

# Software to enable ocean discoveries: a case study with ICESat-2 and Argo

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## Abstract

Increased anthropogenic stressors (e.g., warming, acidification, wildfires and other extreme events) present complex observational challenges for Earth science, and no one sensor can ‘do it all.’ While many remote sensing technologies are available at present, scientific disciplines are often trained to use only a specific subset, greatly limiting scientific advancements. Here we present open-source software (‘icepyx’) that lowers the barrier for entry for two remote platforms offering vertically-resolved information about the ocean’s subsurface: ICESat-2 (Ice, Cloud, and land Elevation Satellite 2) and Argo floats. icepyx provides object-oriented code for querying and downloading ICESat-2 and Argo data within a single analysis workflow. icepyx natively handles ICESat-2 data access and read-in; here we introduce the Query, Unify, Explore SpatioTemporal (QUEST) module as a framework for adapting icepyx to easily access and ingest other datasets and present Argo data as the initial use case. Seamless retrieval of coincident data from ICESat-2 and Argo enables improved targeted and exploratory studies across the cryosphere and open ocean realms. We close with recommendations for future work, a discussion of the value of open science, relevance of our work to upcoming satellite missions, and an invitation to join our programming community.

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# 1 **Software to enable ocean discoveries: a case study with ICESat-2 and Argo**

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## 12 13 **Key Points**

- 14
- 15 • We present open source-software that allows easy access to ICESat-2 and Argo data
- 16 • This software enables observations of vertical profiles in the ocean
- 17 • Additional data streams are planned with community input

18  
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20 extreme events) present complex observational challenges for Earth science, and no one sensor  
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25 ICESat-2 (Ice, Cloud, and land Elevation Satellite 2) and Argo floats. icepyx provides object-  
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27 workflow. icepyx natively handles ICESat-2 data access and read-in; here we introduce the  
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30 retrieval of coincident data from ICESat-2 and Argo enables improved targeted and exploratory  
31 studies across the cryosphere and open ocean realms. We close with recommendations for future  
32 work, a discussion of the value of open science, relevance of our work to upcoming satellite  
33 missions, and an invitation to join our programming community.

34  
35 **Plain Language Summary** Earth is changing rapidly due to human actions, and many different  
36 observations are needed to meet the challenges of the 21<sup>st</sup> century. Scientists are often trained to  
37 only use a particular subset of tools, but there are other relevant tools that go unused. Here we  
38 provide software (QUEST, within icepyx) to bring together two sensors that are commonly  
39 associated with two different communities. The ICESat-2 satellite was launched primarily to  
40 improve understanding of icy regions, and Argo floats were invented to overcome sampling gaps  
41 in the ocean. Both tools provide up-to-date information about the water column on a global scale.  
42 We wrote software in an open-source language (Python) to ease the access of using these  
43 complex tools and advance scientific discovery for all disciplines while also growing a  
44 community of users. By virtue of the software being open source, anyone can join the  
45 community and make contributions, including to incorporate data from other sources. Ultimately,

46 we hope to grow the community, enabling more scientific discoveries to support societal  
47 solutions.

48

## 49 1. Introduction and background

50

51 Advances in remote sensing technologies across different sectors of Earth science offer a  
52 tremendous opportunity to explore multiple observations over a shared place and time. However,  
53 the historical separation between disciplines, even within earth sciences, presents a substantial  
54 challenge for user access and science implementation. In some cases, scientists trained within a  
55 specific discipline may not even be aware of other relevant data products that are publicly  
56 available for use. Although the oceanography community has made substantial progress in  
57 understanding the marine system with ocean-dedicated satellites starting with the Coastal Zone  
58 Color Scanner (Antoine et al., 1996), these platforms are limited to sunlit, cloud-free conditions,  
59 and limited information about the water column can be obtained. More advancements are  
60 possible by combining technologies intended for ocean work with those that were initially  
61 created for different purposes, ideally enabled by an open-source framework (Hostetler et al,  
62 2018). For example, the recent use of an atmospheric lidar sensor (the Cloud-Aerosol Lidar with  
63 Orthogonal Polarization, CALIOP, on Cloud-Aerosol Lidar and Infrared Pathfinder Satellite  
64 Observations, CALIPSO) in ocean studies led to exciting discoveries, including observing diel  
65 vertically migrating zooplankton from space (Behrenfeld et al., 2019), as well as advances in  
66 understanding that will improve conventional technologies (i.e., a seasonal bias in NASA ocean  
67 color data, Bisson et al., 2021a, 2023).

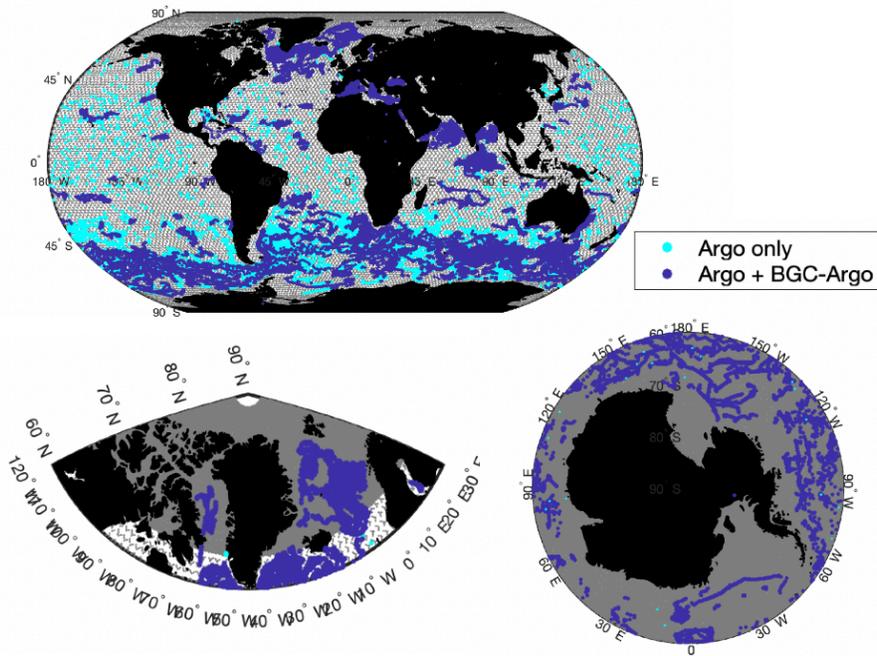
68 Two such technologies that have apparently different purposes yet strong compatibilities  
69 and applications in oceanography are Argo floats (Argo and biogeochemical (BGC), Argo, 2000)  
70 and the Ice Cloud, and land Elevation Satellite-2 (ICESat-2, Markus et al., 2017) mission  
71 launched in 2018. Argo floats move vertically within the water column as they drift in a semi-  
72 lagrangian manner with the currents, primarily offering vertical profiles of temperature, salinity,  
73 and depth. An additional group of Argo floats (BGC) are equipped with biological sensors to  
74 measure chlorophyll concentration, nitrate, oxygen, the particulate backscattering coefficient at  
75 700 nm, and in some cases, photosynthetically active radiation (PAR) and spectral downwelling  
76 irradiance. A portion of Argo floats will transit underneath sea ice (Hague and Vichi, 2021),  
77 capturing precious data not possible using conventional methods, especially from satellites. The  
78 invention and deployment of Argo floats have transformed our understanding of ocean physics  
79 and biology, especially during times and in places inaccessible from ocean color satellite  
80 observations (e.g., wildfires, Tang et al., 2021; under-ice blooms, Horvat et al., 2022). Until  
81 recently, Argo floats were the only tool available to capture the structure of the upper water  
82 column on global scales.

83 In 2018, ICESat-2 was launched with a primary goal of studying polar regions, but it has  
84 technical capabilities to observe terrestrial and ocean ecosystems worldwide. The Advanced  
85 Topographic Laser Altimeter System (ATLAS), the sole instrument onboard ICESat-2 and the  
86 only powerful photon-counting lidar altimeter in orbit, contains a 532 nm laser with a pulse  
87 repetition rate of 10 kHz with three pairs of beams on the ground (Markus et al., 2017). Over the  
88 ocean, ICESat-2 data have been used to generate vertical profiles of particulate backscattering  
89 and light attenuation (Lu et al., 2020, 2021), map bathymetry accurate to ~0.5m (Parrish et al.,  
90 2019), and extract sea ice thickness data for contextualizing under ice phytoplankton phenology  
91 (Bisson and Cael, 2021), the latter of which was accomplished using software described herein.

92 With CALIPSO decommissioned, the only lidar satellite available for ocean observations  
93 presently flying is ICESat-2 (Behrenfeld et al., 2023).

94 Compared to ocean color data, which are typically manageable in aggregate because they  
95 are of relatively small size (available at <https://oceancolor.gsfc.nasa.gov>; note each day of data is  
96 ~1 GB or less), photon data from ICESat-2 are complex, large datasets that cannot be easily  
97 downloaded and stored for local use without substantial manipulation (e.g., just one day of  
98 ICESat-2's ATL03 data product is ~300 GB). While other missions (e.g., MODIS-Aqua,  
99 CALIPSO) have higher-level ocean data products, ICESat-2 ocean products are in development,  
100 and many ocean applications of ICESat-2 rely on lower-level ATL03 photon cloud data to derive  
101 subsurface optical information about the water column. Without open-source, collaborative  
102 software programs and community resource sharing, a substantial amount of prior knowledge is  
103 needed in order to appropriately and efficiently access and use ICESat-2 data for ocean  
104 applications. None of the recent studies using CALIOP for ocean particle and biology studies  
105 have made their code openly available or in an open-source language, limiting the degree to  
106 which satellite lidar analyses in the ocean can be reproduced and proliferated for different needs  
107 (Behrenfeld et al., 2013, 2017, 2019, 2022, Lu et al 2020, 2021, Lacour et al., 2020, Bisson and  
108 Cael, 2021, Bisson et al., 2021a,b, 2023).

109 To enable novel studies of coupled ICESat-2 and ocean data, we introduce an open-  
110 source Python module QUEST, housed and packaged within the icepyx library, a community  
111 and Python software library that simplifies the process of 'querying, obtaining, analyzing, and  
112 manipulating ICESat-2 datasets to enable scientific discovery' (Scheick et al., 2019, 2023). The  
113 module includes testing, documentation, and a tutorial for accessing coincident Argo and  
114 ICESat-2 data using QUEST. Our goal is to lower the access barrier to combining multiple  
115 datasets to advance our understanding of ocean/sea ice processes from polar to global scales  
116 (Figure 1). Here, we discuss the cultural and scientific value of collaborative approaches to  
117 working across disciplines and sensors (§2), including best practices for writing open source  
118 code, based on the authors' experiences in developing this workflow. Our software (§3) is  
119 object-oriented and written with flexibility so future datasets of interest can be included with  
120 ease (§4) for improved scientific application. We close with recommendations for future  
121 software capabilities, and we invite those interested to join our community and participate in  
122 ongoing efforts.



123  
 124 Figure 1. Location of ICESat-2 reference ground tracks over the ocean (grey lines), Argo floats  
 125 equipped with physical (i.e., temperature, salinity) sensors (cyan), and Argo floats with both  
 126 biogeochemical and physical sensors (BGC, dark blue) globally and over both poles. ICESat-2  
 127 produces data from September 2018 to present, Argo (physical parameters) from 1999 to present,  
 128 and BGC-Argo from 2016 to present.

129  
 130 2. Approach to programming and teamwork  
 131 2.1 Open science

132 The United States White House Office of Science and Technology Policy (OSTP) and  
 133 National Science and Technology Council (NSTC) formally define “open science” as “*The*  
 134 *principle and practice of making research products and processes available to all, while*  
 135 *respecting diverse cultures, maintaining security and privacy, and fostering collaborations,*  
 136 *reproducibility, and equity.*” (U.S. OSTP and NSTC, 2023). Released in January 2023, this  
 137 federal definition coincides with the recognition of 2023 as the Year of Open Science, a concept  
 138 galvanized and promoted through NASA’s Transform to Open Science (TOPS) Mission  
 139 (<https://science.nasa.gov/open-science/transform-to-open-science>) which is part of the agency’s  
 140 broader Open-Source Science Initiative (OSSI) ([https://science.nasa.gov/open-science-](https://science.nasa.gov/open-science-overview)  
 141 [overview](https://science.nasa.gov/open-science-overview)). While necessarily broad, this definition highlights the overarching principles that lead  
 142 to many practices long ago adopted by many communities, and the open-source software  
 143 community specifically. Here we highlight one of the many scientific achievements enabled by  
 144 this type of trans-disciplinary, cross-platform, collaborative approach and hope to persuade  
 145 readers to learn about and adopt relevant open science practices in their own teams and  
 146 workflows. Our motivation stems from wanting to enable more cross-disciplinary discoveries  
 147 through open science, in part because some of our previous work was not open. Developing  
 148 QUEST provided a space to learn and exercise open science practices.

## 150 2.2 Our team

151 Our team met at the University of Washington’s ICESat-2 2020 Virtual Hackweek  
152 (Arendt et al., 2020; Huppenkothen et al., 2018). During this event, project teams formed to  
153 collaborate on a pressing technical or research challenge. We identified a growing gap between  
154 ocean and cryosphere studies, namely the lack of ease with which one could download ICESat-2  
155 data simultaneously with other data products of interest. We quickly created a proof of concept  
156 for combining Argo and ICESat-2 data. With no previous collaborations and hailing from  
157 different academic cultures, disciplines (ocean biology, glaciology, sea ice physics, physics), and  
158 time zones (from Pacific Time to Central European Standard Time), working together as a  
159 project group during the week-long event catalyzed a practice of virtual collaboration and  
160 support. At the time, only a few team members had experience working in Python and/or using  
161 version control tools (e.g. git, GitHub) to write code collaboratively. After the hackweek, the  
162 group continued meeting to create what ultimately became the QUEST module presented herein.  
163 To minimize the burden on already full schedules, we intentionally met for only an hour weekly,  
164 setting appropriately rigorous benchmarks for success while performing most of the work during  
165 these meetings. Importantly, during these supportive co-working online sessions, we not only  
166 wrote software but engaged in coding and collaboration best practices, building skills and  
167 learning from one another. In this way we created a culture of trust and transparency that enabled  
168 us to share our skill sets, make research and personal progress, and address challenges in real  
169 time.

170

## 171 2.3 Object-oriented development overview

172 A first step of our team’s collaborative work was reformatting existing code to fully  
173 leverage the benefits Python’s object-oriented structure has to offer. Details of changes to  
174 icepyx’s architecture are outlined in §3.3. Object-oriented programming (OOP) is a common  
175 implementation feature of many popular open-source languages, including Python and JAVA,  
176 that organizes code through an object-centric perspective. An object is any “entity” possessing  
177 unique attributes and behaviors (Supplementary Figure 1). For example, a “person” object might  
178 include “name,” “age,” and “eye color” attributes and “sleep,” “eat,” and “express joy”  
179 behaviors. In the context of oceanography, a “water column” object would have “temperature,”  
180 “salinity,” and “chlorophyll,” among other attributes. Structuring code in this object-oriented  
181 way has several benefits, most notable of which is modularity. Independent segments of code can  
182 be written simultaneously (“orthogonality” as defined by Thomas and Hunt, 2019) and then  
183 brought together like building blocks that interlink. This modularity enables multiple developers  
184 to individually write code segments independently and combine them later so long as there is an  
185 agreed upon input and output format (“Design by contract,” Thomas and Hunt, 2019) between  
186 them. The modularity of OOP is conducive to easy maintenance because if one code segment  
187 needs to be modified, changes can be made without also propagating revisions through other  
188 segments, as long as the input/output criteria are met (see §3.3).

189

## 190 3. icepyx and QUEST: open-source software for ICESat-2 and Argo

### 191 3.1 What is icepyx?

192 icepyx is an open-source Python software package and community designed to enable  
193 collaboration and work with the large and complex data products from ICESat-2. icepyx was  
194 created at the first ICESat-2 Hackweek held in June 2019, less than a year after the launch of the  
195 satellite. During that event, data access methods were presented ad hoc, with new users required

196 to carefully format tens of lines of code to submit a valid data access request or manually  
197 download individual files through a web browser. Since then, the package’s capabilities have  
198 expanded as more users contribute their work. It now provides data access via download or in the  
199 cloud, visualization, and read-in capabilities. Critically, the software package provides a citable,  
200 tested, shared development framework that is publicly available and easily installable via GitHub  
201 (<https://github.com/>), PyPI (the Python Package Index; PyPI, 2023), and Conda (Anaconda,  
202 2023), while the community provides a safe, supportive, communal learning space to build the  
203 skills required to effectively collaborate on code.

### 204 3.2 Specific software functionality

205 The entire process of querying and downloading (or accessing in the cloud) ICESat-2  
206 data can be achieved with icepyx in three steps: (i) initialize the search with the ‘Query’ class,  
207 (ii) log into NASA Earthdata, and (iii) call the download functionality (or begin cloud reading).  
208 Below, we describe a few key programmatic features with which the user can interact. We  
209 encourage potential users to explore the icepyx documentation  
210 (<https://icepyx.readthedocs.io/en/latest/>) and examples (e.g.,  
211 [https://icepyx.readthedocs.io/en/latest/example\\_notebooks/IS2\\_data\\_access.html](https://icepyx.readthedocs.io/en/latest/example_notebooks/IS2_data_access.html)) to explore the  
212 full range of functionality available within the software. Users need a free Earthdata account  
213 (<https://www.earthdata.nasa.gov>) to download any ICESat-2 data from the National Snow and Ice  
214 Data Center Distributed Active Archive Center (NSIDC-DAAC) or access it in the cloud; icepyx  
215 provides multiple authentication options for an individual to enter their credentials, including an  
216 in-notebook login. These options are showcased in the documentation and are not further  
217 addressed here.

218 The Query data object within icepyx allows the user to define their study parameters.  
219 Input variables include a string for the ICESat-2 product of interest (e.g., ‘ATL03,’ ‘ATL07’), a  
220 spatial extent that can be represented as a bounding box or polygon (coordinates or geospatial  
221 polygon file), and a time window. A maximum of one spatial bounding box or search polygon is  
222 allowable per Query object instance, a limitation imposed by the data archive center but easily  
223 addressed with multiple Query objects. Additional search filters can be added for ICESat-2  
224 queries if the user wishes to search for a specific product version, cycle, or reference ground  
225 track. The user can generate a map of their search region and view summary information about  
226 the data product using the methods available on the Query object  
227 ([https://icepyx.readthedocs.io/en/latest/example\\_notebooks/IS2\\_data\\_access.html](https://icepyx.readthedocs.io/en/latest/example_notebooks/IS2_data_access.html)).

228 Configuration parameters required to search for and access data products are  
229 automatically generated by the software. The user can manually create, view, and update these  
230 parameters, but it is not required. After creating a Query object, the user can view the search  
231 results and metadata (e.g. `avail_granules()`). During data ordering and downloading, the user can  
232 additionally subset the file for specific parameters of interest (Supplementary Material) and  
233 supply options to change the file type (e.g., HDF5 to NetCDF4-CF (see `show_custom_options()`)  
234 in the Query object for more details on available subsetting options).

### 235 3.3 QUEST

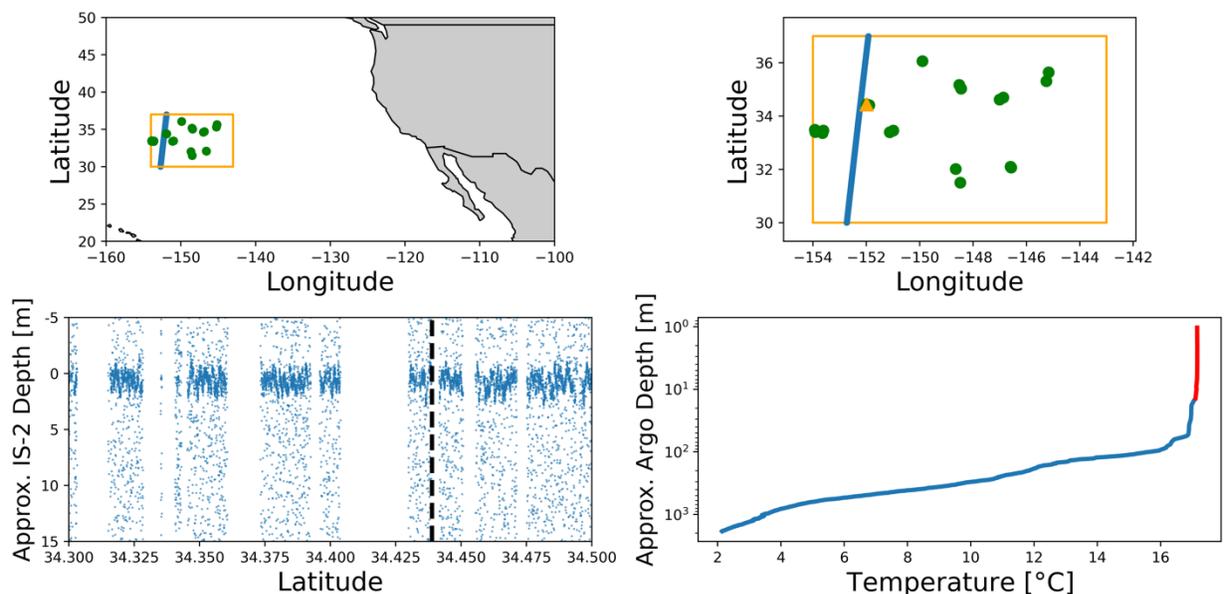
236 Here we present the Query Unify Explore SpatioTemporal (QUEST) module, which is an  
237 expansion of the icepyx Query class (§3.2). From the original icepyx Query object  
238 implementation, we modified the architecture to create a super class object called GenQuery.  
239 Parameters not specific to ICESat-2, such as spatial and temporal information, were isolated to  
240

242 be handled instead by GenQuery, making this information directly accessible to the QUEST  
243 module independent of the ICESat-2 Query functionality. In turn, QUEST uses this super class  
244 GenQuery to handle spatial and temporal data while also housing basic properties and  
245 functionalities common to all datasets (such as preparing data for plotting). These underlying  
246 changes are invisible to the user and take advantage of OOP's ability for high-level organization.

247 The QUEST module is designed to easily query, download, and perform simple  
248 operations on datasets complimentary to and including ICESat-2. Users specify spatiotemporal  
249 bounds for their investigation through creating a QUEST object. The user then utilizes this  
250 higher-level framework to call on subsets of the framework defined specifically for each type of  
251 dataset, providing any additional parameters important for obtaining or manipulating their  
252 dataset of interest (e.g., variables of interest). Attributes and behaviors that are common to all  
253 datasets and required by this higher-level framework are indicated in a template-like Dataset  
254 class and its per-dataset subclasses, with which the user is not intended to interact directly. This  
255 hierarchal system defines a structure for future developers to add functionality for additional  
256 datasets (§4, Supplementary Figure 1).

### 257 258 3.4 QUEST use case: Argo

259 Argo data are available for physical (pressure, temperature, salinity) and biogeochemical  
260 (chlorophyll-a, nitrate, dissolved oxygen, particulate backscatter, downwelling irradiance)  
261 parameters and in a range of data modes (i.e., real-time vs delayed). Real-time data are not  
262 quality controlled whereas delayed-mode data usually are, although some variates, including the  
263 particulate backscattering coefficient ( $b_{bp}$ ), are not strictly quality controlled and need to be  
264 further examined by the user. Argo floats are numerous and the full dataset can be downloaded  
265 from two Global Data Assembly Centers (GDAC); GDAC data access does not permit a user to  
266 search and download for particular floats of interest unless the specific float number is known a  
267 priori (<https://biogeochemical-argo.org/data-access.php>). Downloading the entire Argo dataset is  
268 not feasible for users working locally on their computers due to size constraints, and working  
269 with numerous individual files is less efficient than working within a merged dataframe.  
270 Recently, Tucker et al. (2020) developed an application program interface (API) to query and  
271 download Argo data programmatically based on space/time windows through their web  
272 interface, Argovis. Here, we utilize the Argovis API within QUEST to query, download, and  
273 format delayed-mode Argo data of interest with minimum effort from the user. In this way, the  
274 user does not need to download Argo separate from their ICESat-2 Query, nor does the user need  
275 to download a static dataset from the GDAC. We present an example use case in the North  
276 Pacific, where ICESat-2 and Argo data are available < 5 days apart (Figure 2). In this case, the  
277 depth information available from ICESat-2 appears representative of the rough mixed layer depth  
278 (given by the temperature profile). While ICESat-2 has been used to generate vertical profiles in  
279 the ocean, it is not clear that these signals can be wholly attributed to phytoplankton, because  
280 particles, bubbles, and surface glint also have a role. By coupling nearby Argo observations with  
281 ICESat-2 data, one can more rigorously assess both datasets in tandem, improving the use of  
282 ICESat-2 to address ocean biology and biogeochemistry (Table 1). In the future, it may be  
283 possible to assess stratification in the upper water column from ICESat-2 photon clouds, but  
284 ancillary data such as Argo are needed to facilitate these comparisons and identify uncertainties.



285  
 286 Figure 2. (Top left) Map of ICESat-2 (blue) and Argo (green) data within the icepyx bounding  
 287 box (yellow). (Top right) Zoomed in view of spatial area with closest Argo profile selected in the  
 288 yellow triangle. (Bottom left) Height versus latitude of ICESat-2 photons in the subsurface, with  
 289 Argo location (black dashed line). (Bottom right). Depth versus temperature from Argo profile,  
 290 with ICESat-2 vertical extent highlighted in red.

291  
 292 4. Steps and scientific value of adding a new dataset to icepyx

293 We anticipate many current and future datasets can be included within QUEST to greatly  
 294 amplify the opportunity for scientific discovery at the nexus of disciplines. For example, PACE  
 295 (the Plankton, Aerosols, Clouds, Ocean Ecosystems) mission (Werdell et al. 2019) will supply  
 296 hyperspectral and polarized data on global scales, and GLIMR (Geosynchronous Littoral  
 297 Imaging and Monitoring Radiometer, Salisbury, 2022) will provide hourly data and thereby  
 298 increase the likelihood of synergies with ICESat-2 in the Gulf of Mexico region, where GLIMR  
 299 is targeted to observe. Future progress may be enabled by cloud computing and subsetting  
 300 procedures (described herein) that minimize the computational fluency required by the user to  
 301 access data. We designed the QUEST module of icepyx to leverage object-oriented strengths in  
 302 large part so that additional datasets can easily be added so long as an API is available, and a  
 303 roadmap for adding a new dataset is provided in Figure 3.

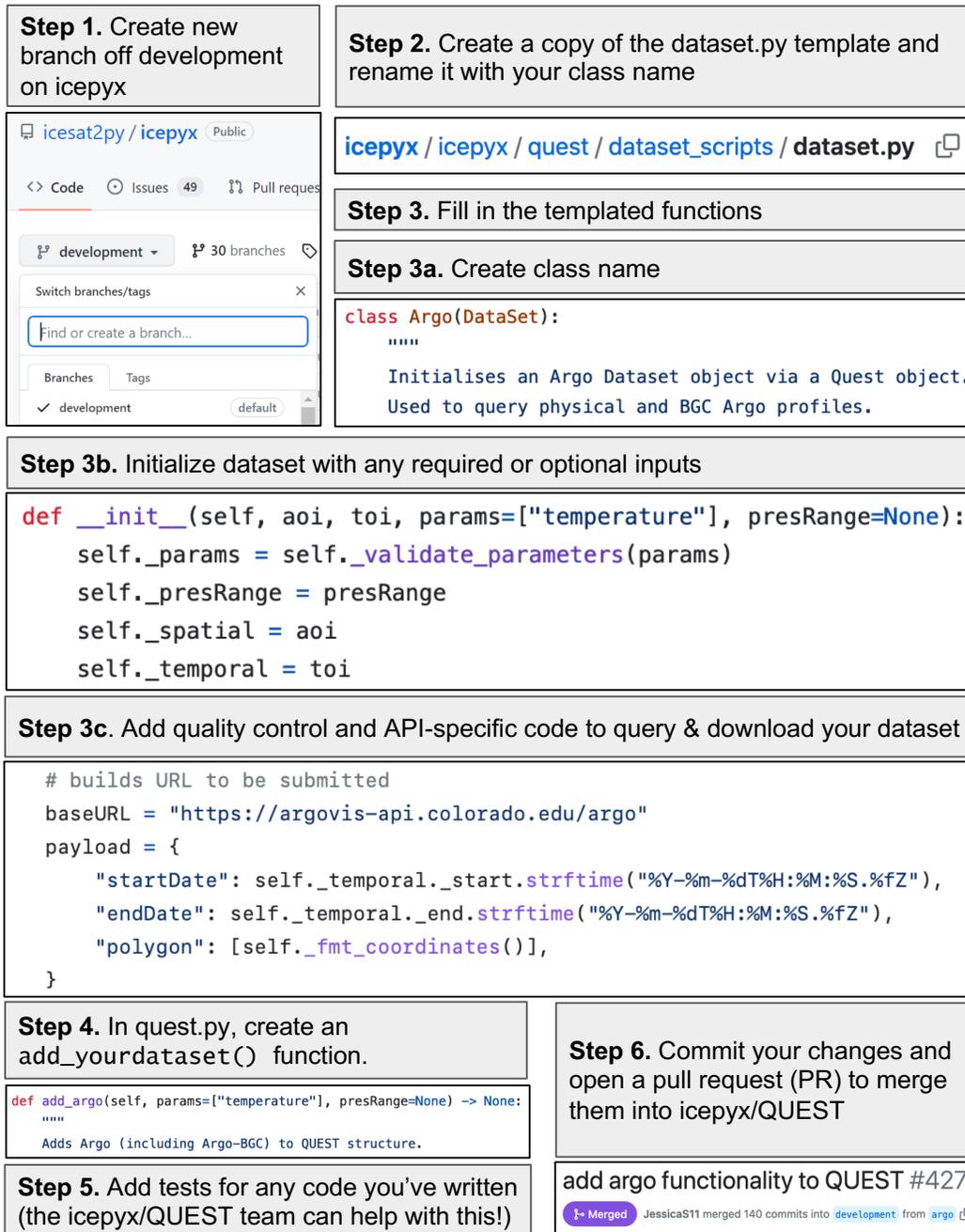
304 The software we describe herein can be used to facilitate a number of targeted and  
 305 exploratory studies across the interface of cryosphere and ocean studies (Table 1). For example,  
 306 Argo profiles provide temperature and salinity that can be used to contextualize and test  
 307 suspected sea ice melting events, and the optical sensors on Argo floats can be used to quantify  
 308 glacial silt in tandem with ICESat-2 measurements of glacial activity. Argo floats also provide an  
 309 important link between sea ice physics and ocean biology, which is needed given the rapid rate  
 310 of Arctic warming (Rantanen et al., 2022) and associated biological changes (Ardyna and Arrigo,  
 311 2020). ICESat-2 and Argo data could also be used in tandem to generate vertical profiles of light  
 312 attenuation or particulate backscattering in the ocean, which would enable fine scale exploratory  
 313 studies in the upper-ocean. Fundamentally, icepyx facilitates direct comparison with ICESat-2  
 314 and Argo observations, which will only become more plentiful in the coming years.

316 Table 1. List of ICESat-2 products relevant for ocean studies

<b>Product</b>	<b>What is it?</b>	<b>Used for?</b>	<b>References (Ocean focus)</b>
<b>ATL03</b>	Global geolocated photon data	<ul style="list-style-type: none"> <li>• Deriving optical information (light attenuation coefficient, <math>b_{bp}</math>) in coastal &amp; global waters</li> <li>• Bathymetry in shallow waters</li> </ul>	Lu et al. 2020, 2021 Eidam et al, 2022, 2023  Parrish et al, 2019
<b>ATL07 (ATL20)</b>	Polar sea ice elevation (Gridded sea ice freeboard)	<ul style="list-style-type: none"> <li>• Sea ice freeboard</li> <li>• Sea ice lead identification</li> </ul>	Bisson and Cael, 2021 Horvat et al, 2022
<b>ATL12 (ATL19)</b>	Ocean Elevation (Gridded sea surface height)	<ul style="list-style-type: none"> <li>• Sea surface height</li> </ul>	Bagnardi et al, 2021

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## Adding a new dataset to QUEST



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Figure 3. Workflow illustrating steps of adding a new dataset to QUEST module.

### 5. A note on best practices

Python is one of the more forgiving languages in which to code, and this increased flexibility reduces both learning barriers and development time; however, sometimes more rigidly formatted code can benefit a project. Access modifiers are one such element that offer more rigidity but are not formally supported in the Python language. As the name suggests, access modifiers are syntax which modify access to objects. An object may be public, protected, or private. Public objects may be accessed anywhere in the program. Protected objects are only

328 accessible within a class and its subclasses. As an example within the context of icepyx,  
329 “Dataset” is a high-level object from which more specific datasets extend including “Argo” and  
330 “ICESat-2”. An attribute common to all datasets is the geographical location at which the data  
331 were collected. The region of interest is an attribute that the user will specify, regardless of the  
332 dataset being queried. API calls require geographic boundaries to be formatted in a specific way.  
333 Requiring the user to manually reformat the geographical region for each API call would be both  
334 tedious for the user and leave unnecessary room for error. This reformatting is best done on the  
335 backend via a function `_fmt_coordinates()`, with which the user should never interact. It is  
336 therefore best practice to designate this function as protected. That is to say, the higher-level  
337 “parent class”, Dataset, possesses a generic `_fmt_coordinates()` function that is inherited by its  
338 “child classes”, ICESat-2 and Argo. The specific child classes have access to the generic  
339 functionality, though the developer may also override `_fmt_coordinates()` within the child class  
340 itself to cater the formatting to the API being called. The take-away from this is that  
341 `_fmt_coordinates()` can be inherited by children of a class, but should not be called outside of the  
342 (sub)class itself.

343 The most restrictive access modifier is “private.” This prohibits access to an object  
344 outside of a class. There are no private variables in icepyx at this time, in part because objects in  
345 Python are public by default and there is no true way of restricting access to objects. Access  
346 modifiers are built on a type of “honor system” in which the programmer is expected to respect  
347 access recommendations. Protected objects are prefixed with a single underscore, and private  
348 objects are prefixed with a double underscore. The end user is expected not to interact with  
349 objects with private or protected designations.

350 The best practices used in the development of icepyx extend beyond those visible in the  
351 code. Test Driven Development (TDD) is a school of software development whereby the  
352 program is written in response to test cases. This process begins with establishing the desired  
353 functionality, writing test cases to reflect that functionality, and finally writing code to achieve  
354 that functionality. Test cases are often thought to simply verify the program is behaving as  
355 expected; however, TDD encourages the developer to consider how the end product will be used.  
356 “Design by contract” and “orthogonality” are among the recommendations presented by Thomas  
357 & Hunt (2019) used explicitly in icepyx’s QUEST module. The term “Orthogonality” signifies  
358 segments of code which are independent of one another. That is to say the inner workings of one  
359 segment should not affect the behavior of another segment. “Design by contract” offers a  
360 framework through which orthogonal code segments may interact. The developer decides on a  
361 contract of preconditions and post conditions to which the program should adhere. In the context  
362 of QUEST, ICESat-2 and Argo objects are independent of one another. There is, however, an  
363 agreed upon contract established by the higher-level “Dataset” class that exists solely on the  
364 backend which enforces input and output types expected by each of the two specific datasets.  
365

## 366 6. Summary, and the value of open-source science to facilitate cross-disciplinary collaborations 367

368 Here we have introduced and described our efforts to build the QUEST module within  
369 icepyx, including architectural modifications to meet software development best practices and  
370 provide a superclass structure to readily accommodate future geophysical datasets. We have  
371 illustrated the science possibilities enabled by QUEST by incorporating physical and  
372 biogeochemical Argo data with ICESat-2 tracks as a case study. Future advancements will come  
373 by adding other datasets to QUEST and expanding upon this initial exploration of coincident

374 data. The science community needs to embrace the philosophy that integrating technologies is  
375 required for ground-breaking advances, not only to achieve closure in the measured parameter of  
376 interest, but also to greatly extend what's possible from any one sensor alone. ICESat-2 and  
377 Argo are the only platforms that offer near real-time, global scale, vertically-resolved subsurface  
378 information about ocean biology and biogeochemistry at present; future missions will be easily  
379 included through our creation of shared, open computational pipelines and infrastructure.

380 Open-source science (OSS) is a powerful concept offering free and unlimited data access,  
381 fully documented open software and algorithms, fully transparent processes and reproducibility,  
382 and a teaching culture (<https://www.earthdata.nasa.gov/esds/open-science>). OSS and its adoption  
383 catalyzes cross-disciplinary conversations surrounding best practices for collaboration,  
384 ultimately enhancing community and scientific rigor. Proprietary software, lack of code sharing,  
385 and ambiguous methodologies hurt our potential for meaningful collaborations. As more  
386 technologies are developed and innovated, the need for transparency and data sharing will only  
387 grow. As we have described here, the QUEST module within icepyx provides a generalized  
388 framework such that future studies incorporating multiple sensors are not only possible, but  
389 could become routine and accessible even for novice developers.

390  
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395 **Open Research** Our software is freely and openly available at  
396 <https://github.com/icesat2py/icepyx>, and was used to download ICESat-2 and Argo data in this  
397 use case. Data from ICESat-2 used in this study are freely available at <https://nsidc.org/home> and  
398 are accessed through our software program, icepyx (Scheick et al., 2019, 2023), Argo data were  
399 collected and made freely available by the International Argo Program and the national programs  
400 that contribute to it (<http://doi.org/10.17882/42182>). The Argo Program is part of the Global  
401 Ocean Observing System.  
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