



Decadal and spatially complete global surface chlorophyll-a data record from satellite and BGC-Argo observations

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- 10 **Abstract.** Decadal-scale satellite-based climate data records of chlorophyll-a (chl-a), an essential climate variable, are now readily available at high accuracy and precision. These data are being extensively used for research and, increasingly, for operational services. However, these observations rely on availability of sunlight and the satellite sensor being able to view the ocean, so there are gaps in data due to the presence of clouds and more widely during the polar winter. This is an issue when spatially complete data are needed for global climate studies, or as inputs to machine learning methods and for data
- 15 assimilation. Whilst addressing cloud cover is well studied, methodologies to overcome missing data due to the polar winter has received little attention and simple approaches to overcome these gaps can lead to unrealistic values. Biogeochemical Argo (BGC-Argo) floats have widely been deployed, and they represent an opportunity to address these gaps. We present an approach that combines BGC-Argo data and a satellite chl-a climate data record to produce a spatially and temporally complete, global monthly chl-a record between 1997 and 2023 at 0.25° spatial resolution. Clouds gaps were filled using an
- 20 established spatial kriging approach. Polar wintertime chl-a were reconstructed using relative changes between the wintertime BGC-Argo chl-a, and the previous autumntime or next springtime satellite observations, for individual hemispheres. Uncertainties were calculated on a per-pixel basis to retain the underlying uncertainty fields in the climate data record and were modified to account for the uncertainties related to the gap filling. The seasonal cycles in the resulting polar data are consistent with light availability. Clear interannual and inter-hemisphere variability in the wintertime chl-a were
- 25 observed. Independent assessment of solely the gap filled wintertime chl-a estimates against *in situ* data (N = 204 total) indicates that the accuracy and precision of the underlying satellite data, a key component of a climate data record, are maintained. The 25 year global and spatially complete chl-a data, that are consistent with the underlying climate data record can be downloaded from Zenodo (Ford et al., 2025b).

30 1. Introduction

Chlorophyll-a (chl-a), the dominant photosynthetic pigment in phytoplankton, has been identified as an essential climate variable by the Global Climate Observing System for assessing current and future changes to oceanic global bio-





geochemical cycles (GCOS, 2021). Satellite-ocean-colour-based synoptic chl-a fields of the surface and near-surface ocean (varying from a few millimetres depth to tens of metres dependent upon the water constituents) have routinely been
produced since the launch of Sea-viewing Wide Field-of-view Sensor (SeaWiFS) in September 1997 and the more advanced satellite ocean colour sensors that have followed. The ocean colour signal at different wavelengths of light can be related to *in situ* chl-a concentrations and used to estimate synoptic scale chl-a (e.g. Gohin et al., 2002; Hu et al., 2012; O'Reilly & Werdell, 2019). These observations from multiple satellites that cover different time periods and often with different sensor characteristics, are now routinely merged into continuous climate data records, the main effort of which results in the Ocean
Colour Climate Change Initiative (OC-CCI) (Sathyendranath et al., 2019). These records are essential for assessing global and regional changes in phytoplankton abundance and primary production (Kulk et al., 2020). Additionally they are routinely used for ecosystem monitoring, understanding biogeochemistry, supporting fisheries management, water quality monitoring and operational ocean forecasting (Sathyendranath et al., 2023b).

However, ocean-colour observations of chl-a have the limitation of data gaps due to cloud cover, and high sun zenith and viewing angles which routinely occur during polar winter. Multiple methods have been developed to fill the data gaps due to cloud cover on both regional and global scales. For example, Saulqiun et al. (2019) used an optimum interpolation technique (commonly used in sea surface temperature records) to gap fill a merged chl-a record. Liu and Wang (2018) used the Data Interpolating Empirical Orthogonal Functions (DINEOF), which reconstructs the missing chl-a based on empirical orthogonal functions, to fill Visible Infrared Imaging Radiometer Suite (VIIRS; one of the inputs to the multi-sensor OC-CCI record) observations. Recently, Hong et al. (2023) used a convolution neural network that ingests environmental information, including sea surface temperature and photosynthetically active radiation, to aid in the reconstruction of chl-a underneath clouds between ~50°N and ~50°S within the OC-CCI record. These methods show differing accuracies, but they are generally effective at reconstructing gaps due to cloud cover (Stock et al., 2020). However, none of these studies attempt to reconstruct the persistent gaps at high latitudes that occur during the polar winter.

These missing high-latitude polar winter data often make the exploitation of the overall chl-a record more challenging or result in assumptions being made about the missing wintertime chl-a concentrations. For example, within efforts to reconstruct the global ocean carbon dioxide (CO₂) sink, these missing data are often manually filled with a fixed value (e.g., Chau et al., 2022; Gregor & Gruber, 2021), or the gaps mean that chl-a data are avoided for the input variables used to interpolate other data which means that any explicit biological signal within the interpolation is omitted (Ford et al., 2024a). Example fixed values include Gregor and Gruber (2021) who use a fixed value of 0.3 mg m⁻³ for all missing polar wintertime data, whereas Chau et al. (2022) use a value of 0.0 mg m⁻³. These practical choices likely influence the underlying interpolation and reconstructions of the data (in this case the ocean CO₂ sink) and are unlikely to be scientifically applicable across all times and geographic locations as they overlook regional and temporal variations and create unnatural boundaries or characteristics (e.g., the Arctic and Southern Ocean likely have different bio-geochemical characteristics). The



expanding availability of autonomous BGC-Argo profilers with chl-a sensors (Roemmich et al., 2019) that collect observations within the polar winter provides an opportunity to generate a data-driven reconstruction of these missing wintertime chl-a. Whilst able to provide data during polar winter, the BGC-Argo chl-a data have reduced accuracy with respect to the satellite observations, so using them to directly gap-fill the higher accuracy climate data record presents some challenges.

We present a methodology for producing a spatially complete monthly chl-a record between October 1997 and December 2023 at a spatial resolution of 0.25° with spatially resolved uncertainties. Cloud gaps were initially filled using an established 75 spatial kriging approach. The missing polar wintertime chl-a data were then filled using relationships between BGC-Argo measured chl-a and the first spring or last autumntime observations within the satellite record. Relative changes between the satellite record and BGC-Argo chl-a were used rather than relying on the absolute values to overcome the difference in depth relevance of the BGC-Argo chl-a versus the satellite record. The relationships were constructed for both the Northern Hemisphere (which includes all of the Arctic Ocean) and Southern Hemisphere (containing the Southern Ocean) separately, which highlights the bio-geochemical differences evident in these different wintertime chl-a response.

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2. Data and Methods

2.1. BGC-Argo Chl-a data

BGC-Argo profilers have been deployed globally, and at the time of writing ~400 (~60 %) of these have fluorometric chl-a sensors. Delayed mode BGC-Argo profile data (2008 to 2023, last ingestion: 1st October 2024) were retrieved from the Argo 85 Global Data Assembly Centers (GDAC) for the Southern Hemisphere (south of 40°S) and the Northern Hemisphere (north of 40°N). These delayed mode profiles have undergone automatic processing, and quality control within the GDAC following Schmechtig et al. (2015) and Schmechtig et al. (2023). For each BGC-Argo profile the quality flagging was applied to only retain the highest quality data (quality flag 2), and the mean chl-a value was extracted from the first 20 m of each profile. 90 The mean was calculated in log₁₀ space due to the logarithmic distribution of chl-a (Campbell et al., 2002). The spatial and temporal distributions of the resulting chl-a profiles in the Southern and Northern Hemispheres are displayed in Figure 1. The BGC-Argo chl-a data were then gridded (mean in \log_{10} space) into monthly 0.25° composites to match the resolution of the satellite observations described in the next section, using existing publicly available software (Ford et al., 2024b).

95 2.2. Satellite observational data

The OC-CCI (v6) chl-a data were retrieved at daily and monthly temporal resolution at their native spatial resolution (4 km) between October 1997 and December 2023 (Sathyendranath et al., 2019, 2023a). The OC-CCI monthly composites were





aggregated after log₁₀ transformation, to compute mean values at 0.25° degree spatial resolution using existing publicly available software (Ford et al., 2024b). The uncertainties (1 sigma; given as the root mean square difference; RMSD) provided with the OC-CCI product were converted to a 0.25° resolution by calculating the mean of the 4 km uncertainties that contribute to each 0.25 grid cell, which assumes spatial uncertainties within adjacent cells are dependent and spatially correlated (Taylor, 1997). Daily sea ice concentration at ~25 km spatial resolution were obtained from *Ocean and Sea Ice Satellite Application Facility* (OSISAF) (OSISAF, 2022). The daily OSISAF sea ice concentrations were combined into monthly composites and regridded to the same spatial grids as the monthly OC-CCI data, by using the same software (Ford et al., 2024b).

To assess the impact of gridding the BGC-Argo and OC-CCI data, a comparison between the daily OC-CCI at 4km and the individual BGC-Argo chl-a profiles was conducted, following standard ocean colour comparison protocols (Bailey and Werdell, 2006; Ford et al., 2021). Each BGC-Argo profile was matched daily to the OC-CCI record (i.e., coincident day), and the mean chl-a (in log₁₀ space) extracted from a 3-by-3 pixel grid (which represents ~12 km by 12 km region at the equator). The same analysis was then repeated for the monthly 0.25° BGC-Argo and OC-CCI data. A standard suite of statistics was calculated in log₁₀ space for both the daily 4km and the monthly 0.25° data and the results were then compared. The metrics included the bias (accuracy), root mean square deviation (RMSD; precision) and the slope and intercept of a Type II regression. This analysis assessed the impact of averaging the BGC-Argo and OC-CCI observations to monthly 0.25°

115 composites (Supplementary Figure S1) and indicated that the averaging had limited effect on the retrieved unweighted bias (accuracy) and RMSD (precision) for the Southern and Northern Hemisphere (i.e., the bias and RMSD results for the daily matches were similar to the monthly 0.25° gridded data). The high intercept values at both 4 km and 0.25° (Supplementary Figure S1), particularly for the northern hemisphere, illustrate why the absolute values of the BGC-Argo data cannot be used to directly fill the satellite record.







Figure 1: Spatial and temporal distribution of the BGC-Argo chlorophyll-a profiles used. (a) Geographical distribution of the individual profiles (i.e., individual profilers appear multiple times). (b) Temporal distribution in years of the number of profiles used for the Southern Hemisphere (<40°S) and Northern Hemisphere (>40°N). (c) Temporal distribution in months of the profiles used for the Southern Hemisphere (<40°S) and Northern Hemisphere (>40°N). Basemap in (a) from Natural Earth v4.0.0 (https://www.naturalearthdata.com/).



2.3. Spatial Kriging for cloud gap filling

- Ocean-colour sensors on board polar orbiting satellites collect data at multiple wavebands in the visible domain, which is 130 used to estimate the chl-a concentration. Clouds are optically thick in the visible spectrum, and so they block the sensor's view of the ocean, leading to missing data within the ocean-colour chl-a data record. The use of monthly composites of ocean-colour-based chl-a reduces the gaps due to cloud cover as clouds tend to evolve (i.e., appear to move) faster than the ocean conditions. Multiple daily observations within the one-month allows the impact of the faster moving clouds to be averaged out. But aggregating data over multiple days cannot help in regions where clouds can be more prevalent, such as the inter-tropical convergence zone. Stock et al. (2020) evaluated multiple approaches to fill data gaps due to cloud cover,
- suggesting that approaches including spatial kriging or DINEOF were the most accurate. Therefore, here we implement a spatial ordinary kriging approach to fill cloud cover gaps.

To perform the kriging, a semi-variogram was computed for each monthly timestep in the timeseries using SciKit-Gstat v1.0.0 (Mälicke, 2022) with the 'martheon' estimator and an exponential function. A visual inspection of the semi-variogram

- output was used to optimise the estimator and function. The semi-variogram was fit to a ~5% subset of the OC-CCI observations that were equally distanced in space, for a monthly varying latitude band where at least 20% of the OC-CCI observations are available. The subset size was a computational choice because the number of pairwise distances that must be calculated by the semi-variogram is a n^2 function, where *n* is the number of locations. Setting the monthly varying latitude limits (i.e latitude band where at least 20% of the OC-CCI observations are available) prevents the kriging from filling data that are missing due to the polar winter and not due to cloud cover. The ordinary kriging was applied only to the missing data
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locations (i.e., the original OC-CCI observations are left unchanged).

2.4. BGC-Argo Wintertime filling

The approach developed with the BGC-Argo profilers to reconstruct the wintertime observations is based on the assumption that wintertime chl-a will decline due to lower light availability before then increasing again as the light returns in the spring. Therefore, the wintertime chl-a would be lower than the last available OC-CCI observations in autumntime and first available observations in springtime. Thus, the decline in chl-a during the polar winter can be estimated using the BGC-Argo profiler chl-a as an observational constraint. The two sets of observations (satellite sensor versus Argo), dependent upon the water constituents, overlap in terms of their depth relevance. However, the BGC-Argo chl-a measured by in vivo fluorescence are considered less accurate than high performance liquid chromatography (HPLC) chl-a predominantly used for the calibration and evaluation of ocean colour data (Long et al., 2024; Roesler et al., 2017). These differences could lead to an underlying bias between the OC-CCI and the BGC-Argo chl-a observations (e.g., see supplementary Figure S1). To minimise these differences, the BGC-Argo chl-a were bias corrected (in log₁₀ space) with respect to the OC-CCI data where coincident observations were available, by determining a temporally fixed bias (the median of all individual float biases for



- 160 each hemisphere). The Northern and Southern Hemisphere bias corrections were 0.02 and 0.30 log₁₀(mg m⁻³) respectively (Supplementary Figure S1c,d). The bias correction does not assume that the OC-CCI record is the 'truth', but our objective is to fill gaps in the OC-CCI data using relative changes to the BGC-Argo chl-a which requires the two datasets to be consistent.
- 165 Next, for each BGC-Argo observation, we count backwards in time to the last autumntime observation up to nine months prior to the BGC-Argo observation time. For example, a time lag of zero indicates a coincident OC-CCI observation with the BGC-Argo, and a lag of one month indicates the OC-CCI observation occurred in the previous month to the BGC-Argo. As the cloud gap filling approach was applied before this step, the "OC-CCI observation" is likely to be an original OC-CCI retrieval but may in some instances actually be a cloud-filled value. For each time lag, the median percentage difference was
- 170 calculated between the OC-CCI and bias-corrected BGC-Argo chl-a in mg m⁻³ (to avoid the switch from positive to negative values within the log₁₀ transformed values) on a pixel-by-pixel basis. This constructs a relative change relationship between the autumntime OC-CCI and BGC-Argo chl-a observations in terms of the time to the OC-CCI observation. The procedure was applied to the Southern and Northern Hemispheres separately, which allows for the known biogeochemical differences between the two polar regions (Ardyna and Arrigo, 2020; Deppeler and Davidson, 2017). Although the process was applied
- up to nine months back in time, in practice the majority of data are filled within ± 4 month (Supplementary Figure S2).

The whole procedure was then applied in reverse, counting forwards to the first springtime observation. This provides both a backwards looking and forwards looking relationship over the wintertime period for each hemisphere. The obtained relationships between OC-CCI and BGC-Argo data were then used to gap fill the gridded wintertime OC-CCI data. For each wintertime pixel, the time lag between the autumntime and springtime OC-CCI observations was calculated, and the relationship with the lowest time lag was used (i.e., either the forward or backward in time relationship). If both had the same time lag, the autumntime relationship was used in preference as these were generally constrained by more BGC-Argo observations (N = 1023; Figure 2a) than the springtime relationship (N=723; Figure 2b).

185 Chl-a concentrations in regions with a sea ice coverage greater than 95 % as indicated by the OSISAF sea ice concentrations were set to a fixed value of 0.1 mg m⁻³ (-1 log₁₀(mg m⁻³)). We selected this value from literature (e.g. Boles et al., 2020; Randelhoff et al., 2020), based on wintertime chl-a concentrations from under ice regions that are not experiencing an significant or enhanced under ice phytoplankton growth, but we acknowledge the potential for highly heterogenous under ice chl-a concentrations.

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Any remaining pixels that were not gap filled by any of the previous procedures are filled with a final kriging pass, following the same methodology as in section 2.3, but globally. This final step was mainly applied in regions of partial sea ice coverage (i.e., those with ice coverage between ~10 and 95%). A breakdown of the pixels filled by each stage in the gap



filling methods are given in Supplementary Figure S3, and the BGC-Argo relationship month lags are given in Supplementary Figure S2.

An implication of applying the BGC-Argo gap filling approach to monthly resolution data leads to artificial latitude banding due to the month lag relationship changing at each latitude. This banding in the monthly gap-filled record is highlighted here as it is dependent upon the methodological choices and data limitation issues. The month lag relationships could instead be linearly interpolated and applied to 8-day composites and then averaged to monthly composites which would likely reduce this banding. But constructing the BGC-Argo relationships using 8-day composites is currently not feasible due to limited BGC-Argo data availability, especially at the higher time lags.

2.5. Uncertainty propagation (1 standard deviation; 1σ)

- 205 The cloud gap filling kriging approach uses observations in the vicinity of the empty pixel (based on the semi-variogram described in section 2.3) to construct the missing chl-a. The uncertainties arising from using the ordinary kriging are a combination of: (1) the underlying OC-CCI uncertainties in the measurements and (2) those arising from the method used to estimate the missing chl-a. Therefore, the accompanying OC-CCI uncertainty fields were also kriged using the same semi-variogram estimated from the chl-a observations producing uncertainty values for each gap filled pixel.
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The polar wintertime data filled with the BGC-Argo relationships use the spring- and autumntime observations which are then multiplied by the percentage reduction in chl-a. Therefore, two sources of uncertainty combine to form the total uncertainty: (1) the uncertainty in the OC-CCI spring- and autumntime observations (1σ), and (2) the uncertainty in the percentage difference estimated from the BGC-Argo profiler (1σ). We estimate the uncertainty in the percentage difference by calculating the median absolute deviation (MAD) and convert this to a standard deviation equivalent. Using the MAD reduces the sensitivity to "outliers" within the percentage differences. Both sources of uncertainty were propagated through the analysis using a Monte Carlo uncertainty approach with 1,000 ensembles, assuming they are independent and uncorrelated, and the resulting spatially varying uncertainty are provided in log₁₀(mg m⁻³) units for each of the polar wintertime filled pixels.

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The under ice chl-a uncertainty was set to $0.4 \log_{10}$ (mg m⁻³), owing to the complex dynamics under sea ice based on a range of sources (Ardyna and Arrigo, 2020; Arrigo et al., 2012, 2014; Boles et al., 2020; Randelhoff et al., 2020) – see the discussion section for further details on this decision. The uncertainties are provided alongside the gap-filled chl-a data, providing consistent spatially and temporally varying uncertainties.





2.6. Independent accuracy and precision evaluation

To independently assess the accuracy and precision of the gap filled wintertime chl-a concentrations we used the OC-CCI chl-a validation dataset (Valente et al., 2022; v3). These data provide the chl-a concentration measured on ships by either HPLC or fluorometric approaches. This dataset is used routinely to assess the accuracy and precision of the OC-CCI record 230 (but are not used to tune the algorithms used). Furthermore, the wintertime values remain independent as these cannot be matched to the original OC-CCI record as there are gaps in the original satellite data record. The individual chl-a observations were gridded onto the same monthly 0.25 ° grid (mean in \log_{10} space) as the gap-filled OC-CCI record, separately for the HPLC and fluorometric chl-a observations. The gridded in situ observations were then compared with the gap-filled OC-CCI data record at the locations where the BGC-Argo relationships were applied (i.e the polar wintertime 235 filled data) for the Northern Hemisphere and Southern Hemisphere, separately. The standard suite of statistics described in section 2.2 were calculated to assess the accuracy and precision of the gap filled wintertime chl-a against these independent

3. Results

in situ observations.

- 240 The relationships between the autumntime (backwards; Figure 2a, c) and springtime (forwards; Figure 2b, d) OC-CCI and wintertime BGC-Argo profilers showed clear differences between the Southern (Figure 2a, b) and Northern Hemisphere (Figure 2c, d). The Southern Hemisphere indicated a slower decline in the chl-a concentration from the previous autumntime compared to the Northern Hemisphere. For example, the one-month lag showed a median 24 % decrease in chl-a for the Southern Hemisphere compared with a median 71 % decrease for the Northern Hemisphere. The springtime comparison also 245 showed similar regional differences (Figure 2b). The forward relationships both indicate similar percentage differences for month lags 1 to 5. The backward and forward relationships at month lags greater than 5 showed more variability, which is likely due to the lower number of available data to construct the relationships (Figure 2).
- Applying both the spatial kriging to fill the cloud gaps, and then BGC-Argo approach to fill the wintertime polar chl-a, 250 allowed for the production of a globally complete observation-based gap-filled chl-a dataset (Figure 3). Using monthly composites reduced the need to broadly apply the cloud gap filling approach and it was mainly applied in earlier years of the timeseries when SeaWiFS was the only ocean colour satellite available (1997-2002; see Supplementary Figure S2). Focusing on further analysis of polar regions where the BGC-Argo wintertime approach was applied, five exemplar locations showed regional differences in the chl-a wintertime concentrations (Figure 3b-f). The selected locations in the Northern Hemisphere 255 (Figure 3b, d) generally showed larger decreases in the wintertime chl-a, although concentrations in the North Atlantic
- Ocean (Figure 3d) had a much larger decline than in the North Pacific Ocean (Figure 2b). The Southern Hemisphere also showed regional difference across the three selected locations (Figure 3c, e, f). These timeseries highlight that the approach





- was able to produce a consistent timeseries that captured interannual variability in the wintertime chl-a (e.g., particularly evident in Figure 3e, f). Condensing the full timeseries into a multi-year monthly climatology illustrates the full coverage
 and spatial and temporal variability of the wintertime period that has been filled by the BGC-Argo approach (Figure 4). These multi-year monthly climatologies show the advantage between using only OC-CCI observations and the gap-filled data, especially at the beginning and end of the winter period, where the cloud gap filling approach aids in reconstructing the seasonality (Figure 4b, d, e). They also reinforce the regional differences in the magnitude of the chl-a decline during winter.
- Total uncertainties in the wintertime chl-a were ~ $0.6 \log_{10}$ (mg m⁻³) in the Northern Hemisphere (Figure 4) where this value is 265 driven mainly by the uncertainty in the relationship determined via the BGC-Argo profilers. The higher uncertainty in the relationship was a combination of fewer Argo profiles, which in turn effects the constraint of the complex wintertime chl-a response in the Northern Hemisphere (Figure 3c, d). The Southern Hemisphere has lower total uncertainties of $\sim 0.4 \log_{10}$ (mg m^{-3}) (Figure 4) that contained more equal contributions to the uncertainties from the BGC-Argo relationship and the 270 underlying spring- and autumntime OC-CCI chl-a uncertainty. The accuracy and precision of the wintertime chl-a (ie the polar gap filled data) was assessed against independent *in situ* chl-a observations, determined either by HPLC (Figure 5a, c) or fluorometric methods (Figure 5b, d). Comparisons to the in situ HPLC chl-a concentrations show higher numbers of coincident observations for the Northern Hemisphere (N = 128; Figure 5a) compared with the Southern Hemisphere (N = 76; Figure 5c). Both hemispheres show good accuracy and precision between the in situ observations and wintertime chl-a, with 275 small biases (less than 0.1 log₁₀(mg m⁻³)) and RMSD of ~0.4 log₁₀(mg m⁻³). Comparison with the *in situ* fluorometric chl-a resulted in insufficient coincident observations to draw conclusions for the Southern Hemisphere (N = 8; Figure 5d). For the Northern Hemisphere, the accuracy of the wintertime chl-a is consistent to the previous comparisons to the BGC-Argo chl-a displaying the same regional biases (N = 2202; Figure 5b; Supplementary Figure S1 d). Although, the precision is larger as highlighted by the RMSD values ~ $0.6 \log_{10}$ (mg m⁻³) compared to ~ $0.4 \log_{10}$ (mg m⁻³) for the comparison to the BGC-Argo 280
- chl-a (Supplementary Figure S1 d). These precision estimates for the Southern Hemisphere (~0.4 log₁₀(mg m⁻³); Figure 5c) and Northern Hemisphere (~0.6 log₁₀(mg m⁻³); Figure 5b) support the validity to the propagated uncertainty estimates for the Southern Hemisphere of ~0.4 log₁₀(mg m⁻³) and the Northern Hemisphere of ~0.6 log₁₀(mg m⁻³). In the Southern Hemisphere these uncertainties are of similar magnitude with the OC-CCI uncertainties for the region, however they are larger within the Northern Hemisphere.







Figure 2: (a) Boxplots indicating the percentage difference between the Ocean Colour Climate Change Initiative (OC-CCI) and bias-corrected BGC-Argo chlorophyll-a (chl-a) based on time lag since the last autumntime observation in the Southern Hemisphere. Red line indicates the median, the box indicates the 25% and 75% quartiles, and circles indicate data considered as outliers. In axis abbreviations are number of samples (N) and median bias (Med). (b) same as (a), but for the Southern Hemisphere springtime relationship. (c) same as (a), but for the Northern Hemisphere autumntime relationship. (d) same as (a), but for the Northern Hemisphere springtime relationship. Y-axis limits have been selected to emphasise the lower time lags, where the higher time lags are constrained by less data and have limited use in the methodology.







Figure 3: (a) Ocean Colour Climate Change Initiative (OC-CCI) chlorophyll-a (chl-a) with gap filling approach applied to the full timeseries climatology (1997 – 2023). (b) Chl-a timeseries extracted for the location marked by arrow between 1997 and 2023. Blue line indicates the OC-CCI timeseries without gap filling and black lines indicate the gap filled data. Grey shaded region indicates the 1σ uncertainty in chlorophyll-a. (c), (d), (e) and (f) same as (b) but for their respective locations. Basemap in (a) from Natural Earth v4.0.0 (https://www.naturalearthdata.com/).







300 Figure 4: (a) Ocean Colour Climate Change Initiative (OC-CCI) chlorophyll-a (chl-a) with gap filling approach applied to the full timeseries climatology (1997 - 2023). (b) Monthly climatology calculated at the location marked by the arrow. Blue line indicates the monthly climatology for the OC-CCI timeseries. Black line indicates the monthly climatology for the gap-filled OC-CCI, where the grey shading indicates one standard deviation of the gap-filled climatology. Dashed blue line indicates a chl-a value of 0.3 mg m⁻³ (~0.5 log₁₀(mg m⁻³)) and is referred to in the text. (c), (d), (e) and (f) same as (b), but for their respective locations. Basemap in 305 (a) from Natural Earth v4.0.0 (https://www.naturalearthdata.com/).







Figure 5: (a) Comparison between monthly 0.25° -gridded *in situ* HPLC chl-a concentrations and the wintertime gap-filled chl-a data in the Northern Hemisphere (in \log_{10} mg m⁻³). Solid line is 1:1 and dashed blue line indicates a Type-II linear regression. In text the abbreviations for the statistical measures are root mean square difference (RMSD) and number of samples (N). (b) Comparison between monthly 0.25° -gridded *in situ* fluorometric chl-a concentrations and the wintertime gap-filled chl-a in the

Northern Hemisphere. (c) Same as (a), but for the Southern Hemisphere. (d) same as (b), but for the Southern Hemisphere.



4. Discussion

The exploitation of satellite-based chl-a data records can be hampered by missing data due to cloud cover and missing data during the polar winter due to low solar elevations. In this study, we have presented an observation-based approach to gap filling the missing polar wintertime chl-a data within a satellite climate data record, using the relative change in BGC-Argo profiler chl-a data as an observational constraint. This process has been preceded by using a relatively simple kriging approach to fill cloud-related missing data, which is then used again as a final step (after the polar data have been filled) to fill any remaining missing data which ensures an ocean-colour-based chl-a data record with full global coverage. The cloud gap filling based on a spatial kriging approach used in this study could be regarded as a simple method. Stock et al. (2020) showed that spatial kriging performed well for cloud gap filling, when compared to more complex methods, such as

- DINEOF. In this study the use of monthly composites does limit the number of observations that need to be gap-filled by the cloud gap filling approach (Supplementary Figure S2). Applying the full methodology to generate a higher-temporal resolution dataset (e.g., by using 8-day composites instead of monthly composite) is possible but could present challenges when larger regions are covered by clouds. This may suggest that more complex methodologies, such as those proposed by
- 325 Hong et al. (2023), using a convolution neural network (that considers the physical and biological conditions), could be more applicable to filling larger cloud cover gaps. It is important to note that spatial gap filling methods make assumptions about the missing data, which may lead to under- or overestimation of chl-a concentrations in regions with persistent cloud cover over time and space.
- The data gaps in optical satellite data due to the polar winter have so far received little attention within gap filling methodologies. The approach within this study provides an observation-based gap filling that exploits the expected underlying temporal signal due to light availability and the fundamental requirement for biological growth to need light. The results appear consistent with previous studies of wintertime chl-a variability. For example, Randelhoff et al. (2020) showed a decline in chl-a to ~0.03 mg m⁻³ (-1.5 log₁₀(mg m⁻³)) in January in Baffin Bay in the Arctic Ocean. We showed wintertime chl-a consistent to these observations (Figure 3d, 4d) during January. Ko et al. (2024) showed wintertime values of ~0.15 mg
- m^{-3} (~-0.8 log₁₀(mg m⁻³)) in the Chuckhi Sea, which would be consistent with the observations near the shelf in the North Pacific Ocean (Figure 3b, 4b). These comparisons to earlier results in the literature indicate that the BGC-Argo relationships applied to the OC-CCI data are able to capture the wintertime chl-a concentrations and their regional differences. The independent assessment conducted using the OC-CCI in situ chl-a validation dataset (Valente et al., 2022) in this study
- 340 reinforces that the wintertime chl-a values are consistent with the observations (Figure 5) and that they maintain any potential regional biases in the underlying OC-CCI dataset. However, both the comparisons to literature and the validation dataset are limited by the number of *in situ* measurements collected during winter.





The decline in chl-a during winter as identified by the BGC-Argo relationships indicate clear differences between the Southern and Northern Hemisphere (Figure 2). This appears to be consistent with our understanding of biogeochemical differences between the two regions (Arteaga et al., 2020; Deppeler and Davidson, 2017). For example, the Southern Hemisphere showed a slower decline in chl-a during the winter compared with the Northern Hemisphere (Figure 2). The difference may reflect the competing limitations of light and iron availability on the evolution of phytoplankton chl-a (e.g., Arteaga et al., 2020) and the associated variations in phytoplankton bloom phenology across a relatively large geographical area (Sallée et al., 2015; Turner et al., 2024) in the Southern Ocean. In the Northern Hemisphere, which includes the Arctic Ocean, phytoplankton growth is closely related to the retreat of sea ice and the subsequent availability of light. Macronutrients (nitrate, phosphate and silicate) are rapidly depleted by phytoplankton growth in the sunlit layer during the spring bloom and remain depleted until wintertime mixing replenishes these from deeper waters (e.g., Manizza et al., 2023), at which time phytoplankton growth becomes light limited (Ardyna and Arrigo, 2020). These limitations at the onset of

355 winter may produce the steeper decline in chl-a concentrations in the Northern Hemisphere, from the spring- and autumntime chl-a. The relationships determined from the BGC-Argo profilers would therefore appear consistent with our understanding of the seasonal variability in phytoplankton.

Interannual variability in the response of the wintertime chl-a was apparent, particularly in the Southern Hemisphere (Figure 360 3e, f). Although the observation-based approach developed here does appear to capture interannual variability in the winter chl-a response, it is potentially underestimated. Reasons for this include the possibility that the BGC-Argo relationship may not fully capture the interannual variability between the autumn or springtime chl-a and the wintertime response. Alternatively, the mean interannual relationship will inherently be weighted towards the years (and their conditions) in which more BGC-Argo profiles were available during winter, i.e., the 2014 and 2018 periods (Figure 1). We do not see this as a limitation of the gap filling method as the differences are likely to be captured within the calculated uncertainties. As the BGC-Argo network reaches the intended ~1,000 profilers (Roemmich et al., 2019; although not all of these could have chl-a

- BGC-Argo network reaches the intended ~1,000 profilers (Roemmich et al., 2019; although not all of these could have chl-a sensors), the interannual differences in the BGC-Argo chl-a wintertime relationships could be further investigated. However, at the time of writing there are ~700 BGC-Argo floats globally, of which ~400 floats have chl-a sensors.
- The exploitation of satellite-based chl-a data records within, for example, ocean CO_2 sink assessments, is currently hampered by the missing data due to both cloud cover and in polar regions during wintertime. Within these assessments, the biological component has been shown to be an important predictor variable in approaches to estimate the in-water CO_2 concentrations (Ford et al., 2022). However, currently to exploit chl-a (or primary production) data within these assessments the missing polar winter data are filled with fixed chl-a concentrations. For example, Gregor and Gruber (2021) set a fixed value of 0.3
- 375 mg m⁻³ (~-0.5 log₁₀(mg m⁻³); blue dashed line in Figure 4). Here, the results show that the use of fixed values for wintertime chl-a concentrations overlooks the regional variability in wintertime chl-a and can in some cases lead to an elevated chl-a concentration above that of the spring bloom during wintertime (Figure 4e, f). These fixed values will also not capture the





interannual variability in the wintertime data, which could lead to discontinuities in the chl-a data record and the predicted in-water CO₂ concentrations. The approach and resulting data presented here could therefore be used for these studies as it provides a gap-filled chl-a data record that is consistent with the underlying ocean colour satellite climate data record.

Although we advocate for dynamic values and using observation-based approaches, the under-ice regions were filled with a fixed value of 0.1 mg m⁻³. The observational chl-a information under ice coupled with no availability of satellite ocean-colour data inherently limits our ability to assign a dynamic value for these under-ice regions. Many studies have identified
localised under ice phytoplankton blooms that can reach chl-a greater than 1 mg m⁻³ (Arrigo et al., 2012, 2014; Boles et al., 2020), but their prevalence over the larger synoptic scales is unclear. Capturing these dynamics will rely on further advances in our understanding of these under-ice environments. BGC-Argo profilers have been deployed with ice avoidance systems (Randelhoff et al., 2020), which could be more widely deployed in sea ice regions to provide an in situ constraint to these under ice environments. Within our approach, the choice of a fixed under-ice chl-a value will have different effects
depending on the application. But it likely has limited effect on the ocean CO₂ sink approaches previously mentioned due to the current assumptions of no CO₂ exchange occurring in regions of high ice concentrations (see references within Watts et al., 2022).

The OC-CCI provides a climate-quality and consistently produced chl-a data record that performs well at the global scale 395 (Sathyendranath et al., 2019). For our approach, the BGC-Argo chl-a were bias-corrected to the OC-CCI observations to maintain the consistency within the wintertime gap filled values, with respect to the observational record. Although the approach could be applied without first bias-correcting the BGC-Argo chl-a, this would introduce a bias 'step' that could impact the retrieval of the seasonal cycle and the determination of trends within the record (Van Oostende et al., 2022). A bias 'step' would reduce the consistency with the OC-CCI observations and the whole record which is a key component of a climate data record. The ability to produce consistent wintertime data with the underlying satellite data record (Figure 2 and

3) also allows the methods to be transferred to other data records (e.g., Hong et al., 2023).

Our results would indicate further *in situ* observations within the Southern Hemisphere and North Pacific Ocean would improve the ability to incorporate and assess the accuracy of approaches for estimating wintertime chl-a concentrations. But equally, it reinforces the need for continued development of the OC-CCI record, and underlying chl-a retrieval algorithms

(e.g., O'Reilly & Werdell, 2019).



5. Conclusion

- In this study, we present an observation-based approach to fill gaps in the polar wintertime chl-a satellite data using BGC-410 Argo profiler observations. We apply the approach, alongside a cloud gap filling approach based on spatial kriging, to monthly 0.25 ° composites of chl-a from the Ocean Colour Climate Change Initiative (OC-CCI) climate data record to produce a gap-filled and spatially complete data record between 1997 and 2023 along with the propagated uncertainties. Data from BGC-Argo profilers during the polar winter were used to construct relationships between the wintertime chl-a and the last available autumntime and first available springtime satellite observations. The BGC-Argo based gap filling approach
- 415 retains the accuracy of the underlying dataset, as assessed with independent *in situ* observations, to produce a coherent timeseries. The resulting data identifies biogeochemical differences in the wintertime chl-a response between the Southern and Northern Hemispheres, whereby the Northern Hemisphere showed a faster and larger decline in chl-a than that in the Southern Hemisphere. These differences appear consistent with our understanding surrounding the seasonality of phytoplankton in these biogeochemical different regions.
- 420 Applying the polar winter gap filling approach indicated that the gap-filled timeseries correctly captures the wintertime decline in chl-a and the interannual variability in the wintertime chl-a. The regional variability in the wintertime chl-a illustrated that the use of fixed values (as often used in the literature) to fill polar wintertime data is likely unsuitable and will result in misleading analyses and could even result in wintertime chl-a concentrations higher than those observed during the spring when concentrations peak. The gap filling approach could be applied to any satellite based chl-a timeseries, and
- 425 theoretically, for any biogeochemical variable that displays a similar wintertime response (e.g., particulate organic carbon or primary production). This study therefore provides a gap-filled coherent timeseries that can be exploited by communities that require spatially complete, gap-filled timeseries, for example as needed by machine learning approaches.

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Data and Code Availability

The monthly 0.25° gap-filled OC-CCI record are available from Zenodo (Ford et al., 2025b). The OC-CCI climate data record (v6) were retrieved from <u>https://doi.org/10.5285/5011D22AAE5A4671B0CBC7D05C56C4F0</u> (Sathyendranath et al., 2023a), and the 2023 extension from <u>https://www.oceancolour.org/</u>. The OSI-SAF sea ice concentrations (v3) were retrieved

445 from <u>https://doi.org/10.15770/EUM_SAF_OSI_0013</u> (OSI SAF, 2022). The code supporting this work is available at <u>https://github.com/JamieLab/SCOPE-ArgoChla</u> and archived at Ford et al. (2025a).

Competing Interests

The authors declare no competing interests.

Author Contributions

450 DJF and JDS conceived the study. DJF developed the methodology with inputs from JDS, GK and SS. DJF wrote the original draft. All authors contributed to reviewing and editing the manuscript.

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