Alternate History: A Synthetic Ensemble of Ocean Chlorophyll Concentrations

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Abstract Internal climate variability plays an important role in the abundance and distribution of phytoplankton in the global ocean. Previous studies using large ensembles of Earth system models (ESMs) have demonstrated their utility in the study of marine phytoplankton variability. These ESM large ensembles simulate the evolution of multiple alternate realities, each with a different phasing of internal climate variability. However, ESMs may not accurately represent real world variability as recorded via satellite and in situ observations of ocean chlorophyll over the past few decades. Observational records of surface ocean chlorophyll equate to a single ensemble member in the large ensemble framework, and this can cloud the interpretation of long-term trends: are they externally forced, caused by the phasing of internal variability, or both? Here, we use a novel statistical emulation technique to place the observational record of surface ocean chlorophyll into the large ensemble framework. Much like a large initial condition ensemble generated with an ESM, the resulting synthetic ensemble represents multiple possible evolutions of ocean chlorophyll concentration, each with a different sampling of internal climate variability. We further demonstrate the validity of our statistical approach by recreating an ESM ensemble of chlorophyll using only a single ESM ensemble member. We use the synthetic ensemble to explore the interpretation of long-term trends in the presence of internal variability and find a wider range of possible trends in chlorophyll due to the sampling of internal variability in subpolar regions than in subtropical regions.

1. Introduction

The ocean biosphere strongly influences biogeochemical cycling, carbon export, and air-sea carbon flux. Although phytoplankton constitute a relatively small reservoir of carbon, their ability to photosynthetically fix carbon from the atmosphere enhances the ocean's role as a carbon sink, allowing the ocean to store 45 times more carbon than the atmosphere (Friedlingstein et al., 2019). The efficiency and strength of the ocean biological pump can influence atmospheric carbon dioxide concentrations; in the absence of the ocean biosphere, atmospheric carbon dioxide concentrations would increase by approximately 50% of pre-industrial values (McKinley et al., 2017).

Internal climate variability plays an important role in the abundance and distribution of phytoplankton in the global ocean. Modes of internal climate variability, such as the El Niño Southern Oscillation (ENSO), the Southern Annular Mode (SAM), and the North Atlantic Oscillation (NAO), alter the physical and chemical environment for, and thus the abundance of, phytoplankton on timescales ranging from interannual to multi-decadal (Chavez et al., 1998; Lovenduski & Gruber, 2005; Thomas et al., 2009; Zhai et al., 2013). Correlations between these climate indices and marine phytoplankton have been demonstrated on regional and local scales using several decades of remotely sensed and in situ observations (Behrenfeld et al., 2001; Chavez et al., 1998; Lovenduski & Gruber, 2005; Thomas et al., 2009; Zhai et al., 2013). For example, bio-optical data from moorings in the Central Equatorial Pacific revealed a reduction in phytoplankton biomass coincident with the 1997–1998 El Niño event, driven by the reduced upwelling of nutrients and subsequent declines in phytoplankton productivity (Chavez et al., 1998). Modes of internal climate variability have also been shown to affect regional upwelling, and thus phytoplankton productivity, in Eastern Boundary Upwelling Systems such as the California and Humbolt Current Systems (Thomas et al., 2009). These studies
demonstrate that the phasing and magnitude of internal climate variability has a measurable imprint on
the ocean chlorophyll record.

Multiple studies have used coupled Earth system models (ESMs) or stand-alone ocean biogeochemical mod-
els to illustrate the influence of internal climate variability on biological processes, often through the lens
of air-sea carbon flux (Bopp et al., 2013; Hauck et al., 2013; Le Quéré et al., 2000; Lenton & Matear, 2007;
McKinley et al., 2018; Wang & Moore, 2012). For example, several modeling studies suggest that SAM has
a marked influence on phytoplankton productivity in the Southern Ocean (Hauck et al., 2013; Lenton & 
Matear, 2007; Wang & Moore, 2012) while ENSO has been demonstrated to impact net primary production
(NPP) in tropical regions (Kwiatkowski et al., 2017). Globally, an analysis of upper ocean dissolved inor-
ganic carbon (DIC) revealed correlations between modeled phytoplankton abundance and ENSO, SAM, and
NAO (Long et al., 2013). Mechanisms of the connection between modes of variability and phytoplankton
biomass have been explored using biogeochemical models to attribute regional changes in biomass to
internal variability driven fluctuations in nutrient supply and light availability (McKinley et al., 2018). Thus,
ESMs are an important tool for developing an understanding of the impact of internal variability on the
abundance and distribution of marine phytoplankton.

Large initial condition ensembles of ESMs are a recently developed research tool for the representation
and analysis of internal variability in the climate system (Bengtsson & Hodges, 2019; Dai & Bloeker, 2019;
Deser et al., 2020; Kumar & Ganguly, 2018). In this approach, each ESM simulation or ensemble member is
initialized slightly differently and thus produces a phasing of internal climate variability that is not identical
to the other ensemble members. Analyses of variability in global air temperature and precipitation using a
subset of initial condition large ensembles conducted with the Coupled Model Intercomparison Project
Version 5 (CMIP5) models reveal that internal variability accounts for approximately half of the spread in
projected climate trends across North America and Europe over the next half century (Deser et al., 2020;
Hawkins & Sutton, 2009, 2011). Additionally, regional differences in the range of internal variability have
also been reported from large ensembles, with subtropical regions experiencing a relatively lower range of
coupled ocean-atmosphere variability (Deser et al., 2010, 2020).

Several recent studies have demonstrated the utility of large ensembles of ESMs for the study of marine
phytoplankton (Frölicher et al., 2016; Krumhardt et al., 2017; Rodgers et al., 2015). Krumhardt et al. (2017)
used the Community Earth System Model 1 Large Ensemble (CESM1-LE) to quantify the contribution
of internal climate variability to uncertainty in projections of NPP. Their analysis revealed that internal
climate variability challenges our ability to quantify the role of emissions mitigation for end-of-century
NPP changes, especially at regional scales. Other studies have identified NPP as a biogeochemical quantity
whose anthropogenic signal is slow to emerge from internal variability using the GFDL Earth System Model
2M (ESM2M; Frölicher et al., 2016; Rodgers et al., 2015; Schlunegger et al., 2019). The important role of
internal variability in NPP contributes to improved predictability of NPP relative to other biogeochemical
variables (Séférian et al., 2014). Thus, large initial condition ensembles of ESMs demonstrate the important
role of internal variability in the long-term changes in marine phytoplankton abundance and productivity.

Observational records of surface ocean chlorophyll concentration from satellite and in situ datasets equate
to a single ensemble member in the large ensemble framework. As such, the observational record cap-
tures only one of the many possible trajectories through climate space that could have occurred, even given
the same physical constraints and boundary conditions. For example, the multi-decade record of remotely
sensed ocean color from the Moderate Resolution Imaging Spectroradiometer (MODIS) recorded the re-
duction in chlorophyll concentration in the Eastern Equatorial Pacific associated with the dramatic 2015–2016
El Niño event (Coria-Monter et al., 2018). Due to this event occurring towards the end of our observational
record, it will have an outsized impact on our estimation of a linear trend. However, had a La Niña event
occurred, rather than an El Niño event, the linear trend estimated over the same period may have been
positive. With a single observational record it can thus be challenging to interpret changes in chlorophyll
concentration or phytoplankton productivity even over long-term (multi-decadal) timescales due to sam-
ppling of internal variability. A complementary approach to quantifying internal variability in phytoplankton
abundance is to construct an observationally constrained synthetic ensemble by statistically emulating the
observational record. This “observational large ensemble” allows us to simulate how phytoplankton would
respond given a different phasing of internal variability, illustrating a range of possible long-term chlorophyll trends.

In this study, we place the observational record of surface ocean chlorophyll concentration into the large ensemble framework by constructing a synthetic ensemble of observed chlorophyll. Much like a large initial condition ensemble generated with an ESM, the synthetic ensemble represents multiple possible evolutions of ocean chlorophyll concentration, each with a different phasing of internal climate variability (ENSO, PDO, and other climate noise). We use statistical emulation techniques to illustrate the importance of internal climate variability for the interpretation of trends in the observational record. We further evaluate our synthetic ensemble methodology in the context of a large initial condition ensemble generated with an ESM to demonstrate that our approach is valid.

2. Data and Model Output

In our analysis, we construct a synthetic ensemble of surface ocean chlorophyll concentration using both remotely sensed and in situ observations. We then evaluate our statistical method using a large initial condition ensemble of an ESM as a testbed. Here, we describe the observational data and the model testbed. We describe the generation of the synthetic ensemble in Section 3.

2.1. Observations

2.1.1. Ocean Color Datasets

Marine phytoplankton have been observed over the past several decades by multiple satellite instruments with varying spatial and temporal coverage. Here, we utilize the global ocean chlorophyll concentration estimated by the MODIS ocean color dataset, as it provides the longest continuous record of global ocean chlorophyll concentration, with coverage from 2002 to present. Analyses of the MODIS ocean color data set were conducted using level 3 composites of 8 day mean output at 9 km resolution of chlorophyll a concentration (mg m\(^{-3}\)) obtained from the NASA Ocean Color Archive (http://oceancolor.gsfc.nasa.gov/). The OCI algorithm was used to convert ocean color measurements to total chlorophyll concentration in mg m\(^{-3}\). The data set was averaged to monthly and coarsened to 1° resolution for comparison with output from the CESM1-LE.

2.1.2. Ocean Time-Series Measurements

We additionally use in situ surface ocean chlorophyll measurements from the Hawaii Ocean Time Series (HOT). Photosynthetic pigment concentrations are measured both in situ using a fluorescence sensor attached to a CTD instrument which is lowered through the water column and through High Performance Liquid Chromatography (HPLC) analysis of water samples which are collected at discrete depth intervals in the water column (Tupas et al., 1997). This observational dataset provides the longest continuous record of surface ocean chlorophyll, with coverage from 1989 to 2018 (Karl & Lukas, 1996). In contrast to the MODIS ocean color data set which provides a shorter record and global coverage, the HOT dataset provides a longer record at a discrete location. Analyses of the HOT dataset were conducted using chlorophyll a concentration (mg m\(^{-3}\)) obtained from the HOT Data Organization and Graphical System (https://hahana.soest.hawaii.edu/hot/). Chlorophyll a concentration is measured using HPLC analysis. The data set has been resampled at monthly intervals using linear interpolation between measurements and averaged over the upper 10 m for comparison with output from our modeling tool, described next.

2.2. Community Earth System Model Large Ensemble

We evaluate our statistical methodology using output from the Community Earth System Model 1 Large Ensemble (CESM1-LE; Kay et al., 2015). CESM1 is a fully coupled climate model that provides simulations of Earth's past climate and projections of Earth's future climate under historical and Representative Concentration Pathway 8.5 external forcing by simulating the evolution of the atmosphere, ocean, land, and sea ice component models (Hurrell et al., 2013). The ocean physical model is the ocean component of the Community Climate System Model version 4 (Danabasoglu et al., 2012). The model has a nominal 1°
resolution and 60 vertical levels. The biogeochemical-ecosystem ocean model consists of an upper-ocean ecological module which incorporates multi-nutrient co-limitation on phytoplankton growth and specific phytoplankton functional groups (Moore et al., 2004), and a full-depth ocean biogeochemistry module which incorporates full carbon system thermodynamics and a dynamic iron cycle (Doney et al., 2006; Moore & Braucher, 2008).

The CESM1-LE models the spatiotemporal evolution of the climate system by simulating multiple ensemble members, each with slightly different initial conditions. Each member is branched from a multi-century 1850 control simulation with constant pre-industrial forcing (Lamarque et al., 2010). The ocean model in the control simulation was initialized from observations (January mean climatological potential density and salinity data from the Polar Science Center Hydrographic Climatology), while the other component models were initialized from previous CESM1 simulations (Danabasoglu et al., 2012). Once the control simulation climate achieved quasi-equilibrium with the 1850 forcing, the first ensemble member was initialized from a January 1, year 402 in the control run. Ensemble member 1 was integrated forward from 1850 to 2100. The remaining ensemble members were integrated from 1920 to 2100 using slightly different initial conditions generated by round-off level differences in their initial air temperature fields from January 1920 of ensemble member 1 (Kay et al., 2015). Due to the chaotic nature of the atmosphere, the small differences in initial conditions quickly propagate through the atmosphere and lead to each ensemble member experiencing a different evolution of internal variability. A total of 40 ensemble members were generated in this fashion for the CESM1-LE experiment. Six CESM1-LE members had corrupted ocean biogeochemistry, therefore, we use the 34 CESM1-LE members with valid ocean biogeochemistry. Analyses of model output were conducted using monthly mean output at 1° resolution over the historical period (1920–2005) due to its realistic volcanic forcing. We consider chlorophyll concentration in the uppermost model layer (10 m) by summing each of the three phytoplankton functional types (diatoms, diazotrophs, and small phytoplankton).

3. Creating a Synthetic Ensemble of the Observational Record

We create a synthetic ensemble to highlight the role of internal variability in historical, observed surface ocean chlorophyll. To generate the synthetic ensemble, we build upon the statistical model developed in McKinnon and Deser (2018) and McKinnon et al. (2017) and additionally described in Elsworth et al. (2020), with slight modifications to the approach. We model chlorophyll concentration as:

$$X_{it} = \beta_i + \beta_S m(t) + \beta_F F + \beta_{\text{ENSO}} M_{\text{ENSO}} + \beta_{\text{PDO}} M_{\text{PDO}} + \epsilon_{it},$$  

where $X$ is the chlorophyll concentration at the location $i$ and time $t$, and $m(t)$ indicates the month associated with time $t$. In this model, chlorophyll is described as a linear combination of the mean state $\beta_i$, seasonality $\beta_S m(t)$, the assumed spatially uniform response to external forcing $\beta_F$, response to climate modes $\beta_{\text{ENSO}} M_{\text{ENSO}}$ and $\beta_{\text{PDO}} M_{\text{PDO}}$, and residual internal climate variability $\epsilon_{it}$. Importantly, the $\beta_i$ term in Equation 1 represents the response to external forcing, while $\beta_{\text{ENSO}} M_{\text{ENSO}}$ and $\beta_{\text{PDO}} M_{\text{PDO}}$ and $\epsilon_{it}$ capture the role of internal climate variability in chlorophyll concentration. The time series $M_{\text{ENSO}}$ and $M_{\text{PDO}}$ represent the evolution of the climate modes ENSO and PDO, respectively, which have been shown to influence chlorophyll concentration (Gregg & Conkright, 2002; Radenac et al., 2012; Yoder & Kennelly, 2003). The Niño 3.4 and PDO indices were obtained from the National Oceanographic and Atmospheric Administration Climate Prediction Center. As in McKinnon and Deser (2018), we address the covariance between ENSO and PDO by creating two orthogonal time series via principal component analysis of the original observed temporal evolution of ENSO and PDO from 1880 to 2020.

3.1. HOT

To illustrate our approach, we create a synthetic ensemble of chlorophyll concentration averaged over the upper 10 m of the water column at HOT, a discrete location in the Subtropical North Pacific. The synthetic ensemble is created in a two-step process (Figure 1). First, we estimate the parameters ($\beta$’s in Equation 1; top panel, Figure 1). Second, we simulate alternate evolutions of chlorophyll over time given different phasings in the climate modes (ENSO and PDO) and by resampling the residuals ($\epsilon$ in Equation 1; bottom panel, Figure 1).
To develop the synthetic ensemble of chlorophyll at HOT, we first remove the mean state, $\beta_0$, from the time-varying chlorophyll, such that the resulting anomaly time series centers around zero (Figure 1a). We then remove the monthly climatology, $\beta_S$, by removing the monthly average in chlorophyll concentration from the anomaly time series (Figure 1b). Note that for this illustration, we assume that the externally forced trend, $\beta_F$, is zero. Finally, we estimate the dependence of chlorophyll on the climate modes ENSO and PDO, $\beta_{\text{ENSO}}$ and $\beta_{\text{PDO}}$, by assuming a linear relationship and calculating the ordinary least squares regression of the deseasonalized anomalies with the ENSO and PDO indices (Figure 1c). The regression coefficients, $\beta_{\text{ENSO}}$ and $\beta_{\text{PDO}}$, are then multiplied by the observed indices, $M_{\text{ENSO}}$ and $M_{\text{PDO}}$, and subtracted from the deseasoned anomalies, leaving us with chlorophyll residuals, $\epsilon$ (Figure 1d).

We apply two techniques to simulate alternate evolutions of chlorophyll concentration over time at HOT. First, the residuals, $\epsilon$, are resampled 1,000 times using the nonparametric moving block bootstrap (MBB) in time (Figure 1e). The MBB captures high frequency temporal variability by resampling the data set with a block length sufficiently large compared to the temporal autocorrelation scale but sufficiently small to generate variability between bootstrapped samples. In this context, the residuals are resampled using a block length of 12 months which encapsulates the seasonal cycle in global chlorophyll concentration variability.

Although block bootstrapping tends to underestimate trend variability when the data are positively correlated and the data record is short, the validation of the statistical method using a large ensemble of an ESM suggests that the methodology does not generally underestimate trend variability (McKinnon et al., 2017). Second, the response of chlorophyll concentration to different possible evolutions of the climate modes over time is incorporated by generating 1,000 surrogate climate modes of ENSO and PDO using the iterative adjusted amplitude Fourier transformation (IAAFT) method (Figure 1f; Schreiber & Schmitz, 1996). This surrogate data approach produces an ensemble of time series with the same amplitude distribution and spectra as the original climate mode time series. The surrogate climate modes are multiplied by the regression coefficients, $\beta_{\text{ENSO}}$ and $\beta_{\text{PDO}}$, estimated from the observed record to create time series of chlorophyll that could have occurred given a different temporal evolution of ENSO and PDO. We combine the block

$$X_i = \beta_0 + \beta_S + \beta_F + \beta_{\text{ENSO}} M_{\text{ENSO}} + \beta_{\text{PDO}} M_{\text{PDO}} + \epsilon_i$$
bootstrapped anomalies and the response to the surrogate climate modes with $\beta_0$ and $\beta^S_{\text{im}1}$ to produce multiple distinct synthetic ensemble members at HOT (Figure 1g).

Figure 2 illustrates the temporal evolution of 10 synthetic ensemble members for the surface ocean chlorophyll concentration at HOT. Each ensemble member has a unique phasing of internal climate variability that results in a distinct temporal evolution for surface ocean chlorophyll at this location. Yet, our method ensures that each ensemble member has similar statistical properties to the original observed time-series. This synthetic ensemble can thus inform our interpretation of the chlorophyll record at HOT by simulating how phytoplankton would respond given a different phasing of internal variability. The phasing of such variability will influence trend estimates of chlorophyll, potentially moderating conclusions regarding the observed trend over the observational record. However, a limitation of the statistical methodology remains that the variability in the observational record will be emulated in the synthetic ensemble by the statistical model. It is appropriate for us to expand the method to a broader spatial scale, and we explore this using satellite chlorophyll observations in the next section.

3.2. MODIS

We demonstrate the role of internal variability on chlorophyll across the global ocean by generating a synthetic ensemble at every $1^\circ \times 1^\circ$ grid cell. We begin with monthly chlorophyll concentration collected over the MODIS mission from 2002 to 2020. In regions with high cloud coverage such as the high latitudes, chlorophyll concentration is linearly interpolated to prevent a sparsity of observations. Although the method of modeling internal variability over the full spatial grid is similar to modeling internal variability at a discrete location, there are two key differences. First, we approximate the externally forced signal, $\beta^F_t$, as the linear trend in global-mean chlorophyll concentration ($2.75 \times 10^{-5}$ mg m$^{-3}$ yr$^{-1}$ from 2002 to 2020), assuming that the global-mean trend is most representative of the externally forced component. Second, our method produces spatially varying regression coefficients, $\beta_{\text{ENSO,PDO}}^{\text{im}_1}$ (Figure S1), that can then be multiplied by the observed indices, $M_{\text{ENSO,PDO}}$, to model the direct influence of climate modes. Due to the sparsity of the ocean color record at high latitudes, the estimation of $\beta_{\text{ENSO}}^{\text{im}_1}$ and $\beta_{\text{PDO}}^{\text{im}_1}$ may be less reliable in these regions. The coefficients are combined with the synthetic climate mode time series to produce a spatially coherent pattern in the synthetically generated chlorophyll for a given time in a given ensemble member.

Figure 2. Temporal evolution of chlorophyll a concentration in mg m$^{-3}$ averaged over the upper 10 m at the Hawaii Ocean Time Series (HOT). The original time series is shown in the black line and 10 synthetic ensemble members generated from the record are shown in the gray dashed lines. The range of possible evolutions displayed by the synthetic ensemble members illustrates the importance of internal climate variability on observational records, even over relatively short timescales.
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The synthetic ensemble of the MODIS ocean color record thus represents multiple possible alternative evolutions of ocean chlorophyll over time at every 1° x 1° grid cell.

We showcase the synthetic ensemble by mapping the anomalous chlorophyll concentration in the Equatorial Pacific Ocean in December 2015, during the observed 2015–2016 El Niño event (Figure 3). Anomalous chlorophyll concentrations are calculated as the difference between the December chlorophyll concentration in 2015 and the average December chlorophyll concentration over the period 2002 to 2020. Observed anomalies in chlorophyll concentration from the MODIS ocean color record show anomalously low chlorophyll concentrations in the Eastern Equatorial Pacific due to regional changes in the distribution of nutrients (Figure 3c). In contrast, synthetic ensemble member 73 displays anomalously high chlorophyll concentrations in this region, as this ensemble member experiences a La Niña-like event during December 2015, promoting an influx of nutrients to the surface and enhanced phytoplankton productivity (Figure 3a). Synthetic ensemble member 427 displays an intermediate magnitude of anomalous concentration, reflective of its ENSO neutral conditions (Figure 3b). Differences between the synthetic ensemble members and the observational record illustrate how internal variability can play an important role in chlorophyll concentration in this region. We also observe large differences between the synthetic ensemble and the observational record outside of this region, where other components of internal variability such as the PDO or other climate noise dominate (not shown).

4. Evaluating the Synthetic Ensemble Methodology Using CESM1-LE

Supplied with chlorophyll concentration from only a single ensemble member of an ESM large ensemble, can we reproduce the variability in the other ESM large ensemble members using our statistical methodology? In other words, can we produce a valid ensemble from a single record, analogous to producing an ensemble from our single observational record? To answer this question, we apply the statistical approach outlined above (Figure 1) to the surface ocean chlorophyll concentration from individual ensemble members of the CESM1-LE over the historical period (1920–2005). We generate 1,000 synthetic ensemble members for each of the 34 members of the model ensemble by removing the global-mean ensemble mean linear trend ($-4.88 \times 10^{-6}$ mg m$^{-3}$ from 1920 to 2005; $\beta_0^s$), the monthly climatology ($\beta_{1-12}^s$) of each individual ensemble member, and the contribution linearly related to the climate modes ENSO and PDO ($\beta_{ENSO,PDO}^s M_{ENSO,PDO}$). Climate modes are sourced for each individual ensemble member using the Climate Variability Diagnostics Package (CVDP), an analysis tool that calculates major modes of climate variability in the CESM1-LE (Phillips et al., 2014). Synthetic ensemble members are generated by combining the block bootstrapped residuals and the surrogate climate modes with the terms previously removed. The synthetically generated ensembles are then evaluated against the full model ensemble to determine the robustness of the statistical method.

The interannual standard deviation in global-mean surface ocean chlorophyll concentration from the model-based, synthetically generated ensemble members exhibits a close correspondence to that of the full CESM1-LE. This is illustrated by similarities in the temporal evolution of global-mean chlorophyll concentration of the synthetic ensemble generated from ensemble member 14 (solid purple line and dashed light blue lines) and the original CESM1-LE ensemble (solid dark blue lines) over the historical period (Figure 4a). However, the statistical model mimics the internal variability in the CESM1-LE ensemble member used to create the synthetic ensemble, highlighting a limitation of applying our approach to a...
limited record. As such, ensemble members with relatively narrower ranges of internal variability, such as CESM1-LE ensemble member 3, produce synthetic ensembles with relatively narrower ranges of internal variability (light blue curve) compared to the full CESM1-LE model ensemble (dark blue curve; Figure 4b). In contrast, CESM1-LE ensemble members with relatively wider ranges of internal variability, such as ensemble member 22, produce synthetic ensembles with relatively wider ranges of internal variability (orange curve) compared to the full CESM1-LE model ensemble (dark blue curve; Figure 4b). This mismatch in interannual standard deviation is 0.002 mg m\(^{-3}\) at its largest (Figure 4b), which is small (4.1%) compared to the mean interannual standard deviation.

The interannual standard deviation in the surface ocean chlorophyll produced synthetically from the CESM1-LE compares favorably to that of the original CESM1-LE across a large fraction of the global ocean (Figure 5a). To illustrate this point, we estimate the fractional error in interannual standard deviation between the CESM1-LE and the synthetic ensemble generated from a randomly selected ensemble member (number 10) as \((\sigma_{\text{CESM1-LE}} - \sigma_{\text{SE}})/\sigma_{\text{SE}}\). Although regional differences exist in the relative underestimation (blue regions) or overestimation (red regions) of the standard deviation in our synthetic ensemble when compared to the original CESM1-LE, the fractional error of the synthetic ensemble is relatively low over the historical period (Figure 5a). Similarly low fractional errors are found for synthetic ensembles generated from other CESM1-LE members (not shown).

We repeat our approach for a period of 20 years near the end of the historical period (1987–2005) of the CESM1-LE, which is comparable to the length of the MODIS ocean color dataset and the HOT record. When compared to the model ensemble, the synthetic ensemble generated from ensemble member 10 exhibits a relatively higher fractional error over shorter timescales than longer timescales (Figure 5b). This result illustrates the limitations in applying this statistical method over shorter periods of time. Observations can provide a strong constraint on uncertainty related to internal climate variability over time, but only in cases where the dominant timescales of variability are resolved within the observed record.

5. Implications for the Interpretation of Observational Records

The synthetic ensemble can be used to illustrate how variable phasing in climate modes can produce different trends over the observational period, both at a discrete location and across the full spatial grid as in Elsworth et al. (2020). For example, Figure 6 illustrates the temporal evolution of two synthetic ensemble...
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members generated from the HOT dataset. Each member displays a trend of opposite sign over the observational period due to a different sampling of climate variability. Synthetic ensemble member 4 displays a trend of $4.01 \times 10^{-5}$ mg m$^{-3}$ yr$^{-1}$ while member 8 displays a trend of $-3.00 \times 10^{-5}$ mg m$^{-3}$ yr$^{-1}$. The range of trends for 1,000 synthetic ensemble members is between $6.40 \times 10^{-5}$ and $-5.43 \times 10^{-5}$ mg m$^{-3}$ yr$^{-1}$. Differing linear trends across the various synthetic ensemble members demonstrate an important role for internal variability in HOT chlorophyll trends.

Figure 7 displays the spatial pattern of the linear trend in annual-mean chlorophyll concentration for two distinct synthetic ensemble members generated from the MODIS record. Observed trends in real-world chlorophyll concentration (Figure 7c) show decreasing chlorophyll over time in the subtropical oceans and
the California Current Eastern Boundary Upwelling System, increasing chlorophyll over time in parts of the subpolar North Atlantic and Southern Oceans, and a statistically significant (hatched; determined by a t-test with a p-value less than 0.05) negative trend in the Equatorial Pacific. In contrast, synthetic ensemble members 16 (Figure 7a) and 45 (Figure 7b) exhibit trends of opposite sign from the observations across much of the ocean. For example, in the Eastern Equatorial Pacific, synthetic ensemble member 16 displays a trend toward increasing chlorophyll concentrations over time, while synthetic ensemble member 45 displays a statistically significant trend toward decreasing chlorophyll. This mismatch of trends is also apparent in the California Current Eastern Boundary Upwelling System, and parts of the subpolar North Atlantic, Indian, and Southern Oceans. Thus, results from our synthetic ensemble suggest that internal variability can cloud the interpretation of chlorophyll trends across much of the ocean, consistent with Elsworth et al. (2020), even when the trends are deemed statistically significant (as in the Equatorial Pacific), although we note that our MODIS results rely on a short record, which affects the performance of our method (Figure 5b).

Across much of the global ocean, different synthetic ensemble members produce dramatically different long-term trends (Figure 7). From this, we can infer that processes external to the climate system are challenging to detect in the observational record of chlorophyll in the majority of the ocean. Our findings thus complement those of several other studies that use a range of statistical methods to comment on detectability of the effects of anthropogenic climate change in the ocean biosphere (Beaulieu et al., 2013; Gregg & Rousseaux, 2014; Hammond et al., 2020; Henson, 2014; Henson et al., 2010, 2016).
Internal variability creates a wider range of possible chlorophyll trends in subpolar regions than in subtropical regions (Figure 8). A synthetic ensemble generated from the observed chlorophyll concentration averaged over the subpolar biomes generates a broader distribution of linear trends than a synthetic ensemble generated from observed chlorophyll concentration averaged over the subtropical permanently stratified biomes (cf. blue and orange curves in Figure 8; biomes defined as in Fay & McKinley, 2014), due to higher \( \sigma_{\text{var}} \) at high latitudes in our statistical model. This means that if we observe large absolute magnitude trends in chlorophyll in subpolar regions, they are much more likely to be driven by internal processes than in subtropical regions. This regional variation in internal trends can help to decode the likely causes of trends in chlorophyll from the observational record (e.g., Behrenfeld et al., 2007), especially between regions of relatively high productivity (subpolar regions) and regions of relatively low productivity (subtropical regions).

6. Conclusions

We place the observational record of surface ocean chlorophyll into the large ensemble framework by constructing a synthetic ensemble of observed chlorophyll using the HOT and MODIS datasets. The synthetic ensembles represent multiple possible evolutions of ocean chlorophyll concentration, each with a different phasing of internal climate variability. Our approach illustrates the importance of internal climate variability for the interpretation of trends in the observational record, and our findings can help to decode the causes of observed changes in chlorophyll across various oceanic regions. When applied to the CESM1-LE from 1920 to 2005, we are able to reproduce the variability in surface ocean chlorophyll concentration of the full model ensemble using our statistical methodology. However, our assumption that ENSO and PDO are linearly related to chlorophyll may not be a robust assumption. Additional assumptions underpinning our statistical model, such as the approximation of the global mean being representative of the externally forced trend and the residual variability being encapsulated by a block length of 12 months, may affect the interpretation of our results.

Limitations exist when applying this statistical method over shorter timescales, especially those comparable to the length of existing continuous observational datasets for surface ocean chlorophyll. Additionally, the approach assumes internal variability does not change with time, which may not be a valid expectation as the climate continues to change due to anthropogenic influence (Resplandy et al., 2015; Thompson et al., 2015). However, the synthetic ensemble can be used as an effective tool to illustrate the important role of internal variability in the evolution of a variety of ocean biogeochemical parameters provided a sufficient length of continuous observations are available. Future work can utilize this statistical methodology to compare the range of internal variability observed over the observational record with the range of internal variability generated in large ensemble modeling studies.

**Data Availability Statement**

HOT chlorophyll data are available at [https://hahana.soest.hawaii.edu/hot/hot-dogs/interface.html](https://hahana.soest.hawaii.edu/hot/hot-dogs/interface.html). The MODIS chlorophyll data were obtained from the National Aeronautics and Space Administration Ocean Color Archive at [https://oceancolor.gsfc.nasa.gov/](https://oceancolor.gsfc.nasa.gov/). The Niño 3.4 and PDO indices are available from the National Oceanographic and Atmospheric Administration Climate Prediction Center [https://www.cpc.ncep.noaa.gov/data/indices/](https://www.cpc.ncep.noaa.gov/data/indices/). CESM-LE output is available from the Earth System Grid at [http://www.cesm.ucar.edu/projects/community-projects/LENS/data-sets.html](http://www.cesm.ucar.edu/projects/community-projects/LENS/data-sets.html). Synthetic ensembles generated from the HOT and MODIS datasets are available at [https://osf.io/52c3s/](https://osf.io/52c3s/).
Acknowledgments
The authors thank the HOT research team for their sustained efforts collecting oceanographic data. CESM computing resources were provided by CSLI at NCAR; NCAR is sponsored by NSF. The authors are grateful for funding from NSF (OCE-1558225 and OCE-1752724).

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10.1029/2020GB006924
