned to the nearest and zero to the rest. The graphical result of these definitions is 272 shown in Fig. 4. By definition, these classes do not carry information on spectral similarity. Every spectrum always has a total membership equal to one, no matter how the spectral shape differs 273 274 from those of the FU. However, a real spectrum is never going to have a random shape. We show 275 later in the article that the optical variability in the world's surface waters is limited and is well 276 described by the hue angle to a first order.

### 277 3. Results and discussion

### 278 **3.1. Color distribution of global reflectances**

The dimensionality reduction from (x,y) to the hue angle as a color descriptor implies some loss of information unless the interdependency between x and y is very strong, i.e., case 1. Fig. 5 plots the (x,y) (panel a1)) and the ( $\alpha$ ,s) polar coordinates (panel b1)) of the ESA-OC-CCI v2.0 global climatological monthly R<sub>rs</sub>. The frequency distributions of the (x,y) coordinates are shown in panels a2) and a3), whereas the respective for ( $\alpha$ ,s) are shown at panels b2) and b3).



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Fig. 5 Distributions of the global climatological ESA-OC-CCI v2.0  $R_{rs}$  on the (x,y) plane and in polar coordinates ( $\alpha$ ,s). Panel a1) log-density plot of (x,y) distribution, with dot color indicating increasing data density. The moving median of y for every x as thick line, and the 25<sup>th</sup> and 75<sup>th</sup> percentiles as band boundaries, are plotted on top. a2) distribution of x. a3) distribution of y. a4) same band as panel a1) but setting the moving median of y as ordinates origin. Panels b1) to b4) are equivalent to a1) to a4) but replacing x by s and y by  $\alpha$ .

291 Fig. 5 shows that all global variability occupies a very limited area in the (x,y) and ( $\alpha$ ,s) planes, 292 distributing along a trail from deep blue until green-brown color. More importantly, this trail is very 293 narrow and, to a first order, it is distributed along a line (thick lines in panels a1) and b1)), evidencing 294 a strong inter-dependency. Therefore, for a given  $\alpha$ , an average s can be predicted. This statement is 295 especially true for the bluest waters (panels a4) and b4)), confirming the hypothesis that a single 296 parameter condenses well all optical information. On the other hand, the trail progressively spreads 297 with increasing x or decreasing  $\alpha$ , illustrating an increasing optical complexity. At some point, for 298 green-brown waters, a given hue angle can be associated to a wider range of saturations (and 299 spectral shapes) with correspondingly different constituent concentrations, as happens in case 2 300 waters. These results show that there is not a clear threshold for the separation between case 1 and 301 case 2 waters, although the band thickness  $\Delta s$  appears to remain relatively stable from the blue waters until  $\alpha \approx 214^{\circ}$ , staying  $\Delta s < 2 \cdot 10^{-3}$  and then sharply increasing. This boundary falls in the class 302 303 FU=3 (blue waters) and could be defined as separator between case 1 and case 2 waters. Around 80 % of the world's surface waters fall under this case 1 classification (see frequency distribution of the 304 305 hue angle in panel b2)), including all oceans and big seas. Description of annual variability of selected 306 marine areas is provided further on.

#### 307 **3.2. Class memberships based on the hue angle**

Seasonal variation of the class memberships 2 and 4 (C2 and C4) is shown in Fig. 6 for the Mediterranean and Black Seas, using also the ESA-OC-CCI v2.0 global climatological monthly R<sub>rs</sub>. Class memberships are functions of the hue angle. They have value one when the hue angle of a pixel is equal to that of the FU classes 2 and 4, respectively, and fall linearly to zero when the hue angle is that of the adjacent FU classes (Fig. 4). Classes are defined such as a pixel has non-zero membership for a maximum of two adjacent classes, so pixels showing non-zero values for C2 and C4 are disjoint sets and can be plotted on the same map.



315

Fig. 6 Color maps of membership to class 2 and class 4 of the Mediterranean Sea for the climatological months of January, April, July and October, based on the ESA-OC-CCI v2.0 global climatological monthly R<sub>rs</sub>.

319 The map of January clearly distinguishes between the eastern and the western Mediterranean: 320 the eastern Mediterranean has medium C2 membership, increasing towards the more oligotrophic 321 areas, whereas the western displays C4 membership and has higher values towards the coastal areas. 322 The Black Sea has zero values for C2 and C4, indicating a dominance of higher classes. From spring to 323 summer, water becomes bluer in both basins, as indicated by higher C2 values for the eastern and 324 western Mediterranean, with the exceptions of the Alboran Sea and the bloom at the gulf of Lion. 325 The Black Sea shows increased C4 membership. In July, eastern Mediterranean waters are very blue 326 which leads to reduced C2 membership, and more dominance by C1, while the western have higher 327 values and almost no presence of C4 membership. The Black Sea displays the highest C4 membership 328 values, except the northern coastal areas, whose waters are greener. In October, water is tending 329 back towards greener colors, which translates in higher C2 memberships in the western 330 Mediterranean, while the Black Sea starts to reduce the C4 membership and tends to higher classes.

### 331 **3.3. Global maps of seasonal Forel-Ule variability**

Application of the FU algorithm to the ESA-OC-CCI v2.0 global climatological monthly R<sub>rs</sub> (Fig. 7) reveals a vast majority of zones falling on the lowest FU classes. 94 % of the surface waters belong to FU between 1 and 4 and 99% belong to the first 10 classes. The ultra-oligotrophic zones are permanently classified in FU=1, although their extension does have seasonal variability. FU=2 zones have an overall higher surface area. Equatorial, coastal and middle to high latitude seas occupy higher FU values. All oceanic zones are restricted to FU from 1 to 4.



338



The FU OWTs (Fig. 8) are constructed by clustering all R<sub>rs</sub> belonging to a particular FU index. By using the climatological satellite data to build the OWTs, a good representation of average marine reflectances is ensured.



344

Fig. 8 Remote-sensing reflectances corresponding to the first 10 FU water types, obtained from the ESA-OC-CCI v2.0 global climatological monthly R<sub>rs</sub>. Bold traces correspond to median values and bands extend between the 25<sup>th</sup> and 75<sup>th</sup> percentiles. Data of all classes can be found at Table A1.

The FU OWTs nicely represent many different water types: the first numbers are typical of clear oceanic waters, displaying decreasing R<sub>rs</sub> values at blue wavelengths and increasing at the green with increasing FU. As FU increases beyond 5, R<sub>rs</sub> are more characteristic of green coastal waters and include higher ranges of concentrations and shapes.

Given that FU estimations can be made visually or with simple instruments like photographic cameras (Busch et al. 2016), and also given the existence of long-term FU records, it is of value to provide indicators of optical descriptors that are common in optical oceanography, like diffuse attenuation coefficient ( $K_d$ ), Secchi disk depth ( $z_{SD}$ ), and chlorophyll concentration ( $C_a$ ).



356

Fig. 9 Diffuse attenuation coefficient of downwelling irradiance of the first 9 FU classes, representing the median in bold line and the interval between the 25<sup>th</sup> and 75<sup>th</sup> percentiles in shaded band. For a

359 complete description, the reader is referred to Table A2.

The FU-related K<sub>d</sub> classes are calculated by deriving K<sub>d</sub> on a pixel basis (Lee et al. 2002; Lee et al. 2013) and clustering them based on FU. They are shown in Fig. 9. K<sub>d</sub> increases monotonically at every band as FU increases, with a red shift of the window of maximum light penetration, relevant for  $z_{SD}$  calculations (Lee et al. 2015). FU=1 has the minimum at 443 nm, FU=2 to 4 have the minimum at 490 nm, FU=5 has the minimum at 510 nm, and FU=6 to 10 have the minimum at 555 nm.

Light extinction in the ocean is an important parameter for heat budget calculations and ecosystem modeling, and can be linked to underwater visibility. Modelers who need to assume a light extinction model can take advantage of this classification by downloading these climatological FU maps and adjusting light extinction models to their specific zone and season. If models already predict light extinction, cross-checking with this climatology can provide indication about the accuracy of the modeling.



371

Fig. 10 Secchi disk depth histograms for each FU class. Each histogram aggregates all z<sub>sD</sub> derivations
 (Lee et al. 2015) from the ESA-OC-CCI v2.0 global climatological monthly R<sub>rs</sub> whose per-pixel
 associated FU have the same value. Statistical descriptors can be found in Table A3.

375 Secchi disk depth generally decreases as FU increases. The class FU=1 has a  $z_{SD}$  distribution 376 with a very wide and asymmetric shape due to its dead-end position, until  $z_{SD}$ =60 m. Its shape 377 suggests that it may be composed of a multipolar distribution, which may be related to separate 378 oceans. This case exemplifies well that FU=1 is very ambiguous for representing an average 379 oligotrophic ocean. The next low FU distributions are bell-shaped for oceanic waters, but as FU 380 reaches 6, a second population appears at the left of the bell shape: these observations are linked to 381 coastal zones with different optical properties, where sediments and CDOM reduce transparency.



382

Fig. 11 Chlorophyll concentration histograms for each FU class. Each histogram aggregates all C<sub>a</sub> data the ESA-OC-CCI v2.0 global climatological monthly C<sub>a</sub> dataset whose per-pixel associated FU have the same value. Statistical descriptors can be found in Table A4.

The histograms of chlorophyll concentration for every FU class (Fig. 11) reveal a similar but inverted shape than  $z_{SD}$  for oceanic waters, as expected, though having a general Gaussian shape, even for optically-complex waters, perhaps suggesting that the left tails of the  $z_{SD}$  distributions for FU 8 to 10 were caused by sediments and CDOM.



390

Fig. 12 Chlorophyll concentration and Secchi disk depth box plots for each FU optical water type. The median is plotted as a dot inside a white circle. The interquartile range is delimited by the box around the median. Whiskers extend until three times the interquartile range below and above the first and third quartile, respectively. Data beyond the whiskers range are considered outliers and are plotted as dots. Statistical descriptors can be found in Tables A3-A4.

Box plots of chlorophyll concentration and Secchi disk depth for every FU condense well the information in the former histograms. The progression is the expected for the blue-green range, with  $C_a$  increasing and  $z_{SD}$  decreasing until FU=17. From this point on,  $C_a$  starts a sharp decrease. Here, very high CDOM concentrations are expected to decrease light availability for the primary producers and thus limiting  $C_a$ .  $z_{SD}$  does not show significant variations at the highest FU classes.

#### 401 **3.5.** Seasonal variability of selected marine areas

Fig. 13 shows a map of series-averaged C<sub>a</sub>. This map highlights the five ultra-oligotrophic gyres. These are characterized by anticyclonic circulation, downwelling and thick thermoclines. Depressed nutricline levels limit the algal development and subsequent biogeochemical processes. While their biological activity is small compared to other areas, their vast size makes their contribution to the global productivity and biogeochemistry significant (Morel et al. 2010). Other zones display higher C<sub>a</sub> values. Middle-to-high oceans are subject to nutrient-rich currents. Shelf seas are more sensitive to 408 terrestrial runoff and bottom resuspension, and upwelling coastal areas are known for the high
409 phytoplankton biomass. Enclosed and semi-enclosed seas follow their own dynamics (Colella et al.
410 2016; Kopelevich et al. 2004; Pitarch et al. 2016).

For a more detailed study about color variability across the globe, we defined twenty-one zones (Table 2, Fig. 13) that represent a wide range of optical variability. The most oligotrophic inner cores of the gyres were selected. Other marine zones were also included, from the equatorial pacific to mid-latitude oceanic zones, enclosed seas, shallow seas and coastal zones. For each zone, the median of all valid pixels was calculated. The goal here is to understand how the optical variability in each region is resolved by increasingly simplified optical descriptors, from (x,y) to the hue angle, to FU.



418

419 Fig. 13 Selected marine zones for the study of the seasonal color variability, over a map of the series-

420 averaged chlorophyll-a concentration.

## 421 Table 2 Acronym and bounding coordinates of the study zones (see Fig. 13)

Zone	Acronym	East (° E)	West (° E)	South (° E)	North (° N)
North Atlantic subtropical gyre	NASG	-65	-52	24	26.5
South Atlantic subtropical gyre	SASG	-30	-23	-19	-15.5
North Pacific subtropical gyre	NPSG	148	160	11	15
South Pacific subtropical gyre	SPSG	-126	-112	-29	-23
Indian Sea gyre	IND	75	87	-29	-24.5
North Atlantic	NA	-45	-20	37	44
South Atlantic	SA	-40	0	-44	-37
Equatorial Pacific	EQP	-160	-120	-2	2
Off south east Greenland	GREE	-32	-25	60	67
Eastern Mediterranean Sea	EMED	24	33	32.5	34
Western Mediterranean Sea	WMED	4.5	7.5	38	41.5
Black Sea	BLAC	42.2	44	30	38
Persian gulf	PERS	52.4	53.8	25	26.2
Arabian Sea	ARAB	54	63	10.5	14.5
Caspian Sea	CASP	47	54	35	47
Yellow Sea	YELL	121.5	125.5	33	35.5
Southern Baltic Sea	BAL	19.6	20.8	57	59.5
Azov Sea	AZOV	36.2	37.4	45.5	46.3



Fig. 14 Hue angle climatological annual variability of selected marine zones (see Fig. 13 and Table 6).
The boundaries between consecutive FU classes are also indicated.

425 Fig. 14 plots the hue angle annual variability of all selected marine zones in Fig. 13 (see Table 2 for boundaries and nomenclature). They all show  $\alpha$ >229 °, and are above the boundary between 426 427 FU=1 and FU=2. Despite being saturated to FU=1, all gyres present a clear hue angle seasonal cycle, 428 with a minimum (greenest) in winter and a maximum (bluest) in summer. Lower winter hues are 429 related to vertical mixing that allows some underlying waters, richer in nutrients, to reach lower 430 depths. Higher hues are associated with a decline in phytoplankton, which is limited by lack of nutrients due to a strong pycnocline formation that stabilizes the water column, limiting the vertical 431 432 mixing, and thus, nutrient supply to the surface. In the NPSG, nutrient supply during winter mixing seems to be hampered, so that seasonality is smooth. NA and SA, as well as both Mediterranean 433 434 basins show the same trend, with maxima in winter and minima in summer, though with different 435 dynamic ranges and lower hues, caused by a higher nutrient availability. NA and WMED have the 436 widest variability and SA and EMED the lowest, all crossing between FU 1-3. Somewhat expected, the 437 EQP has very little seasonal variability, crossing the border between FU=2 and 3 across the seasons. Here, nutrients are horizontally advected to this region (Dave and Lozier 2015), causing higher 438 439 biomass and greener waters. Our data suggests that this process is somewhat higher during the 440 boreal summer, leading to a slight seasonal cycle.

ARAB has the bluest waters in May and the greenest in August, and a secondary blueness peak in November. Phytoplankton blooms in the northwest Arabian Sea during August-September. They are driven by the seasonal monsoon, that triggers upward nutrient fluxes to the euphotic zone, forced by the physical processes of coastal upwelling and offshore Ekman pumping (Brock and McClain 1992). GREE follows the dynamics of a boreal sea, displaying blue waters with the maximum hue in winter and the minimum in August, during the summer bloom. Production starts in March and increases slowly because of low temperature. The spring bloom occurs in about May. However, over the summer, nutrient limitation may set in and limit production in concert with a rapid decline in insolation. Thus, the phytoplankton in the open Greenland Sea may be controlled by nutrients replacing light as the limiting factor for phytoplankton production during summer (Richardson et al. 2005).

JAP displays a high oscillation with general characteristics of an oligotrophic sea, with higher pigment concentrations in winter than in summer, plus two characteristic blooms, one in spring, that lowers the hue down to FU=5, and a weaker fall bloom. Kim et al. (2000) explained bloom occurrence as the result of the changing balance between the critical depth and the mixed layer depth. The different bloom intensity can be related to different light availability in both seasons.

458 Despite its shallow bottom, PERS shows FU values consistent with tropical and subtropical 459 seas. The highest  $C_a$  in the open-water region of the Gulf take place in winter, while lower 460 concentrations were observed in both spring and summer. A sharp bluing of the water in April is 461 caused by low  $C_a$  in April, driven by nutrient depletion (Al-Naimi et al. 2017).

YELL displays a huge range of variability, from FU=4 in winter till FU=7 in summer. Sediment resuspension caused by seasonal currents plays a role (Yamaguchi et al. 2012) but the area is also affected by strong summer blooms due to high (and increasing) nutrient discharge (He et al. 2013). Similar dynamics are present in BOH displays, but accentuated due to a lower distance to land and much shallower waters.

BLAC is a semi-enclosed sea, affected by terrestrial influence, which leads to significant particle backscattering even in open areas (Kopelevich et al. 2004). Its color dynamics is that of a temperate sea, and is driven by Ekman pumping (Kubryakov et al. 2016), with greener hues in winter around 175 °, corresponding to FU=5, and bluer in summer, around 200 °, corresponding to FU=4.

471 CASP shows on average the highest hues in June and the lowest in September, consistent with 472 previous results using three years of SeaWiFS data (Kopelevich et al. 2004), although the lack of in-473 situ data in their study could not confirm if the seasonal low hue was caused by  $C_a$  or other 474 constituents.

SBAL displays seasonal dynamics influenced by an intense summer bloom (Pitarch et al. 2016)
that leads to a green-brown color (FU=8-9). The rest of the year, color is dominated by high amounts
of CDOM. Note here the absence of data during the darkest winter months due to low sun zenith
angles.

Finally, two edge examples have been found at AZOV and PLAT, known for the high turbidity of their waters. While AZOV shows the highest hues in May and the lowest in August, PLAT shows the highest FU in July and lowest in February. In both cases, seasonality is likely to be a mixture of riverborne sediments and phytoplankton phenology. Dogliotti et al. (2016) documented a seasonal cycle of turbidity at the southern end of the estuary of PLAT that followed the same trends as shown here.

484 The latter analysis showed the ability of the hue angle to monitor ecosystem variability in a 485 wide range of marine waters. The hue angle compresses all R<sub>rs</sub> information into a single color indicator, which is theoretically enough in case 1 waters. When sediments and dissolved organic 486 487 matter vary independently to C<sub>a</sub>, the spectrum can show a wider variety of shapes. As already 488 commented in the methods section, the hue angle does not carry information on the saturation. High 489 saturation can happen in zones with high sediment concentrations where spectrum shows a broader 490 shape, or high CDOM zones, where the magnitude of the full spectrum is low. Saturation can 491 therefore be a second indicator describing optically complex waters.

492

#### 493 **3.6. Optical water types comparison**

494 Projecting global  $R_{rs}$  and various OWTs on the CIE (x,y) space provides a good graphical 495 assessment of how the latter are representative of the former. There is however, not a clear criterion 496 to judge the goodness of any OWT set applied over a given dataset. So far, their definition and their 497 number has remained arbitrary. Generally, if the purpose is to describe ecosystem variability, the 498 OWTs must cover all the observed variability and have a fine enough resolution across the dynamic 499 range. If the purpose is algorithm delimitation, the number of classes can be tailored to the number 500 of applicable algorithms. Although there is an increasing number of OWTs sets for marine and inland waters, or for specific regions, we restrict our study to those OWTs published for global marine 501 502 waters, in particular for M15, W16 and J17.



503

Fig. 15 Top panels show various OWTs projected in the (x,y) plane (panel a1)) and in polar coordinates (panel b1)). The log-density plot of the coordinates derived from global climatological ESA-OC-CCI v2.0 R<sub>rs</sub> is shown, with the running median and the intervals determined by the 25<sup>th</sup> and 75<sup>th</sup> percentiles. Bottom panels represent the differences with respect to the running median.

508 All OWTs (Fig. 15) fall approximately onto the trail formed by the global R<sub>rs</sub> across all the range 509 except the original FU scale (blue). This scale was designed to visually match the hue of perceived 510 color above water, but whose spectra do not have to match the shape of R<sub>rs</sub>. Instead, the coordinates 511 of the FU-derived R<sub>rs</sub> classes (green) fall very precisely on the trail formed by the marine waters, 512 because they were derived after clustering the same R<sub>rs</sub> forming the data cloud, being the original FU 513 classes only used as discriminators based on the hue angle. The FU R<sub>rs</sub> classes cover very evenly the dynamic range although fall short in reaching the bluest waters (see insets in Fig. 15a1,b1). FU=1 is 514 515 located between the third and the fourth J17 classes.

The M15 classes were derived from global imagery over coastal waters, although their definition of coastal waters was not based on optics and included very blue waters. Therefore, their clearest class has the color of the bluest Indian Ocean waters and even of the North Atlantic subtropical gyre. At the other extreme, their highest in terms of hue angle is near FU=11, like the turbid coastal waters of the Azov Sea. 521 The W16 classes cover a wide dynamic range. The bluest class has the color of the gyres, 522 except the pacific, and the brownest has a hue angle of 39 °, which represent a class close to FU=16. 523 This appears then suitable not only for clear marine waters, but also for very turbid and yellow 524 coastal and inland waters.

525 The J17 OWTs cover the optical variability of the oligotrophic oceans better than the other 526 OWTs because they were generated directly from the CCI global reflectances with the aim of 527 representing the bluest waters that were missing in the original OWTs (Moore et al. 2001). At the 528 most turbid end, Jackson et al. (2017) noticed that they had fell short in describing turbid waters, 529 since their contribution in their dataset was overwhelmed by that from the clearest ones. For this 530 reason, they decided to add three more spectra, consisting of sediment-laden waters of increasing 531 concentrations. These new classes have very similar hue angle and in the (x,y), they fall nearly on the 532 top of each other. This can be explained by the fact that same sediment type was the same, only 533 varying in concentration. In terms of the science of colorimetry, the last three J17 classes differ in 534 brightness but not in color.

The bluest W16 class and the three bluest J17 waters differ from the oceanic R<sub>rs</sub> (see lower panels of Fig. 15). These classes have significantly lower saturation (broader spectra) than the R<sub>rs</sub> they should be representing. This result is unexpected for J17, as J17 OWT were generated from OC-CCI v2.0 R<sub>rs</sub>, as the marine data of this article. A possible explanation might be related to the training data extraction in that J17, coming from four daily product file per year of the OC-CCI series, one in the middle of each season, and geographically sampled from a series of two-by-two degree squares, distributed across the Longhurst provinces.

542 Higher M15 and W16 classes follow pathways with a sort of zig-zag patterns starting from the 543 green waters, unlike FU and J17, that appear to follow a line along the trail formed by all the marine 544 variation. This is due to the fact that M15 and W16 classes were generated from normalized R<sub>rs</sub>, 545 which made their R<sub>rs</sub> dataset more sensitive to shape differences, that is different color saturations 546 for a given hue. This pattern is even more pronounced for the W16 dataset. This finding is consistent 547 with the fact that W16 used data collected from a number of specific sites and so might be biased 548 toward conditions related to those sites. Interestingly, the zig-zag pattern does not exist for the bluest M15 and W16 classes, that are well confined inside the average marine variability (Fig. 15, 549 550 panels a2) and c2)), proving that normalized or non-normalized R<sub>rs</sub> contain the same information in 551 blue waters. For greener waters, there are spectra than can have a similar hue angle but different spectral shapes: see for instance classes 7 and 8 of M15: both have a very similar hue angle (215.1 552 553 and 215.6 degrees, respectively), but completely different spectral shapes: class 7 is characteristic of 554 coastal zones with moderate chlorophyll and little sediment, while class 8 can be related to little chlorophyll but higher sediment concentrations. With their classification based on non-normalized 555 556 R<sub>rs</sub>, J17 obtain a single class in this region (their number 9) whose spectra looks somewhat in the middle of classes 7 and 8 of M15. 557

#### **3.7. Forel-Ule scale expansion in blue waters**

559 The previous sections have shown how the FU OWTs exceed the dynamic range of marine waters at the green-yellow end, but fall short at the bluest waters. This feature is nevertheless not a 560 561 shortcoming for algorithm determination. J17 found that the optimal chlorophyll-a algorithm for their first seven classes was OCI (Hu et al. 2012). However, if the purpose is to monitor variability, 562 563 then additional resolution can be added, by the addition of a new bluest class, " $FU_0$ ". Here, we 564 provide a demonstrative example of this addition. First step is to assign a hue angle to this new class. Based on Fig. 14, we choose the boundary between the classes FU<sub>1</sub> and FU<sub>0</sub> at 232 °, that lays in the 565 middle of the variability within the gyres. Thus, 232  $^{\circ}$  is the point of equal distance between FU<sub>1</sub> and 566 FU<sub>0</sub>, which leads to  $\alpha_0$ =234.55 °. Interestingly, this value is above the maximum recorded, which will 567

avoid class memberships saturated at the lowest FU. With this choice, even the bluest pixels will have some membership to  $FU_1$ .

570 To fully define the color properties, a saturation value must be given. Fig. 16a shows that the 571 original 21 FU classes follow a path in the ( $\alpha$ ,s) plane. Therefore, we obtain an analytical expression 572 with spline curves and extrapolate this trajectory until 234.55 °. This leads to: s<sub>0</sub>=0.2621. Conversion 573 to rectangular coordinates leads to (x<sub>0</sub>,y<sub>0</sub>)=(0.1813, 0.1198), shown in Fig. 16b.





Fig. 16 a) Polar coordinates ( $\alpha$ ,s) of the 21 original FU classes, after Novoa et al. (2013), with derived spline curve and coordinates ( $\alpha_0$ ,s<sub>0</sub>) of the new class FU<sub>0</sub>. b) The CIE 1931 color space in the (x,y) coordinates, with the coordinates of the 21 FU colors (2013) and the new FU<sub>0</sub> (red dot).

The new class  $FU_0$  has a bluish-purple color and is representative of the clearest oceanic 578 579 waters. To show enhanced detail in these kind of waters, we have repeated the analysis of Fig. 7, i.e., 580 mapping the global FU variability across a climatological year, but now with the added class, FU<sub>0</sub>. 581 Now the color variability inside the oligotrophic gyres becomes evident. The gyres are alternating 582 between the classes 0 and 1. SPSG displays the highest extension of FU=0 in the austral summer, 583 converting almost completely to FU=1 in winter. NPSG displays the second greatest extension of 584 FU=0 areas whereas the NASG is the greenest of all gyres, displaying only small extensions of FU=0 585 during the boreal summer.



586

587 Fig. 17 Global FU-extended annual variability based on the ESA-OC-CCI v2.0 climatological R<sub>rs</sub>.

588



589

Fig. 18 Climatological chlorophyll-a maps for the months a) February and b) August. The contour lines
 are the boundaries between FU classes, including the newly developed FU<sub>0</sub>.

Fig. 18 shows climatological  $C_a$  maps for the months of February and August. The yearly oscillation is clearly evidenced here: low to mid latitudes display lower  $C_a$  values in summer and higher in winter while some higher latitudes like the North Atlantic or North Pacific display higher productivity in summer. The boundaries between the corresponding FU classes overlap in both maps and provide clear evidence that  $C_a$  is driving color at the oceanic scale to a first order. The FU scale is highlighted as an effective delimitator of regions like the oceanic gyres, the equatorial pacific, upwelling zones and oceanic fronts.

599 The addition of a new lower class can have benefits for tracking the progression of the surface 600 of the most oligotrophic oceanic areas over a given time period. This could be achieved by running 601 the algorithm on the full CCI series. On the other hand, an altered FU scale would have reduced 602 significance when linking to historic measurements because the new class 0 takes pixels from the old 603 class 1. Consequently, IOPs and AOPs associated to FU=1 are altered, and shifted towards a greener 604 type, and therefore, all figures and tables displaying aggregated quantities would need to be rebuilt. 605 Classes 2 and higher would remain unaltered.

## 606 4. Conclusions

607This work has performed for the first time a thorough evaluation of the hue angle and FU608products over global oceanic waters. The projection of monthly climatological  $R_{rs}$  of selected marine609zones onto the CIE (x,y) plane depicted a continuous trail, that formed a rather compact curved line

for the oligotrophic zones, suggesting a good description using a single parameter (case 1) while the trail showed increasing spread as hue angle decreased, as expectable for case 2 waters. The FU scale falls short in describing optical variability of the oligotrophic zones, with all oligotrophic gyres shown as FU=1. For mid-latitude zones, coastal zones and productive seas, ranges encompassed two, three, up to even five FU classes. We showed that the FU scale can be expanded to better characterize variability in oligotrophic waters.

616 Considering the FU index as a clustering variable of satellite ocean color data allowed the 617 determination of median chlorophyll, Secchi disk depth and diffuse attenuation coefficient, for every 618 FU, providing a physical basis for the FU scale and allowing the association of water color to relevant 619 parameters for primary production, ocean heating or visibility. This approach is methodologically 620 different to that presented in Wang et al. (2019), which combined radiative transfer modelling and 621 empirical relationships to relate z<sub>SD</sub> and FU data to modern IOPs.

622 The FU OWTs form a clear sequence from bluest to greenest waters, with increasing  $C_a$ , 623 increasing  $K_d$  and decreasing  $z_{SD}$ . As FU increases, so does the spread within each class, indicating an 624 increasing optical diversity and decreasing representativeness of an average class. Comparatively, the 625 classes proposed in Jackson et al. (2017) show similar characteristics except with a broader range for 626 blue waters, a slight mismatch in color with respect to the FU classification, and three upper classes 627 that do not add further dynamic range in the context of color (not brightness). Contrary to these two 628 classifications, classes by Mélin and Vantrepotte (2015) and Wei et al. (2016) highlight R<sub>rs</sub> shape 629 differences within the average marine waters and identify clusters of similar hue but different 630 saturation.

The FU optical water types are a clearly ordered set in terms of the hue angle. Similar firstorder behavior was found for the global marine R<sub>rs</sub>, which supported the definition of class memberships as functions proportional to the angular distances to the two nearest FU, having the properties of adding up to one at a given hue angle. This methodology sets the basis for an intuitive yet rigorous algorithm blending procedure.

636 Projection of a spectrum onto the (x,y) plane has the limitation of being sensitive only to 637 spectral information within the visible range, with the bands 412 nm and 670 nm already having a 638 minimal weight. An expectable effect is the possible inability to respond to CDOM changes in marine 639 waters that are independent to  $C_a$ . Any other outside this range is not detectable.

640 The direct relationships between color, transparency and phytoplankton are representative of 641 average marine conditions and thus less frequent events are not represented. Examples of these 642 situations are glacial flour-rich lakes or marine coccolithophore blooms. In both cases, turbidity is 643 much higher than described by the average relationships shown here, given their hue angle. This 644 anomaly is caused by the kind of particles present in the water, that highly increase the brightness 645 and saturation of the spectrum without increasing the hue angle very much, compared to average 646 marine cases. If such anomalous spectra are to be included in optical water types, they can be 647 manually extracted from selected images (Moore et al. 2012).

648 In this article, we have studied the global traits of optical variability. FU classes showed internal 649 variability that is expected to relate to different zones of the ocean. Future work could aim at 650 clustering data within each FU class and identify similarities and differences between these "second-651 order classes" within each FU. This approach would provide more insights of optical variability within 652 distinct optical ranges in the world's oceans.

In addition to all the characteristics of any OWT classification (i.e., tool for uncertainty assessment and for variability monitoring), the FU scale adds the advantage of being linkable to historic measurements. This approach can allow us to continue to monitor long-term change in optical diversity over the global ocean color by stitching together in situ FU data collected over the 657 past century with the satellite era. The approach can be used to bridge, in a consistent manner, satellite data from two different periods (e.g. 1970-80's CZCS and 1997-onward) using in situ FU data 658 659 over the two periods. The FU climatology can be the basis for quality control of in-situ global FU data. 660 For instance, in-situ values that would be highly off the climatological values could be flagged. Nevertheless, any study linking satellite FU to historic in-situ FU from visual observation will need to 661 deal with the issue that FU observations over a Secchi disk appear greener than those over an 662 optically deep water column (Pitarch 2017). Another issue is that satellite FU are calculated from 663 bidirectionally-corrected R<sub>rs</sub>, whereas in-situ FU come from upwelling radiance in air, for any 664 665 illumination conditions. An added difficulty is that archived FU data provide no information on the 666 atmospheric conditions. This is likely to add unknown biases, whose effect will need to be tested, 667 potentially using coupled atmospheric and marine optical modelling.

Increasingly, bio-optical modules are being added to global biogeochemical models (Baird et al. 2016; Dutkiewicz et al. 2019) to look at impacts of climate change. Our approach can be integrated and used to verify early 20th century model simulations through comparison with in situ FU data collected at the time.

As a final remark, the FU scale and the hue angle are powerful quantities for outreach and educational purposes, easy to understand by a broader audience. They are intuitive quantities that help provide clear messages to spread scientific developments to mass media (McGrath 2019) and are ideal for developing citizen-science projects and events on water quality and ocean state, and engaging citizens in becoming actively involved in environmental monitoring (Citclops 2015). For these reasons, this topic will deserve further attention by the community in the coming years.

## 678 **5. Acknowledgements**

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## Annex A

Table A1 Percentiles 25<sup>th</sup>, 50<sup>th</sup> (median, bold) and 75<sup>th</sup> of the global climatological R<sub>rs</sub> associated to every FU, times 1000. The median values are defined as the FU-R<sub>rs</sub> OWTs. The normalized root mean square deviation (RMS difference over the mean value) is provided, as useful to show the indicating ability of the FU classes.

	FU	1	2	3	4	5	6	7	8	9	10	11
	p25	11.016	7.6593	5.1896	3.0242	2.0882	1.8225	1.8049	1.8266	1.9182	1.9442	1.98
Rrs412	p50	12.329	8.5122	6.2162	3.7662	2.617	2.4442	2.7722	2.9814	3.1359	3.0965	3.0594
	p75	13.974	9.3271	7.2776	4.7273	3.4246	3.6636	4.7479	5.2498	5.3063	4.9788	4.6239
	NRMSD	1.015	1.01	1.0299	1.0651	1.1313	1.2469	1.2781	1.2447	1.2227	1.234	1.2113
	p25	8.6404	6.2396	4.6492	3.1004	2.2515	1.9935	1.938	1.8995	1.9182	1.8737	1.8876
Rrs443	p50	9.5296	6.8382	5.3101	3.6612	2.7782	2.7521	3.2024	3.4217	3.6301	3.5116	3.4768
	p75	10.509	7.4576	6.0966	4.3471	3.4871	4.2209	5.7998	6.5377	6.5895	5.974	5.6509
	NRMSD	1.0109	1.0089	1.022	1.0538	1.1401	1.2967	1.3244	1.2772	1.2559	1.2494	1.2138
	p25	5.8257	5.1678	4.3647	3.3709	2.7683	2.7701	3.0024	3.1455	3.3634	3.4142	3.3941
Rrs490	p50	6.0535	5.4362	4.8643	3.8807	3.3763	3.9066	5.0333	5.5882	5.9554	5.8866	5.9312
	p75	6.2898	5.8069	5.5613	4.5166	4.273	6.1066	8.6594	9.6985	9.8765	9.189	8.8311
	NRMSD	1.0019	1.0056	1.0183	1.0553	1.1491	1.2867	1.2829	1.2257	1.1976	1.1857	1.1601
	p25	3.3605	3.3238	3.197	2.9027	2.7305	2.8937	3.2379	3.5284	3.8503	3.9345	3.9762
Rrs510	p50	3.452	3.5105	3.5085	3.2798	3.206	3.8828	5.1885	5.936	6.4656	6.4735	6.6164
	p75	3.5417	3.8112	4.062	3.7775	3.942	5.8699	8.7139	10.103	10.484	9.9153	9.679
	NRMSD	1.0014	1.0073	1.0157	1.043	1.1201	1.2667	1.2738	1.2147	1.1877	1.1758	1.1492
	p25	1.3324	1.6903	1.9171	1.9069	2.0619	2.642	3.4487	4.1836	4.8803	5.3384	5.7549
Rrs555	p50	1.4244	1.7983	2.1416	2.3059	2.6044	3.6976	5.677	7.1528	8.3388	8.8767	9.5032
	p75	1.5162	1.9409	2.5022	2.8087	3.363	5.796	9.9198	12.528	13.643	13.424	13.614
	NRMSD	1.005	1.009	1.0228	1.067	1.1588	1.3068	1.287	1.2232	1.1906	1.1746	1.1417
	p25	0.11575	0.20267	0.27558	0.33067	0.42649	0.5958	0.86331	1.1943	1.6244	2.0202	2.434
Rrs670	p50	0.1381	0.23461	0.31794	0.39102	0.51361	0.79461	1.3832	2.1484	2.9874	3.6123	4.2298
	p75	0.15994	0.27929	0.36992	0.46855	0.65003	1.2289	2.6012	4.2451	5.4503	6.0559	6.7456

	NRMSD	1.2668	1.0955	1.1143	1.1665	1.2474	1.3947	1.4083	1.324	1.2779	1.2483	1.
	FU	12	13	14	15	16	17	18	19	20	21	
	p25	2.1197	2.0982	1.822	1.6582	1.4503	1.2418	2.4601	2.6281	2.6736	2.726	
Rrs412	p50	3.2555	3.1541	2.8373	2.4001	2.2218	2.0205	3.7438	4.5718	4.0693	4.09	
	p75	4.7566	4.6344	4.4183	4.0482	4.3232	4.0885	6.3204	6.8928	5.9646	6.3058	
	NRMSD	1.1802	1.2483	1.3069	1.3969	1.4731	1.4947	1.3101	1.3621	1.5667	1.3586	
	p25	2.0314	2.0856	1.7557	1.6059	1.3862	1.2079	1.121	1.3204	1.3676	1.9248	
Rrs443	p50	3.8131	3.4769	2.9685	2.3936	1.9916	1.6222	1.7061	2.0445	2.3149	2.703	
	p75	5.7045	5.4325	4.7963	3.6119	3.182	2.3284	2.7541	3.1021	3.4514	3.8792	
	NRMSD	1.187	1.1635	1.1871	1.1873	1.2276	1.235	1.2388	1.1704	1.1819	1.1378	
	p25	3.5876	3.5896	3.1898	2.9658	2.7174	2.4875	2.1467	2.3665	2.4254	2.6363	
Rrs490	p50	6.4911	6.0634	5.1716	4.3417	3.6841	3.2129	2.9514	3.4086	3.3791	3.8462	
	p75	9.0113	8.894	7.9498	6.2245	5.648	4.3436	4.3871	4.8753	5.4314	5.3633	
	NRMSD	1.1419	1.1292	1.1487	1.1446	1.1591	1.1561	1.1848	1.1206	1.1458	1.1189	
	p25	4.1664	4.0729	3.7157	3.5196	3.1648	2.8301	2.4476	2.7354	2.6382	2.7343	
Rrs510	p50	7.2172	6.9098	5.8867	4.8914	4.2153	3.6276	3.3718	3.5378	3.6699	3.7573	
	p75	9.9667	9.9684	8.9431	6.9559	6.2093	4.7851	4.8224	5.0719	5.2375	5.0109	
	NRMSD	1.1334	1.1221	1.1428	1.1374	1.1538	1.1494	1.1743	1.1067	1.1201	1.0986	
	p25	6.1767	6.3959	5.522	5.1835	5.0568	4.837	3.8859	3.4678	2.8018	2.7691	
Rrs555	p50	10.635	10.605	9.0728	7.5442	6.7783	6.1927	4.91	4.8775	4.5105	3.8885	
	p75	14.285	14.794	13.832	10.829	9.83	8.0257	7.2041	6.5843	6.0834	5.3058	
	NRMSD	1.1261	1.1169	1.1403	1.1368	1.149	1.1259	1.1621	1.1217	1.1354	1.1191	
	p25	3.0533	3.5946	3.7649	4.2492	4.6733	5.1744	4.5067	5.1961	5.0864	5.9692	
Rrs670	p50	5.4807	5.9337	5.955	6.0316	6.1105	6.3767	6.2091	6.7818	7.5231	9.2302	
	p75	7.966	8.8898	9.2645	8.6642	9.1095	8.4577	9.1568	9.8671	10.705	14.236	
	NRMSD	1.1761	1.1506	1.153	1.1403	1.1605	1.1781	1.2532	1.178	1.1338	1.1663	

	FU	1	2	3	4	5	6	7	8	9	10	11
	p25	0.23311	0.40351	0.61743	0.99557	1.5997	2.5404	3.7856	5.26	6.923	8.5758	10.478
K-1412	p50	0.27214	0.45567	0.68526	1.1108	1.7946	2.9014	4.5755	6.8669	9.3814	11.416	13.631
K0412	p75	0.31207	0.50638	0.77756	1.2672	2.0607	3.4524	6.0573	9.0605	11.865	14.359	17.237
	NRMSD	2.1856	1.0975	1.1303	1.1414	1.1293	1.1157	1.0993	1.0845	4.1994	1.572	1.2451
	p25	0.21923	0.37833	0.56149	0.84521	1.3034	2.0496	3.2057	4.7788	6.466	8.4062	10.385
	p50	0.25397	0.42218	0.61886	0.93445	1.4466	2.3205	3.7689	5.6536	7.7139	9.7158	11.796
KU445	p75	0.2909	0.4667	0.68972	1.0503	1.6452	2.7145	4.8566	7.3267	9.5562	11.499	13.54
	NRMSD	2.1759	1.106	1.155	1.1792	1.1727	1.1363	1.0974	1.0693	5.9628	2.3567	2.4504
	p25	0.2391	0.34442	0.46394	0.62704	0.88519	1.3046	2.0014	2.8814	3.8921	5.0359	6.2936
	p50	0.26435	0.37208	0.50163	0.69349	0.99186	1.5046	2.424	3.7216	5.1437	6.4702	7.8106
K0490	p75	0.2886	0.40154	0.54818	0.77454	1.1385	1.8514	3.4808	5.4275	7.1152	8.381	9.7
	NRMSD	1.894	1.1119	1.1842	1.2193	1.2177	1.1864	1.1463	1.1149	3.5436	2.0634	1.7912
	p25	0.34987	0.44773	0.55419	0.65786	0.84909	1.2106	1.7937	2.5411	3.4007	4.3922	5.5362
	p50	0.37117	0.47472	0.58412	0.72562	0.95279	1.4047	2.2063	3.3727	4.711	5.8709	7.0752
Kasio	p75	0.3942	0.50367	0.6258	0.80303	1.096	1.7272	3.2787	5.1116	6.6317	7.7952	8.9982
	NRMSD	1.5937	1.0944	1.1573	1.2162	1.2352	1.2046	1.1629	1.1312	3.5052	2.0447	1.7857
	p25	0.64078	0.67407	0.71933	0.78785	0.92853	1.1878	1.6027	2.1107	2.7101	3.4177	4.227
VAEEE	p50	0.6477	0.68427	0.73637	0.8252	0.99168	1.316	1.8829	2.8126	3.8351	4.6947	5.5864
KU555	p75	0.655	0.69618	0.75918	0.87064	1.0816	1.5465	2.8237	4.3112	5.5437	6.4191	7.3657
	NRMSD	1.3502	1.0747	1.1333	1.1977	1.2257	1.2109	1.1726	1.1474	3.0054	2.0954	1.7355
	p25	4.4218	4.4374	4.4523	4.4637	4.4957	4.5851	4.8157	5.7764	6.4168	6.978	7.496
	p50	4.4257	4.4421	4.4622	4.4848	4.5303	4.7031	5.6579	6.403	7.1268	7.7938	8.4176
K0870	p75	4.43	4.4483	4.4776	4.5122	4.5917	5.4211	6.4101	7.4338	8.3182	8.9809	9.7265
	NRMSD	1.0011	1.0007	1.0008	1.0022	1.0074	1.0198	1.0247	1.036	1.1755	1.1854	1.1131
	FU	12	13	14	15	16	17	18	19	20	21	

Table A2 Percentiles 25<sup>th</sup>, 50<sup>th</sup> (median, bold) and 75<sup>th</sup> of the global climatological K<sub>d</sub> associated to every FU, times 10. The normalized root mean square deviation (RMS difference over the mean value) is provided, as useful to show the indicating ability of the FU classes.

	p25	12.561	15.06	17.503	20.374	23.062	24.332	14.705	14.778	20.097	28.152
Kd412	p50	17.002	19.704	23.33	28.573	35.881	44.401	25.318	30.187	33.621	47.229
K0412	p75	21.107	24.732	30.012	36.348	46.893	60.39	44.505	48.403	45.808	81.003
	NRMSD	1.6738	1.3966	1.3086	1.156	1.214	1.2899	1.6725	1.3671	1.4809	1.2808
	p25	12.965	15.36	18.926	24.121	30.631	39.774	35.749	35.418	34.581	40.869
	p50	14.327	17.147	21.194	26.663	35.124	47.237	46.933	46.74	44.33	57.268
Ка443	p75	16.454	19.494	23.608	29.666	39.764	54.438	59.792	64.021	61.65	89.374
	NRMSD	1.9455	1.3505	1.1479	1.1199	1.1845	1.2116	1.4048	1.1932	1.2071	1.2511
	p25	8.1397	9.8644	11.846	14.858	18.641	23.254	23.332	24.239	25.039	29.665
K-1400	p50	9.5778	11.469	13.454	16.447	20.608	26.404	27.609	28.837	30.027	39.258
Ka490	p75	11.66	13.589	15.788	18.134	22.661	29.649	31.286	35.38	38.47	60.902
	NRMSD	1.6288	1.3164	1.1192	1.0558	1.173	1.1608	1.3247	1.1662	1.1121	1.2154
	p25	7.2671	8.7353	10.515	13.28	16.726	20.955	21.711	22.538	23.514	28.739
	p50	8.764	10.393	12.2	14.763	18.653	23.818	24.858	26.199	28.209	37.063
KUSTO	p75	10.886	12.618	14.673	16.834	20.62	26.943	28.686	32.529	35.651	59.132
	NRMSD	1.7645	1.4163	1.1319	1.0577	1.1734	1.1663	1.3169	1.1672	1.1115	1.2
	p25	5.5589	6.5013	7.7544	9.5196	11.811	14.749	15.731	18.549	21.907	27.284
KAFFF	p50	6.8638	8.0561	9.3377	10.992	13.332	16.398	18.191	22.279	25.468	36.082
KUSSS	p75	8.8048	10.308	12.025	13.463	16.208	18.736	22.956	27.761	29.868	54.655
	NRMSD	2.0277	1.5756	1.162	1.077	1.3994	1.2599	1.3941	1.1584	1.1231	1.1923
	p25	8.1899	8.8514	9.5956	10.713	12.215	13.912	13.053	12.815	12.921	14.104
Vdc70	p50	9.3909	10.147	10.884	11.926	13.507	15.523	15.28	15.513	15.755	17.549
KUD/U	p75	10.779	11.724	12.911	13.711	15.238	17.172	17.556	19.369	19.596	25.417
	NRMSD	1.0907	1.0821	1.0406	1.0278	1.0536	1.1009	1.1981	1.1115	1.0671	1.1282

	FU	1	2	3	4	5	6	7	8	9	10	11
	p25	32.372	23.287	17.087	12.224	8.8563	6.0818	3.2734	2.1256	1.6475	1.4228	1.2387
<b>z</b> <sub>SD</sub>	p50	36.328	25.121	18.668	13.626	9.9518	7.1701	4.9728	3.3197	2.4166	1.9708	1.664
	p75	41.942	27.129	20.175	15.061	11.156	8.0045	5.8624	4.444	3.4578	2.7442	2.2155
	NRMSD	1.0151	1.0052	1.0079	1.0151	1.0222	1.0379	1.0627	1.078	1.0838	1.0804	1.0796
	FU	12	13	14	15	16	17	18	19	20	21	
	p25	1.0407	0.90981	0.79518	0.72428	0.62745	0.54247	0.53398	0.48152	0.47913	0.35545	
<b>z</b> <sub>SD</sub>	p50	1.3471	1.1539	1.0148	0.87076	0.73187	0.60557	0.64912	0.65251	0.60483	0.53912	
	p75	1.6804	1.4332	1.2139	1.0038	0.82917	0.6997	0.78487	0.79595	0.7583	0.6962	

Table A3 Percentiles 25<sup>th</sup>, 50<sup>th</sup> (median, bold) and 75<sup>th</sup> of the global climatological Secchi disk depth (m) associated to every FU. The normalized root mean square deviation (RMS difference over the mean value) is provided, as useful to show the indicating ability of the FU classes.

Table A4 Percentiles 25<sup>th</sup>, 50<sup>th</sup> (median, bold) and 75<sup>th</sup> of the global climatological chlorophyll concentration (mg m<sup>-3</sup>) associated to every FU, times 10. The normalized root mean square deviation (RMS difference over the mean value) is provided, as useful to show the indicating ability of the FU classes.

	FU	1	2	3	4	5	6	7	8	9	10	11
	p25	0.46307	1.2509	2.1864	4.425	8.7668	13.94	20.894	28.132	33.139	38.031	42.706
C	p50	0.6565	1.4427	2.596	5.4827	11.118	17.455	25.262	33.517	39.333	46.663	54.02
Ca	p75	0.84922	1.6638	3.1611	6.9951	14.551	22.852	31.987	41.528	49.975	63.165	72.947
	NRMSD	1.1273	1.0394	1.1318	1.1294	1.1245	1.1211	1.0937	1.088	1.092	1.1066	1.1244
	FU	12	13	14	15	16	17	18	19	20	21	
	p25	45.197	50.166	55.438	61.792	69.495	79.281	30.209	22.509	15.373	10.27	
C	p50	57.852	63.985	66.21	72.651	83.516	111.07	93.542	46.123	32.199	16.328	
Ca	p75	76.392	89.26	86.299	86.811	106.12	140.47	133.3	105.66	67.183	36.89	
	NRMSD	1.164	1.1949	1.1835	1.1468	1.1179	1.1052	1.2145	1.3589	1.4264	1.6297	

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# List of Figure Captions

Fig. 1 The CIE standard observer color matching functions and the sum of all.

Fig. 2 The CIE 1931 color space in the (x,y) coordinates. The coordinates of the 21 FU colors after Novoa et al. (2013) are plotted as blue dots. The white point W lays on (1/3,1/3). An arbitrary spectrum is represented as point P, having polar coordinates ( $\alpha$ ,s) and laying between FU 3 and 4.

Fig. 3 Discretization errors  $\Delta x$  and  $\Delta y$  in the computation of the (x,y) coordinates as a function of x' for the IOCCG synthetized dataset, and corresponding fitted curves  $c_x$  and  $c_y$  (Table 1).

Fig. 4 Class membership functions as function of the hue angle.

Fig. 5 Distributions of the global climatological ESA-OC-CCI v2.0  $R_{rs}$  on the (x,y) plane and in polar coordinates ( $\alpha$ ,s). Panel a1) log-density plot of (x,y) distribution, with dot color indicating increasing data density. The moving median of y for every x as thick line, and the 25<sup>th</sup> and 75<sup>th</sup> percentiles as band boundaries, are plotted on top. a2) distribution of x. a3) distribution of y. a4) same band as panel a1) but setting the moving median of y as ordinates origin. Panels b1) to b4) are equivalent to a1) to a4) but replacing x by s and y by  $\alpha$ .

Fig. 6 Color maps of membership to class 2 and class 4 of the Mediterranean Sea for the climatological months of January, April, July and October, based on the ESA-OC-CCI v2.0 global climatological monthly  $R_{rs}$ .

Fig. 7 Global FU annual variability based on the ESA-OC-CCI v2.0 global climatological monthly R<sub>rs</sub>.

Fig. 8 Remote-sensing reflectances corresponding to the first 10 FU water types, obtained from the ESA-OC-CCI v2.0 global climatological monthly  $R_{rs}$ . Bold traces correspond to median values and bands extend between the 25<sup>th</sup> and 75<sup>th</sup> percentiles. Data of all classes can be found at Table A1.

Fig. 9 Fig. 19 Diffuse attenuation coefficient of downwelling irradiance of the first 9 FU classes, representing the median in bold line and the interval between the 25<sup>th</sup> and 75<sup>th</sup> percentiles in shaded band. For a complete description, the reader is referred to Table A2.

Fig. 10 Secchi disk depth histograms for each FU class. Each histogram aggregates all  $z_{SD}$  derivations (Lee et al. 2015) from the ESA-OC-CCI v2.0 global climatological monthly  $R_{rs}$  whose per-pixel associated FU have the same value. Statistical descriptors can be found in Table A3.

Fig. 11 Chlorophyll concentration histograms for each FU class. Each histogram aggregates all  $C_a$  data the ESA-OC-CCI v2.0 global climatological monthly  $C_a$  dataset whose per-pixel associated FU have the same value. Statistical descriptors can be found in Table A4.

Fig. 12 Chlorophyll concentration and Secchi disk depth box plots for each FU optical water type. The median is plotted as a dot inside a white circle. The interquartile range is delimited by the box around the median. Whiskers extend until three times the interquartile range below and above the first and third quartile, respectively. Data beyond the whiskers range are considered outliers and are plotted as dots. Statistical descriptors can be found in Tables A3-A4.

Fig. 13 Selected marine zones for the study of the seasonal color variability, over a map of the seriesaveraged chlorophyll-a concentration.

Fig. 14 Hue angle climatological annual variability of selected marine zones (see Fig. 13 and Table 6). The boundaries between consecutive FU classes are also indicated.

Fig. 15 Top panels show various OWTs projected in the (x,y) plane (panel a1)) and in polar coordinates (panel b1)). The log-density plot of the coordinates derived from global climatological

ESA-OC-CCI v2.0  $R_{rs}$  is shown, with the running median and the intervals determined by the 25<sup>th</sup> and 75<sup>th</sup> percentiles. Bottom panels represent the differences with respect to the running median.

Fig. 16 a) Polar coordinates ( $\alpha$ ,s) of the 21 original FU classes, after Novoa et al. (2013), with derived spline curve and coordinates ( $\alpha_0$ ,s<sub>0</sub>) of the new class FU<sub>0</sub>. b) The CIE 1931 color space in the (x,y) coordinates, with the coordinates of the 21 FU colors (2013) and the new FU<sub>0</sub> (red dot).

Fig. 17 Global FU-extended annual variability based on the ESA-OC-CCI v2.0 climatological R<sub>rs</sub>.

Fig. 18 Climatological chlorophyll-a maps for the months a) February and b) August. The contour lines are the boundaries between FU classes, including the newly developed FU<sub>0</sub>.