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Putting It All Together: Adding Value to the Global Ocean and Climate Observing Systems With Complete Self-Consistent Ocean State and Parameter Estimates

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In 1999, the consortium on Estimating the Circulation and Climate of the Ocean (ECCO) set out to synthesize the hydrographic data collected by the World Ocean Circulation Experiment (WOCE) and the satellite sea surface height measurements into a complete and coherent description of the ocean, afforded by an ocean general circulation model. Twenty years later, the versatility of ECCO's estimation framework enables the production of global and regional ocean and sea-ice state estimates, that incorporate not only the initial suite of data and its successors, but nearly all data streams available today. New observations include measurements from Argo floats, marine mammal-based hydrography, satellite retrievals of ocean bottom pressure and sea surface salinity, as well as ice-tethered profiled data in polar regions. The framework also produces improved estimates of uncertain inputs, including initial conditions, surface atmospheric state variables, and mixing parameters. The freely available state estimates and related efforts are property-conserving, allowing closed budget calculations that are a requisite to detect, quantify, and understand the evolution of climate-relevant signals, as mandated by the Coupled Model Intercomparison Project Phase 6 (CMIP6) protocol. The solutions can be reproduced by users through provision of the underlying modeling and assimilation machinery. Regional efforts have spun off that offer increased spatial resolution to better resolve relevant processes. Emerging foci of ECCO are on a global sea level changes, in particular contributions from polar ice sheets, and the increased use of biogeochemical and ecosystem data to constrain global cycles of carbon, nitrogen and oxygen. Challenges in the coming decade include provision of uncertainties, informing observing system design, globally increased resolution, and moving toward a coupled Earth system estimation with consistent momentum, heat and freshwater fluxes between the ocean, atmosphere, cryosphere and land.

Keywords: ECCO, global ocean inverse modeling, optimal state and parameter estimation, adjoint method, ocean observations, coupled Earth system data assimilation, ocean reanalysis, global ocean circulation

1. BACKGROUND

The central goal of the ECCO consortium is the production of global ocean state and parameter estimates in support of climate research. ECCO requires dynamical and kinematical consistency of its products, in particular, conservation of mass, heat, and salt throughout the estimation period. Avoiding shortcomings identified in atmospheric reanalysis (e.g., Bengtsson et al., 2004, 2007) and making optimal use of the sparse observational coverage calls for the use of smoothing methods from optimal estimation theory (Wunsch and Heimbach, 2007, 2013; Stammer et al., 2016). The ECCO method exploits information contained in observations both forward and backward in time, while avoiding unphysical perturbations of the time-evolving state that is being constrained. It is the only method that has been found to be practical and that avoids the shortcomings of reanalyses and combines the very diverse ocean data sets that we now have and will continue to collect. The underlying model serves as a "dynamical interpolator" between and beyond the often sparse and heterogeneously sampled observations (in space and time) of various types.

Among ECCO's early accomplishments was the production of the first generation of near-global ocean state estimates, covering the years 1992–1997 (Stammer et al., 2002, 2004; Stammer, 2003). The latest ECCO solution can be used to produce climatologies, based on most data available from the global observing system since the early 1990s, not only for temperature and salinity, but which also provides consistent three-dimensional flow fields and connected dynamical variables (e.g., sea level and bottom pressure), consistent surface forcing fields, and property budgets to explore the underlying dynamics (e.g., Ekman and Sverdrup transports, mixing, and vorticity fluxes) (Fukumori et al., 2018). Self-consistency among the range of state variables is invaluable for depictions of the global ocean, e.g., in terms of its overturning circulation (Cessi, 2019).

2. THE PRESENT

2.1. The ECCO Central Production

The ECCO estimation framework in production today has undergone a number of significant improvements and updates. Extending over the period 1992–2015 (an update to 2017 is currently under way), the latest product, ECCO version 4 release 3 (ECCOv4, Forget et al., 2015a; Fukumori et al., 2017), has increased horizontal and vertical resolution and covers the entire globe. The estimation framework has been extended to account for uncertain model parameters that are now routinely part of the inversion (Forget et al., 2015b). The production of the next-generation ECCO version 5 at higher spatial resolution is currently ongoing.

Observational data streams have vastly expanded (Fukumori et al., 2017), and the ways in which these are ingested into the estimation framework have been refined. The space-based backbone consists of daily along-track sea level anomalies from satellite altimetry (Forget and Ponte, 2015) relative to a mean dynamic topography (Andersen et al., 2016), monthly ocean bottom pressure anomalies from GRACE mascon solutions (Watkins et al., 2015), monthly sea surface temperature fields from passive microwave radiometry (Reynolds et al., 2002), monthly sea surface salinity fields from Aquarius (Vinogradova et al., 2014), and daily sea ice concentration fields (Peng et al., 2013; Meier et al., 2017). Major *in-situ* observing systems used in ECCO include the global array of Argo floats (Roemmich et al., 2009; Riser et al., 2016), ship-based CTD and XBT hydrographic profiles and gridded monthly climatological temperature and salinity fields from the World Ocean Atlas 2009 (WOA09, Antonov et al., 2010; Locarnini et al., 2010), tagged marine mammals (Roquet et al., 2013; Treasure et al., 2017), and ice-tethered profilers (ITPs) in the Arctic (Krishfield et al., 2008). The versatility of the estimation framework enables the inclusion of novel data sets, such as satellite and *in-situ* inferred electric conductivity as a measure of ocean heat content changes (Trossman and Tyler, 2019). Ocean mixing parameters have been inferred from a subset of Argo, ITP, and hydrographic observations (Cole et al., 2015; Whalen et al., 2015), and are starting to be included in the observational data streams [Trossman et al., in revision].

2.2. Selected Science Applications

Numerous scientific studies have been conducted with various ECCO solutions, leading to new insights into the ocean's role in climate. Partial summaries are in Wunsch et al. (2009), Wunsch and Heimbach (2013), and Fukumori et al. (2018). Here, we highlight two research areas and related studies that have been afforded by the latest ECCO solution. This review only allows for a compressed discussion.

2.2.1. Ocean Heat Content Changes During the Recent Surface Warming Slowdown (SWS) Period

Much attention has been given, both in the scientific literature and in public media to the apparent warming slowdown in global mean surface temperature (GMST) over the first decade of the twenty-first century compared to the 1990s (e.g., Medhaug et al., 2017). The focus on surface temperatures distracted from the fact that a volumetric index such as vertical integrals of heat content changes is a physically more complete climate indicator than (surface) area-based indices. In this context, Nieves et al. (2015) identified issues with several ocean reanalysis products in providing reliable vertical profiles of temperature changes. **Figure 1** shows decadal trends in global mean ocean temperature as a function of depth over the periods 1993–2001, 2002–2010, and the difference between the two, from ECCOv4 and two ocean hydrographies. Decadal difference profiles are not available for Argo, which only reached its global coverage in about 2006. The figure is adapted from Nieves et al. (2015), which did not provide any uncertainty estimates for the hydrographies. Compared to the ocean reanalysis trends analyzed by Nieves et al. (2015), which exhibits large deviations from hydrography, ECCOv4 shows a more credible fit to hydrography trends over much of the depth range 0–1,500 m. ECCO's depicted uncertainty (gray shading) represents the formal standard error computed from a least squares linear trend fit to the monthly ECCO values and scaled to account for the effective degrees of freedom (i.e., residual autocorrelation) assuming the residuals of the fit behave as a first-order autoregressive (AR1) process. Note further that the two hydrographics are markedly different in the upper 800 m. ECCOv4 also reproduces the apparent slowdown in surface temperature trends as compared to an optimally interpolated blend of *in-situ* and satellite SST data. The analysis is set against the larger backdrop of full-depth ocean heat content changes over the last few decades. The latest ECCOv4 estimate produces a global mean heating rate of 0.48 $\pm$ 0.16 W m^{-2}, which includes a 0.095 W m^{-2} geothermal flux (Wunsch, 2018). All uncertainties quoted are likely at lower bounds as they do not account for systematic errors. A full-depth analysis of vertical heat transport by Liang et al. (2017) shows the global mean heat flux imbalances to be small residuals of regionally large anomalies that underly contributions from multiple centers of action, that cooling layers at depths may result from adjustment to surface forcing centuries ago (Gebbie and Huybers, 2019), and the need for accurate budget closure. The use of Argo data since roughly 2006 and satellite altimetric data from 1993 onward in combination with dynamical consistency provides powerful constraints on the ECCO solution over the estimation period.

2.2.2. Origins of North Atlantic Water Mass Volumetric Variability

Quantifying Atlantic water mass variability in terms of its volumetric composition over time provides a powerful diagnostic for determining the relative role of diabatic (locally forced) vs. adiabatic (induced via advection) processes (Forget et al., 2011; Speer and Forget, 2013). An approach is to consider the volume of water contained within temperature classes, following Walin (1982). Such a study has been conducted by Evans et al. (2017) over the period 2004–2011, which

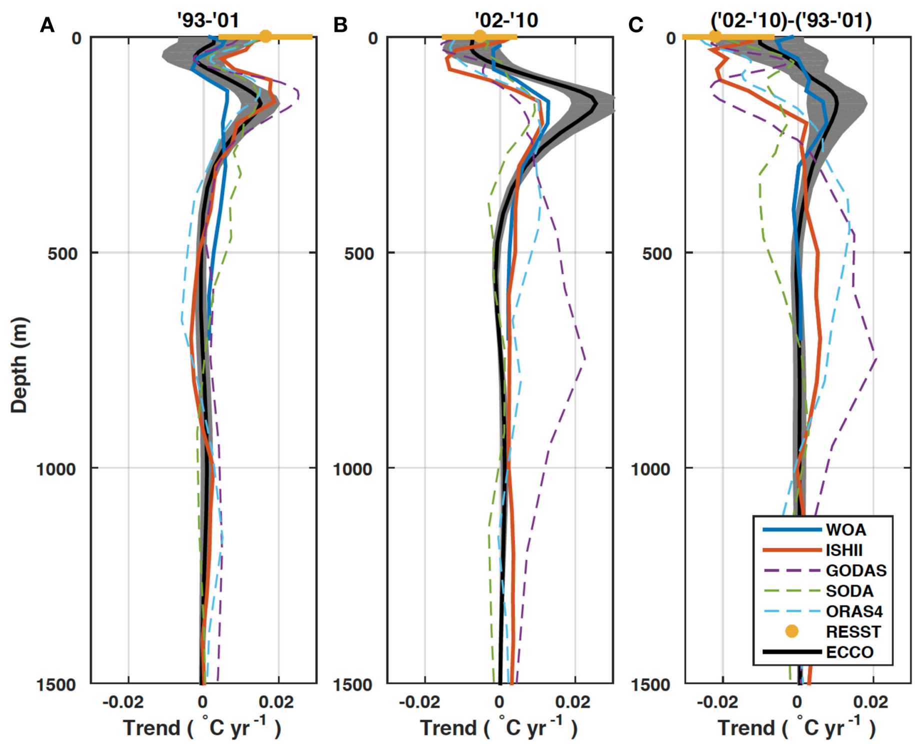

FIGURE 1 | Decadal trends in global mean potential temperature as function of depth over the periods 1993–2001 **(A)**, 2002–2010 **(B)**, and their difference **(C)**, inferred from two hydrographies, three ocean reanalysis and the ECCOv4 state estimate. Black: ECCOv4 (gray shading indicates formal standard error, see main text), dark blue: WOA (Levitus et al., 2012); red: Ishii (Ishii et al., 2005); purple: GODAS (Huang et al., 2010); green: SODA (Carton and Santorelli, 2008); light blue: ORAS4 (Balmaseda et al., 2012); yellow: SST (Reynolds et al., 2002). Adapted from National Academies of Sciences, Engineering, and Medicine (2016) (their Figures 4, 23).

includes the marked reduction in the Atlantic Meridional Overturning Circulation (AMOC) inferred at 26 N from the RAPID mooring array (Roberts et al., 2013). Water mass volume anomalies in temperature classes, $V(\theta, t)$, between 26 and 45 N (**Figure 2**, top panels) were derived from a gridded Argo product (Roemmich-Gilson Argo Climatology, RGAC; Roemmich and Gilson, 2009) and ECCOv4. Both products reflect seasonal exchange of volume between the warmer surface waters ($\theta > 18°$C) and mode/central waters (θ between 10°C and 18°C), as well as interannual variability in volumetric contributions of subtropical mode water ($\theta \sim 18°$C), among others. Determining water mass transformation rates between temperature classes, $\mathrm{d}V/\mathrm{d}t$, proves difficult for RGAC (**Figure 2c**), conceivably due to aliasing when sampling the mesoscale eddy field, but is feasible for ECCOv4 (**Figure 2d**). The analysis reveals negative volume anomalies during the winters of 2009/10 and 2010/11. For temperature classes larger than 15°C these anomalies are consistent with diabatic changes inferred from air-sea heat flux diagnostics (**Figure 2e**). However, for temperatures below 15°C, the adiabatic component as diagnosed from ECCOv4 (**Figure 2f**) explains the bulk of the volumetric census anomalies. The study provides compelling evidence that wind-driven transport anomalies led to a southward shift in the mean structure of the interior subtropical gyre circulation, weakening northward volume transport at 26 N. Evidence for the role of such advective signals has previously been gathered across an isolated line of latitude from the RAPID mooring array at 26 N (Cunningham et al., 2013).

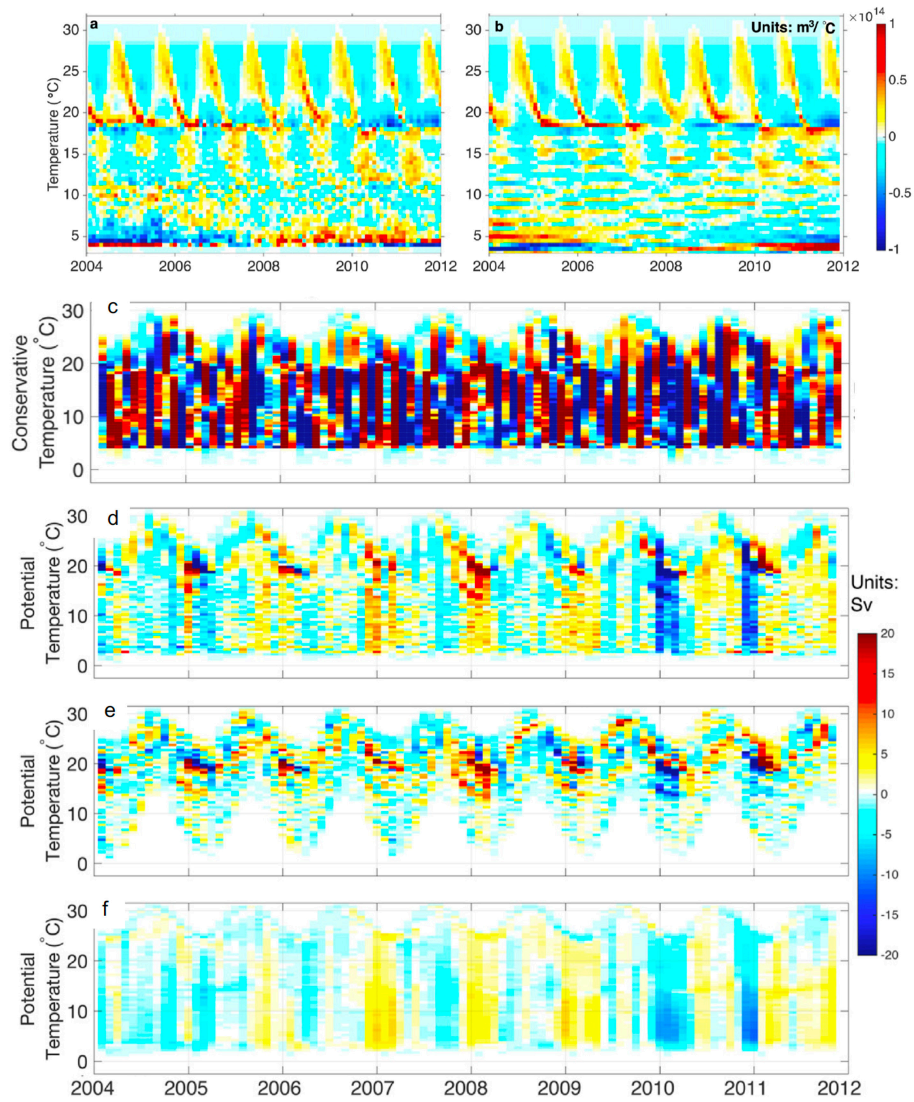

FIGURE 2 | Top panels: Volume anomaly in temperature classes, $V(\theta, t)$, with respect to the time mean in the North Atlantic between 26 and 45 N from **(a)** RGAC and **(b)** ECCOv4. Lower panels: Total monthly $\mathrm{d}V/\mathrm{d}t$ between 26 and 45 N from **(c)** RGAC and **(d)** ECCOv4. Also shown in **(e)** is the diabatic contribution to **(d)** inferred from monthly diathermal transformation due to air-sea heat fluxes, and **(f)** the adiabatic transformation in **(d)** implied by the volume change per temperature class due transport divergence between 26 and 45 N. For details, see Evans et al. (2017). ©American Meteorological Society. Used with permission.

2.3. Regional and Extended-Period Efforts

The tremendous computational cost involved in conducting the nonlinear least-squares optimization problem as well as the occurrence of strong nonlinearities have so far prevented the production of global eddy-resolving decadal state estimates. Instead, regional eddy-permitting estimates of limited duration have spun-off. These include the Southern Ocean State Estimate (SOSE, Mazloff et al., 2010), the Arctic Subpolar gyre sTate Estimate (ASTE, Nguyen et al., 2017), as well as estimates of the California Current System (Verdy et al., 2014), the tropical Pacific (Hoteit et al., 2010; Verdy et al., 2017), and the Gulf of Mexico (Gopalakrishnan et al., 2013). The versatility of the underlying ECCO infrastructure has facilitated these spin-offs. In turn, experience gained in the regional efforts has benefited the global estimation. Other non-ECCO related regional estimation efforts are summarized by Edwards et al. (2015).

An emerging emphasis has been on coupled ocean-sea ice estimation to account for Arctic and Southern Ocean sea ice. Dedicated efforts to develop a dynamic/thermodynamic sea ice model that fits within the estimation framework (Menemenlis et al., 2005; Heimbach et al., 2010; Losch et al., 2010; Fenty and Heimbach, 2013) led to an initial attempt at the global-scale coupled problem (Fenty et al., 2015). A major focus of ASTE is the finding of data used in Arctic research that are not necessarily part of global data repositories and assessing their use in state estimation (Nguyen et al., 2017). Emerging challenges are the use of satellite observations of sea ice (and snow) thickness, as well as remotely sensed drift data to constrain sea ice velocities.

Restricting estimates to the period with available satellite altimetric data limits the applicability of ECCO products for studies of decadal variability. This issue led to a dedicated effort by the German ECCO (GECCO) partners to extend the estimation period back to 1952 (Köhl and Stammer, 2008). Now in its second generation, GECCO2 has extended the period to cover the entire span of the available NCEP reanalysis, but at the cost of sparse observational coverage to constrain the solution prior to the 1990s. On these long timescales, there are issues with convergence of the optimization, which requires splitting the period into a number of smaller assimilation windows (Köhl, 2014). The challenge of quantifying uncertainties in the estimates that go along with changes in the observing system is exacerbated in the long state estimates.

2.4. Estimation Infrastructure, Data Access and Analysis Tools

A key enabling technology of ECCO is the ability to generate an adjoint version of the Massachusetts Institute of Technology general circulation model (MITgcm) for various configurations by means of algorithmic differentiation (Marotzke et al., 1999; Heimbach et al., 2005). Adjoint code generation via the open-source tool OpenAD (Utke et al., 2008) is being pursued. All ECCO state estimates are free-running solutions to the MITgcm and, as such, can be independently reproduced by users interested in performing new experiments (e.g., ocean response to idealized atmospheric wind stress forcing), determining the impact of new data constraints, and generating problem-specific model output (e.g., tracer dispersion). Extending the existing set of model-data misfit constraints is facilitated by the "generic cost" code framework introduced in ECCO v4. Instructions for re-running the model and complete model configurations (including parameters, initial conditions, atmospheric boundary conditions) are provided alongside the solutions (see **Table 1**).

ECCO products can be accessed via the ECCO webpage (ecco.jpl.nasa.gov). We are currently working to host the standard output fields on NASA's Physical Oceanography Distributed Data Center (PO.DAAC, podaac.jpl.nasa.gov), which will allow users to access the state estimate using several different technologies, including a new secure FTP-like interface (PO.DAAC Drive), Open-source Project for a Network Data Access Protocol (OPeNDAP), Thematic Realtime Environmental Distributed Data Services (THREDDS), and so-called web services enabling access via API protocols. A list of links to data products, model configurations, analysis tools and documentation is summarized in **Table 1** in the *Data Availability Statement* below.

3. THE FUTURE

With the increasing accuracy and skill of the ECCO state estimates, new scientific frontiers come into view. Most of these are related to capturing coupled variability, representing secular changes, and closing property budgets across different

TABLE 1 | Links to ECCO products, configurations, and documentation.

ECCO Products	
Latest product (ECCO v4,r3)	https://ecco.jpl.nasa.gov/products/latest/
All ECCO products	https://ecco.jpl.nasa.gov/products/all/
ECCOv4 release 3 documentation	
User guide (website)	https://ecco.jpl.nasa.gov/products/latest/user-guide/
Evaluating tracer budgets	http://hdl.handle.net/1721.1/111094
Reproduction (on premise or AWS cloud)	https://eccov4.readthedocs.io/en/latest/
Data constraints	http://hdl.handle.net/1721.1/120472
ECCOv4 release 3 analysis tools	
gcmfaces (Matlab)	https://gcmfaces.readthedocs.io/en/latest/
ecco-v4-py (Python)	http://ecco-v4-python-tutorial.readthedocs.io/
xmitgcm (Python)	https://xmitgcm.readthedocs.io/en/latest/
MITgcm (source code)	https://mitgcm.readthedocs.io/en/latest/

components of the Earth system (Buizza et al., 2018). In the following, we sketch several coupled problems that appear on the horizon.

3.1. Increased Horizontal Resolution

An increase in horizontal resolution in future ECCO products is targeted to begin resolving the geostrophic eddy field and its impact on the mean circulation. A drawback is the increased degree of nonlinearity of the underlying estimation problem, and the question over which time period the linearization was implied by the adjoint model remains valid. Possible limitations to long assimilation windows have been raised by Lea et al. (2000) and Köhl and Willebrand (2002), among others. A number of computational and practical solutions in the context of estimating statistical properties rather than nonlinear features ("eddy-fitting") and stabilizing the adjoint to improve controllability at high resolution have been proposed, e.g., by Hoteit et al. (2005), Abarbanel et al. (2010), Wang et al. (2014), and Gebbie and Hsieh (2017). Given the desire within ECCO for maintaining long assimilation windows, i.e. dynamical consistency, these methods are actively being pursued.

3.2. Coupled Ocean-Atmosphere Estimation

A natural extension of ECCO consists in the coupled ocean-atmosphere estimation problem, an avenue pursued by many reanalysis groups today (see Penny et al. [this issue] for a detailed review). Reasons include (i) the ability to close property budgets across the coupled system, (ii) to enable dynamical feedbacks, (iii) to obtain adjusted air-sea fluxes that are consistent with both ocean and atmosphere dynamics, (iv) to infer a coupled state that is balanced with respect to the underlying modeling framework and thus potentially more suitable for initializing extended predictions A major challenge consists in the disparity between oceanic and atmospheric time scales, the time window of validity of the model linearization, which in the atmosphere amounts to synoptic time scales (and in the ocean to resolved eddy turnover time scales), and implications for adjoint model stability for long assimilation windows.

Initial efforts at extending the ECCO capabilities to a fully coupled Earth system model are being conducted using intermediate complexity atmosphere/land models, such as the PlaSim model (Fraedrich et al., 2005; Blessing et al., 2014). This coupled model, called CEN Adjoint Model (CENAM), was put together such that an algorithmic differentiation tool can be used to construct its adjoint for state and parameter estimation purposes. Stammer et al. (2018) present a pilot study for computing adjoint sensitivities of the coupled climate system. To overcome strong nonlinearities, synchronization with observations approaches from dynamical systems theory are being explored to stabilize the adjoint model (Abarbanel et al., 2010; Lyu et al., 2018).

Complementary efforts to understand sensitivities of the ocean to the atmospheric state from a high-end atmospheric model are being conducted in preparation for coupling (Strobach et al., 2018). Other avenues using weak or hybrid coupled assimilation as well as approximate adjoints are also being pursued.

3.3. Coupled Ocean-Ice Sheet Estimation

There is mounting evidence that the increased mass loss from the polar ice sheets, Greenland (WCRP Global Sea Level Budget Group, 2018) and Antarctica (The IMBIE team, 2018), observed over the last two decades is linked to ocean circulation changes that have brought about warmer waters to the grounding zones of marine-terminating glaciers and ice shelves. Concerns over the implications of rising sea levels call for the joint treatment of the coupled ocean-ice sheet system. Substantial progress is being made, both with asynchronous coupling between the MITgcm and the Ice Sheet System Model (ISSM, Seroussi et al., 2017) as well as with synchronous, property-conserving coupling between the MITgcm's ocean and ice stream/shelf model (Goldberg et al., 2018; Jordan et al., 2018). The availability of adjoint models of all of these components, along with at least annually resolved satellite observations at Antarctica's marine margins, offer the prospect of developing a tightly coupled, skillful estimation system.

3.4. Coupled Ocean-Biogeochemistry and Ecology Estimation

The advent of profiling floats equipped with biogeochemical (BGC) sensors presents a revolution in data density for constraining BGC and ecosystem models. The software exists to assimilate these measurements along with remote sensing of ocean color into models (e.g., Gregg et al., 2009; Song et al., 2016; Verdy and Mazloff, 2017). BGC ocean property observations constrain many aspects of the Earth system, such that coupling not only informs the carbon system and ocean health, but also improves many other components of the Earth system models. Another thrust is the development of the ECCO-Darwin project, which combines physical and biological observations with the coupled framework of the eddy-permitting ECCO and Darwin ecosystem models (Follows and Dutkiewicz, 2011), but with significant remaining obstacles (Dutkiewicz et al., 2018).

3.5. Uncertainty Quantification (UQ) and Optimal Observing Network Design

Although formally an integral part of state and parameter estimation, deriving formal uncertainties accompanying the optimal estimates adds another level of computational complexity (National Academies of Sciences, Engineering, and Medicine, 2012). This has so far prevented most ocean reanalysis (or estimation) projects from dealing comprehensively with UQ. In the context of derivative-based estimation, identification of key metrics (or quantities) of interest enables the development of a formal chain that propagates the uncertainties from observations and uncertain parameters (priors) through the inference (i.e., posterior uncertainties at the optimal estimate) to the derived metrics of interest (Kalmikov and Heimbach, 2014, 2018). This Hessian-based framework lends itself to conducting optimal observing system design studies (see Fujii et al., under review) that provide valuable information on the optimal placement of available observational assets to maximize their utility in constraining key oceanographic quantities of interest (Köhl and Stammer, 2004).

3.6. Synergistic Use of Products and Model

While the state estimates are the central product of ECCO estimation, the virtue of their physical consistency is best realized by their analysis in conjunction with the underlying ocean general circulation model. The state estimates provide descriptions of the ocean, whereas the model affords its explanation; e.g., why is the ocean state what it is and why does it change as it does? As experience is gained, application of state estimation is expanding from drawing inferences from sampling the estimates akin to observations to quantitatively analyzing processes by utilizing the complete physics embodied in the model. Examples of such include analyses of property budgets that are closed without unresolved components (e.g., Buckley et al., 2015; Piecuch et al., 2017; Ponte and Piecuch, 2018), tracing origins and fate of ocean water masses (e.g., Fukumori et al., 2004; Gao et al., 2011; Qu et al., 2013) and quantifying causal mechanisms controlling the ocean (e.g., Fukumori et al., 2015; Pillar et al., 2016, 2018; Jones et al., 2018; Smith and Heimbach, 2019). The model's adjoint offers a unique tool in such efforts by providing an efficient means to evaluate physical dependencies among different quantities of interest. While the fidelity of state estimation will continue to evolve, existing systems provide a means to understanding and explaining what they do already resolve of the ocean. The full exploitation of state estimation requires a holistic approach and is ripe for innovation.

4. CONCLUDING REMARKS

The past two decades have seen substantial progress in the development and production of rigorous global ocean state and parameter estimates in support of climate research. That development has relied in part on the availability of continuous climate-quality records of quasi-global coverage, beginning with satellite altimetry (since 1992), satellite gravimetry (since 2003), and hydrographic profiles from the Argo float program (globally since ca. 2006). Sustaining such observing systems over long periods of time to build a climate record is a key imperative of ocean and climate monitoring (National Academies of Sciences, Engineering, and Medicine, 2017). The underlying computational estimation approaches used in the model-data synthesis serve several purposes: (i) they extract optimal information from the sparse and heterogeneous observational streams that constitute the Global Ocean Observing System (GOOS), (ii) they provide a quantitative framework for hypothesis testing and model parameter calibration, and (iii) they enable a quantitative understanding of the underlying dynamical and physical processes that have been learned jointly from observations and models. Much of what these approaches offer, for rigorous climate model calibration and initialization, remains under-explored. Realizing their full potential faces substantial practical hurdles but is indispensable for tackling important issues in ocean climate science. Increasing horizontal resolution and moving toward a comprehensive coupled Earth system estimation framework are major thrusts for the decade ahead.

DATA AVAILABILITY

ECCO strives to make all of its products available online to the scientific community. This includes the state estimates, ancillary fields to perform accurate budget calculations, the complete model configuration to reproduce the state estimate, analysis tools, as well as documentation. **Table 1** provides a comprehensive list of links to these resources.

AUTHOR CONTRIBUTIONS

All authors listed have made a substantial, direct and intellectual contribution to the work, and approved it for publication.

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