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1 **A Software Package for an Adaptive Satellite-based Sampling for**
2 **Oceanographic cruises (SPASSOv2.0): tracking *fine scale* features for**
3 **physical and biogeochemical studies.**

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13 ABSTRACT: During the past decade increasing interests arose in understanding the role of fine-
14 scales (processes of the order of 10s of km) on ocean energy and biogeochemical budgets. However,
15 *in situ* evidence of these processes remains poorly documented and represents only few specific
16 ocean conditions. To fill this gap, new adaptive sampling feature-oriented strategies need to be
17 developed. A possible approach is to target fine-scale features, identified from space, with *in situ*
18 surveys. The SPASSO (Software Package for an Adaptive Satellite-based Sampling for Oceanographic
19 cruises) package provides real-time analysis of satellite-derived products and diagnostics
20 to identify fine-scale biophysical dynamics of any given study area. Besides the visualization
21 of satellite products, the software computes a large variety of Eulerian and Lagrangian diagnostics
22 inferred from near-real time altimetry to accurately direct oceanographic sampling towards
23 fine-scale features. Over the last decade, this adaptive sampling methodology was successfully
24 developed as showcased by several previous cruise examples. In 2023, the groundbreaking SWOT
25 mission fosters the development of a new, improved and fully automated version of the software
26 (SPASSOv2.0) to address the need to target SWOT-scales during *in situ* experiments.

27 1. Introduction

28 Ocean dynamics play a key role in the Earth system by distributing properties and matter
29 around the globe. Ocean processes span a wide range of spatio-temporal scales from the global
30 thermohaline circulation (\sim years - hundreds of kilometers) to the microscale of turbulent mixing
31 (\sim hours/minutes - meters). In between stands the mesoscale (\sim months - hundred kilometers) and
32 submesoscale (\sim days - few kilometers) dynamics characterized by the formation, transport and
33 dissipation of features such as eddies, meanders, filaments or fronts (McWilliams 2006). These
34 two regimes are closely associated, being defined by their transient nature as well as by respectively
35 a dominant or non-negligible role of geostrophy (Lévy et al. 2012) and therefore nowadays often
36 referred together as the *fine scale*. The *fine scales* have a central role in the physical, biogeochemical,
37 and ecological dynamics of the ocean, strongly modulating in the horizontal and vertical the energy
38 and transport pathways of the ocean, the exchanges at its interfaces, and shaping the dynamical
39 “seascape” in which marine biota live (Kavanaugh et al. 2016; Mahadevan 2016; McGillicuddy Jr
40 2016; Taylor and Thompson 2023). Although empirical evidence of strong intermittent ocean
41 circulation below $\Theta(100\text{km})$ emerged since the 60s (e.g., Gill et al. 1974; Wyrтки et al. 1976), eddies
42 and filaments still present today a major challenge in terms of their observability. During their life
43 cycle, these structures may drift on distances that make several times their horizontal dimension.
44 An observational network capable of fully resolving the spatial and temporal variability of one of
45 these structures should therefore offer a precision of less than 1 km in the horizontal, of few meters
46 in the vertical, on a region hundreds of kilometer large and hundreds of meter deep, for a period
47 up to several months.

48 In the 1980’s the first interdisciplinary studies based on *in situ* observation specifically focused
49 on mesoscale features were carried out in the North Atlantic in the vicinity of the Gulf Stream
50 and well-known Gulf Stream rings. Several mesoscale *in situ* mappings, such as the POLYGONE
51 (Brekhovskikh et al. 1971), POLYMODE (McWilliams et al. 1983), MODE (Group et al. 1978)
52 and Tourbillon (Tourbillon 1983) experiments were conducted in about 100×100 km areas,
53 chosen ahead the field experiment for their intense mesoscale activity. At that time sampling
54 strategies usually consisted in large scale surveys of the mapping area including CTD, expendable
55 bathythermographs (XBT) profiles and floats deployment on a nearly uniform grid to target as
56 precisely as possible the location of mesoscale features. After the completion of such large scale

57 survey, some higher resolution feature-oriented mapping was performed to observe fine-scale
58 characteristics of a specific mesoscale feature.

59 At the same time, advances in satellite infrared imagery allowed for mapping large areas of sea
60 surface temperature (SST). These near-real time images proved to be very useful for mesoscale
61 feature identification and tracking, as thermal signature reveals the formation and circulation of
62 warm and cold rings. Indeed several pioneering *in situ* cruises determined their sampling location
63 and strategy using advanced very high resolution radiometer (AVHRR) data. The "Ring group"
64 used these images to identify, track and sample several Gulf Stream cold rings for about a year
65 (including four cruises) to describe both the physical and biological interactions during the rings'
66 lifetime (Ring Group 1981). Similarly warm-core eddies in the Gulf of Mexico (Biggs 1992)
67 and Algerian eddies in the Mediterranean Sea (Millot et al. 1997; Taupier-Letage et al. 2003)
68 have been chosen from infrared images to study the mesoscale feature properties and associated
69 phytoplankton dynamics. However, the success of such strategies relied on the availability of
70 exploitable (i.e. cloud-free) sets of images.

71 This limitation is partially overcome since the 2000's thanks to the emergence of altimetry
72 derived products (sea surface height (SSH) and surface velocities). This technology provide
73 global observation of the ocean surface dynamics at mesoscale resolution (~ 75-100 km; Abdalla
74 et al. 2021). In parallel, the first ocean color images (chlorophyll concentration, Chl) revealed
75 clear biological mesoscale patterns (McClain 2009). The spectacular advances in remote sensing
76 observations both in terms of horizontal resolution and temporal data availability widened the
77 mesoscale feature detection capabilities. Indeed not only satellite-derived data were made available
78 over the entire globe in a quasi near-real time, offering the possibility to track features directly from
79 space, but also the variety of satellite products extensively diversified the approaches to identify
80 mesoscale processes. While some spatial technologies provide cloud-free snapshots of mesoscale
81 features (altimetry or micro-wave SST), others offer the opportunity, when sky is clear, to observe
82 submesoscale heterogeneity by highlighting local tracer gradients at remarkable scales of few
83 meters to kilometers (infra-red SST or ocean color). The submesoscale nature of phytoplankton
84 patchiness, as seen by satellite-derived Chl, results from advection and stirring effect of small-
85 scale ocean circulation as shown by several studies (Gower et al. 1980; Peláez and McGowan 1986;
86 Mahadevan and Campbell 2002; d'Ovidio et al. 2010).

87 The *fine scale* surface transport information provided by satellite-derived products can be sup-
88 plemented by Eulerian and Lagrangian analysis inferred from velocity fields. Eulerian diagnostics,
89 such as kinetic energy (KE) or Okubo-Weiss (OW) criterion analyze local properties of the flow
90 from instantaneous snapshot of the velocity field (Okubo 1970; Weiss 1991). On the other hand,
91 Lagrangian diagnostics provide a finer measure of the dynamics experienced by a water parcel
92 transported by a time-dependent flow field. By essence, the chaotic advection of water parcels
93 reveals transport structures below the resolution of the velocity field. This is achieved by estimating
94 sub-grid tracer filaments that are produced by the resolved features of the velocity field through
95 stirring. For instance, a field of eddies with radii of 100 km and resolved at a resolution of 10 km
96 can be used to initialize a Lagrangian model at 1 km resolution, and stir a numerical tracer into
97 filaments at this finer resolution. This characteristic makes Lagrangian diagnostics powerful tools
98 to investigate *fine scale* processes (d’Ovidio et al. 2009). For instance, the finite-size or finite-time
99 Lyapunov exponents (FSLEs and FTLEs), a widely used Lagrangian diagnostic measuring the
100 dispersal rate of advected particles, were proved to compare well with fine scale distribution of
101 SST and satellite-derived phytoplankton niches (Lehahn et al. 2007; Rossi et al. 2008; d’Ovidio
102 et al. 2010).

103 By combining the analysis of available near-real time satellite resources with derived Eulerian
104 and Lagrangian diagnostics in an automated way, Petrenko et al. (2017) set up a new approach
105 for real-time adaptive *fine scale* sampling strategy during the LATEX10 cruise in 2010. An
106 automated algorithm, the Software Package for an Adaptive Satellite-based Sampling for Oceano-
107 graphic cruises (SPASSO), was developed to provide on-board teams with daily maps of: near-real
108 time satellite-derived surface currents, SST and Chl concentration and altimetry-derived Eulerian
109 and Lagrangian diagnostics. This methodology filled the need for assessing in real-time a de-
110 tailed description of the sampling area to opportunely study various biophysical processes such
111 as the dynamic of an hyperbolic point and associated dispersion processes (LATEX10 cruise;
112 Petrenko 2010), biogeochemical budgets associated with mesoscale phytoplankton bloom (OUT-
113 PACE cruise; Moutin and Bonnet 2015), natural iron fertilization in the Southern Ocean (KEOPS-II
114 cruise; Queguiner 2011), or fine scale biophysical coupling (OSCAHR cruise; Doglioli 2015).

115 The new Surface Water and Ocean Topography (SWOT) satellite mission, launched in late 2022,
116 offers a one of a kind opportunity to investigate the *fine scale* dynamics of the upper ocean, at

117 unprecedented horizontal and temporal resolutions, and to address the *fine scale* influence on
118 the global energy budget in the ocean (d’Ovidio et al. 2019). Indeed during the calibration
119 and validation (CalVal) period, from March to July 2023, the satellite recorded cloud-free SSH
120 observations along both SWOT swaths (120 km wide) with a 1-day repeat: the 1-day orbit, or *fast-*
121 *sampling* phase (Morrow et al. 2019). An international effort, conducted in the framework of the
122 SWOT-Adopt-A-Crossover (AdAC) consortium, was carried out to coordinate *in situ* observations
123 at orbit crossover points, hence visited twice a day during the fast-sampling phase. Endorsed
124 by CLIVAR in 2019, this initiative encompasses more than 20 *in situ* experiments planned in a
125 variety of ocean regions during the CalVal phase. The need to uniformly support all SWOT-AdAC
126 cruises in their sampling strategies motivated the development of an updated version (v2.0) of the
127 SPASSO software aiming to: 1) easily enable the code configuration for simultaneous multiple
128 fields experiments during SWOT fast-sampling phase; 2) facilitate its autonomous use by a wide
129 range of oceanographers; 3) develop new diagnostics designed to address innovative biophysical
130 issues.

131 In the following we provide a complete description of the SPASSOv2.0 software architecture
132 and functioning. Examples of SPASSO-generated maps are displayed and the computation of
133 available Eulerian and Lagrangian diagnostics is detailed (Section 2). To illustrate the software
134 capabilities and efficiency to guide future successful *fine scale* biophysical studies, we present
135 several case studies of previous SPASSO-based *in situ* sampling experiments which occurred in
136 various oceanic regions (Section 3).

137 **2. Material and methods**

138 *a. Software architecture and philosophy*

139 A key characteristic of the new SPASSOv2.0 framework is to provide a complete Python environ-
140 ment that encapsulates a set of functionalities to: 1) download ocean data; 2) perform dynamical
141 analysis; 3) visualize and save ocean parameters. The tool is designed following modern scientific
142 engineering software development and considering two main concepts:

143 *(i) Ease of use:* Software usage must be accessible to various oceanographers from different fields
144 that are not always familiar with complex model computation. Therefore, a standard configuration

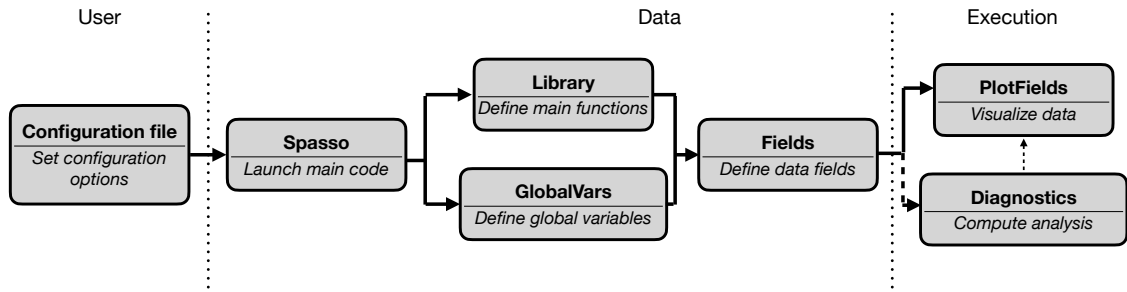


FIG. 1. Functionalities and structure of the SPASSOv2.0 algorithm.

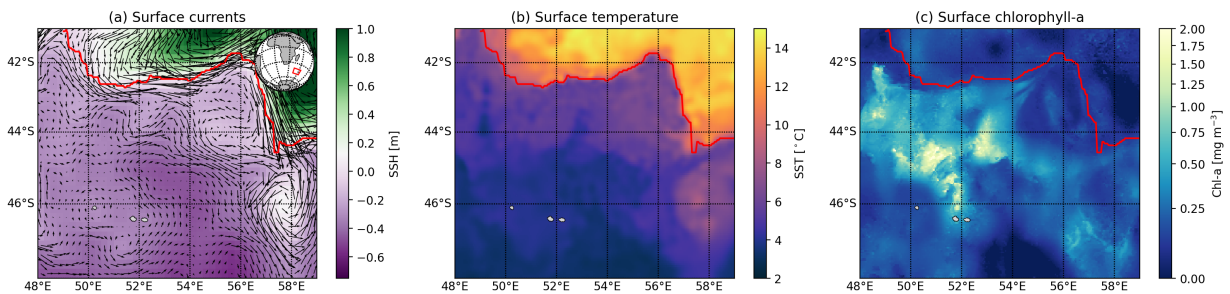
145 of the software is openly accessible through Github (<https://github.com/OceanCruises/SPASSO>)
 146 and can be implemented by modifying a unique file controlling the algorithm main options.

147 (ii) *Modularity and flexibility:* The algorithm is designed to allow for the addition of various
 148 specialized sub-components (data, plotting options, outputs) to match different ocean sampling
 149 objectives without modifying the core code.

150

151 The main code ([Spasso.py](#)) first reads a text configuration file ([config_*.ini](#)) containing all
 152 the necessary options to run SPASSOv2.0 (Fig.1). In the configuration file, the user sets specific
 153 options related to his configuration such as: the cruise name and domain, the type of configuration
 154 (near-real time or delayed-time), the list of the desired satellite products and associated parameter
 155 limits, the list and parameter details for Eulerian and Lagrangian configuration and some output
 156 file options. The configuration file is the ONLY file the user needs to modify for a standard
 157 configuration of the code. After reading the configuration file, SPASSOv2.0 loads the necessary
 158 functions ([Library.py](#)) and global variables ([GlobalVars.py](#)) requested from the configuration
 159 file options. Then, the satellite data required by the user are downloaded and stored by [Fields.py](#).
 160 A second layer is then in charge of plotting the downloaded data for visualization ([PlotFields.py](#))
 161 and optionally computing some diagnostics for dynamical analysis ([Diagnostics.py](#)). The data
 162 used by SPASSOv2.0 are mainly satellite-derived physical and biogeochemical ocean variables
 163 (surface currents, SSH, SST, Sea Surface Salinity and surface Chl concentration) freely available,
 164 in near-real time, distributed by different platforms such as the European Copernicus marine data
 165 store (CMEMS). A novel option available in SPASSOv2.0 allows for the use of delayed-time
 166 available data to perform climatological and post-sampling analysis.

167 Figure 2 shows an example of three typical maps generated by SPASSOv2.0 configured to use
 168 SSH, surface currents, SST and Chl from CMEMS near-real-time products in the Indian sector of the
 169 Southern Ocean. These datasets provide some satellite-derived contextual information for spring
 170 2011 (Queguiner 2011, KEOPS-II cruise). The satellite image analysis highlights the circulation
 171 of the major branch of the Antarctic Circumpolar Current, north of the Crozet Plateau, associated
 172 with the SubAntarctic Front (SAF) (Fig. 2a and b). For this specific example, we show the SAF
 173 position as detected by the local maxima of the SST gradient magnitude following a traditional
 174 gradient-based front identification method (see more detail in Wang et al. (2023) Supplementary
 175 Material). An intense phytoplankton bloom, constrained in cold waters to the south by the SAF,
 176 is visible on the chlorophyll-a image (Fig. 2c). The horizontal distribution of the bloom around
 177 the Crozet Plateau is structured by the surface currents measured by altimetry. The analysis of
 178 this coupling can be extended by computing some classical Eulerian and Lagrangian diagnostics
 179 ([Diagnostics.py](#)) provided by an embedded complementary software package coupled with
 180 SPASSOv2.0.



181 FIG. 2. Satellite-derived (a) Sea Surface Height and velocities (colorscale, m); (b) Sea Surface Temperature
 182 (colorscale, °C); (c) Surface Chlorophyll-a concentration (colorscale, $\text{mg}\cdot\text{m}^{-3}$) for October 14th, 2011. Red line
 183 shows the SubAntarctic Front (SAF) defined as the local maxima of satellite-derived SST gradient magnitude.
 184 Data were retrieved from the Copernicus Marine Data Store for the following products: (a) velocities and SSH:
 185 <https://doi.org/10.48670/moi-00148>; (b) SST: <https://doi.org/10.48670/moi-00168>; Chl-a: [daily cmems_obs-oc_glo_bgc-plankton_my_14-gapfree-multi-4km_PID](https://doi.org/10.48670/moi-00168)
 186 <https://doi.org/10.48670/moi-00168>

187 *b. Eulerian and Lagrangian analysis: LAMTA software*

188 SPASSOv2.0 is coupled with a Python Lagrangian software (LAgrangian Manifolds Tracking
189 Algorithm, LAMTA included in the `Diagnostics.py` file) that computes some Eulerian and La-
190 grangian diagnostics to provide statistics of the considered velocity field. Lagrangian diagnostics
191 are derived from the trajectories of virtual particles analyzed to provide a complementary hydro-
192 dynamical description of the sampled region flow. Lagrangian ocean analysis are now widely
193 used by the marine scientists community to track water masses, coherent structures, marine debris
194 or biological dispersion (Van Sebille et al. 2018). LAMTA has been developed to advect virtual
195 particles in horizontal 2-D time-evolving velocity fields and process the resulting trajectories to
196 provide insights on the ocean circulation and dynamics (d’Ovidio et al. 2015). The Lagrangian
197 diagnostics, including tracer advection, Lagrangian Coherent Structure (LCS) detection and water
198 masses Lagrangian age, are provided as daily surface fields. These quantities are of particular
199 interest for planning oceanographic sampling since they include history on the horizontal motion
200 of seawater parcels. In the following, we describe the Eulerian diagnostics, the particle trajectory
201 computation and the derived Lagrangian diagnostics computed by the LAMTA software.

202 *Eulerian diagnostics:*

203
204 The surface **kinetic energy (KE)** estimated from altimetry-derived geostrophic currents is often
205 used to study the variability of surface ocean currents and eddies. We define KE at a given time
206 as the total kinetic energy, including mean flow and eddy contributions. KE thus represents the
207 amount of energy due to flow motion (Fig. 3a). It is expressed as the sum of the squared velocities
208 (u, v) , in $cm^2.s^{-2}$:

$$KE = u^2 + v^2 \quad (1)$$

209 The identification of ocean mesoscale eddies is particularly useful since they are believed to
210 play significant roles in ocean heat and salt exchanges (Jayne and Marotzke 2002; Dong et al.
211 2014; Zhang et al. 2014) as well as on primary production, intermediate trophic levels and large
212 predators (Falkowski et al. 1991; Cotté et al. 2007; Gaube et al. 2018; Della Penna and Gaube
213 2020). Different eddy detection methods have been developed and compared to identify mesoscale
214 features (Souza et al. 2011). One of them is based on the **Okubo-Weiss parameter (W)** which

215 compares at a given point (i, j) the intensity of the strain (S) to the vorticity (ω) (i.e. the importance
 216 of deformation *versus* rotation in $days^{-2}$):

$$W_{i,j} = Sn_{i,j}^2 + Ss_{i,j}^2 - \omega_{i,j}^2 \quad (2)$$

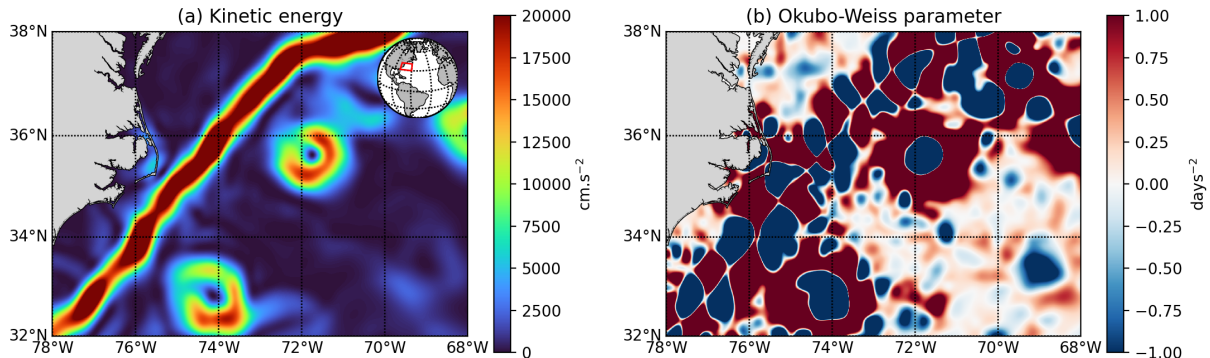
217 where $Sn_{i,j}$ is the normal strain, $Ss_{i,j}$ is the shear strain and $\omega_{i,j}$ is the relative vorticity. These
 218 quantities are evaluated from the derivative of the daily surface geostrophic velocity fields (u, v)
 219 derived from altimetry:

$$Sn_{i,j} = \frac{\partial u}{\partial x_{i,j}} - \frac{\partial v}{\partial y_{i,j}}$$

$$Ss_{i,j} = \frac{\partial u}{\partial y_{i,j}} + \frac{\partial v}{\partial x_{i,j}}$$

$$\omega_{i,j} = \frac{\partial v}{\partial x_{i,j}} - \frac{\partial u}{\partial y_{i,j}}$$

220 Negative values of W identify regions of recirculation that can be associated with eddy cores,
 221 while positive W locate prevailing stretching areas (Fig. 3b). Isolines of W can be used to identify
 222 Eulerian eddy boundaries. However, since this diagnostic does not consider the temporal variability
 223 of the velocity field, it fails at representing the complex filamentous structures associated with eddy
 224 stirring. These *fine scale* characteristics of the flow can be more reliably assessed in a Lagrangian
 225 framework involving numerical particle trajectories computation.



226 FIG. 3. (a) Kinetic energy (colorscale, $cm.s^{-2}$) and (b) Okubo-Weiss parameter (colorscale, $days^{-2}$) computed
 227 with satellite-derived geostrophic velocities from July 24th, 2022 (<https://doi.org/10.48670/moi-00148>).

228 *Off-line trajectory calculation:*

229

230 Particle trajectories are computed off-line using horizontal 2-D velocity fields either stored from
231 altimetry or Eulerian model outputs. Trajectories can be computed in a forward or backward
232 in-time mode. Since water parcels history is traced back in SPASSOv2.0, LAMTA is set up by
233 default in a backward mode.

234 Virtual particles can either be seeded from a list of locations (x, y) and times (t) provided by the
235 user or can be initialized over a regular 2-D horizontal grid with a predefined resolution δ_s at a
236 certain time t . The default seeding is over the entire domain and at the time of observation. A
237 fine spatial seeding resolution (i.e. small δ_s) results in higher horizontal resolution Lagrangian
238 diagnostics but also exponentially increases computing time. A trade-off between resolution and
239 computing time must be considered when choosing δ_s , especially for large regions of interest.

240 Particle advection is then performed by (1) interpolating in space and time the gridded velocity
241 field to each individual particle position; (2) integrating in time the trajectory. LAMTA's archi-
242 tecture allows users for coding their preferred methods for spatial interpolation and explicit time
243 stepping. In the following we detail the default LAMTA set-up for a typical SPASSOv2.0 use.
244 Each individual particle position $X(t)$ is updated by time-stepping the velocity at $X(t) = x$:

$$\mathbf{X}(t + \Delta t) = \mathbf{X}(t) + \int_t^{t+\Delta t} v(\mathbf{x}(\tau), \tau) d\tau \quad (3)$$

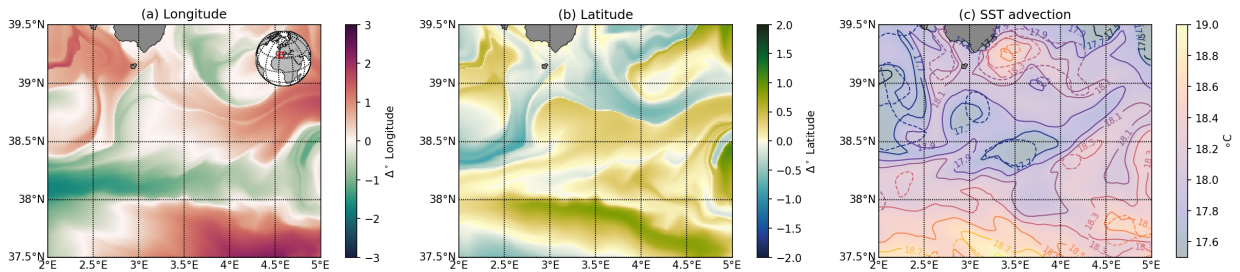
245 To accurately estimate the particle displacement, a fourth-order Runge-Kutta method is used for
246 the integration of Eq.3: the interpolated velocity field is evaluated every 6 hours. Within grid cells,
247 velocities are estimated using a linear 2-D interpolation. Once computed, the resulting trajectories
248 are used to derive several Lagrangian diagnostics such as tracer advection, Lagrangian Coherent
249 Structures and transit times.

250 *Tracers advection:*

251

252 Computed in non-divergent flows, Lagrangian tracer patches conserve mass and volume. Several
253 Lagrangian tools have been developed to map volume transport pathways by attributing small
254 amount of transport, conserved along the trajectories, to each virtual particle (Blanke and Raynaud

255 1997; Döös et al. 2017). Similarly, tracers' dispersion can be studied by attributing a portion of a
256 tracer quantity assumed to be conserved for a given period equal to the virtual particle advection
257 time.



258 FIG. 4. (a) Longitude (left) and (b) latitude (right) advection computed from Lagrangian trajectories initiated
259 on May 11, 2018 on a 0.01 degree grid and advected backward in time for 15 days using altimetry derived
260 velocities (Mediterranean product from Copernicus Marine Data Store: <https://doi.org/10.48670/moi-00141>).
261 (c) SST advected (shaded colormap and plain contours) backward for 3 days from May 11, 2018. The dashed
262 contours show the SST field on May 11, 2018 before advection (SST product from Copernicus Marine Data
263 Store: METOFFICE-GLO-SST-L4-REP-OBS-SST).

264 Another way to study content advection is to map the difference between the tracer value at
265 the initial and final position of the virtual particle. Tracer/content values are defined from the
266 satellite-derived value identified at the time and location of the particle (Barceló-Llull et al.
267 2021). In SPASSOv2.0 tracer advection maps (SST, SSS or chlorophyll-a) can be computed with
268 this method. A default advection time of 3 days is considered for these non-conservative tracers:
269 Figure 4c shows a map of temperature advection from a satellite derived SST field. Advection maps
270 of longitude or latitude can also help identifying water masses origin. This diagnostic measures
271 the difference in longitudes (or latitudes) between each initial and final particle position. A typical
272 value of 12 to 15 days for particle advection is recommended for these diagnostics to assume that
273 water masses conserved the initial characteristics they had at their origin. Figure 4a,b show an
274 example of longitude and latitude advection maps computed south of the Balearic Islands in the
275 Mediterranean Sea. Green patches identify regions where water parcels were located anywhere east
276 of the grid cell 15 days before; whereas red areas indicate a western origin. Similar conclusions can
277 be inferred from the latitude advection map in the North-South direction: blue (yellow) patches
278 reveal a northern (southern) origin respectively. Strong gradients of these advectons can also

279 be used to detect frontal areas between potentially different water masses moving in opposite
280 directions.

281 *Lagrangian Coherent Structure detection:*

282

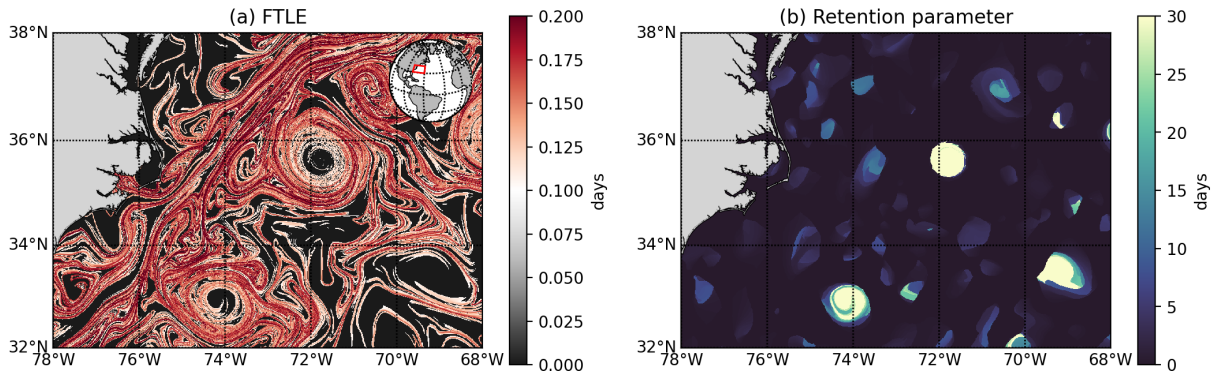
283 Coherent structures such as eddies, jets and fronts are ubiquitous features in the ocean that drive
284 the distribution of ocean tracers and impact ocean biogeochemistry (Smith et al. 2016; Mahadevan
285 2016; Zhang et al. 2019). The Lagrangian Coherent Structures (LCS) theory relies on the detection
286 of distinct coherent regions, separated by clear boundaries, based on Lagrangian trajectory analysis.
287 One empirical diagnostic of LCSs is the Finite Time Lyapunov Exponent (FTLE) which identifies
288 attracting and repelling material structures (Lapeyre 2002). FTLE (λ) computed from a backward
289 in time integration measures the exponential rate of separation between water parcels initially at a
290 close distance from one another, and is defined as (Eq. 4):

$$\lambda = \frac{1}{2} \frac{\log\left(\frac{d_f}{d_i}\right)}{T} \quad (4)$$

291 with d_f the final particle separation (distance), d_i the initial particle separation (distance) and T
292 the integration time (i.e. number of days of integration).

293 The backward FTLE diagnostic identifies attracting LCSs along which water parcels tend to
294 accumulate due to horizontal stirring even if they were originally located at large distance apart.
295 Because of that, the ridges (i.e. local maxima) of Lyapunov exponents, computed from altimetry
296 data, can be used to identify stirring regions where water masses are relatively quickly elongated.
297 Figure 5a shows FTLEs associated with the highly energetic Gulf Stream and related rings: the
298 current and eddy boundaries intensely stir the water masses, as revealed by the FTLEs filaments.
299 These features can thus be used to identify frontal regions acting like barriers to the flow. On the
300 contrary, regions of low or null FTLEs, highlighted in black on Figure 5a emphasize zones with low
301 stirring effect. Several studies have already shown the correlation between the detected structures
302 from Lyapunov exponents and the distribution of tracer gradients (Lehahn et al. 2007; d'Ovidio
303 et al. 2009; Rousselet et al. 2018), or the location of biological niches (d'Ovidio et al. 2010;
304 De Monte et al. 2012; Della Penna et al. 2017). These previous studies computed the so-called
305 Finite Size Lyapunov Exponent (FSLE): the lyapunov exponent is calculated only for particle pairs

306 when they reach a d_f equal or greater than a predefined distance (or size, as its name suggests). The
 307 FSLE computation can take an infinite time if we wait for all particles to reach the final distance.
 308 The FTLE theory instead computes Lyapunov exponents for all particles advected for a finite time,
 309 regardless of their final separation. In this version of LAMTA, we chose to compute FTLE rather
 310 than FSLE because the FSLE concept particle integration needs to be bounded in time anyway.



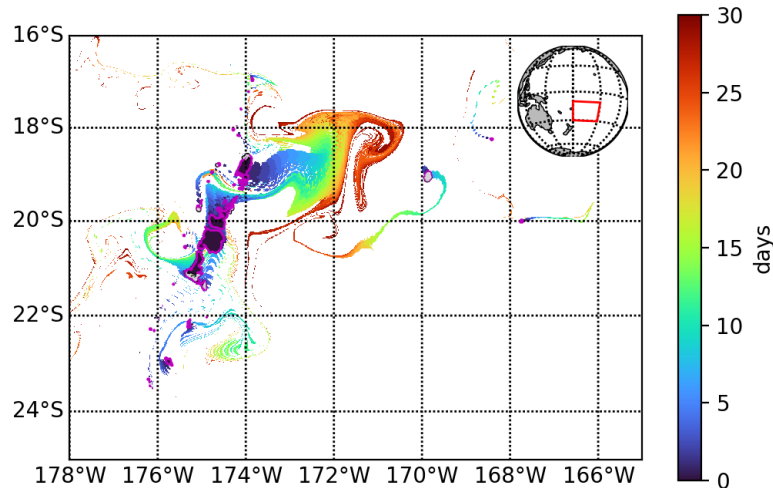
311 FIG. 5. (a) Finite-Time Lyapunov exponents (colorscale in days⁻¹) (FTLE). (b) Retention parameter (colorscale,
 312 days) computed from 30 days backward trajectories initiated on a 0.01 degree grid on July 22nd, 2022 using
 313 altimetry derived velocities (<https://doi.org/10.48670/moi-00148>).

314 Other significant coherent structures commonly tracked are oceanic mesoscale eddies, due their
 315 ability to trap and transport water masses and their biotic and abiotic contents. If the Lyapunov
 316 exponents can detect enclosed filaments associated with some eddy cores, they fail at estimating the
 317 trapping nature of eddies. One crucial information to understand some of the biological dynamics
 318 related to ocean eddies is in fact the timescale of eddy trapping. d'Ovidio et al. (2013) have
 319 defined the Retention Parameter (RP) that evaluates the time a water parcel recirculates within
 320 an eddy. Unlike traditional eddy tracking algorithm usually based on the detection of sea level
 321 anomaly, vorticity or streamlines closed contour (Haller 2015; Le Vu et al. 2018; Laxenaire et al.
 322 2018), the RP calculation is an hybrid Eulerian-Lagrangian method based on the evaluation of the
 323 OW parameter along backward Lagrangian trajectories. As long as the OW parameter remains
 324 successively negative, the particle is considered trapped in an eddy core. Once the OW parameter
 325 changes sign (i.e. becomes positive), the particle is treated as out of the eddy. Therefore the RP is

326 defined as the time of persistence of a negative OW value. Compared to the Eulerian OW parameter
327 diagnostic, the RP identifies only structures able to trap water in their core (Fig. 3c).

332 *Lythogenic water masses age and transit:*

Nutrient enrichment of water masses by contact with a topographic feature such as coasts, shelf



328 FIG. 6. Water parcels lythogenic age (colorscale in days) since they were in contact with isobath $z = -200$ m
329 marked by magenta contours. Lagrangian trajectories were initiated on a 0.01 degree grid resolution and
330 computed from 30 days backward advection starting on March 8th, 2015 using using altimetry derived velocities
331 (<https://doi.org/10.48670/moi-00148>).

333
334 breaks, sea mounts or hydrothermal vents is a crucial physical process leading to biological
335 enhancement. A Lagrangian approach developed by d'Ovidio et al. (2015) considers the time
336 since the last contact with an isobath ('water age') chosen according to the topographic element
337 depth. Technically, 2-D backward-in-time trajectories are checked for crossing any area where ocean
338 depths are shallower than the selected isobath anytime during the time integration. If a trajectory
339 never reaches a region above the chosen isobath then it is discarded from the water age calculation.
340 The time taken by the particle to reach the isobath is assigned to the initial particle grid cell. This
341 means the water parcel located in this area was in contact with the topographic feature, defined
342 by the isobath threshold, X days ago. Theoretically this lythogenic water age diagnostic allows
343 for the identification of water patches potentially nutrient-enriched by contact with coastal or deep
344 sediments. Figure 6 shows an example of a water patch previously in contact with the Tonga

345 islands in the southwest Pacific: the waters located at 172°W and 18°S were near the Tonga island
346 coasts 20 days prior 8 March 2015. This diagnostic has been previously matched with the surface
347 distribution of satellite-derived Chl patches and surface drifters (d’Ovidio et al. 2015; Sanial et al.
348 2014, 2015; Sergi et al. 2020; Chabert et al. 2021).

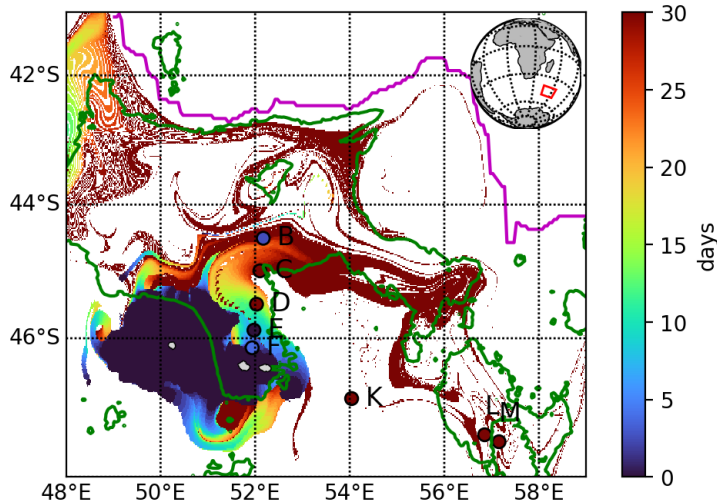
349 **3. Biophysical applications**

350 In its early stages, SPASSO was used to specifically track *fine scale* processes and features such
351 as the evolution of the dynamics associated with persistent mesoscale eddies (LATEX cruises,
352 Petrenko et al. 2017), or to monitor the impact of horizontal advection in regulating the salinity
353 maximum within the subtropical gyre (STRASSE cruise, Reverdin et al. 2015). However it rapidly
354 proved to be quite useful for biophysical applications of growing interests lately. This section
355 reviews how SPASSO can help design sampling strategies to elucidate biophysical processes at
356 *fine scales*. We selected the following examples as they span a large variety of oceans and seas
357 (Atlantic, Pacific, Southern Ocean and Mediterranean Sea) as well as physically and biologically
358 contrasted environments: productive boundary current, open ocean oligotrophic areas or High-
359 Nutrient, Low-Chlorophyll (HNLC) region.

360 *a. Natural ocean fertilization effect on phytoplankton blooms*

361 Phytoplankton blooms are episodic and rapid population increase events often driven by an
362 unusual supply of limiting nutrients. In the case of seasonal blooms, the simultaneous availability
363 of light energy along with nutrient resources (or a rapid decrease in grazing pressure) is also required
364 for photosynthesis and phytoplankton growth. Submesoscale horizontal and vertical transport is
365 one among the physical processes (restratification, solar forcing, surface heating) participating in
366 enhancing phytoplankton blooms whether they occur in coastal, oligotrophic or HNLC regions
367 (Mahadevan 2016; Lévy et al. 2018).

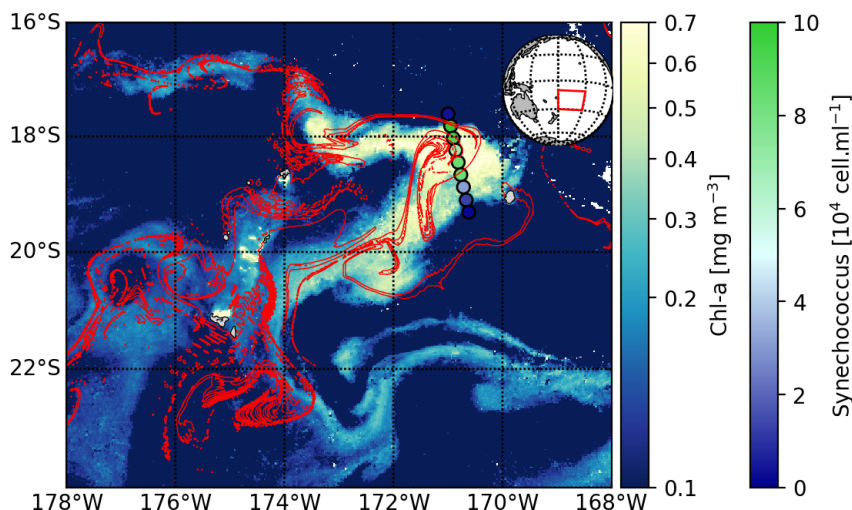
374 The main goal of the KEOPS-2 campaign was to study the potential influence of natural iron
375 fertilization on phytoplankton blooms off the Crozet Plateau around the Kerguelen islands in the
376 Southern Ocean (Queguiner 2011). SPASSO outputs were perfectly suited to identify such a bloom
377 from space and plan *in situ* sampling. SPASSO maps of surface Chl were used to locate the bloom
378 and displayed a surface patch expanding from the Crozet Islands (~46°S-52°E) further north until



368 FIG. 7. Reproducing Sanial et al. (2014) results: Water ages (colorscale, days) since lying above the 2000 m
 369 isobath (isobath limit is shown by the limit of initial age = 0 days). The Lagrangian trajectories are advected from
 370 October 14th, 2011 for a maximum of 80 days using the satellite-derived velocities ([https://doi.org/10.48670/moi-](https://doi.org/10.48670/moi-00148)
 371 00148). The magenta line marks the SAF front identified by the maximum SST gradient (Fig. 2). The green line
 372 contours satellite chlorophyll-a concentration above $0.25 \text{ mg}\cdot\text{m}^{-3}$. Colored dots (same color scale, days) show
 373 the apparent radium ages of surface waters derived from $^{224}\text{Ra}/^{228}\text{Ra}$ ratios (more details in Sanial et al. (2014)).

379 restricted by the SubAntarctic Front (SAF, Fig. 2c). The bloom extension and SAF position are
 380 also shown by the green and magenta lines respectively on Figure 7. The water mass ages were
 381 also estimated from the 2000 m isobath to mimic the potential deep-ocean iron fertilization. The
 382 water mass age patch distribution matches the distribution of significantly high values of surface
 383 Chl (Fig. 2c and green contour on Fig. 7). SPASSO output analysis thus suggests that the seasonal
 384 phytoplankton bloom has been triggered by a deep-water iron enrichment: the relatively good
 385 overlay between both independent estimates of Chl-a concentration and Lagrangian lythogenic
 386 water mass age indicates a potential influence of physical processes in driving and shaping the
 387 bloom. In order to validate the lythogenic water mass age diagnostic, Sanial et al. (2014) estimated
 388 the age of surface waters from radium isotopic ratios. The colored dots on Figure 7 show an
 389 increase in water age with the distance from the Crozet Islands. However the farthest station (B) is
 390 characterized by relatively younger waters (~ 8 days old) indicating a more recent interaction with
 391 the shelf sediments than stations (C,D) located closer to the islands. This pattern is probably due to

392 a small-scale circulation stirring a tongue of young waters in contact with the northern boundary
393 of the Plateau further east. This tongue is actually visible on the lithogenic water age at around
394 45°S-51°E but does not extend east enough probably because of the poor accuracy (at that time)
395 of altimetry-derived geostrophic currents near the coast.



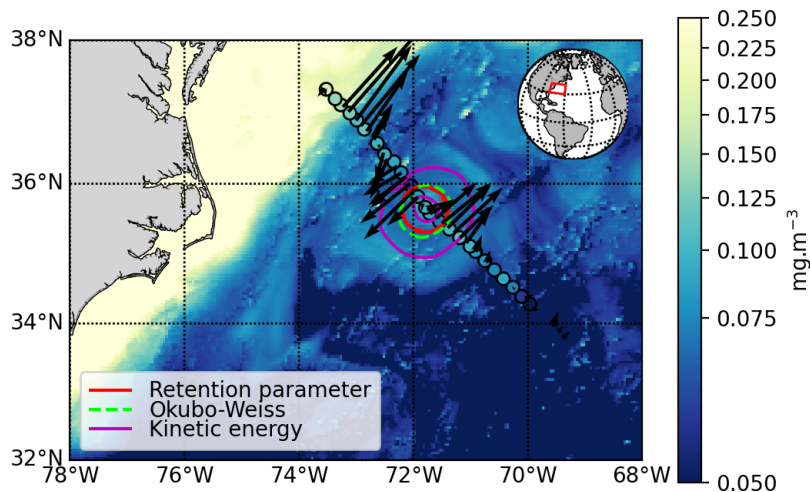
396 FIG. 8. Satellite-derived surface chlorophyll-a concentration (colorscale in mg m^{-3}) on March 8th, 2015
397 extracted from de Verneil et al. (2017) and Rousselet et al. (2018) results. Contours of "enriched" water patches
398 derived from water age diagnostic (Fig 6) are shown in red.

399 Another phytoplankton bloom has been sampled in the ultra-oligotrophic South Pacific ocean
400 during the OUTPACE cruise (Moutin et al. 2017). The main objectives of OUTPACE were to char-
401 acterize the distribution of biogeochemical elements and biological diversity along an oligotrophic
402 gradient (i.e. depleted nutrient environments). Halfway through the cruise, SPASSO images re-
403 vealed a spectacular unusual phytoplankton bloom marked by relatively high Chl concentration in
404 the vicinity of Tonga Islands (Fig. 8). *In situ* high-resolution biological sampling confirmed the
405 location of the bloom (Rousselet et al. 2018) as shown by the *Synechococcus* abundances on Figure
406 8. The patch of lithogenic water ages (red contours) initiated at 200 m (i.e. around the Tonga
407 Islands) matched the surface distribution of satellite-derived Chl suggesting the bloom could be
408 induced by a near-surface coastal nutrient enrichment. This hypothesis have then been confirmed
409 by further Lagrangian analysis and the mechanism in place has been defined as a delayed island

410 mass effect (IME) where mesoscale circulation create a hotspot of productivity by transporting
411 nutrient enriched waters (de Verneil et al. 2017; Messié et al. 2020).

412 *b. Eddy influence on primary production*

413 Gulf Stream rings are certainly the most studied eddies in ocean research history since the
414 pioneer observations in the 1970's (Richardson et al. 1978). Although several studies already
415 fully describe the formation, evolution and biological implications of warm-core and cold-core
416 Gulf Stream rings, a substantial knowledge can be derived by sampling a Gulf Stream eddy with
417 high frequency multiplatform sampling technologies and methods. The FIGURE-CARING cruise
418 (Benavides and Carracedo 2022) was guided by SPASSO to a large mesoscale eddy with a non-
419 negligible Chl signature, while heading towards the North Atlantic to cross-sample the Gulf Stream
420 (Fig. 9).



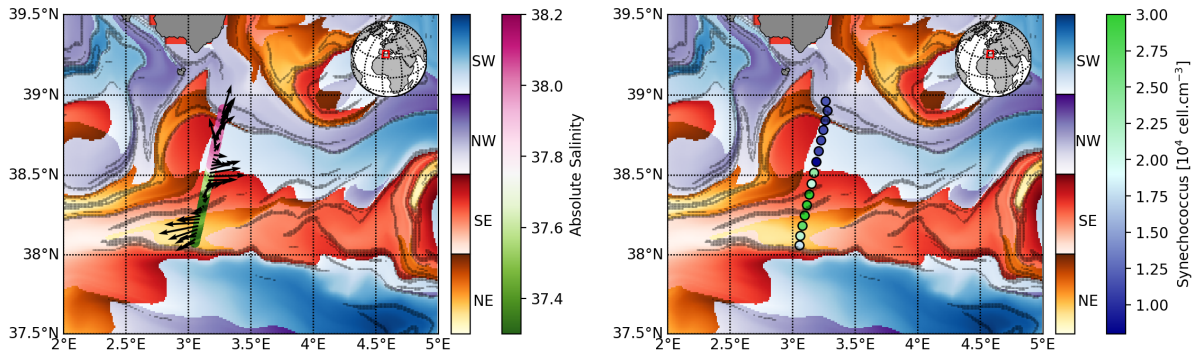
421 FIG. 9. Satellite-derived chl concentration (color scale, mg.m^{-3}) for 24 July 2022 (product from Copernicus
422 Marine Data Store: cmems_obs-oc_glo_bgc-plankton_myint_14-gapfree-multi-4km_PID). Contours of reten-
423 tion parameter (25 days) in red, Okubo-Weiss parameter (-1 days^{-2}) in dashed green and kinetic energy (7000
424 cm.s^{-2}) in magenta. Arrows show surface currents from ADCP (first level at 27 m). Colored dots show surface
425 chl concentration (color scale, mg.m^{-3}) from underway sea water system every 3 minutes for visualization
426 purposes.

427 A high resolution biophysical cross-eddy sampling was planned based on SPASSO diagnostics
428 information. The core and eddy center were accurately determined using several Eulerian and
429 Lagrangian-based diagnostics (KE, OW and FSLE) as revealed by the surface current measured
430 by the hull-mounted vessel ADCP (Fig. 9). High-frequency sampling (every 5 seconds) of
431 the surface Chl concentration displays a similar gradient of surface Chl as the one detected by
432 satellite. High-resolution measurements of N₂ fixation rates conducted across the eddy revealed
433 substantially higher eddy-induced rates, associated with consistent detection of Trichodesmium
434 cells, than previously reported in the western North Atlantic (Hoerstmann et al. 2023). Overall,
435 these feature-oriented observations demonstrate that eddies contribute significantly to diazotrophy
436 and thus to reactive nitrogen input in the western North Atlantic.

437 *c. Fronts and biological niches*

438 The few observations focusing on frontogenesis influence over phytoplankton diversity usu-
439 ally took place in persistent and intense fronts generated by energetic boundary currents or
440 coastal upwellings (Ribalet et al. 2010; Clayton et al. 2017). However, most of the global
441 ocean is characterized by weakly energetic and short-lived features. One of the main objectives
442 of the PROTEVSMED-SWOT cruise was to observe (sub)mesoscale circulation and associated
443 ageostrophic dynamics in the moderately energetic open Mediterranean Sea (Dumas 2018). Based
444 on SPASSO analysis, simultaneous physical and biological high-frequency measurements were
445 performed, south of the Balearic Islands, in a potential frontal area marked by a surface Chl gradi-
446 ent (Tzortzis et al. 2021). The analysis of FTLE distribution and water mass origins also suggested
447 the presence of a front separating biogeochemically contrasted areas.

454 Figure 10 shows a global water mass origin map produced during post-processing by combining
455 both longitude and latitude advection maps from Figure 4. Each color map refers to a relative
456 orientation on a compass rose (SouthWest, NorthWest, SouthEast and NorthEast) and follows the
457 wind direction formalism (i.e. coming from). Figure 10 thus highlights that most of the waters
458 in the 38.5°N-39°N band are globally coming from the west whereas waters in the 38.5°N-38°N
459 travel from East to West. This contrast in water mass origins is confirmed by the hydrological
460 characteristics measured at high-frequency with a CTD mounted on a towed vehicle (see Tzortzis
461 et al. (2021) for more details). For example the salinity dramatically changes at the boundary of the



448 FIG. 10. Water parcels origin computed from longitude and latitude advections shown in Figure 4. The
 449 colorscale indicate geographical origin direction from the grid cell position (SW: SouthWest; NW: NorthWest;
 450 SE: SouthEast; NE: NorthEast). Black arrows show the current velocities measured by a vessel-mounted ADCP
 451 on May 11th, 2018 at 25 m depth. Near-surface absolute salinity measured with a SeaSoar vehicle along the
 452 cross-front transect is also shown with the green to pink colorscale and the Synechococcus concentration with the
 453 blue to green colorscale (more details about *in situ* data acquisition and treatment in Tzortzis et al. (2021)).

462 two different water masses: northern saltier waters travel east whereas southern cooler waters flow
 463 west. The Lagrangian-based water mass origins and directions are coherent with surface currents
 464 estimated from the hull-mounted ADCP. A FTLE-derived front also matches with the change in
 465 direction from surface currents. The distribution of phytoplankton abundances (*Synechococcus* on
 466 Figure 10) shows an across front contrast in phytoplankton diversity: some groups are dominant
 467 on one or the other side of the front thus creating biological niches. SPASSO analysis allowed for
 468 sampling a contrasted front whose 3D fine-scale biophysical description and history was completed
 469 by post-cruise investigations (see Tzortzis et al. 2021, 2023).

470 4. Conclusions

471 In this paper, we have introduced the new user-friendly Python version of the SPASSO software
 472 and detailed the Eulerian and Lagrangian diagnostics available for near-real time ocean analysis.
 473 We have also documented potential biophysical applications and assess the current code accuracy
 474 based on previous scientific experiments that were conducted using previous less well-developed
 475 SPASSO version. This represent a benchmark for future usages especially in the context of the new
 476 altimetric SWOT mission and field experiments conducted in the framework of the SWOT-AdAC

477 consortium (<https://www.swot-adac.org>). Future evaluation of SPASSO-based strategies will
478 arise from the analysis of the *in situ* SWOT-AdAC sampling experiments that will provide a large
479 overview of the *fine scales* in diverse oceans and regions (coastal vs. open ocean, eutrophic vs.
480 oligotrophic, highly vs. weakly energetic). Additionally, future versions of SPASSO will benefit
481 from the new high-resolution SWOT products, when available, enabling for the first time very *fine*
482 *scale* features detection.

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489 *Code availability.* The code for SPASSO is licensed under the MIT licence and version 2.0 is
490 available through GitHub at <https://github.com/OceanCruises/SPASSO/>.

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