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Sensitivity analysis of a bio-optical model for Italian lakes focused on Landsat-8, Sentinel-2 and Sentinel-3

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Abstract

We analysed the sensitivity of a Case-2 bio-optical model where the water reflectance is computed as a function of concentrations of three optical water quality parameters (WQPs) of three Italian lakes (Garda, Mantua and Trasimeno) and their specific absorption and backscattering coefficients. The modelled reflectance is computed based on the spectral characteristics of three optical sensors, on-board Landsat-8, Sentinel-2 and Sentinel-3. The variance-based analysis was able to quantify the lake-dependence for all (50,000 runs) the simulated reflectance. The results confirmed that Sentinel-3 water reflectance is sensitive to WQPs in all the trophic conditions investigated.

Keywords: Sensitivity analysis, bio-optical model, water quality parameter, inland water.

Introduction

Multi- and hyper- spectral remote sensing provides a robust analytical tool to analyse temporal changes in water quality over wide areas by studying the interaction between electromagnetic radiation and the water body [Brando et al., 2003, 2009; Giardino et al., 2007; Bresciani et al., 2012a,b; Olmason et al., 2013]. This interaction is mainly due to pure water and the optical active parameters such as Chlorophyll-a (Chl-a), Suspended Particulate Matter (SPM), Coloured Dissolved Organic Matter (CDOM) which control the extinction of radiation in the water column [Lindell et al., 1999; Pasterkamp et al., 1999; Dekker et al., 2001; Babin et al., 2003; Strömbeck et al., 2001]. The inversion of biooptical modelling is a well-known method to retrieve these parameters in inland and coastal waters [Dekker et al., 1995; Lee et al., 1999; Cracknell, 2001; Brando and Dekker, 2003; Dall'Olmo et al., 2005; Odermatt et al., 2012]. In the forward mode, the reflectance spectra simulated by bio-optical models depend on [e.g. Pierson and Strömbeck, 2001; Kutser et al., 2005] the concentrations of water components (e.g., Chl-a, SPM and CDOM), on the specific inherent optical properties (SIOPs), and on the downwelling light field. The biooptical model simulation takes into account the wavelength-dependence of the reflectance spectra, which can be described according to the spectral channels of satellite sensors.

The latest satellite missions, such as Landsat Data Continuity Mission (LDCM) and Sentinels 2 and 3 [Donlon et al., 2012; Drusch et al., 2012] that carry new sensors, will enhance the research and monitoring of water environments by their temporal and spatial coverage, as well as the accuracy of retrieving water variables by their spectral and spatial resolution [Malenovsky et al., 2012].

Pahlevan et al. [2014] analysed the radiometric performance of Operational Land Imager (OLI), on board Landsat 8 [Irons et al., 2012], for water quality applications [e.g., Vanhellemont and Ruddick, 2014].They identified local gain factors for radiance and reflectance to improve the retrieval of in-water products by considering in situ measurements and other ocean colour satellites as a benchmark. The Ocean and Land Colour Instrument (OLCI), an improved continuation of Medium Resolution Imaging Spectrometer (MERIS) [Donlon et al., 2012], on-board Sentinel-3, is a useful satellite for monitoring waters environments which leaves the moderate spatial scale unchanged (300 m) [Aschbacher et al., 2012; Malenovsky et al., 2013; Palmer et al., 2014]. The Multi Spectral Instrument (MSI) on board Sentinel-2 has fewer bands and a wider bandwidth than OLCI [Drusch et al., 2012]. It thus provides high-resolution optical images for marine biodiversity and habitat analysis in coastal and inland areas [Malenovsky et al., 2012].

The sensitivity evaluation of models to retrieve the concentrations of water quality parameters (WQP) when applied to the spectral configurations of different sensors (and water types) fully exploits data gathered from these new satellite missions. The sensitivity analysis (SA) investigates the uncertainty of the input factors compared to the uncertainty in the model response [Saltelli et al., 2004]. The SA procedures are classified into three main groups: one-factor-at-a-time (OAT) [Morris, 1991], regression-based [Manache and Melching, 2008] and variance-based methods [Sobol, 1993; Saltelli et al., 2000, 2010; Lilburne et al., 2009].

The OAT method applied to the bio-optical model works by varying one WQP at a time and constraining the other variables [Uferman and Robinson, 2002]. Hence, the sensitivity index of a specific parameter depends on the central values of the other parameters, and the interactions among variables are omitted [Saltelli et al., 2006].

Garver and Siegel [1997] applied a linear regression sensitivity method to study the time series of IOP measurements of the Sargasso Sea in order to determine the best IOP model configuration. The definition of partial derivatives of the quasi-analytical algorithm (QAA) [Lee et al., 2002] enabled the uncertainties of the derived IOPs and the relative importance of the analysed parameters to be investigated [Lee et al., 2010]. A variance-based method was also applied to the Hydrolight [Mobley, 1994] simulated spectra of above-water remote sensing reflectance $(Rrs(\lambda))$ demonstrating the sensitivity of the semi-analytical inversion model to both the concentrations of water constituents [Duarte et al., 2003] and to geometric and bottom effects [Gerardino-Neira et al., 2008].

In this work, a variance-based procedure [Saltelli et al., 2010] was applied to study the sensitivity of a bio-optical model which simulates the water reflectance of three Italian lakes - Garda, Mantua and Trasimeno - with different trophic conditions by analysing the main effect of single WQPs and their interactions. The water reflectance was simulated according to a four-components model defined in Brando and Dekker [2003], by considering

the SIOPs typical of each lake and the spectral band definitions of Landsat8, Sentinel-2 and 3, which can be potentially applied for lakes [Irons et al., 2012; Malenovsky et al., 2012; Vanhellemont and Ruddick, 2014; Lobo et al., 2014].

In the first part of the paper we describe the three Italian lakes used as test areas. We then outline the bio-optical analytical model used to simulate the water reflectance and to run the sensitivity analysis. Finally, the results are presented for the sensitivity indices of water reflectance for three water types/trophic conditions, according to the new generation of multi-spectral sensors.

Materials and methods

Study area

Lakes Garda, Mantua and Trasimeno were selected as representative of different trophic levels; for these lakes long-term data of in situ measurements on water quality characteristics are also available. The main morphological and trophic characteristics are summarized in Table 1. Lake Garda is the largest lake in Italy, located in a subalpine region and characterized by deep water. It is an important tourist site with oligo-mesotrophic waters and occasional cyanobacteria blooms during the fall, according to recent limnological studies [Salmaso and Mosello, 2010]. In Mantua the lakes are formed by three shallow fluvial lakes (fed by the river Mincio, the emissary of Lake Garda). Located in the centre of the Padana plain, their water status is strongly affected by pressure both from agriculture and industry. Excess growth of macrophyte vegetation and dystrophic water conditions makes the waters of the Mantua lakes very productive; the most intense phytoplankton blooms, characterized by high biomass in surface, occur in the summer [Bresciani et al., 2013]. The third test area is Lake Trasimeno, the largest in central Italy, characterised by shallow waters with recurrent wind-induced resuspension of bottom sediments and increasing water turbidity. A high amount of nutrients [Cingolani et al., 2005] induced by agricultural and zoo-technical activities, combined with meteorological conditions and tourism-related activities keep the level of the lake in between the meso- and eu-trophic status.

In situ data

In situ data (WQPs and SIOPs) used to simulate water reflectance and to perform the sensitivity analyses rely on data gathered from recent fieldwork in the study areas (see Tab. 2). The data were all collected during summer (including previous and subsequent weeks), so as to be able to describe the usual conditions that can be found in the three lakes at this time of the year. Overall, WQP measurements were more numerous than SIOPs (e.g., Chl-a concentrations for Lake Garda) because WQPs were also achieved by traditional limnological campaigns, where the optical properties were not measured. For Lake Garda, in situ measurements were collected between July and October [Bresciani et al., 2012a and references therein] over 11 years; for the Mantua lakes, the samples were collected during the summers of 2007, 2008, 2010 and 2011 [Bresciani et al., 2013 and references therein]; for Lake Trasimeno in situ data were collected between May and September 2008 and 2009 [Giardino et al., 2014 and references therein].

The same methods were used to collect water samples and to perform the subsequent laboratory analysis on WQPs. The water samples were collected in the euphotic layer of the water column, water samples were filtered by GF/F filters of 47 mm, and the material retained was analysed by applying a spectrophotometric method adopting acetone for Chla extraction [Lorenzen, 1967]. SPM measurements were performed by the gravimetric method [Van der Linde, 1998] and CDOM was measured by spectrophotometry at 440 nm [Babin et al., 2003]. Figure 1 shows the WQPs ranges over the three test sites.

Figure 1 - WQP box-plot comparison of the three sites in semi-logarithmic scale. Green refers to Chl-a values, blue the SPM and yellow the CDOM. Red and blue asterisks are the average and extreme values of distributions, respectively.

For the SIOPs the following methods were applied in each lake. The absorption spectra of particles retained on the filters $a_p(\lambda)$, were obtained using the filter pad technique [Strömbeck and Pierson, 2001] and were calculated according to Babin et al. [2003]. Filters were then treated with acetone to extract pigments and the absorption spectra of these bleached filters were measured to assess tripton $(a_{TR}(\lambda))$, the inorganic particulate matter suspended in bodies of water. The absorption spectrum of phytoplankton $a_{nb}(\lambda)$ was derived by subtracting $a_{TR}(\lambda)$ from $a_p(\lambda)$ spectra. The spectrophotometric determination and processing of the absorption spectra of CDOM, $a_{\text{CDOM}}(\lambda)$, were derived according to Babin et al. [2003]. The backscattering coefficients of the particles $(b_{bn}(\lambda))$ were derived from HydroScat-6 measurements [Maffione and Dana, 1997].

Lake	Water quality parameter			Inherent Optical Properties	Sampling period		
	$Chl-a$	SPM	CDOM	absorption	backscattering		
Garda	493	131	51	20	20	July-October $(2002 - 2003 - 2013)$	
Mantua	43	31	24	38		Summer 2011	
Trasimeno	38	38	38	31		May - September $(2008 - 2009)$	

Table 2 - Number of samples collected per lake and their relative sampling periods.

SIOP data were spectrally resampled according the spectral response (Fig. 2) of Landsat 8 [Barsi et al., 2011] and satellite band definitions of the central wavelength and bandwidth for Sentinel-2 and Sentinel-3 [Drusch et al., 2012; Donlon et al., 2012] in the range of 400- 740nm, which is sensitive to water reflectance (Fig. 3).

Figure 2 - Bandwidth for Landsat 8, and central wavelength and width for Sentinel-2 and Sentinel-3 sensors. Red refers to all bands adopted during the simulations in the range 400-740 nm. [Barsi et al., 2011; Drusch et al., 2012; Donlon et al., 2012].

Figure 3 - SIOP values in the three study areas.

Bio-optical analytical modelling

The bio-optical model used in this study was similar to previously published Case-2 models [Brando and Dekker 2003; Dekker 2001; Pierson and Strömbeck, 2001], where the subsurface irradiance reflectance $R(0, \lambda)$ is calculated as a function of absorption and backscattering coefficients and of the shape of illumination light field according to [1]:

$$
R(0-\lambda) = f(\lambda) \cdot \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)} \quad [1]
$$

With:

 $b_{b}(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda) = b_{bw}(\lambda) + [SPM] \cdot b_{bp}^{\dagger}(\lambda)$ $a(\lambda) = a_w(\lambda) + a_p(\lambda) + a_{\text{CDOM}}(\lambda) = a_w(\lambda) + [\text{Chl-a}] \cdot a_{ph}^*(\lambda) + [\text{TR}] \cdot a_{TR}^*(\lambda) + [\text{CDOM}] \cdot a_{\text{CDOM}}^*(\lambda)$

 $b_b(\lambda)$ is the spectral total backscattering coefficient, $a(\lambda)$ is the spectral total absorption coefficient and $f(\lambda)$ is a function of the ratio of the average cosine of the downwelling light to that of the upwelling light [Mobley, 1994].

The $b_b(\lambda)$ e a(λ) coefficients are given as a sum of the contribution of water and the *i-th* component. Each $b_{bi}(\lambda)$ and $a_i(\lambda)$ are defined by multiplying the concentrations of each single WQP ([Chla], [CDOM], [SPM]) by its relative SIOPs. $a_w(\lambda)$ and $b_{hw}(\lambda)$ are absorption and backscattering contributions of pure water. The concentration of tripton [TR] was retrieved from [Chl-a] and [SPM] according to Brando and Dekker [2003] and Giardino et al. [2007] [2]:

$$
[TR] = [SPM] - 0.07 [Chl - a] \qquad [2]
$$

Sensitivity analysis

The SA of the above analytical model was performed with the algorithm [Zambrano-Bigiarini, 2013] based on the variance method described in Saltelli et al. [2010]. The algorithm is implemented in the open-source software package SIMLAB developed at the Joint Research Centre [Saltelli et al., 2004].

The variable values are produced by the quasi-random number generator [Dutang and Savicky, 2013] covering the being set determined from the available in situ measured WQPs. The sample distribution is assumed as normal with a confidence level of 68% to ensure an interval large enough to cover the real variability of all the WQP concentrations. To represent all the input combinations, the quasi-random sequence of each variable is combined with the other variables; at first, two sets of input values are sampled producing two matrices (A and B). To complete the possible permutations, a third matrix is obtained by the radial sampling of values by matrixes A and B [Saltelli, 2002].

The SA of the model output $(Y=f(x))$ to the variables involved $(x=(x_1,...,x_i,...x_k))$ and their coupling is performed by varying each *i-th* variable (from 1 to *k*) separately, first order, $f_i(x_i)$, and together, second order $f_{ij}(x_i, x_j)$ [3].

$$
R(0-, \lambda) = f(x) = f_0 + \sum_{i=1}^k f_i(x_i) + \sum_i \sum_{j>i} f_{ij}(x_i, x_j) + ... + f_{1,2,...,k}(x_1, x_2,...,x_k)
$$
 [3]

Firstly, two WQPs are constrained and the third variable is the variable of the model. The runs then involve two variables with the third WQP constrained. This running mode analyses the sensitivity of the model to each variable and to each variable-coupling. The single output represents the simulated water reflectance of which the total variance (V(Y)) is composed of single and coupling contributions of the quasi-random sequences of the variables, according to the following general equation expressed for a specific wavelength [4]:

$$
V(Y) = \sum_{i} V_{x_i} + \sum_{i < j} V_{x_i x_j} + \sum_{i < j < m} V_{x_i x_j x_m} + \dots + V_{12 \dots k} \tag{4}
$$

 $V(Y)$ is the simulated reflectance variance, V_i is the single contribution to the total variance due to the i-th variable (x_i) and, in our case, represents the sensitivity of the output model, R(0-, λ), to the specific WQP. The coupling contribution, V_{xixi} , is due to the two-variable (i-j) interaction. The k index is the number of variables (model input) and n the number of runs [Saltelli et al., 2010; Lilburne and Tarantola, 2009].

With the based-variance method, the sensitivity indices can be retrieved. The single contribution is described by the main effect (S_i) , representing the first order of sensitivity index determined for each variable [5]:

$$
S_i = \frac{V_{x_i}}{V(Y)} \quad [5]
$$

If the sum of the main effects of the WQP is less than 1, the output variability is partly due to the coupling variables. The orders higher than one represent the variable interactions (V_{12}) $+ V_{13} + V_{23} + V_{123}$. Where there is no interaction in the model, these terms will be close to 0. The total sum of all sensitivity indices is 1 [Saltelli et al., 2010] [6].

$$
1 = \sum_{i} S_{i} + \sum_{i} \sum_{j>i} S_{ij} + \sum_{i} \sum_{j>i} \sum_{m>j} S_{ijm} + \dots \quad [6]
$$

The total sensitivity index (S_i) is the sum of all sensitivity indices involving the i-WQP. For instance, in the case of three parameters, the total indices are $S_{t_1} = S_1 + S_{12} + S_{13} + S_{123}$, $S_{12} = S_2 + S_{12} + S_{23} + S_{123}$, $S_{13} = S_3 + S_{13} + S_{23} + S_{123}$. S_{11} describes the single and couplingvariable contribution of each WQP to the model response. The $S_{\rm ti}$ - S_i measures the couplingvariable contribution per *i-th* variable, the higher this value, the more the coupling-variables contribute to the output.

To estimate S_i and S_i for all the parameters, the total number of model runs (n) depends on the sample size (N) and variable amount (k) according to the Equation [7]:

$$
n = (N * (k + 2)) \quad [7]
$$

The Sobol' sensitivity analysis also provides the most significant interactions between pairs of variables by calculating the second order sensitivity indices (S_{ij}) [Saltelli et al., 2006].

Results

The bio-optical model simulation was performed on 10000 samples (N) per WQP (i.e. Chl-a, SPM and CDOM) obtaining 50000 simulated reflectances (*n*) per lake, sensor and sensitivity indices, according to Eq. [7].

Focusing on simulated reflectances, according to the spectral configuration of OLI, OLCI and MSI for the three lakes, Fig. 4 highlights that reflectance values, have peak in the green region (about 550 nm), which is typical in turbid productive waters, such as those in the Mantua and Trasimeno lakes [Bresciani et al., 2013; Giardino et al., 2014]. In Lake Garda the simulated spectra are lower due to the lower concentrations of SPM of Lake Garda compared to Mantua and Trasimeno.

The lower reflectance in the blue (± 0.03) is due to Chl-a and CDOM. This shape is clear for the Sentinel-3 sensor, which has four bands in the blue region from 400 to 490 nm (Fig. 4). The OLCI sensor on board Landsat 8, which has two bands in the blue, is also able to capture this behaviour. In addition Sentinel-2 holds great potential for assessing Chl-a in productive turbid waters by considering the last two bands at 705 and 740 nm [Gitelson et al., 2007].

Figure 4 - Simulated reflectance and relative variation in the study areas according to the spectral characterization of sensors.

Once the variability of the modelled reflectance in different inland water environments had been assessed, the model variability due to changes in these environmental conditions was analysed. The SA of the analytical model highlighted the contribution of each WQP

considering the status of the lake and wavelengths. The simulated reflectances considering the Landsat 8, Sentinel-2 and Sentinel-3 sensors had different sensitivity indices due to their band spectral definitions.

The quantitative assessment of the SA procedure provided the main effects and coupling effects of the three WQPs per band in all the lakes studied (Fig. 5). The stacked area plot in Figure 5 shows the cumulated total of main effects and interactions (see Sensitivity Analysis section) vs. wavelengths in the lakes and sensors studied (the retrieved Sti-Si is not discussed in this paper because the average value is close to 0, due to the overall low levels of interaction between the WQPs).

Figure 5 - Stacked area plot of the cumulated total of main effects and interactions vs. wavelength in lakes and sensors studied.

The sensitivity indices of Lake Garda (Fig. 5) show that values of main effect of CDOM are high in the bands of the blue region for all sensors, where CDOM has a strong absorption

coefficient [Babin et al., 2003], and small variations in concentrations show a change in water reflectance. S_{Chl-a} has an important weight in the range 442 - 510 nm with higher values than 25%. In this range, at 490 nm, Giardino et al. [2007] identified the maximum variation in the first derivative of reflectance due to Chl-a variation. In terms of longer wavelengths, the bio-optical model is sensitive to variability in SPM with values of S_i increasing up to the peak in the range from 550 to 620 nm, whereas the sensitivity of two other parameters has the opposite behaviour. These results are also similar to a previous analysis in the area with Hyperion [Giardino et al., 2007]. Low coupling effects are mainly under 5% of total variance (Fig. 5).

In Lake Trasimeno, the SPM main effect is generally high according to trophic conditions [Giardino et al., 2010], in particular moving toward the red region for all the sensors. This result highlights how the SPM variability affects water reflectance. Indeed SPM has a spatial pattern concentration, which consequently causes different spectral responses of the water reflectance [Giardino et al., 2014]. In all bands, the sum of the main effects of WQPs in Lake Trasimeno are always lower than 100%, which means that there are coupling effects (4-6%). CDOM and SPM are dominant variables in the coupling effect over the first part of the spectrum, while moving towards the red bands, this effect is mostly due to SPM and Chl-a. In case of eutrophic waters such as the lakes of Mantua, the main effect of Chl-a has a higher averaged sensitivity index than in Garda and Trasimeno in the first bands (25%). This then falls to 708 nm for Sentinel-2 and Sentinel-3 runs. The values of the main effect of CDOM are negligible in all bands. Similar to Lake Trasimeno, the sum of the main WQP effects in the Mantua lakes is never 100%, but always close to 96%.

As expected the model is sensitive to the WQP variations as a function of the trophic condition of the lakes. In all the channels and sites, the SPM has a strong influence in modelling the water reflectance.

The contribution of Chl-a in the simulated reflectance of Mantua (Fig. 4) is clear in S_{Chl-a} (Fig. 5) calculated in the red bands of Sentinel-3. This is consistent with the Gitelson Indices [Gitelson et al., 2007] adopted by Bresciani et al., 2013 who analysed the variability of Chl-a in the same spectral range. In Garda and Trasimeno, Sentinel-2 and Landsat 8 had comparable main effects in terms of Chl-a, CDOM and SPM, particularly in the first part of the spectrum (Fig. 5).

In addition to the WQP sensitivity analysis, the sensitivity analysis for the SIOPs was also performed for the three lakes. The normalized RMSD (root-mean-square-deviation) between the water reflectance simulated with maximum and minimum SIOP values was 54% in Garda, 23% in Trasimeno and 32% in Mantua. The variance-based procedure considering different SIOPs analysed the variability of the main effects of the variables (WQPs) depending on the trophic status. The average results are summarized in Table 3 considering all sensors. Figure 6 shows the variation in the main effects of the WQPs obtained with total environmental variability of the SIOPs considering the Sentinel3 sensor. In the spectrum, CDOM and Chl-a had more variability compared to SPM up to 550nm, whereas with longer wavelengths, the SPM main effect variation is affected more by SIOP variation. The CDOM and SPM main effects are the most sensitive to variations in SIOPs in Lake Garda at 400 nm, with changes in values up to 19%, while their average variability along the spectrum is 9% (Tab. 3). In Trasimeno and Mantua, the main effects of Chl-a are the most sensitive with a variation up to 17% and 13%, respectively.

	$S2-MSI$			S3-OLCI			$L8-OLI$		
	Chl-a	SPM	CDOM	Chl-a	SPM	CDOM	Chl-a	SPM	CDOM
Garda	6%	7%	4%	6%	9%	9%	5%	7%	5%
Trasimeno	4%	7%	8%	13%	8%	9%	17%	9%	10%
Mantova	7%	7%	1%	13%	10%	3%	9%	8%	1%

Table 3 - Averaged variations in main effect for each WQP and sensor.

Figure 6 - Main effect variation considering the total environmental range of SIOPs (*** **refers to the minimum; the point refers to the average, and + to the maximum) for Sentinel3 in the three lakes.**

Conclusions

This work describes the spectral sensitivity of the new remote sensing sensors to the WQP using the water reflectance simulated by analytical modelling applied to three Italian lakes, describing different trophic conditions. The lakes are Garda, Trasimeno and Mantua, which are characterized by different biophysical properties, concentration ranges of water quality parameters and bio-optical parameters. The sensitivity analysis presented in this study and applied to the forward analytical model defines the contribution, both separately and combined, of CDOM, SPM, Chl-a to water reflectance simulation in terms of main effects and interactions.

The results highlight the important role of SPM in describing water reflectance in the three lakes, except in the blue spectral region where Chl-a and CDOM also have significant main effects. The quantitative definition of variable sensitivity indices may be another way to describe lacustrine apparent optical properties. Sentinel-2 seems to show the best

agreement between spatial resolution, spectral definition and sensitivity to variations in three WQPs. The sensitivity results of Sentinel-2 and Landsat 8 in Lake Garda and Trasimeno demonstrate the effectiveness of these sensors for Chl-a analysis (Fig. 3) in terms of mesoeutrophic and oligotrophic status. In addition the combined use of these two sensors may improve the revisit time of the study area with a good spatial resolution (about 30m) and a comparable sensitivity. On the other hand, the higher spectral resolution of Sentinel-3 makes this sensor more sensitive to variations in WQPs in the forward analytical model in the trophic conditions studies.

These results provide important information relating the sensitivity of the new generation sensors to different trophic statuses. In forward analytical modelling, the sensitivity indices of simulated reflectance depend on the spectral response function of the sensor, as shown in Figure 3. This sensitivity classification is useful in terms of the efficiency of a sensor in retrieving water quality parameters (WQP) through inversion bio-optical modelling.

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