



argoFloats: An R Package for Analyzing Argo Data

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An R package named *argoFloats* has been developed to facilitate identifying, downloading, caching, and analyzing oceanographic data collected by Argo profiling floats. The analysis phase benefits from close connections between *argoFloats* and the *oce* package, which is likely to be familiar to those who already use R for the analysis of oceanographic data of other kinds. This paper outlines how to use *argoFloats* to accomplish some everyday tasks that are particular to Argo data, ranging from downloading data and finding subsets to handling quality control and producing a variety of diagnostic plots. The benefits of the R environment are sketched in the examples, and also in some notes on the future of the *argoFloats* package.

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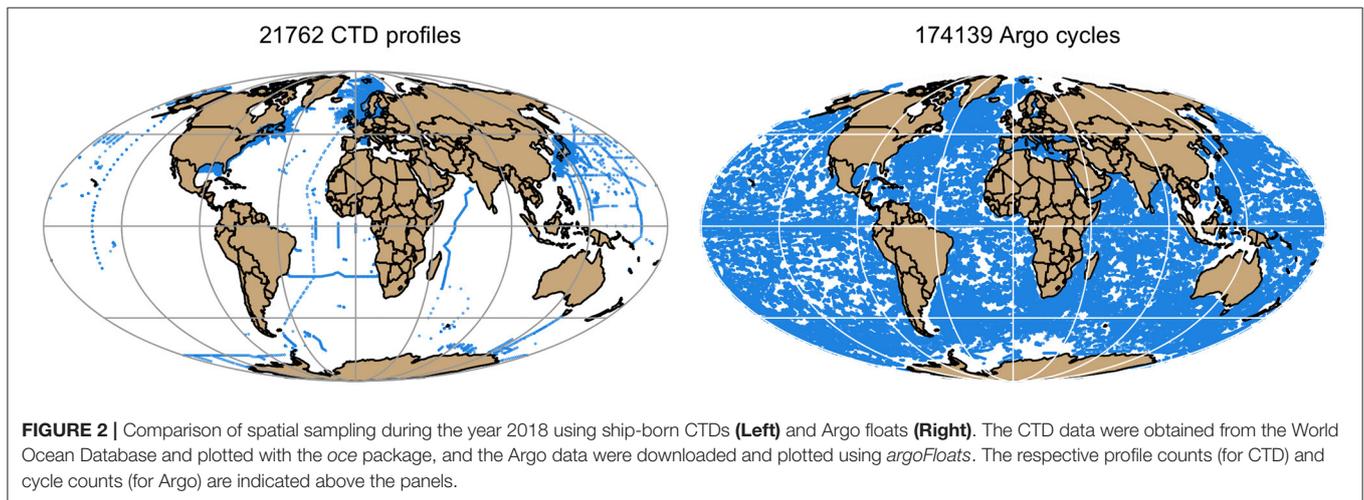
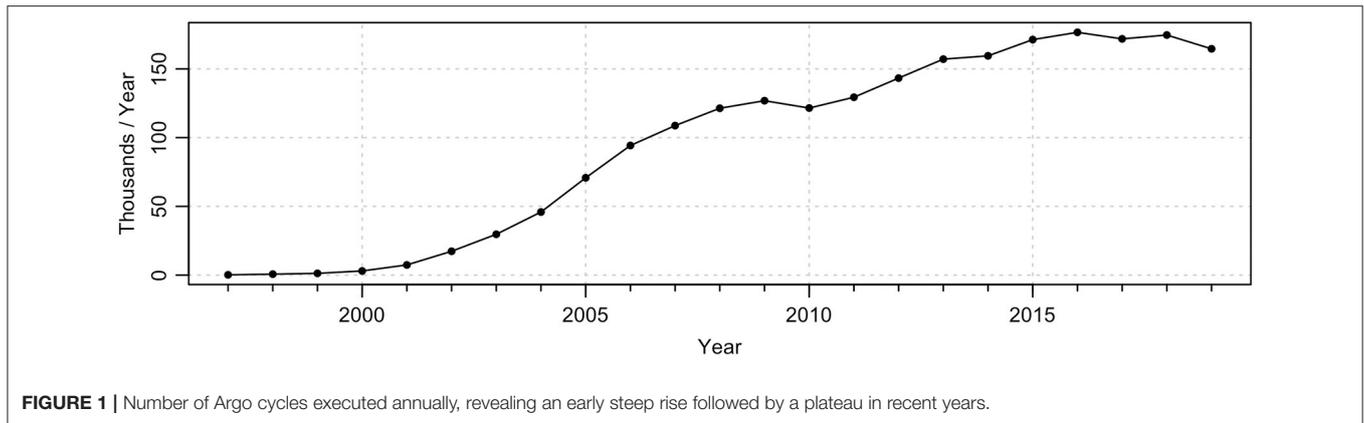
1. THE ARGO PROGRAM

The ocean is not a uniform, static fluid. Rather, its properties vary with both space and time, and these variations are important not just for the ocean itself, but also for ocean-atmosphere interactions. For this reason, measuring variations of seawater properties and currents is a critical prerequisite to understanding and predicting the ocean and its place in the climate system.

Sampling the ocean with ships has proved to be somewhat problematic. Despite the high accuracy of ship-based measurements, the spatial and temporal coverage is limited, with large areas remaining unexamined for decades at a time. At particular isolated locations, the temporal issue is addressed well by moorings. However, traditional moorings provide no data until they are recovered, and so moorings are of little utility in data-assimilative modeling efforts. Satellite imagery provides another alternative to ships, providing good geographical and temporal resolution. However, sensors aboard satellites provide information mainly about surface properties, yielding little direct information about the underlying waters.

These and other limitations of ships, moorings, and satellites have been addressed by the Argo Program of drifting profiling floats, which was initiated in 1999 (see e.g., Roemmich et al., 2009). Argo floats can control their depth by altering their buoyancy, and this is key to their utility. The usual protocol is for a float to remain at a parking depth that is 1 km below the surface (or less, depending on water depth) for approximately 9 days. Then the buoyancy is reduced so that the float descends to 2 km (water depth permitting), after which buoyancy is increased, causing the float to ascend to the surface. The drift-profile pairs are a component of what are called “cycles” in Argo nomenclature.

Argo floats are typically deployed from ships and thereafter drift freely for about 4 years (Carval et al., 2019), making approximately 150 ocean profiles. During those profiles, instruments record pressure, temperature, and electrical conductivity (through which salinity is computed), with the optional addition of other quantities to be described below. These data, along with location inferred



by GPS, are transmitted by the Argos, Iridium, or Orbcomm communication systems to receiving stations (Schmid et al., 2007). (Other, less precise, positioning systems were used in past years.) Thus, Argo floats provide profiling data at the transmitting sites, and an analysis of those site locations permits inferences about currents at the parking depths (Ollitrault et al., 2013).

The original Argo Program (now called the “Core” Program) was extended to address the evolving needs of the research community, forming what is now known as the biogeochemical (“BGC”) Argo Program, which began by deploying optical and oxygen sensors on Argo floats (Roemmich et al., 2019). Today, BGC-Argo floats may carry additional sensors including oxygen, pH, nitrate, downward irradiance, chlorophyll fluorescence, and optical backscattering (Bittig et al., 2019), providing insight about biogeochemical processes in the upper 2 km of the ocean. The BGC initiative was then followed by the “Deep” Argo Program, with floats descending as far as 6 km below the surface, starting with a pilot phase in 2014 (Gasparin et al., 2020). As **Figure 1** shows, there has been a marked increase in Argo sampling since the onset of the program, with a plateau in recent years. As of November 2020, over 16000 Core Argo floats had been deployed,

along with over 1400 BGC floats and over 100 Deep floats (see Argo (2020) for notes on data availability).

By virtue of the large number of floats and the short time between their profiles, the Argo Program provides a valuable supplement to traditional ship-based Conductivity Temperature Depth (“CTD”) instruments. In 2018, for example, there were 8 times as many Argo profiles as there were ship-based CTD profiles recorded in the World Ocean Database (see Boyer et al. (2018) for an introduction to this database). However, this is an underestimate of the significance of the Argo Program, because the ship-based CTD profiles tend to be acquired only in selected regions. This is illustrated in **Figure 2**, which reveals dense Argo sampling in large expanses of the ocean that received little ship coverage. (Although the Arctic is presently sampled poorly by both methods, efforts are underway to develop Argo floats suitable for the Arctic; see e.g., Nguyen et al. (2020) for a discussion.)

The dense spatio-temporal sampling made available by the Argo Program has not gone unnoticed in the scientific community. Increasingly, Argo specialists are being joined by general oceanographers and climate scientists, who see the Argo Program as providing just one of many datasets that they need

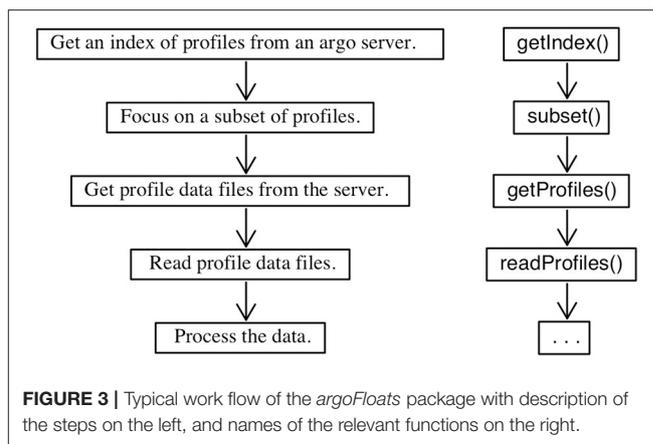
to deal with. This opens up a need for new tools for analyzing Argo data both as a particular focus, for example, the Argovis (Tucker et al., 2020) and Euro-Argo fleet monitor¹ web systems, and the *argopy* Python package (Maze and Balem, 2020), and as a subcomponent of more expansive research programs that employ a spectrum of measurement technologies. In the latter category are analysts who may need more than the standardized plots and analyses that tend to be offered by online Argo tools, particularly when it comes to integrating diverse datasets and performing specialized analyses. These analysts are among those for whom the *argoFloats* package was designed.

2. THE ARGOFLOATS PACKAGE

Increasingly, oceanographers are relying on the R language (R Core Team, 2020) for their data analysis. There are five main reasons for this. First, R offers a comfortable interactive environment, supported by easy linkage with compiled languages for speed and with other interpreted languages, such as Python, for convenience. Second, R provides a vast and unrivaled suite of statistical functions, supported with detailed documentation provided within R itself and in dozens of textbooks. Third, R packages are tested stringently, both when they are first accepted to the system and also at regular intervals thereafter, with the testing being carried out across co-dependent packages, on multiple versions of R and on multiple computing systems. Fourth, R is an inherently cross-disciplinary tool, frequently used by chemical and biological oceanographers. And, fifth, the *oce* package supports many aspects of oceanographic analysis, with specialized functions for computing seawater properties, for reading many native instrument formats, and for creating specialized graphical representations that meet oceanographic conventions. See Kelley and Richards (2020) for more on *oce* and Kelley (2018) for more details of general oceanographic analysis with R.

Although the *oce* package provides tools for dealing with Argo data, it does not identify detailed paths to datasets, nor support the integration of data spread across several downloaded files. This motivated the development of another R package, named *argoFloats*. The prime goal of *argoFloats* is to eliminate the gap between the Argo data and the end user. It allows the user to choose from multiple data sources, to download and cache Argo data files, and to sift through those downloaded data based on float ID, time, geography, variable, profile, etc. It also has tools for producing a range of practical graphical representations, including temperature-salinity diagrams and profile plots, and for handling Quality Control (“QC”) information, as will be highlighted in the following sections.

It is worth noting that *argoFloats* was designed from the start to be suitable for users with widely-ranging coding expertise. For this reason, a number of learning tools were created alongside the package. These include (1) detailed documentation on the functions and datasets within the package, (2) vignettes that sketch using the package in practical applications, (3) a developer website (Kelley et al., 2020a) that has tools for reporting bugs,



requesting features, and viewing changes in the code, (4) a user website (Kelley et al., 2020b) that requires less expertise than the developer website, and (5) Youtube tutorials (links to which are provided in the websites) that offer step-by-step instruction on using the package.

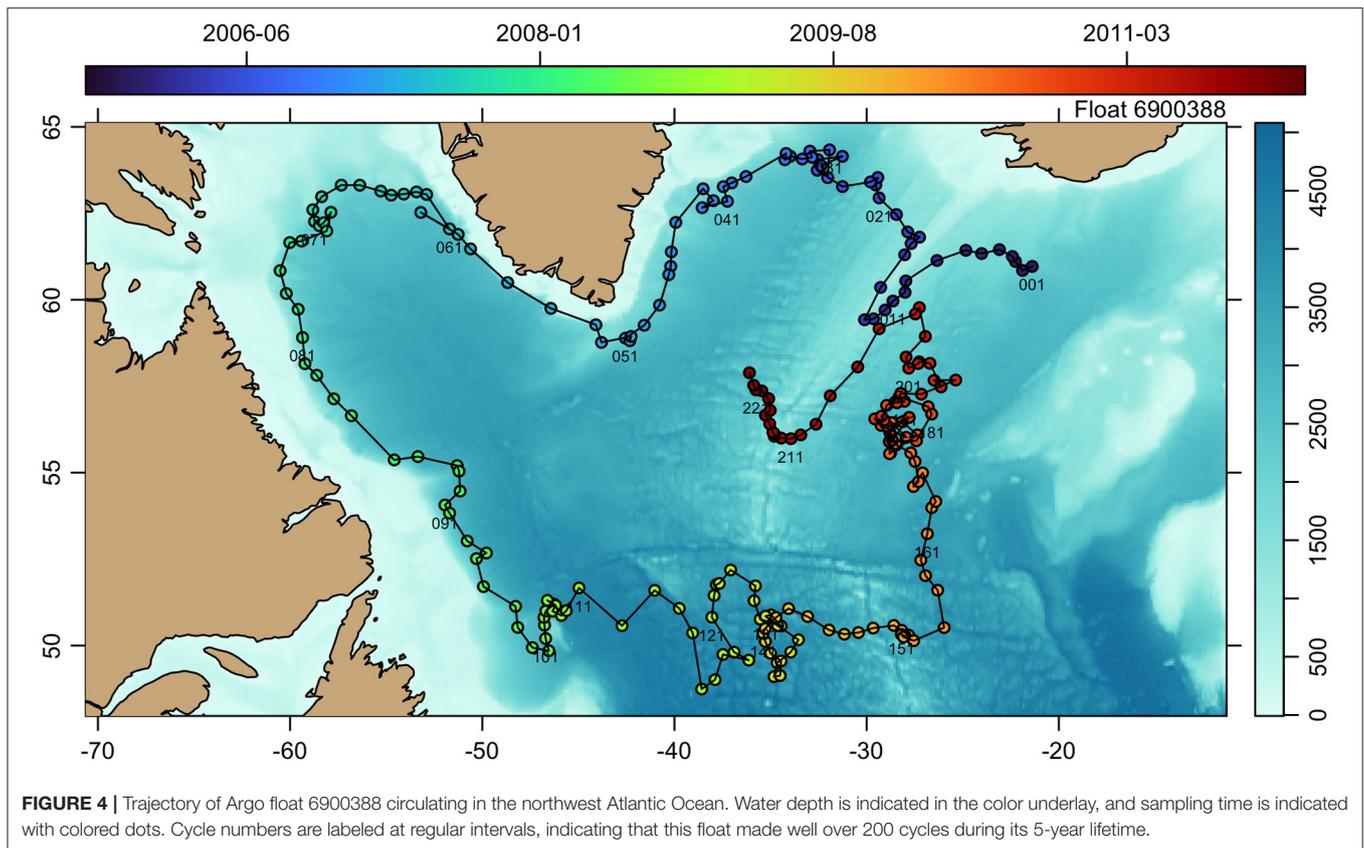
Figure 3 shows the basic steps involved in working with the *argoFloats* package. The procedure normally starts with a call to the `getIndex()` function, which either acquires an index of float files from an Argo server, or gets a pointer to a locally cached index, depending on the age of such a cached index. The default is to limit downloads to once per day, but this can be changed by using an optional argument in the `getIndex()` call. The main item in these index files is a URL fragment that tells where to get the netCDF data files containing float profile data. There are three types of index files that can be acquired by `getIndex()`: one that holds Core and Deep data, a second that holds BGC data, and a third that holds a combination (“synthetic,” in Argo nomenclature) of the first two. These are specified by one of the `getIndex()` arguments, with Core data being the default. Other arguments control the server that will be queried to get the index, the name of a local directory in which to store downloads, and parameters controlling whether the function ought to act silently. Reasonable defaults are set for all of these, e.g., if a server is not specified, `getIndex()` tries the Ifremer server², switching to the USGODAE server³ if the former fails to respond.

Once an index has been downloaded, the next step is usually to subset it according to some criterion. This is accomplished by using a function called `subset()` that specializes a generic R function. (The scheme of specializing generic functions is one of the reasons for the popularity of R, since it makes it easy to guess how to work with new types of data in familiar ways.) The `subset()` operation can be done in many different ways. These include isolating data by float ID, by cycle number, by time, by location, by institution, or by Deep category, etc. It is common to subset sequentially, often performing statistical analyses or producing graphs of the data at each step. To help an analyst keep track of the winnowing that occurs with each `subset()` call, the

²ftp.ifremer.fr.

³usgodae.org.

¹<https://fleetmonitoring.euro-argo.eu/dashboard>.



function prints a note on the fraction of data that were retained. It should be noted that finding subsets is a fast operation, because it does not involve file downloads.

Once a subset of interest has been specified, the next step is to download the netCDF files containing the data of interest, using `getProfiles()`. This function takes as primary input the return value of either `getIndex()` or `subset()`. Since the file sizes are of order 100 KB, this step can be slow if many files are needed. For this reason, `getProfiles()` follows the pattern set by `getIndex()`, caching downloaded files, so that future calls can use local files if they meet an age criterion. Therefore, `getProfiles()` tends to be a fast operation, except at the start of a new project.

The next step, accomplished with `readProfiles()`, is to read the local data. In most cases, this function uses the output of `getProfiles()`, but it is also possible to specify netCDF file names, skipping the previous steps.

Once data have been read, the user has an object in the R session that can be analyzed in a wide variety of ways. Generic functions are provided for some common tasks, with the prime components being as follows.

1. The `summary()` generic function provides an overview of the object.
2. The `[[` generic function retrieves data from within an *argoFloats* object. For example, if *A* is an object returned by `readProfiles()`, then `A[["temperature"]]` returns

an R list object with one element for each profile stored in *A*. At this stage, the user can use standard R methods to perform a profile-by-profile analysis, to string the data together to get an overall view, etc.

3. The `plot()` generic function creates a variety of graphical displays of the data, e.g., maps of the positions of the Argo float(s), temperature-salinity diagrams, time-series plots of QC flags and data, and profile plots. Simple calls to `plot()` created most of the figures that follow in this paper, although some of them are further modified by adding features (extracted with `[[]]` using standard R graphical functions for drawing symbols, lines, polygons, text, images, etc.

Further to the last point, it is worth noting that the use of `[[]` to extract data from *argoFloats* objects gives the user the freedom to use any of the statistical and other functions provided by R and its many thousands of contributed packages. Thus, although it might seem to be simple, the `[[]` function is actually a central contributor to the power and scope of *argoFloats*.

3. ARGOFLOATS WORKFLOW EXAMPLES

3.1. Analysis of Float Trajectories

Figure 4 shows the path of the float 6900388 (that is, the float with World Meteorological Organization number 6900388) in the North Atlantic. Its construction followed the pattern outlined in Figure 3, although there was no need for the `getProfiles()`

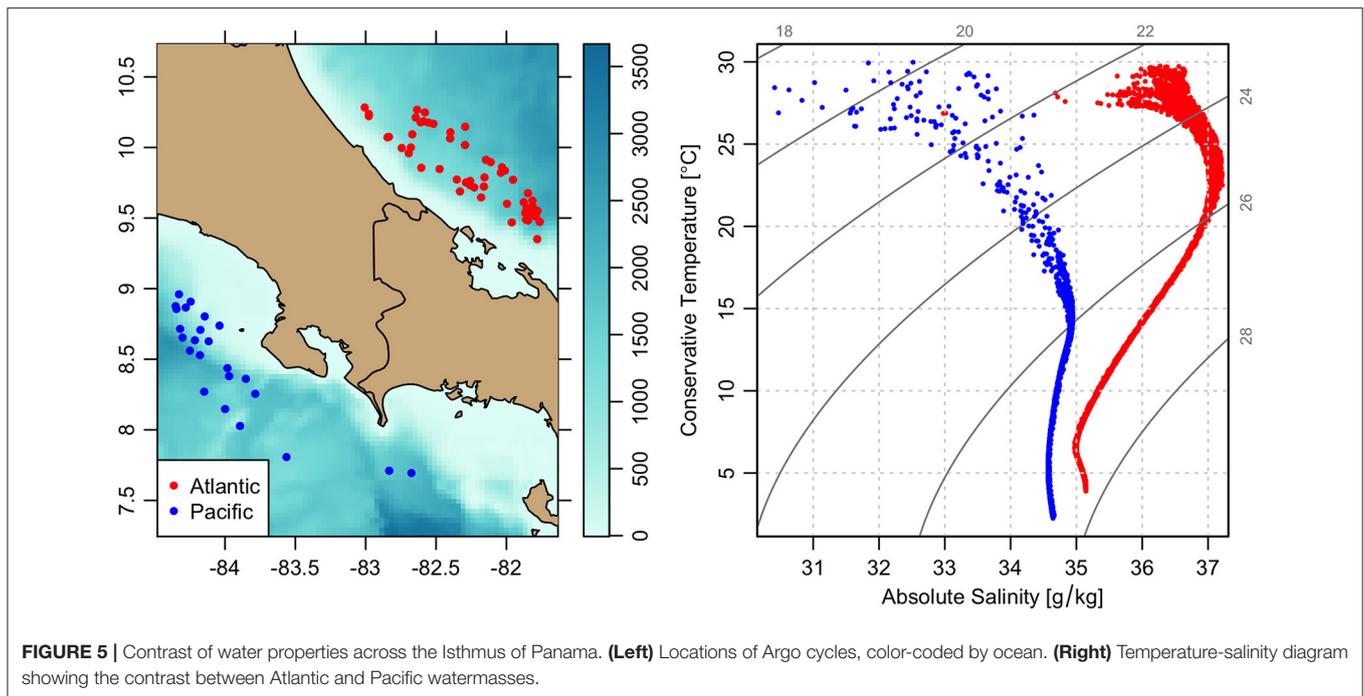


FIGURE 5 | Contrast of water properties across the Isthmus of Panama. **(Left)** Locations of Argo cycles, color-coded by ocean. **(Right)** Temperature-salinity diagram showing the contrast between Atlantic and Pacific watermasses.

or `readProfiles()` stage because Argo index files contain float sampling times and locations, and together these things are all that is required to construct **Figure 4**. A simpler version of the plot, skipping the indication of time, is obtained with

```
library(argoFloats)
index1 <- getIndex()
index2 <- subset(index1, ID="6900388")
plot(index2, bathymetry=TRUE)
```

and readers who run this code will find that the `subset()` call reveals that there are 223 cycles for this float. Two files will be downloaded in the process, one for the Argo index, and another (from a NOAA server) for a bathymetry file tailored to this geographical view. In many applications, the user will already have a local bathymetry file, so the second argument to `plot()` can be altered to use that, speeding up the process.

The main difference between the results of the preceding four-line operation and **Figure 4** is the use of colored symbols to indicate float sampling times and the labeling of cycle numbers at some locations. The relevant information may be obtained with

```
time <- index2[["time"]]
```

and similar steps, after which standard R functions (including `colormap()` and `drawPalette()` from the *oce* package) may be used to add other elements of **Figure 4**. This illustrates how *argoFloats* provide basic functionality for common tasks, while also making it easy for users to extend that functionality to meet their own needs.

It would be simple to extend this with the `geodXy()` function in *oce*, to learn more about ocean velocities at the float parking depth. Some smoothing or regression analysis might be

required to achieve the desired results, and readers who are new to R may be pleased to learn how easy it is to carry out such analyses with standard R functions.

This first example has dealt only with index data, i.e., it has skipped the third and fourth steps in **Figure 3**. Many analyses will be similar to this (see e.g., the later section about a GUI application), but it is also important to illustrate how to download Argo netCDF data files with `getProfiles()` and how to read those data files with `readProfiles()`, as will be done in the next section.

3.2. Watermass Analysis

Temperature-salinity diagrams are a useful tool for watermass analysis, and a common first step is to prepare such diagrams showing water samples obtained in different areas. **Figure 5** is a case in point. The first step in its construction was to use `subset()` to isolate a circle within a 150 km radius of Panama. The region was then subdivided into polygons separating the Atlantic and Pacific waters. The polygons were determined using `plot(..., which="map")` to get a map of the region, then using `locator()` to determine vertices on these selected polygons. (Note that `subset()` can choose data by ocean basin, but this is not accurate in this region, evidently owing to the limited resolution of the polygons used by the Argo processing system to designate ocean basins.) The fact that none of these steps takes more than a minute is an illustration of why people are drawn to R for interactive work. It is also worth noting that R makes it easy to follow such exploratory steps with algorithmic schemes, e.g., defining subsets that trace bathymetric contours or the boundaries of marine protected areas, or that establish Argo-based virtual moorings or ocean transit sections.

The right-hand panel of **Figure 5** was made with `plot(argos, which="TS", col=colBasin)`, where `argos` holds data obtained by applying `readProfiles()` to the output of `getProfiles()` for the relevant geographical regions and `colBasin` was defined to colorize by region. The resultant temperature-salinity diagram should make sense to readers with oceanographic experience, who are aware of a large contrast between Atlantic and Pacific watermass types. However, readers who try the procedure summarized above will find that there are many outliers that make no physical sense. This is because *argoFloats* works with the data as specified in the official data files, and these data are subject to error. As with many oceanographic datasets, Argo data are typically accompanied by QC flags. Using `applyQC()` on an `argo` object containing profiles turns questionable data into NA (missing) values, so they do not appear on the plot. This step was taken in the creation of **Figure 5**. The *argoFloats* package has several tools for the handling of QC flags, and it is important that users become familiar with them, because the official QC flags are not always entirely accurate.

3.3. Quality Control Analysis

Core, BGC, and Deep Argo data all undergo testing to ensure the data found at the Data Assembly Centers (“DACs”) are reasonably accurate. This is done on both “real-time” and “delayed” data. As is explained in the Argo User’s Manual (Carval et al., 2019), real-time measurements are assigned a QC flag within a 24–48 h time frame, and delayed-mode are reexamined within 1–2 years by scientists who apply additional procedures to check the quality. In addition to the designation of QC flags, some data sets may be changed in recognition of the QC analysis or in light of improvements to instrument calibrations, etc., with the results being referred to as “adjusted” data.

It is important to note that even with vigorous testing procedures, QC flags cannot be considered perfect. As described in section 1.3 of the Argo User’s Manual (Carval et al., 2019), the user assumes all risk using Argo data and, as will be demonstrated presently, careful analysts should consider applying their own QC checks to their data.

A three-step process can help with such work. First, use `plot(..., which="QC")` to plot an overview of the QC flags for the parameters of interest. In addition to showing QC flags, this function can also show the `dataStateIndicator` designation, which reveals the level of QC processing performed on individual float cycles. Second, use `applyQC()` to replace suspicious data with NA values, so they will not appear in plots or be considered in calculations, and create some diagnostic plots (e.g., temperature-salinity diagrams, profiles of temperature, salinity, and density) to assess whether `applyQC()` failed to remove some questionable data. Third, if there are such questionable data, use `showQCTests()` to get a summary of the QC tests (if any) that were performed on the data. (Perhaps surprisingly, different QC procedures are sometimes applied to different cycles for a given float.) The first and third of these steps might be skipped for quick work, but they should be carried out for in-depth analysis.

For example, **Figure 6** shows a QC plot for float 1901584. cursory examination indicates that, although the float reported data for nearly 5 years, the quality of those data declined seriously in its final 2 years. Another variant of the plot (not shown) reveals that the “data state indicator” was 2B for each profile made with this float, which according to Reference Table 6 of the Argo User’s Manual (Carval et al., 2019) indicates that automated testing has been done, without additional scrutiny by scientists.

To this end, **Figure 7** shows the impact of removing the “bad” data from this float using `applyQC()`. It will be obvious to anyone with oceanographic experience that the uncorrected data (left-hand panel) are heavily polluted with erroneous values. Indeed, the water properties are so far from typical oceanic values that the `oce` function that produces this plot does not even attempt to draw isopycnal curves across the whole panel. The coloring in this figure indicates that the wildest outliers have been flagged as questionable. The right-hand panel, which is cleared of flagged data, is more reasonable. However, and importantly, it also contains some points that are far from the main data cloud, and that would likely catch the attention of a experienced analyst.

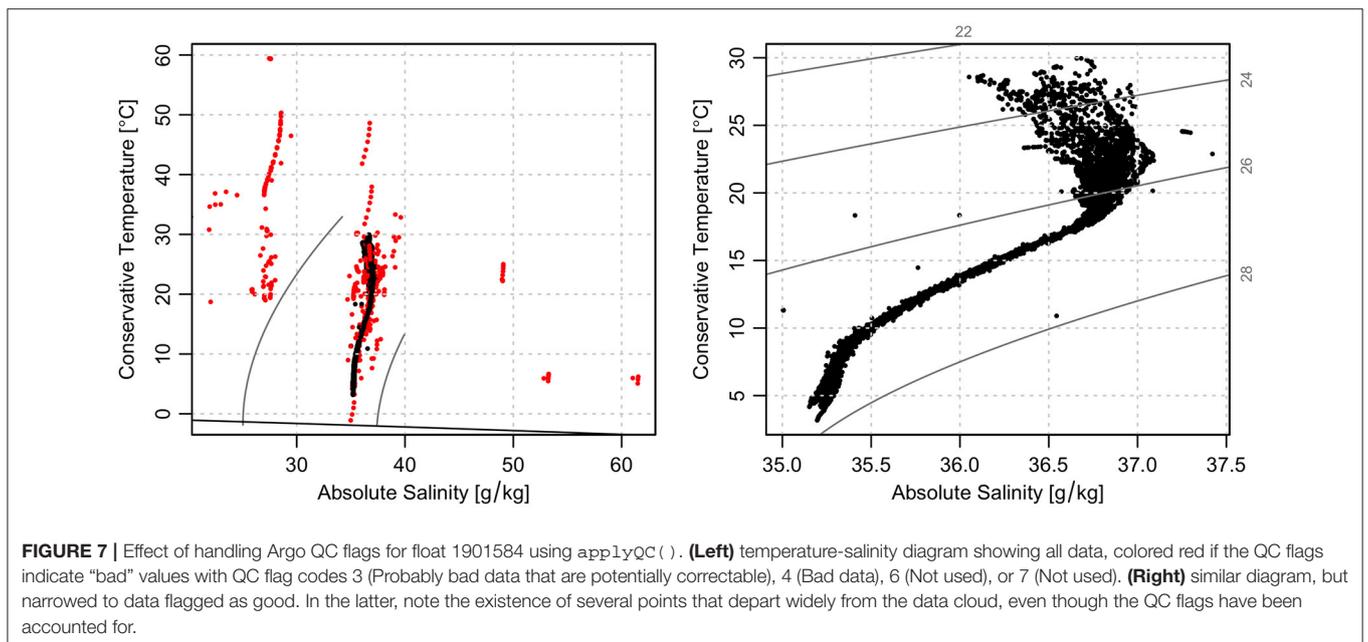
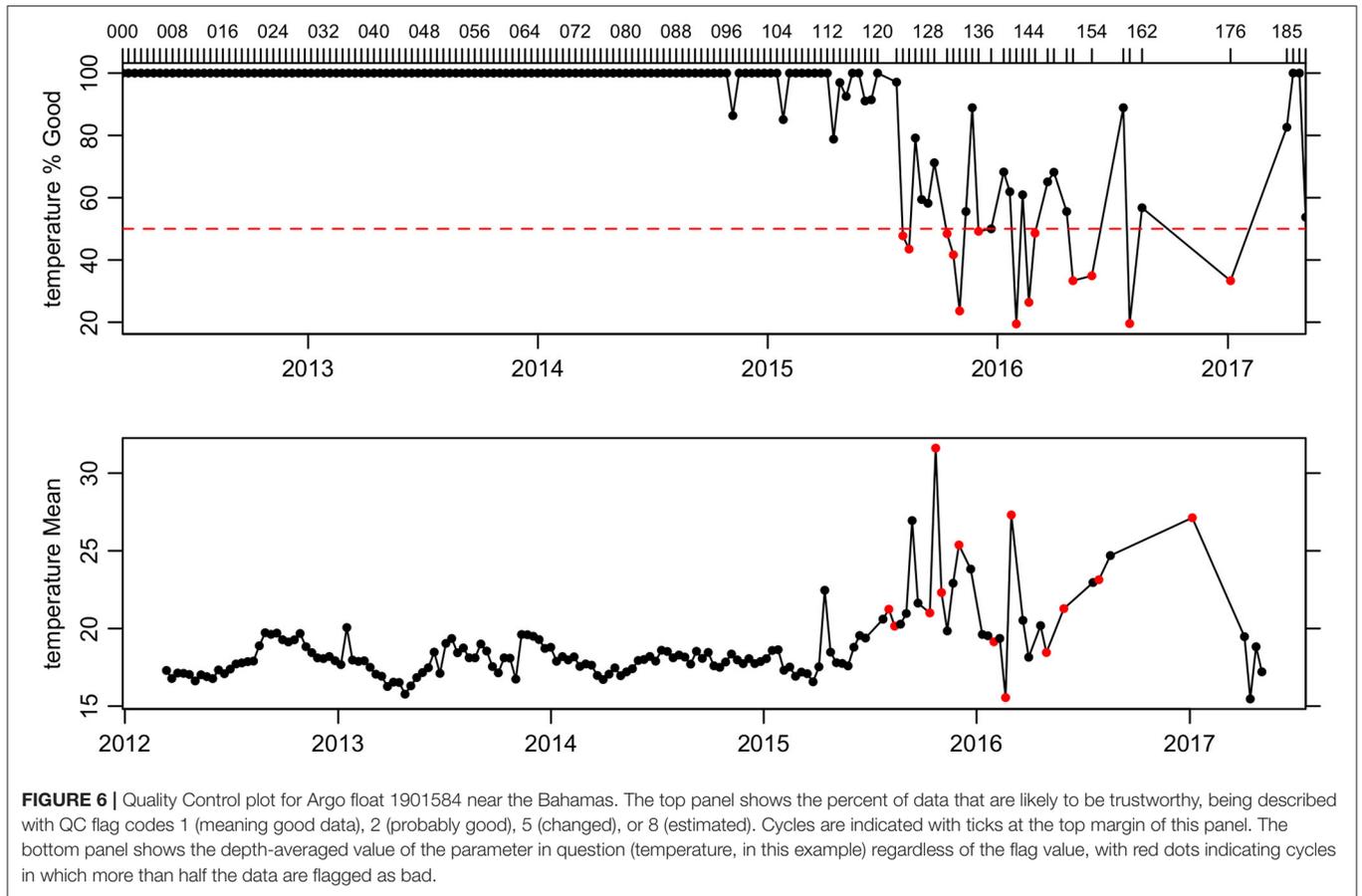
One way to investigate such outliers on a temperature-salinity diagram is to consider the dependence of the seawater property called “spiciness,” which is in some sense orthogonal to density on such a diagram (Flament, 2002; McDougall and Krzysik, 2015). **Figure 8** shows the results of such an analysis, in which a smoothing cubic spline was used to summarize the dependence of spiciness on potential density anomaly. The standard deviation δ of the difference between data and spline was computed, and then points that departed from the spline by more than 5δ were colored. This seems to identify outliers well, as can be seen when the data are redrawn in temperature-salinity space. A reasonable next step might be to compute density-dependent deviation, to account for the (expected) thickening of the data cloud for waters near the surface. There again, the standard R functions will greatly reduce the analysis effort.

Having identified a set of outlying points, either with an algorithm as in **Figure 8** or by any other means, it is easy to determine which profiles contain those points, and then to use `showQCTests()` to learn which QC tests had been performed in each case. This can provide useful clues as to why suspicious data made their way onto the Argo data servers without being flagged. Another good practice is to produce profile plots for each case, highlighting the questionable points as a way to diagnose possible problems with existing QC procedures, and to help frame ideas for new tests, such as our new spiciness test.

3.4. Using Adjusted Data

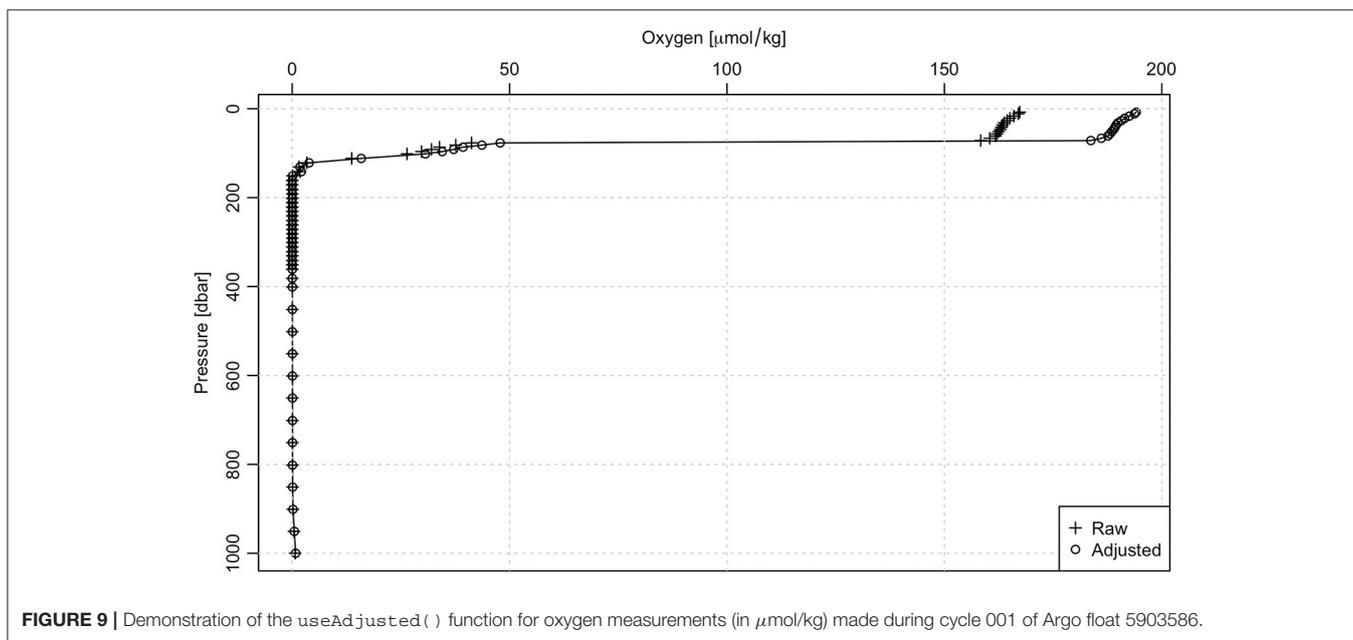
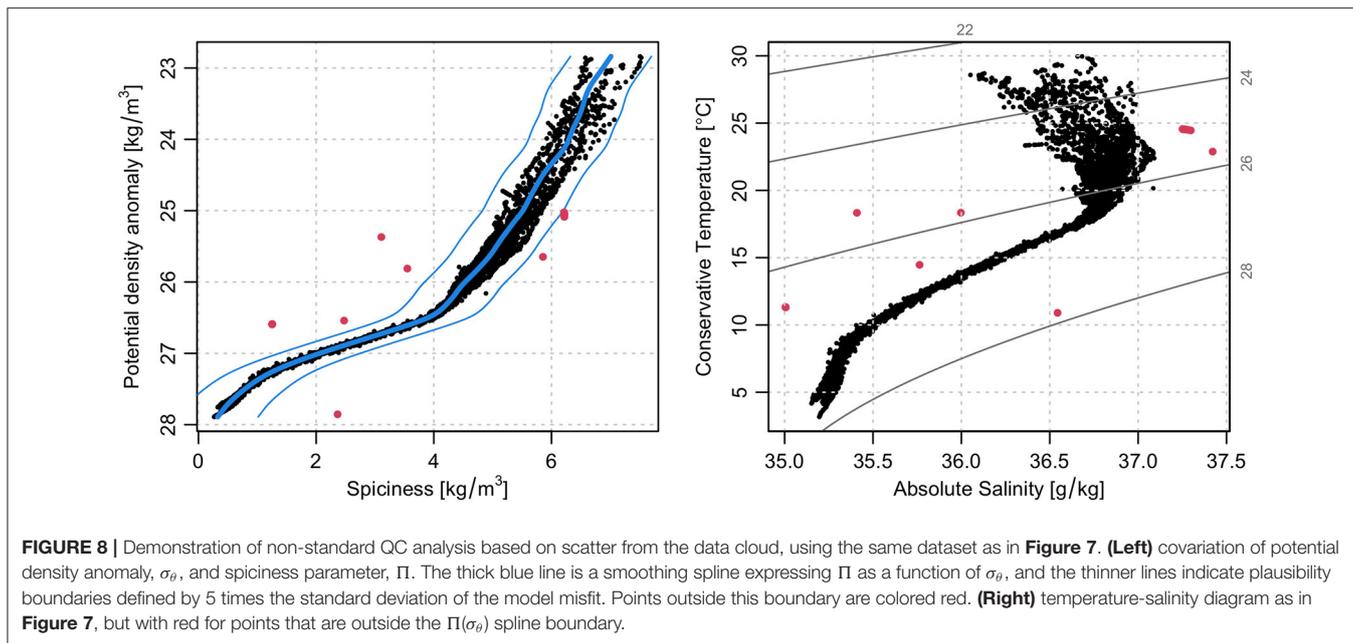
Some data sets undergo adjustments that are made in recognition of the QC analysis or improved calibration, with the adjusted values being stored within data files alongside the raw (original) values. Adjustments tend to be more common with BGC data than with Core data, perhaps owing to issues relating to sensor maturity (Thierry et al., 2018).

The *argoFloats* function named `useAdjusted()` provides a convenient way of dealing with such data. It works by optionally copying adjusted data into the locations that normally store raw data. This causes subsequent calls to `plot` and `[[` to focus



on the adjusted data, as opposed to the raw data. By default, `useAdjusted()` carries out replacement for all fields that have adjusted values. However, the function has an optional argument

that causes it to replace only adjusted- and delayed-mode data, skipping over real-time data. This option can be useful, because real-time adjusted data are always equal to missing



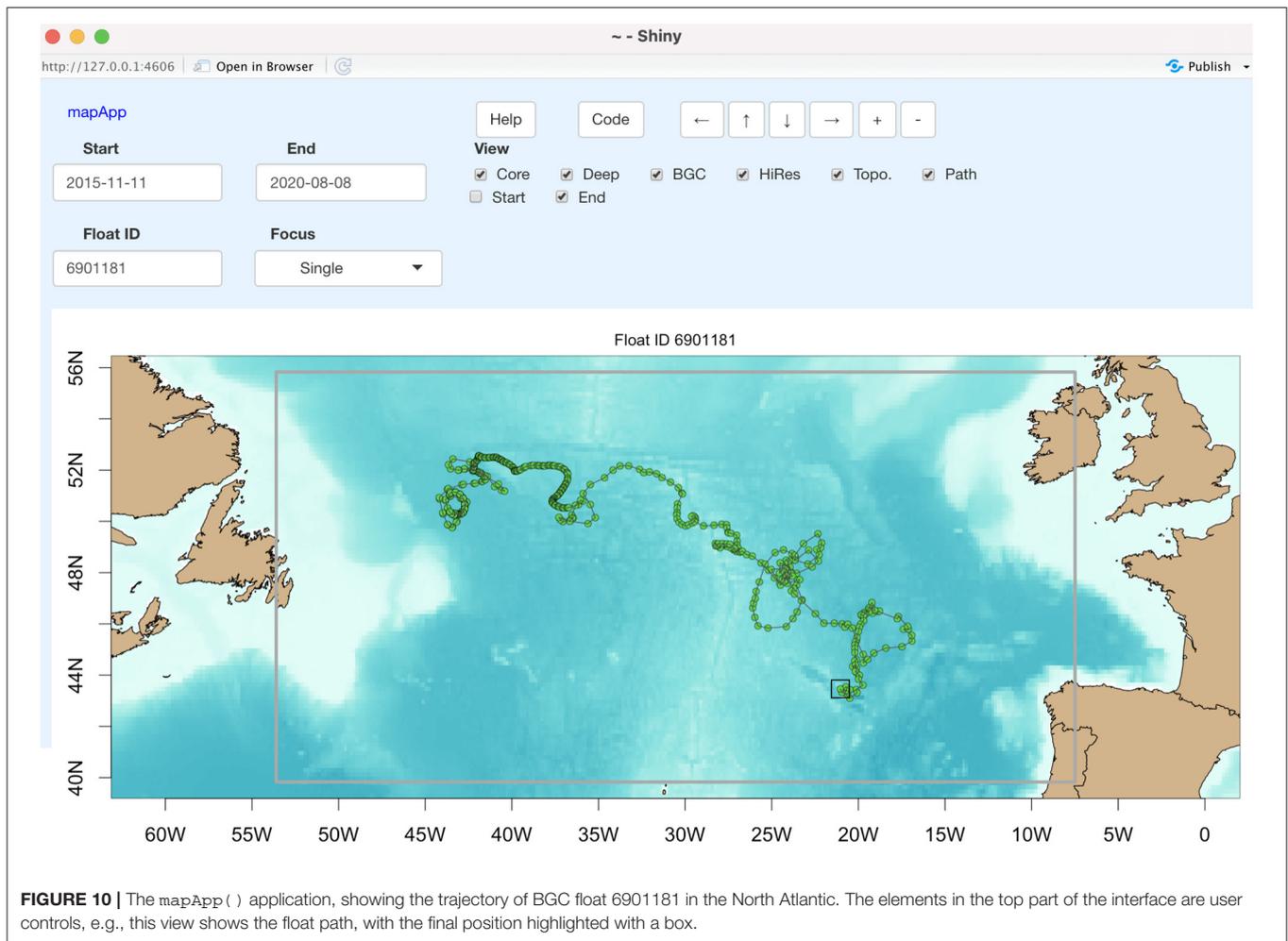
values, leaving spatial/temporal gaps that raw data can help to fill in.

An example of using adjusted values is provided in **Figure 9**, which displays raw and adjusted oxygen profiles for cycle 001 of float 5903586, which sampled for about 2.5 years along the coast of Saudi Arabia. The diagram was made in two steps. First, raw data were read in and plotted with the *argoFloats* version of `plot()`, supplied with arguments indicating to show a profile of oxygen. Second, a new object was created with `adjusted <- useAdjusted(raw)`, so that `[[` would return adjusted values. Then, the adjusted pressure and oxygen concentration were accessed with `[`, and

plotted on the diagram, along with a legend, using standard R function calls. As in the preceding temperature-salinity example, it is worth noting that *argoFloats* is designed to provide only basic plots, with the user relying on standard R functions to add extra features. This eases the burden on users who are familiar with R, and helps to teach others how to use R for general tasks.

4. INTERACTIVE FLOAT MAPPING TOOL

The `mapApp()` function launches a GUI-based application for examining float locations, using the powerful R-shiny system



(Chang, 2020). Initially, this shows a world view, with dots representing the locations of Argo float profiles within a selected time interval. Different colors are used for Core, BGC, and Deep profiles.

Multiple GUI elements make it easy to explore the data. Buttons control which float styles to display, whether to display bathymetry, whether to use low- or high-resolution coastlines, whether to draw line segments joining successive float locations, whether to draw starting and ending points on float trajectories, and so forth. There are also buttons to move the focus view around the earth, and to control the size of the display area. Text-entry fields are used to select a time interval to display, and there is a field in which the user can enter the ID of a particular float of interest. In addition, the system monitors the mouse location, with a click-slide action causing zooming to the indicated region, a hovering action causing a display of information about the nearest float profile, and a double-clicking action causing a float ID to be entered into the ID selection box. There is a simple way to switch from a multi-float view in a given time range to a view of the historical trajectory of a selected float, which can be quite helpful in finding datasets of interest for further exploration.

Other controls permit other actions, all of which are both documented and reasonably self-evident. Of particular note is a button that displays the `argoFloats` code that would produce the indicated view, starting from a `getIndex()` call, followed by `subset()` calls to isolate the data in question, and followed by hints on further actions that the user might undertake, including plots similar to those shown in previous sections of this document.

For example, **Figure 10** shows a view of BGC float 6901181. Entering that float number in the float-ID box will reveal that this float was deployed in November 2015, near the western end of the trajectory, at the 43.6W and 51.0N. The black square by one of the points toward the European continent indicates the latest position of the float, at 20.9W and 43.3N. The complexity of the ocean circulation is revealed clearly in the complex shape of the trajectory between these two locations. Readers interested in exploring this float in more detail might find it helpful to start by using `mapApp()` to reproduce **Figure 10**, after which clicking on the `Code` button will reveal the `argoFloats` function calls needed to isolate the data, and, for example, plot a temperature-salinity diagram.

5. THE FUTURE OF ARGOFLOATS

As sketched above, *argoFloats* already provides a variety of tools for advancing Argo data analysis. However, it is still in a phase of active development, during which the developers are responding to community needs. The core functions, `getIndex()`, `subset()`, and `[]`, have proven to be suitable for everyday work, and are unlikely to change greatly. The same cannot be said of `plot()`, which is likely to continue to gain significant new features soon, to accommodate the fairly wide variety of oceanographic plot styles. Similarly, there are plans to complement the `mapApp()` tool with other tools that provide more in-depth analysis of Argo data.

From the start, *argoFloats* has taken a practical approach to most problems. Newcomers to Argo data tend to find it difficult to download data using FTP tools or the server websites, so `getIndex()` was created to help in this task. Isolation of particular floats for a given purpose is also challenging, and so `subset()` was created. Reading the files that store Argo profile data demands skills not just in reading `netCDF` but also in linking the actual data elements with their associated metadata, such as QC flags and units. Users are relieved of such burdens by `readProfiles()`, which in itself relies on lower-level functions provided by the *oce* package. Similarly, *oce* is relied upon for the various oceanography-specific operations such as the handling of QC flags, computation of Absolute Salinity and Conservative Temperature from measured properties, the construction of temperature-salinity diagrams, etc.

At this time, *argoFloats* handles many practical tasks that are required by a research team of university and government scientists. While this is a good start, we feel certain that the package will benefit from a wider base of users and developers. For this reason, we are employing an open-source model for both coding and collaboration, and we hope this paper will get others interested in this community project.

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DATA AVAILABILITY STATEMENT

The datasets analyzed for this study were downloaded in November 2020 from the Argo servers <ftp.ifremer.fr> and <ftp://usgodae.org/pub/outgoing/argo>.

AUTHOR CONTRIBUTIONS

CR conceived of the idea and secured the initial support for the work and participated in discussions and planning. DK and JH wrote the majority of the code in the package. DK and CR shared in salary support for JH. DK and JH wrote the text. CR helped to edit it. All authors contributed to the article and approved the submitted version.

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