Skillful multiyear predictions of ocean acidification in the California Current System

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Abstract: The California Current System (CCS) sustains economically valuable fisheries and is particularly vulnerable to ocean acidification, due to the natural upwelling of corrosive waters that affect ecosystem function. Marine resource managers in the CCS could benefit from advanced knowledge of ocean acidity on multiyear timescales. We use a novel suite of retrospective forecasts with an initialized Earth system model (ESM) to predict the evolution of surface pH anomalies in the CCS. Here we show that the forecast system skillfully predicts observed surface pH variations multiple years in advance over a naïve forecasting method. Skillful predictions of surface pH are mainly derived from the initialization of dissolved inorganic carbon anomalies that are subsequently transported into the CCS. Our results demonstrate the potential for ESMs to provide predictions relevant to managing the onset and impacts of ocean acidification in this vulnerable region.

Ocean acidification is an ongoing large-scale environmental problem, whereby the absorption of anthropogenic CO_2 by the ocean lowers its pH, impacting ocean ecosystems worldwide[1]. The California Current System (CCS) supports productive fisheries crucial to the US economy and is particularly vulnerable to ocean acidification due to the upwelling of naturally corrosive (*i.e.*, relatively low pH) waters to the surface[2]. The upwelling process results from equatorward winds along the western North American coastline. These winds facilitate both coastal upwelling and curl-driven Ekman suction, forcing waters enriched in carbon and nutrients from beneath the thermocline to the surface[3]. These nutrient subsidies drive high productivity in CCS waters, essential to supporting regional fisheries[4]. However, the upwelled waters are also corrosive due to their high content of remineralized carbon. The air-to-sea flux of anthropogenic CO_2 into the CCS further compounds this natural acidity. Multiple studies over the past decade have observed coastal CCS waters that are anomalously low in pH and undersaturated with respect to calcium carbonate minerals[5–7]. These conditions adversely affect a wide range of organisms that precipitate calcium carbonate shells, such as pteropods, coccolithophores, and shellfish[1]. These organisms are keystone species that support commercial and recreational fisheries which generate approximately $6B in revenue per year[8]. The CCS's intersection between economically valuable fisheries and natural vulnerability to ocean acidification makes it a high-priority region to study for multiyear biogeochemical predictions. With advanced warning of regional pH declines, managers of shellfisheries could select for more favorable sites (*i.e.*, regions forecasted to have more basic conditions) or buffer specific coastal waters with sodium carbonate[9].

Results

Forecasting ocean biogeochemistry in the California Current

Prediction efforts for the CCS have focused primarily on using seasonal forecasts of sea surface temperature[10–12] (SST) and biogeochemical variables[13] (*e.g.,* dissolved oxygen and bottom pH) as inputs into ecosystem forecasting models. A more recent effort demonstrates the potential for initialized predictions of surface chlorophyll in the CCS with two year forecasts[14]. However, no studies have attempted to predict ocean biogeochemistry in the CCS at the multiannual to decadal scale. This temporal scale is critical for fisheries managers, as it aids them in setting annual catch limits, changing and introducing closed areas, and adjusting quotas for internationally shared fish stocks[15]. However, decadal forecasting of ocean biogeochemistry is still in its infancy[16–20]. In the absence of biogeochemical predictions longer than nine months, managers rely upon the assumption that anomalies persist from year to year. These so-called persistence forecasts are commonly used as a baseline to put initialized skill into context and work at lead times commensurate with the decorrelation timescales of the system[10–12,15]. On the other hand, initialized predictions use a physically based modeling framework to advance information from initial conditions forward in time; if the system is predictable (*i.e.*, sufficiently deterministic) and the model skillful, this can yield a powerful forecasting framework. Recent ensemble simulations of initialized ESMs provide the most powerful tool currently available for improving upon decadal persistence forecasts. Their coupling of global physical models of the atmosphere, ocean, cryosphere, and land with the carbon cycle, terrestrial and marine ecosystems, atmospheric chemistry, and natural and human disturbances allows one to deeply investigate how interactions between the physical climate system and biosphere lead to predictability in a complex system such as the CCS[21]. These predictions have the potential to improve upon the persistence management method, pushing the horizon of forecasting ecosystem stressors past a single season or year.

Here we use an initialized global ESM with embedded ocean biogeochemistry, the Community Earth System Model Decadal Prediction Large Ensemble[22] (CESM-DPLE), to make retrospective forecasts of surface pH anomalies in the CCS from 1955 through 2017. The CESM-DPLE employs an ocean model with nominal 1° x 1° horizontal resolution and 60 vertical levels. Forty ensemble members were initialized annually on November 1st from a forced ocean-sea ice reconstruction (hereafter referred to as the "reconstruction") and then the coupled simulations were integrated forward for ten years (Fig. 1, A and B; see methods and supplementary). The reconstruction is skillful in representing surface pH variability on seasonal to interannual timescales in the CCS (Fig. S1). Due to the diverse terminology used in weather and climate forecasting[23], we are careful with our definitions. We use the phrase "potential predictability" when referring to correlations between CESM-DPLE and the reconstruction. High correlation coefficients (*i.e.*, high potential predictability) represent the theoretical upper limit for predictions in the real world, given the chaotic nature of the climate system[24]. We use the phrase "predictive skill" when comparing CESM-DPLE to observations; skill demonstrates our ability to predict the true evolution of the real world with CESM-DPLE. We quantify our ability to predict anomalies with the anomaly correlation coefficient (ACC), and our accuracy in predicting anomaly magnitudes with the mean absolute error (MAE). We compare our initialized forecasts to a simple persistence forecast and the uninitialized CESM Large Ensemble[25] (CESM-LE) mean, which includes the same external forcing (*i.e.*, rising atmospheric CO_2) as the CESM-DPLE. The former assesses whether CESM-DPLE is useful relative to a simple forecasting method, while the latter determines the degree to which initialization engenders predictability beyond that afforded by supplying the model with time-varying forcing. We test predictive skill by comparing the initialized forecasts to a gridded observational product of surface pH from the Japan Meteorological Agency (JMA), which spans 1990–2017[26,27]. This product is based upon empirical relationships derived for alkalinity and pCO_2 as functions of *in situ* measurements, such as SST and sea surface height, which were then used in a carbonate system solver to derive gridded surface pH (see methods). Our focus in this study is on surface pH anomalies within the California Current Large Marine Ecosystem (see Fig. 1C for the spatial domain). We remove a second-order trend from all surface pH time series, since the long-term ocean acidification signal dominates over the 1954–2017 period (Fig. 1A). We aim to test our ability to predict year-to-year variations in CCS surface pH anomalies (Fig. 1B), which act to temporarily accelerate or slow down the ongoing ocean acidification problem.

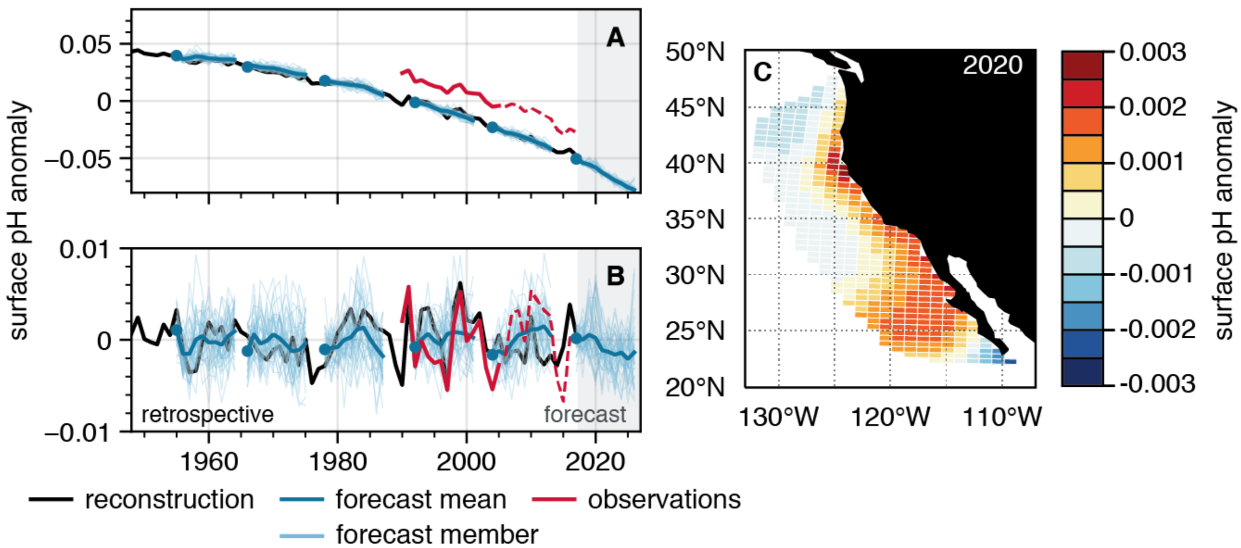

Fig. 1. *CESM-DPLE experimental design and near-future surface pH anomaly forecast.* (**A**) Trended and (**B**) detrended area-weighted annual surface pH anomalies for the (black) reconstruction, (red) observational product, and (blue) CESM-DPLE decadal forecasts initialized in 1954, 1965, 1977, 1991, 2003, and 2017 (other initializations were omitted for visual clarity). The dark blue line is the ensemble mean forecast, and thin blue lines are the individual 40 forecasts. The dashed red lines denote when the model loses observed variability in atmospheric CO_2 forcing (see Fig. S7A). (**C**) 2020 forecast for detrended surface pH anomalies in the CCS, based on the lead year 3 forecast initialized on November 1st, 2017. Positive values denote a basic anomaly (reduction in the ocean acidification trend), while negative values denote an acidic anomaly (acceleration of the ocean acidification trend).

Predictions of simulated and observed surface pH

Retrospective forecasts of detrended annual surface pH anomalies in the CCS suggest a potential to predict multiple years in advance over a simple persistence forecast (Figs. 2 and 3). Although a persistence forecast is valuable at lead year one in parts of the CCS (Fig. 2F), the initialized forecast is statistically significant over persistence nearly everywhere (Fig. 2K). By lead year two, persistence begins to yield negative ACCs in the southern portion of the CCS, while retaining some positive correlation in the north; ACCs become non-significant and weakly negative from lead year three and beyond (Fig. 2, H to J). The initialized forecast, in contrast, retains predictability in the central and southern CCS through lead year five (Fig. 2, A to E). Initialized predictions have higher ACCs than a persistence forecast everywhere out to five-year leads, save for three coastal grid cells along the coastal Pacific Northwest in lead year three (Fig. 2, K to O). An area-weighted perspective of the CCS reveals that the initialized forecast is significantly better than both persistence and the uninitialized forecast through five-year leads (Fig. 3A). The lead year one ACC of 0.72 explains over 50% of the variance in predicted surface pH anomalies and is comparable or better than the skill achieved by seasonal forecasts of SSTs in the CCS[10,11]. The MAE is smaller than both persistence and the uninitialized forecast over all ten lead years (Fig. 3B).

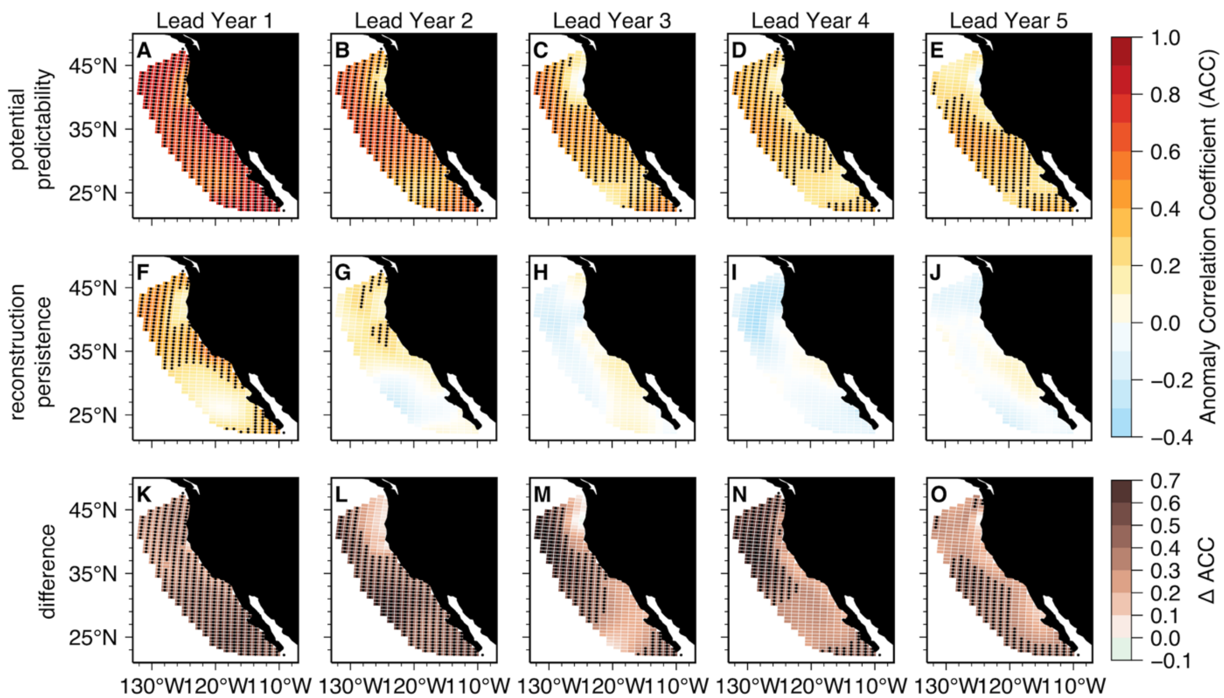

Fig. 2. *Potential predictability of surface pH in the California Current*. (**A** to **E**) CESM-DPLE initialized forecast of detrended annual surface pH anomalies for lead years one through five correlated with the reconstruction. (**F** to **J**) Persistence forecast for the reconstruction for lead years one through five. Stippling in **A** to **J** denotes statistically significant correlations at the 95% level using a *t* test. (**K** to **O**) Difference between the CESM-DPLE forecast ACCs and persistence. Stippling indicates that the initialized prediction is statistically significant over the persistence forecast at the 95% level using a *z* test. Only positive ACCs and ΔACCs are stippled.

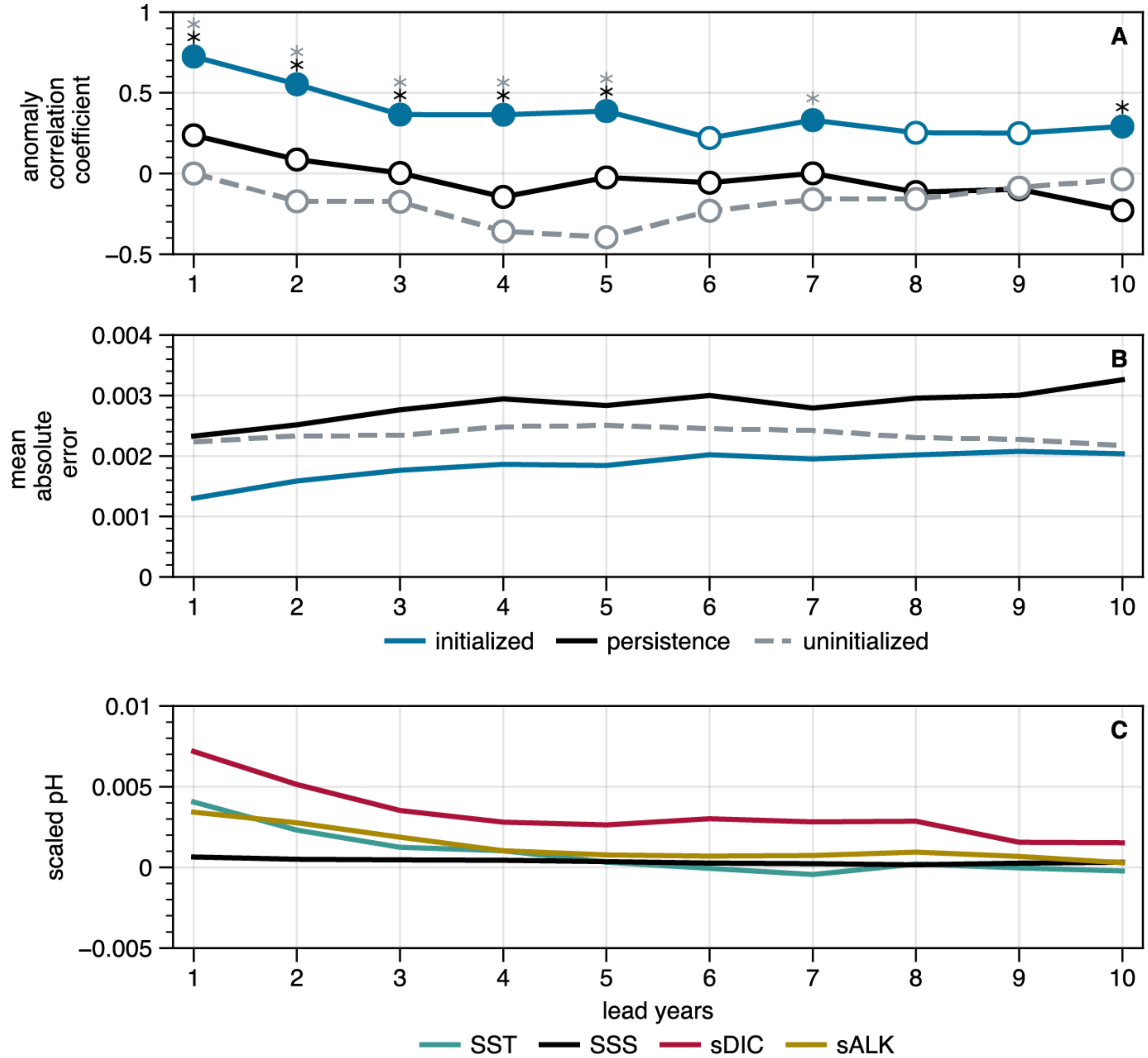

Fig. 3. *Area-weighted potential predictability of surface pH in the California Current and driver variables of surface pH predictability.* (**A**) ACCs for ten lead years for (blue) CESM-DPLE, (black) a persistence forecast from the reconstruction, and (grey) the uninitialized CESM-LE. Filled circles denote statistically significant positive correlations at the 95% level using a *t* test. Black and gray asterisks indicate significant predictability over persistence and the uninitialized forecast at the 95% level using a *z* test, respectively. (**B**) As in (**A**), but for MAE and without significance testing. (**C**) Scaled predictability in common pH units (see supplementary methods) of (black) sea surface salinity, (teal) sea surface temperature, (gold) salinity-normalized alkalinity, and (red) salinity-normalized dissolved inorganic carbon.

Because the reconstruction simulates the mean state, seasonal cycle, and variability of surface pH in the CCS well (Figs. S1 and S2), potential predictability extends to predictive skill relative to the observational product (Fig. 4). Initialized predictions have positive ACCs throughout the CCS at lead year one (Fig. 4A), and have significant skill over persistence through lead year four from Cape Mendocino to Baja California (Fig. 4, K to N). Persistence in the observationally based surface pH estimates is somewhat useful south of Cape Mendocino at lead year one, but yields negative ACCs from lead years two to five throughout most of the CCS (Fig. 4, F to J). Note, however, that virtually none of these correlations are statistically significant. Across all five lead years, ACCs from the initialized predictions are larger than those of observational persistence for most of the CCS (Fig. 4, K to O), with an area-weighted mean ΔACC ranging from 0.17 to 0.48. Skill is lost for the southernmost portion of the CCS by lead year two (Fig. 4B), followed by the Pacific Northwest at lead year three (Fig. 4C). Bias in the initialized predictions of the observational surface pH (as measured by the MAE) are smaller than that of observational persistence for most of the CCS over five lead years (Fig. S5). Our results suggest that CESM-DPLE could be used for multiyear forecasting of surface pH variability in the CCS today. Fig. 1C shows the forecast of surface pH anomalies in the CCS for 2020, which corresponds to a lead year three forecast from the November 1st, 2017 initialization of CESM-DPLE. Our forecast suggests that variability in surface pH will reduce the ocean acidification trend along the coastline and in the southern CCS, but will slightly enhance the trend offshore in the central and northern CCS.

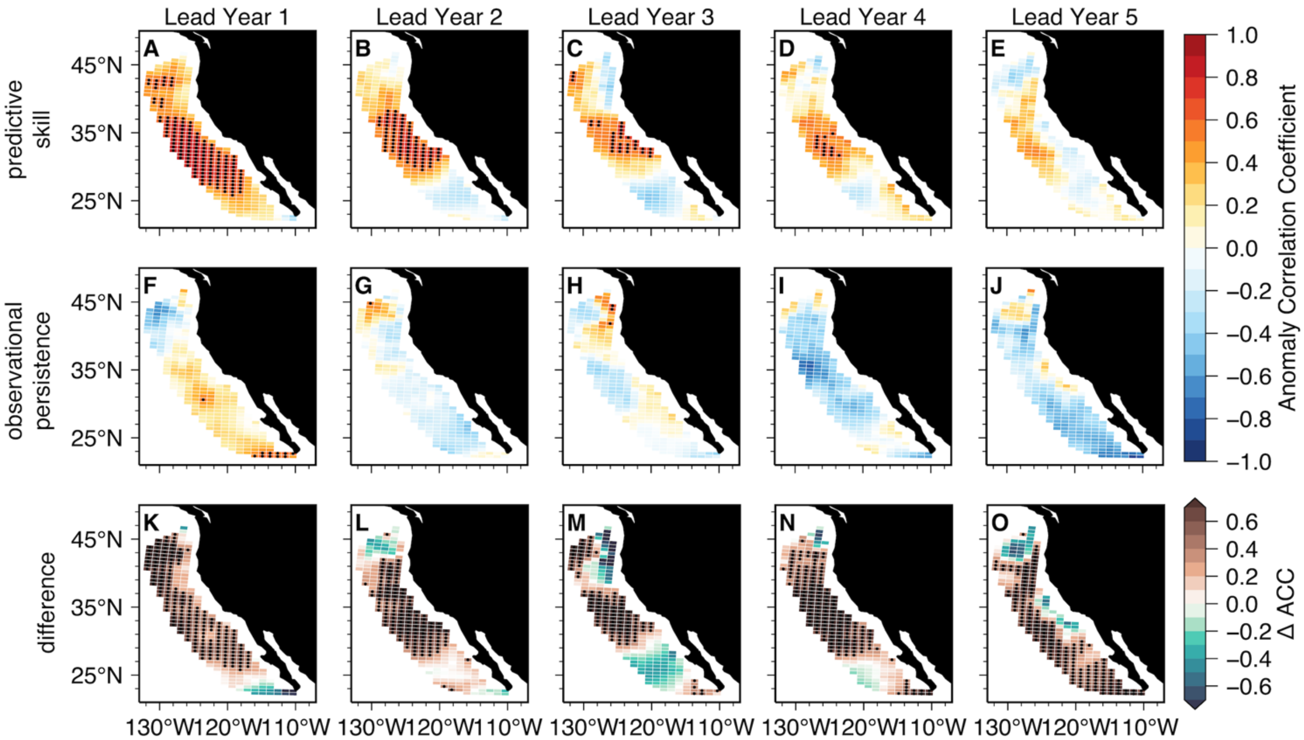

Fig. 4. *Predictive skill of surface pH anomalies in the California Current*. (**A** to **E**) CESM-DPLE initialized forecast of detrended annual surface pH anomalies for lead years one through five correlated with the observational product over 1990–2005. (**F** to **J**) Persistence forecast for the observations for lead years one through five. Stippling in **A** to **J** denotes statistically significant correlations at the 95% level using a *t* test. (**K** to **O**) Difference between the CESM-DPLE forecast ACCs and observational persistence. Stippling indicates that the initialized prediction is statistically significant over the observational persistence forecast at the 95% level using a *z* test. Only positive ACCs and ΔACCs are stippled.

Mechanisms of pH predictability

We are further interested in what lends predictability to surface pH in the CCS. We begin by investigating predictability in the driver variables of pH: temperature, salinity, dissolved inorganic carbon (DIC), and alkalinity. By scaling these variables to common pH units (see supplementary for method), we can deduce which drivers aid the most in predicting surface pH. We find that predictability in salinity-normalized DIC (sDIC) has the largest influence on surface pH predictability over all lead years (Fig. 3C). The combined predictability of both SSTs and alkalinity is roughly equivalent to sDIC over the first five lead years, while sea surface salinity plays a negligible role over all lead years (Fig. 3C). Predictability in sDIC is mainly driven by the persistence of its anomalies, but is enhanced further by initializations (Fig. S3). A budget analysis of DIC in the upper 150m of the CCS suggests that variability in vertical and lateral DIC advection plays a leading role in setting the DIC inventory, as evidenced by the high correlation between the advective flux and total tendency terms ($r = 0.9$; Fig. S4). Source waters for the CCS exhibit substantial interannual to decadal variability and are mainly comprised of subarctic waters transported by the California Current (upper 200 m) and eastern tropical Pacific waters transported by the California Undercurrent (200–300 m), which propagate biogeochemical anomalies into the system[28,29]. Thus, the subsurface and basin-wide initializations of DIC—as well as predictability of meridional and vertical transport variability—are crucial factors in making skillful multiyear predictions of surface pH variability. In turn, enhanced observations or reanalysis of these fields would be necessary for operational forecasting of surface pH in the CCS.

Discussion

While this study presents a very promising first result, there are some caveats worth noting. Simulations were run with a spatial resolution of approximately 100 km x 100 km. In turn, we do not explicitly resolve the fine-scale coastal upwelling of corrosive waters (which occurs within roughly 30 km of the coastline in the CCS), but instead simulate the combined effect of coastal and curl-driven upwelling in nearshore grid cells. Our simulation also uses subgrid scale parameterizations to capture the important process of eddy-induced offshore flux of tracers in the CCS[30,31]. Despite the coarse resolution, previous work has shown that alongshore winds, upwelling, and air-sea CO_2 fluxes are well-represented in this configuration of CESM relative to observations[32,33]. In this study, we only highlight predictability in annual averages of surface pH, since predictability at annual resolution is much higher than that of monthly resolution. However, we do find significant predictability over persistence of surface pH anomalies through June of the upwelling season following initialization, and into May of the following upwelling season (Fig. S6). Lastly, in assessing predictive skill, we are challenged by the limited coverage of gridded surface pH observations. While the observational product used in this study spans 1990–2017, the observational data for atmospheric CO_2 used to force the reconstruction ended in 2005, after which point a smooth scenario-based projection was used (Fig. S7A). This causes a drop-off in the ability of the reconstruction to replicate observed surface pH anomalies (Fig. S7B). Thus, we only assess skill over the 1990–2005 period, limiting our degrees of freedom for statistical significance.

Our results demonstrate for the first time the potential for an initialized ESM to retrospectively predict surface pH multiple years in advance in a complex, sensitive, and economically important oceanic region. Although our study highlights CESM-DPLE's ability to predict surface pH anomalies, other ocean acidification parameters—such as calcium carbonate saturation states—can be expected to be predictable, due to their common dependence on variability in dissolved CO_2. By detrending our simulated and observational products prior to analysis, we show that we have the potential to predict interannual variations in surface pH. As the ocean acidification signal dominates in this region over decadal timescales, multiyear predictions of surface pH variability could aid in forecasting the acceleration or slowdown of ocean acidification in the CCS.

Methods

Model simulations

The Community Earth System Model Decadal Prediction Large Ensemble[22] (CESM-DPLE) is based on CESM, version 1.1, and uses the same code base, component model configurations (Table S1), and historical and projected radiative forcing as that used in its uninitialized counterpart, the CESM Large Ensemble[25] (CESM-LE). This includes historical radiative forcing (with volcanic aerosols) through 2005 and projected radiative forcing (including greenhouse and short-lived gases and aerosols) from 2006 onward. Because CESM-DPLE and CESM-LE have an identical code base and boundary conditions, the two ensembles can be compared directly to one another to isolate the relative influence of initialization and external forcing on hindcast predictability and skill.

CESM-DPLE was generated via full-field initialization each year on November 1st from 1954 to 2017, for a total of 64 initialization dates[22]. An ensemble of 40 forecast members—created by round-off perturbations made to atmospheric initial temperature field—were integrated forward from each initialization for 122 months. The ocean and sea ice model components were initialized from a forced ocean-sea ice reconstruction (referred to as the “reconstruction”; see following section for configuration details), while atmosphere and land components were initialized from the November 1st restart files of a single member of CESM-LE. In particular, the ocean biogeochemical model used in all CESM simulations in this study is the Biogeochemical Elemental Cycling (BEC) model, which contains three phytoplankton functional types (diatoms, diazotrophs, and a small calcifying phytoplankton class), explicitly simulates seawater carbonate chemistry, and tracks the cycling of C, N, P, Fe, Si, and O[34,35]. Note that the ocean biogeochemistry and simulated atmospheric CO_2 concentration are diagnostic, such that there is no feedback onto the simulated physical climate[22]. Further details on drift adjustment and anomaly generation can be found in the supplemental.

The reconstruction simulation was run from 1948–2017 with active ocean and sea ice model components from CESM, version 1.1, with identical spatial resolutions as the freely coupled CESM-DPLE and CESM-LE (Table S1). The ocean and sea ice components were forced by a modified version of the Coordinated Ocean-Ice Reference Experiment (CORE) with interannual forcing[36,37], which provides momentum, freshwater, and buoyancy fluxes between the air–sea and air–ice interfaces. CORE winds were used globally, save for the tropical band (30S–30N), where NOAA Twentieth Century Reanalysis, version 2[38] winds (from 1948–2010) and adjusted Japanese 55-year Reanalysis Project[39] winds (through 2017) were used to correct a spurious trend in the zonal equatorial Pacific sea surface temperature (SST) gradient[22]. No direct assimilation of ocean or sea ice observations was used in the reconstruction; thus, any faithful reproduction of ocean and sea ice climatology or variability is due mainly to the atmospheric reanalysis that drives the simulation[22].

Observational product

We compare initialized forecasts of surface pH to the Japanese Meteorological Agency (JMA) Ocean CO_2 Map product[26,40], which provides monthly estimates of pH from 1990–2017 over a 1° x 1° global grid. Surface pH was computed diagnostically with a carbonate system solver, using estimated surface alkalinity and pCO_2 as inputs. To compute gridded alkalinity, the ocean was divided into five regions, where empirical relationships were derived for *in situ* alkalinity as a function of sea surface height (SSH) and sea surface salinity[26] (SSS). Gridded observations of SSH and SSS (independent of the *in situ* observations) were then input into the empirical equations to derive gridded surface alkalinity. Gridded surface pCO_2 was computed through a multistep process. First, the ocean was divided into 44 regions and relationships between *in* situ pCO_2 and *in situ* SST, SSS, and Chl-*a* were derived by multiple linear regressions in each region for one to three of the variables[40]. The gridded pCO_2 product was then derived by applying these functions to independent gridded observations of SST, SSS, and Chl-*a*. Further details on the datasets used in deriving their product can be found in Takatani et al. 2014 and Iida et al. 2015.

Statistical analysis

We use deterministic metrics to compare the ensemble mean retrospective forecasts to one or both of the following baselines: (1) a persistence forecast, and (2) the uninitialized CESM-LE ensemble mean forecast. The persistence forecast of the reconstruction and observational product assumes that anomalies from each initialization year persist into all following lead years[41]. A comparison of the initialized forecast to the persistence forecast shows the utility of our initialized forecasting system over a simple, low-cost forecasting method; a comparison of the initialized forecast to the CESM-LE ensemble mean shows the utility of initializations (rather than external forcing) in lending predictability to the variable of interest. Unless otherwise noted, forecasts are analyzed at annual resolution. This corresponds to the January–December average following the November 1st initialization. In turn, lead year “one” truly covers lead months 2–14. When considering monthly predictions, lead month “one” corresponds to the November 1st–30th average following initialization.

We compute the anomaly correlation coefficient (ACC) via a Pearson product-moment correlation to quantify the linear association between predicted and target anomalies (where the target is either the model reconstruction, CESM-LE ensemble mean, or the observational product). If the predictions perfectly match the sign and phase of the anomalies, the ACC has a maximum value of 1. If they are exactly out of phase, it has a minimum value of -1. The ACC is a function of lead time[11,42]:

$$ACC(\tau) = \frac{\left(\sum_{\propto=1}^{N}\left(F'_{\propto}(\tau) \times O'_{\propto+\tau}\right)\right)}{\sqrt{\sum_{\propto=1}^{N} F'_{\propto}(\tau)^2 \sum_{\propto=1}^{N} {O'_{\propto+\tau}}^2}}$$

Where *F’* is the forecast anomaly, *O’* is the verification field anomaly, and the ACC is calculated over the period 1955–2017 (N=63) relative to the reconstruction and CESM-LE, and over 1990–2005 (N=16) relative to the JMA observational product. Note that N reduces by one for each subsequent lead year (*i.e.*, the verification window shrinks). We quantify statistical significance in the ACC using a *t* test at the 95%

confidence level with the null hypothesis that the two time series being compared are uncorrelated. We assess statistical significance between two ACCs (*e.g.*, between that of the initialized forecast and a simple persistence forecast for the same lead time) using a *z* test at the 95% confidence level with the null hypothesis that the two correlation coefficients are not different.

To quantify the magnitude of forecast error, or the accuracy in our forecasts, we use the mean absolute error[42] (MAE). The MAE is 0 for perfect forecasts and increases to infinity with the amplitude of the mean absolute difference between the forecasts and target. MAE is used instead of bias metrics such as the root mean square error (RMSE), as it is a more accurate assessment of bias in climate simulations[43].

$$MAE(\tau) = \frac{1}{N}\sum_{\propto=1}^{N} |F'_{\propto}(\tau) - O'_{\propto+\tau}|$$

We follow Lovenduski et al. (2019) to convert predictability in pH driver variables (SST, SSS, salinity-normalized dissolved inorganic carbon (sDIC), and salinity-normalized alkalinity (sALK)) to common pH units:

$$r_x \cdot \frac{dpH}{dx} \cdot \sigma_x$$

Where r_x is the ACC between anomalies in driver variable *x* and target anomalies, $\frac{dpH}{dx}$ is the linear sensitivity of pH to the driver variable, and σ_x is the standard deviation of driver variable anomalies in the reconstruction.

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Author contributions

RXB and NSL designed the study. RXB analyzed the data, prepared figures and tables, and wrote the paper. SGY and KL coordinated and ran CESM-DPLE and FOSI simulations. NSL, SGY, MCL, and KL provided invaluable feedback throughout the study and reviewed the manuscript.

Additional information

The authors of this study are unaware of any competing interests. Output from the CESM-DPLE and reconstruction can be downloaded through the Earth System Grid Federation (https://www.earthsystemgrid.org/dataset/ucar.cgd.ccsm4.CESM1-CAM5-DP.html). The JMA Ocean CO_2 map product can be downloaded online at https://www.data.jma.go.jp/gmd/kaiyou/english/co2_flux/co2_flux_data_en.html. Analysis was performed using climpred, an open source python package developed by the lead author for analyzing initialized forecast models. Documentation is available at https://climpred.readthedocs.io. Post-processed model output and observations as well as Jupyter notebooks used to create all figures in this study will be made available by the lead author on Zenodo and Github following acceptance and publication of this manuscript.

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