1 **Comparison of 4DVAR and EnKF State Estimates and Forecasts in the Gulf**
2 **of Mexico**

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ABSTRACT

15

16 **1. Abstract**

17 An experiment is conducted to compare four-dimensional variational (4DVAR) and ensem-
18 ble Kalman filter (EnKF) assimilation systems and their predictability in the Gulf of Mexico
19 (GoM) using the Massachusetts Institute of Technology general circulation model (MITgcm).
20 The quality of the ocean state estimates, forecasts, and the contribution of ensemble prediction
21 are evaluated. The MITgcm - Estimating the Circulation and Climate of the Ocean (ECCO)
22 4DVAR (MITgcm-ECCO) and the MITgcm - Data Assimilation Research Testbed (DART) EnKF
23 (MITgcm-DART) systems were used to compute two month hindcasts (March – April, 2010) by
24 assimilating satellite-derived along-track sea-surface height (SSH) and gridded sea-surface tem-
25 perature (SST) observations. The estimates from both methods at the end of the hindcast period
26 were then used to initialize forecasts for two months (May – June, 2010). This period was selected
27 because a Loop Current (LC) eddy (Eddy Franklin: Eddy-F) detachment event occurred at the end
28 of May 2010, immediately after the Deepwater Horizon (DwH) oil spill. Despite some differences
29 between the setups, both systems produce analyses and forecasts of comparable quality and both
30 solutions significantly outperformed model persistence. A reference forecast initialized from the
31 $1/12^\circ$ HYCOM/NCODA global analysis also performed well. The EnKF experiments for sen-
32 sitivity to filter parameters showed enhanced predictability when using more ensemble members
33 and stronger covariance localization, but not for larger inflation. The EnKF experiments vary-
34 ing the number of assimilation cycles showed enhanced short-term (long-term) predictability with
35 fewer (more) assimilation cycles. Additional hindcast and forecast experiments at other times of
36 significant LC evolution showed mixed performances of both systems that strongly depends on the
37 background state of the GoM circulation. The present work demonstrates a practical application
38 of both assimilation methods for the GoM and compares them in a limited number of realiza-

39 tions. The overall conclusion showing improved short-term (long-term) predictability for EnKF
40 (4DVAR) carries an important caveat that the results from this study are specific to a few 4DVAR
41 and EnKF LC eddy separation experiments in the GoM and cannot be generalized to conclude
42 the relative performances of both methods, especially in other applications. However, some of the
43 concepts and methods should carry over to other applications.

44 **2. Introduction**

45 Analyzing and predicting the ocean state has long been an important goal of the scientific com-
46 munity. Even though ocean observing platforms have witnessed tremendous developments in the
47 last decade, oceanic observations are still sparse and intermittent compared to the scales needed to
48 completely represent the ocean variability. Numerical models are routinely used to supply extra
49 information in the form of dynamic and kinematic constraints, but also bring uncertainties due to
50 poorly known inputs and parameters, limited resolution, approximate parameterizations of unre-
51 solved physics, and numerics. Efficient combination of numerical models and observations using
52 the framework of data assimilation (DA) is now recognized as the most effective way to forecast
53 the state of the ocean (Ghil and Malanotte-Rizzoli 1991; Wunsch 1996; Edwards et al. 2015).

54 DA methods exploit the model dynamics as an interpolator of the data in space and time. By
55 construction, they also readily provide a dynamical forecasting system that is updated by the ob-
56 servations. The theoretical framework of DA for oceanic problems is now well established and two
57 separate directions are usually followed; the deterministic variational approach and the statistical
58 filtering approach (Edwards et al. 2015). Variational methods seek the model trajectory that best
59 fits the observations by minimizing an objective function measuring the discrepancy between the
60 model predictions and observations by adjusting uncertain model parameters. Adjoint methods can
61 be used to compute the gradients needed for the optimization of the objective function (Le Dimet

62 and Talagrand 1986). Statistical methods proceed by sequentially updating a model prediction
63 every time new observations are available, taking into account their respective uncertainties. En-
64 semble Kalman filters (EnKFs), which are Monte Carlo implementations of the celebrated Kalman
65 filter, are now widely used in the ocean community (Hoteit et al. 2002; Tippett et al. 2003). The
66 readers are referred to a detailed review paper by Edwards et al. (2015) (and references therein)
67 on the historical developments of variational and sequential methods and recent advances in en-
68 semble and four-dimensional variational approaches in the context of regional ocean assimilation
69 systems.

70 DA is used to improve model representations of the ocean circulation at global and regional
71 scales, to test formal hypotheses in models, and to assess observing systems. Examples of ma-
72 jor ocean DA systems include the US NAVOCEANO forecasting system (Smedstad et al. 2003),
73 the Mediterranean Forecasting System (MFS) (Pinardi et al. 2003), the French MERCATOR sys-
74 tem (Brasseur et al. 2005), the Meteorological Research Institute Multivariate Ocean Variational
75 Estimation (MOVE) system (Usui et al. 2006), the Hybrid Coordinate Ocean Model (HYCOM)
76 Nowcast/Forecast system (Chassignet et al. 2007), the Australian Bluelink Ocean Data Assim-
77 ilation System (BODAS) (Oke et al. 2008). All these systems are based on so-called three-
78 dimensional DA methods (Optimal Interpolation - OI and three-dimensional variation - 3DVAR),
79 which are simplified versions of the Kalman filter (KF) operating with static error covariance ma-
80 trices. With progress in computing resources, transition to more advanced four-dimensional data
81 assimilation systems based on Four-Dimensional Variational (4DVAR) methods and the Ensemble
82 Kalman filters (EnKFs) methods is underway. Examples of the ongoing efforts to build advanced
83 4DVAR assimilation systems include the Nucleus for European Modelling of the Ocean (NEMO)
84 incremental variational system based on the observation-space formulation of the weak constraint
85 4DVAR (Mogensen et al. 2009), the Regional Ocean Modeling System (ROMS) 4DVAR with

its three variants: incremental strong constraint 4DVAR (I4DVAR), a dual formulation based on a physical-space statistical analysis system (4DVAR-PSAS), and a dual formulation representation-based variant of 4DVAR (R4DVAR) (Moore et al. 2011c,a,b), and the Estimating the Circulation and the Climate of the Ocean (ECCO) system, which uses the Massachusetts Institute of Technology general circulation model (MITgcm), and is enabled to adjust various model parameters and inputs (“model controls”) (Stammer et al. 2002; Wunsch and Heimbach 2007; Forget et al. 2015). Several other ocean data assimilation projects are designing their assimilation systems based on various flavors of EnKFs. Some examples are the Towards an Operational Prediction system for the North Atlantic European coastal Zones (TOPAZ) (Bertino et al. 2008), the European COastal sea and Operational observing and Prediction system (ECCOP) (Nerger et al. 2005), the POSEIDON monitoring, forecasting and information system for the Greek Seas (Korres et al. 2010), and the global ocean DA system at the Global Modeling and Assimilation Office (GMAO) (Keppenne et al. 2005), and the Red Sea ocean assimilation system (Toye et al. 2017).

The MITgcm-ECCO assimilation system has focused on providing multi-decadal global ocean reanalyses, e.g. Köhl et al. (2007), Wunsch and Heimbach (2007), and more recently Forget et al. (2015). It was also successfully used by Hoteit et al. (2005); Gebbie et al. (2006); Mazloff et al. (2010); Hoteit et al. (2009, 2010) for regional, eddy-permitting configurations. Recently, the MITgcm-ECCO system has been configured for the Gulf of Mexico (GoM) region by Gopalakrishnan et al. (2013b) to produce short-term (two month) analysis and forecasts for the Loop Current (LC) circulation in the GoM.

To equip the MITgcm with more predictive capabilities, the ensemble Data Assimilation Research Testbed (DART) package (Anderson et al. 2009), has been implemented with the MITgcm (Hoteit et al. 2013). DART is a portable software facility employing multiple stochastic and deterministic EnKFs. It has been developed at the National Center of Atmospheric Research (NCAR)

110 and is now used for research and operational weather forecasting problems (Zubrow et al. (2008);
111 Aksoy et al. (2009); Dowell and Wicker (2009), to cite but a few). The MITgcm-DART system
112 has been tested for LC predictability in the GoM by Hoteit et al. (2013), and for predicting the
113 circulation of the Red Sea by Toye et al. (2017).

114 The objectives of these two MITgcm-based assimilation systems, MITgcm-ECCO and MITgcm-
115 DART, are related although their technical approaches differ. One important difference between
116 a variational and an EnKF DA system is that EnKFs provide an efficient dynamical approach to
117 update approximate forecast uncertainties (or background) in time, making them more suitable
118 for forecasting than 4DVAR (Lorenc 2003). Another practical advantage is that 4DVAR requires
119 the implementation of the model adjoint while an EnKF does not, and so is called “non-intrusive”
120 (Lorenc 2003). However, unlike 4DVAR, the EnKF solution is not necessarily consistent with the
121 (non-linear) dynamics of the system, making it less suitable to study ocean dynamical balances
122 (Houtekamer and Mitchell 2005). This is further amplified by the need for adhoc techniques (e.g.
123 localization and inflation) to mitigate rank-deficiency of ensemble covariances due to the use of
124 small ensembles (Song et al. 2010).

125 This study demonstrates the practical application of both 4DVAR and EnKF methods for the
126 GoM, and is the first attempt to quantitatively compare the two DA methods for regional ocean
127 state estimation and prediction. In the weather forecasting community, several studies have re-
128 ported comparisons of variational and sequential DA approaches for different weather-related ap-
129 plications, although few of them were based on realistic model hindcasting and forecasting sys-
130 tems. Zhang et al. (2011) compared EnKF against both 3DVAR and 4DVAR methods with the
131 Weather Research and Forecasting (WRF) model for a warm season over the contiguous United
132 States. The EnKF and 4DVAR forecast errors were comparable at 12-36h lead times and both
133 were substantially smaller than the 3DVAR forecast errors, whereas the longer lead time fore-

cast errors from EnKF were smaller than the 4DVAR/3DVAR forecasts. Lorenc (2003) compared EnKF with 4DVAR for a medium-range mesoscale numerical weather prediction (NWP) system, and found EnKF is less suitable for uncertainty in a wide range of scales and may not use high-resolution satellite data as effectively as 4DVAR, and suggested a EnKF-4DVAR hybrid method. Yang et al. (2009) compared the Local ensemble transform Kalman Filter (LETKF) with 3DVAR and 4DVAR schemes in a quasi-geostrophic channel model and found that, LETKF and 4DVAR solutions are superior to 3DVAR solutions. The LETKF solutions, which account for the flow-dependent background error covariance, are more accurate than 4DVAR within a 12h window, while 4DVAR solutions greatly benefit from longer assimilation windows. Another comparison study between LETKF and 4DVAR with the experimental operational system at the Japanese Meteorological Agency (JMA) by Miyoshi et al. (2010) reported that overall performance of both methods are essentially comparable. Whitaker et al. (2009) compared 4DVAR and 3DVAR systems with ensemble-based data assimilation (EnsDA) in a surface-only, observing system experiment. They found that 4DVAR and EnsDA solutions were comparable, that both were superior to 3DVAR solutions, and that the EnsDA system provided useful estimates of analysis error. An intercomparison study of five different variational and EnKF systems for the Environmental Canada was reported by Buehner et al. (2010) in the context of global deterministic NWP. The forecast quality from that study showed varied skill depending on the flow-dependent EnKF error covariances. The readers are directed to the special collection of papers on intercomparison of both methods at http://journals.ametsoc.org/page/Ensemble_Kalman_Filter.

The main focus of this work is to compare MITgcm-ECCO and MITgcm-DART for eddy-permitting, estimation and prediction of the circulation of the GoM. To produce GoM state estimates, both satellite-derived along-track sea-surface height (SSH) and gridded sea-surface temperature (SST) data are assimilated over a period of two months (March – April, 2010). These

are then used to initialize a forecast for two months (May – June, 2010) starting from the end of the assimilation period. The performance of the assimilation methods are analyzed by computing model-observation root-mean-square-difference (*rmsd*) for the satellite SSH and SST data during both the hindcast and forecast periods. Model forecasts from both assimilation methods are also compared against independent Spray glider (Sherman et al. 2001; Rudnick et al. 2004) measurements of temperature and salinity profiles taken in the northern GoM continental shelf waters. Forecasts from the 4DVAR optimized state, the EnKF ensemble members, and the EnKF ensemble mean analysis are compared over the two month period during a LC eddy (Eddy-F) detachment event in late May 2010. Sensitivity experiments with respect to various MITgcm-DART EnKF parameters, such as the ensemble size, localization length scale, covariance inflation factor, and number of assimilation cycles (hindcast period) are also conducted and their respective impact on the system predictability is assessed. Additionally, MITgcm-ECCO and MITgcm-DART are compared for time periods other than 2010, testing predictability of the system for various LC eddy separation events in the GoM during 2006 (Eddy Yankee), 2013, and 2014 (Eddy Kraken).

3. Model Configuration and Observations

a. MITgcm - Intra-Americas Seas (MITgcm-IAS) Model

The MITgcm Intra-Americas Seas (MITgcm-IAS) model is a regional implementation of the MITgcm (Marshall et al. 1997). The setup of the model, including model initial conditions, open boundary conditions, and atmospheric forcings, is the same as the one implemented in Gopalakrishnan et al. (2013a), and is summarized in Tables 1 and 2. A more detailed description and a forward model evaluation against observations can be found in Gopalakrishnan et al. (2013a).

b. Observations

The observations used in this study are the same as assimilated in Gopalakrishnan et al. (2013b) and are outlined in Table 3. The following description of observations is derived from Gopalakrishnan et al. (2013b) with minor modifications to explain how these are assimilated into MITgcm-ECCO and MITgcm-DART systems.

SSH anomalies were obtained from the Radar Altimetry Database System (RADS, <http://rads.tudelft.nl/rads/index.shtml>). For MITgcm-ECCO, the along-track observations from three satellites: Jason-1 (J1), Jason-2 (J2), and Envisat (N1) with respect to the time-mean dynamic ocean topography (MDT), calculated from the difference between the Danish National Space Center Mean Sea Surface 2008 (DNSCMSS08) and Earth Gravity Model 2008 (EGM08): DNSCMSS08-EGM08 (Andersen and Knudsen 2009; Pavlis et al. 2012), were computed over each day and spatially bin-averaged onto the model grid. For MITgcm-DART, along-track SSH observations from the same three satellites were converted into absolute SSH signal by adding the MDT (DNSCMSS08-EGM08), and were sampled at observation locations within the assimilation window of 3 days (± 1.5 day from the analysis time). Since the current configuration of the MITgcm-IAS model did not include tidal or atmospheric pressure forcing, tidal corrections and inverted barometer correction were applied to the along-track SSH observations.

The SST data were obtained from the daily optimally interpolated product derived from the Tropical Rainfall Measuring Mission’s (TRMM) Microwave Imager (TMI) and the Advanced Microwave Scanning Radiometer for the Earth Observing System (AMSR-E) instruments produced by Remote Sensing Systems Inc. (<http://www.remss.com/>) on a 0.25° longitude $\times 0.25^\circ$ latitude grid. For MITgcm-ECCO, the daily gridded SST data were spatially interpolated onto the model grid (0.10° longitude $\times 0.10^\circ$ latitude grid) prior to assimilation for computational conve-

nience. For MITgcm-DART, the daily gridded SST data were sampled at the observation grid resolution of 0.25° longitude $\times 0.25^\circ$ latitude, and were averaged over the 3-day assimilation window (± 1.5 day from the analysis time).

The time mean of the TMI/AMSR-E SST data for March 1 - April 29, 2010 is shown in Figure 1a. Superposed satellite ground tracks from three satellites: Jason-1 (J1), Jason-2 (J2) and Envisat (N1) for the same period are shown in Figure 1b. In order to ensure the quality of SSH and SST data and to account for expected model representational error, observations near the coast (at water depth < 500 m) were not used for assimilation.

Besides the above observations which are used in the state estimates, temperature and salinity observations from a glider trajectory in the GoM were used for independent data comparison with model forecasts. The SIO and the Woods Hole Oceanographic Institution (WHOI) deployed a Spray glider (Sherman et al. 2001; Rudnick et al. 2004) in the northern GoM continental shelf waters during June 2010 as part of the DwH oil spill monitoring. The glider temperature and salinity data, spanning from the surface to a depth of 500 m, were binned every 6 hours. The glider trajectory is marked by magenta circles in Figure 1a (top panel). Although these glider observations only sampled northern shelf-slope waters which are not representative of the central GoM/LC water masses, they are used here as independent data for assessing the forecasts of subsurface water properties from both methods, to verify that adjustments to the LC state do not degrade the estimate elsewhere.

c. Observation Uncertainty Covariances

The prior estimates of observation uncertainties for both SSH and SST are dominated by model representational errors which include expected error in the atmospheric forcing values that determine the mixed-layer depth (and thus affect modeled SST), coarse time resolution of atmospheric

225 forcing, and expected errors in the parameterizations of mixing in the model, all of which affect
226 the model mixed-layer physics.

227 1) MITGCM-ECCO

228 *SSH*: The MITgcm-ECCO is capable of isolating the uncertainties associated with the time-
229 independent geoid from the generally smaller uncertainties in the anomalies, and the model SSH
230 time mean and anomalies were separately fit to the observed along-track SSH time mean and
231 anomaly with different uncertainties in the two cost functions. The SSH anomaly uncertainty was
232 assumed to be spatially-invariant, at 5 *cm* for Jason-1 (J1), Jason-2 (J2), and 10 *cm* for Envisat (N1)
233 and ERS-2 (E2), and the geoid uncertainty is also assumed to be spatially-invariant at 10 *cm*.

234 *SST*: The SST data uncertainty was set at 5 times the standard deviation (over time) of the mod-
235 eled SST over five-years (forward model solution for 2004 – 2008 taken from Gopalakrishnan
236 et al. (2013a)), and were limited to be between 10° *C* in the deep central GoM to 50° *C* in the shal-
237 low coastal waters. Since the gridded SST data were spatially interpolated to model grid points
238 for computational convenience, relatively high SST observational uncertainty, especially near the
239 coast, is used to account for the redundant interpolated observations and model representational
240 error, which are expected to be high near the coast in relatively shallow water. The detailed de-
241 scription of the observation uncertainty covariances, same as the one used in this study for the
242 MITgcm-ECCO system, can be found in Gopalakrishnan et al. (2013b).

243 2) MITGCM-DART

244 *SSH*: The MITgcm-DART system assimilates absolute (anomaly + MDT) along-track SSH, and
245 the observation error for SSH was assumed to be the same as for the MITgcm-ECCO anomalies:
246 spatially-invariant, at 5 *cm* for J1 and J2, and 10 *cm* for N1 and E2.

247 *SST*: The MITgcm-DART assimilates gridded SST data at observation locations, and the obser-
248 vation error for SST is assumed to be spatially-invariant at $10^{\circ}C$. This high SST error is assumed
249 to include model representational error in the mixed-layer physics and to make it consistent with
250 the prior estimates of SST error in MITgcm-ECCO.

251 *d. Background Uncertainty Covariances*

252 The background uncertainty covariances for both MITgcm-ECCO 4DVAR and MITgcm-DART
253 EnKF systems are based on the model variability over the five-year forward model simulation for
254 the period 2004 - 2008 (Gopalakrishnan et al. 2013a). These uncertainties were treated differently
255 depending on the assimilation systems.

256 1) MITGCM-ECCO

257 For the MITgcm-ECCO 4DVAR, the background uncertainty covariances for the model initial
258 temperature and salinity controls were computed from the standard deviation (over time) of the
259 model variability over five-years (forward model solution for 2004 – 2008 taken from Gopalakr-
260 ishnan et al. (2013a)). These background error covariances were first multiplied by $\sqrt{\frac{dz_{min}}{dz}}$ (dz_{min}
261 is minimum depth level thickness and dz is vertical z -level thickness) to compensate for the larger
262 raw sensitivities at depth levels with large z -level thickness. The MITgcm-ECCO 4DVAR formu-
263 lation assumes the background uncertainty covariances ($\mathbf{Q}$, Equation 1 in Gopalakrishnan et al.
264 (2013b)) to be diagonal, meaning that the background uncertainty was assumed to be independent
265 point-to-point. To keep the adjustment fields appropriately smooth, the MITgcm-ECCO 4DVAR
266 system enforces 2D and 3D smoothness of control variables following Weaver et al. (2003); Forget
267 (2009); Hoteit et al. (2010). We used a decorrelation scale of $50km$ for the smoothed controls in
268 the horizontal, and of $10m$ in the vertical (the vertical scale was set small so that each level was

independent). In order to account for the diagonality assumption and for the smoothing scales, the background uncertainty covariances were increased, by a factor of about 14 for the surface levels (100km horizontal scale corresponds to 10 grid points of 0.10° longitude $\times 0.10^\circ$ latitude model grid, and 10m in the surface consists of two depth levels, which corresponds to a factor of $\sqrt{200}$), and by a factor of about 10 for the depth levels below. These increased background uncertainty covariances also account for the model representational errors, especially near the surface, such as errors due to bad atmospheric forcing or mixed layer physics.

This amplification of background error covariances is required in order to make sufficient adjustments to the initial condition controls to allow the model to fit the observations. Sensitivity experiments scaling these uncertainties by factors of two did not have much effect on the solutions, and the adjustments to temperature and salinity initial condition controls were not overly large near the surface (not shown). Adjustments in depth (greater than 3000 m) were discouraged by low prior variance, since they were not expected to be realistic. A detailed description of the background uncertainty covariances used in this study can be found in Gopalakrishnan et al. (2013b) which used the same MITgcm-ECCO 4DVAR system.

2) MITGCM-DART

The MITgcm-DART EnKF assimilation system starts from an initial ensemble of state vectors that is meant to represent the uncertainties around the initial state estimate. For the MITgcm-DART EnKF, the background error covariances was estimated from an Empirical Orthogonal Function (EOF) analysis of a large set of model realizations (taken from a forward model solution for 2004 – 2008 from Gopalakrishnan et al. (2013a), which was also used in the MITgcm-ECCO 4DVAR background uncertainty covariances). The three-dimensional, multi-variate EOFs are computed from the historic simulation without removing the seasonality, which is assumed to

292 be relatively low in this region. The percentage of variance explained by the first five EOFs are
293 EOF-1) 22, EOF-2) 10, EOF-3) 7, EOF-4) 6, EOF-5) 4, and the cumulative variance explained by
294 the first 50 EOFs is about 90%. This background uncertainty covariance is not diagonal by virtue
295 of multi-variate EOFs. A detailed description of generation of the filter initial ensemble for the
296 MITgcm-DART EnKF system can be found in Hoteit et al. (2013).

297 **4. MITgcm-IAS 4DVAR Framework**

298 The MITgcm-IAS 4DVAR assimilation is based on the ECCO system (Stammer et al. 2002).
299 Although the MITgcm-IAS model and the MITgcm-ECCO 4DVAR state estimation method used
300 in this study are the same as implemented in Gopalakrishnan et al. (2013b), the 4DVAR assimi-
301 lation experiment in this study were re-done with following changes to make it more comparable
302 to the MITgcm-DART EnKF as described below: 1) The length of the assimilation window was
303 reduced to 60 days from 61 in the Gopalakrishnan et al. (2013b) to match the MITgcm-DART
304 experiment. 2) Even though the MITgcm-ECCO system enables a variety of control parame-
305 ters, here we only adjust the model initial conditions for temperature and salinity for a direct and
306 fair comparison with the MITgcm-DART results, while the Gopalakrishnan et al. (2013b) also
307 included open boundary and atmospheric forcing controls. A detailed description of the state esti-
308 mation procedure, including control variables, cost functions for observations, model background
309 uncertainty covariances, observation uncertainty covariances, and the iterative optimization can be
310 found in Gopalakrishnan et al. (2013b).

311 *a. MITgcm-IAS 4DVAR State Estimation Experiment*

312 The satellite-derived along-track SSH, separated into temporal mean and anomalies, and gridded
313 SST data were assimilated using MITgcm-ECCO over an assimilation window of two-months:

314 March 1 – April 29, 2010. The state estimation optimizes the model trajectory by adjusting the
315 model control variables, which in this case are model initial conditions for temperature and salinity.

316 The model initialization for the MITgcm-ECCO control simulation and the treatment of the
317 viscosity and diffusivity parameters in the MITgcm-ECCO forward and adjoint model simula-
318 tions are the same as in Gopalakrishnan et al. (2013b), and the following description is derived
319 from there. The control model simulation (MIT-C) is the forward model solution from iteration 1,
320 which uses initial conditions and boundary conditions from assimilated HYCOM/NCODA 1/12°
321 global daily analysis (<http://hycom.org/dataserver/glb-analysis>), atmospheric forcing
322 from National Centers for Environmental Prediction/National Center for Atmospheric Research
323 Reanalysis-1 (NCEP/NCAR-R1) (Kalnay et al. 1996) surface fluxes and winds, and monthly cli-
324 matological run-off fluxes (freshwater) from ECCO global model state estimate. The initial con-
325 ditions, open boundary conditions, and atmospheric forcing for the MIT-C are the background and
326 “first-guess” for the state estimation.

327 The MITgcm-ECCO adjoint model simulation used increased horizontal diffusivity and vis-
328 cosity terms (second order terms were increased by a factor of 10 and fourth order terms were
329 increased by a factor of 5 of the forward model simulation, refer Table 1), with the KPP mixing
330 parameterization turned off (Hoteit et al. 2005; Gopalakrishnan et al. 2013b). Using an itera-
331 tive minimization procedure via a variable-storage Quasi-Newton M1QN3 algorithm (Gilbert and
332 Lemaréchal 1989), the cost function descent reaches a plateau after 14 iterations with a relatively
333 small slope (less than 1% per iteration) and the sum of the model-observation squared misfits nor-
334 malized by the number of observations and the assumed observation variance were less than 1 for
335 all data types. The total cost function is reduced by 46% after 14 iterations, and the individual
336 observation costs decreased at roughly the same rate as the combined cost function.

337 The optimized state estimate at the end of the assimilation period is used as initial conditions to
338 forecast the ocean state for two months (April 30 - June 28, 2010), using monthly climatological
339 open boundary conditions, atmospheric forcing, and run-off fluxes. Since the forecasts for lateral
340 and atmospheric boundary conditions are generally available only for a period of about 3 days
341 in a real time operational ocean hindcasting/forecasting system, we used monthly climatological
342 forcings for the two-month long forecasts, so the forecast setup does not take advantage of pos-
343 sible predictability in the ocean and atmospheric boundary conditions as would be the case in an
344 optimized system.

345 **5. MITgcm-IAS EnKF Framework**

346 *a. MITgcm - Data Assimilation Research Testbed (MITgcm-DART)*

347 DART is an open-source software facility that provides a variety of algorithms for ensemble
348 DA using both stochastic (e.g. ensemble Kalman filter - EnKF, (Evensen 2006)) and deterministic
349 (e.g. ensemble adjustment Kalman filter - EAKF, (Anderson 2001, 2003)) Kalman filters. DART
350 is also equipped with advanced inflation and localization schemes, very useful for good behavior
351 of an EnKF (Anderson et al. 2009). Whereas localization tries to eliminate spurious correlations
352 due to sampling errors, inflation mitigates for insufficient variance due to the omission of some
353 sources of errors in the filter and in the model (Hoteit et al. 2002). The readers are referred to
354 <http://www.image.ucar.edu/DAReS/DART/> for further information about DART.

355 MITgcm was integrated to DART by Hoteit et al. (2013) and is recently applied in the Red Sea
356 by Toye et al. (2017). MITgcm and DART run as separate executables with no modifications to
357 each code. The exchanges of information between the two codes is handled through a set of in-
358 terface routines. The state vector is exchanged by the two codes via the interface routines and

359 is composed of the model prognostic variables, which in the case of the MITgcm are the salin-
360 ity, temperature, horizontal velocities (U and V), and the two-dimensional SSH. The assimilation
361 system is initialized from an ensemble of state vectors that is meant to represent the uncertainties
362 around the initial state estimate. The MITgcm is then used as a forecast model to integrate the
363 ensemble of state vectors forward in time. The resulting forecast ensemble is then sent to DART
364 for updating with the incoming observations. The forecast-update cycles are then repeated every
365 time new observations become available. A detailed description of the MITgcm-DART interface
366 identical to that used in this study, with its application to the GoM can be found in Hoteit et al.
367 (2013).

368 *b. MITgcm-IAS EnKF State Estimation Experiment*

369 The pre-processed along-track absolute SSH and gridded SST data, sampled over an assimilation
370 window of 3 days, were assimilated sequentially using MITgcm-DART system for a period of 60
371 days (20 3-day assimilation cycles) starting from March 1, 2010 till April 29, 2010.

372 The filter parameters, including ensemble size, covariance inflation factor, localization length
373 scale, and filter initialization are described in detail in Hoteit et al. (2013). We used EAKF and
374 the filter initialization is based on an EOF analysis, as described in the background uncertainty
375 section. The details of atmospheric forcings, open boundary conditions, and run-off fluxes of
376 the MITgcm-IAS model are provided in Table 2. The MITgcm-DART results from the 2010
377 experiment discussed in the next section used 50 ensemble members, a spatially invariant inflation
378 factor of 1.2, and localization radius of 250 km (EnKF2010-N50-I1.2-L250 in Table 4).

379 At the end of the 20 3-day assimilation cycles, an ensemble forecast was initialized using each
380 ensemble member, in addition to a single forecast initialized from the ensemble mean analysis

381 from the last assimilation cycle, for a period of two months (April 30 - June 28, 2010), using
382 monthly climatological open boundary conditions, atmospheric forcing, and run-off fluxes.

383 **6. Comparison of Model Hindcast and Forecast with Observations**

384 The performance of MITgcm-ECCO and MITgcm-DART systems were analyzed by com-
385 paring the solutions with daily-interpolated gridded SSH fields from AVISO analysis ([http:](http://marine.copernicus.eu/)
386 [//marine.copernicus.eu/](http://marine.copernicus.eu/)) and daily gridded SST data from TMI/AMSR-E for hindcasts
387 and forecasts, and with Spray glider temperature and salinity observations for forecasts. The
388 Ssalto/Duacs altimeter product AVISO is produced and distributed by the Copernicus Marine and
389 Environment Monitoring Service (CMEMS) (<http://marine.copernicus.eu/>).

390 *a. Hindcast Comparison*

391 The SSH fields from MITgcm-ECCO (both the optimized solution from iteration 14: MIT-
392 4DVAR, and control “first-guess” solution: MIT-C) and MITgcm-DART (ensemble mean anal-
393 ysis: MIT-EnKF-A and forecast: MIT-EnKF-F) were compared with AVISO analysis and HY-
394 COM/NCODA global daily analysis (HYCOM-GLOBAL). The model-data SSH comparisons at
395 the start (March 1, 2010: Figure 2) and end (April 29, 2010: Figure 3) dates of the two-month hind-
396 cast period are shown for daily-averaged fields over the GoM basin (spatial domain highlighted
397 by the blue curve in Figure 1). At the start, the MIT-4DVAR estimates of the LC shape and its
398 westward and northward intrusion into the GoM basin are very similar to AVISO and HYCOM-
399 GLOBAL analysis. The model control adjustments that produced MIT-4DVAR by the iterative
400 minimization process make only minor SSH changes compared to MIT-C. This means that the
401 “first-guess” (MIT-C) forecast initialized with HYCOM/NCODA global daily analysis and using
402 NCEP/NCAR-R1 forcing and HYCOM/NCODA boundary conditions provides realistic GoM cir-

403 culation features, suggesting that HYCOM/NCODA analysis is remarkably compatible with the
404 MITgcm-ECCO 4DVAR system.

405 The cyclonic Loop Current Frontal Eddies (LCFEs: (Vukovich and Maul 1985; Cochrane 1972;
406 Vukovich et al. 1979; Fratantoni et al. 1998)) on the eastern side at the neck of the LC (cen-
407 tered roughly at 24°N , 276°E), and near the northwestern side of the LC (centered roughly at
408 26°N , 272°E) shown by MIT-4DVAR and MIT-C are also very similar to AVISO and HYCOM-
409 GLOBAL analysis. The presence of these LCFEs plays a determinant role in the LC eddy shedding
410 (Schmitz 2005, 2003). The MIT-4DVAR and MIT-C reproduce the cyclonic eddies and the pre-
411 viously shed, slowly dissipating LC eddy in the southwestern GoM basin seen in the AVISO and
412 HYCOM-GLOBAL analysis. The MIT-EnKF-F starting SSH is the long-term mean of a five-year
413 (2004 – 2008) forward model simulation (Gopalakrishnan et al. 2013a), based on which the en-
414 semble members were generated, and therefore differs from the AVISO and HYCOM-GLOBAL
415 analysis. In order to clearly demonstrate the performance of the MITgcm-DART, and to be con-
416 sistent with the ensemble covariance which is relative to the mean background state, the filter is
417 initialized using EOFs of a large set of MITgcm-IAS forward model realizations which are refer-
418 enced to its long-term mean rather than HYCOM/NCODA $1/12^{\circ}$ global daily analysis used in the
419 MITgcm-ECCO initialization. In spite of these starting differences, MIT-EnKF-A (after the first
420 assimilation cycle) shows many of the AVISO analysis SSH features, especially the location of an
421 older, dissipating LC eddy and the cyclonic eddies in the southwestern GoM basin, and a LCFE on
422 the northwestern side of the LC (centered roughly at 26°N , 272°E). It however fails to reproduce
423 the LCFE on the eastern side near the neck of the LC, likely due to the limited observations in
424 the 3 day window. It is remarkable that the MIT-EnKF-A is able to reproduce most of the AVISO
425 analysis SSH features after only one assimilation cycle.

426 At the end date of the hindcast period, the SSH fields from MIT-4DVAR, MIT-EnKF-A, and
427 MIT-EnKF-F show similar LC northward and westward extent to the AVISO and HYCOM-
428 GLOBAL analysis, but MIT-C differs. Also all estimates except MIT-C reasonably reproduce
429 the size, shape, and location of the older, dissipating LC eddy and cyclonic eddy features in the
430 southwestern GoM basin. It should be noted that there are only small differences between MIT-
431 EnKF-A and MIT-EnKF-F at the end of the hindcast period.

432 The model SST fields were compared with TMI/AMSR-E data and HYCOM-GLOBAL analysis
433 at the end of the hindcast period (Figure 4). Except for MIT-C, SST estimates compare well with
434 TMI/AMSR-E data and HYCOM-GLOBAL analysis, especially the LC shape and temperature,
435 and the cooling of the northern GoM basin. Model SST shows a warmer southwestern GoM basin
436 with a positive bias of $\sim 2^{\circ}$ C compared to TMI/AMSR-E data and HYCOM-GLOBAL analysis.
437 Again, the SST of MIT-EnKF-A and MIT-EnKF-F are very similar at the end of the hindcast
438 period.

439 For more quantitative comparisons, the daily-averaged SSH from the MITgcm-ECCO and
440 MITgcm-DART hindcasts as well as HYCOM/NCODA global daily analysis are compared to the
441 AVISO analysis SSH. For MITgcm-ECCO, the hindcast *rmsd* curves from MIT-4DVAR, MIT-C,
442 model-persistence (MIT-P), and HYCOM-GLOBAL are shown in Figure 5a. The MIT-P solution
443 is assumed to be constant over the whole hindcast period and is equal to the MIT-4DVAR initial
444 state. The MIT-4DVAR hindcast has an overall *rmsd* of 6 cm, lower than the HYCOM-GLOBAL
445 analysis throughout the hindcast period, and shows considerable reduction in the *rmsd* (about 50
446 % near the end of the assimilation period) when compared with MIT-P and MIT-C.

447 The AVISO gridded SSH are estimated by Optimal Interpolation, merging the measurements
448 from the different altimeter missions available, and is the Absolute Dynamic Topography (ADT)
449 which is equal to Sea Level Anomaly (SLA) + time-Mean Dynamic Topography (MDT) with

respect to a twenty-year (1992 – 2012) mean. While the mapped AVISO product is not necessarily the true SSH state, it is a widely-used benchmark and has small differences with the satellite along-track SSH observations. Computing SSH *rmsd* with the assimilated along-track observations from RADS (not shown) gives misfit time-series that are qualitatively similar, but are much less smooth, as well as less homogeneous due to fluctuating numbers of observations from day to day depending on when altimeters sample the domain. The space-time smoothness of the AVISO analysis makes it more convenient as a reference for SSH *rmsd* comparison given that the true SSH is not available.

The SSH hindcast *rmsd* comparison for the MITgcm-DART experiment is shown in Figure 5b. The MIT-EnKF solutions over the 20 3-day assimilation cycles were linearly interpolated between the analyses for the *rmsd* computation. As before, the MIT-P estimate held the MIT-EnKF-A initial state constant over the hindcast period. As expected, the MIT-EnKF-A has the lowest *rmsd*, showing the most *rmsd* reduction compared to MIT-EnKF-F during the first three analysis cycles. Overall, MIT-EnKF-A shows a *rmsd* of 6 cm, lower than HYCOM-GLOBAL throughout the hindcast period. The ensemble standard deviation (spread) (thick dashed lines), and total error (ensemble spread + observation error of 5 cm, thin dashed lines) averaged over the GoM basin for both analysis (red curves) and forecasts (black curves) are also shown in Figure 5b. The ensemble spread starts at 7.5 cm for forecast and 6 cm for analysis, drops to about 2.5 cm after the third analysis cycle for both analysis and forecast, and stays close to this value throughout the hindcast period. The total spread curves for analysis and forecast show that MITgcm-DART fits SSH within the prior estimates of observation error throughout the two-month hindcast period, although it is possible that the spread is too small and the assumed observation error is too large.

In general, both MIT-4DVAR and MIT-EnKF-A solutions show similar *rmsd* during the hindcast period, closely following the HYCOM-GLOBAL analysis and outperforming MIT-P.

473 *b. Forecast Comparison*

474 The SSH fields as forecasted by MIT-4DVAR, MIT-C, MIT-EnKF-Ens, and MIT-EnKF-Ave are
475 visually compared to AVISO and HYCOM-GLOBAL analysis at the end of the first month (May
476 29, 2010) of the two-month forecast period in Figure 6. MIT-EnKF-Ens refers to the forecast
477 initialized from the EnKF ensemble mean analysis (MIT-EnKF-A) at the end of the hindcast,
478 MIT-EnKF-Ave is the mean of forecasted ensemble states, MIT-4DVAR was initialized from the
479 end of the MITgcm-ECCO optimized state, and MIT-C was initialized using the optimized state
480 from HYCOM/NCODA $1/12^\circ$ global daily analysis for the start date of the forecast.

481 MIT-C exhibits a well connected LC, without any formation and detachment of a LC eddy. MIT-
482 4DVAR forecasts a LC eddy (Eddy-F) close to detachment from the LC, and the structure of the
483 LC and the size, shape, and location of the newly-formed eddy compares well with AVISO and
484 HYCOM-GLOBAL analysis. In addition, the MIT-4DVAR forecast shows a small cyclonic LCFE
485 on the eastern side of the LC, between the LC and the newly formed Eddy-F (centered roughly at
486 24°N , 276°E), in agreement with AVISO and HYCOM-GLOBAL analysis. The presence of these
487 cyclonic LCFEs might trigger the LC eddy shedding processes in the GoM (Schmitz 2005, 2003;
488 Le Hénaff et al. 2012; Vukovich and Maul 1985; Cochrane 1972; Vukovich et al. 1979; Fratantoni
489 et al. 1998). Both MIT-4DVAR and MIT-C correctly predict the older, dissipating LC eddy in
490 the western GoM basin, as seen in AVISO and HYCOM-GLOBAL analysis. MIT-EnKF-Ens and
491 MIT-EnKF-Ave predict very similar features of the LC and the newly formed eddy (Eddy-F), and
492 the small-scale cyclonic LCFE on the east side of the LC (centered roughly at 24°N , 276°E) with
493 the Eddy-F just detached, whereas MIT-4DVAR forecast and AVISO analysis suggest Eddy-F is
494 close to detachment from the LC, as previously mentioned. The coarse horizontal resolution (10
495 km) and high viscosity and diffusivity coefficients of the MITgcm-IAS forecast model might cause

the smoother and more circular LC eddy (Eddy-F) relative to AVISO and HYGOM-GLOBAL analysis.

MIT-4DVAR, MIT-C, MIT-EnKF-Ens, and MIT-EnKF-Ave forecasts of the three-dimensional temperature and salinity were also compared with the Spray glider data in the GoM during June 2010 (Section 3). The model forecasts were linearly interpolated in time and space to the glider observations. The glider observations and differences with MIT-4DVAR (obs - MIT-4DVAR), MIT-C (obs - MIT-C), MIT-EnKF-Ens (obs - MIT-EnKF-Ens), and MIT-EnKF-Ave (obs - MIT-EnKF-Ave) are shown in Figure 7. The anomaly root-mean-square-difference: $rmsd_a$ and anomaly correlation coefficient: cc_a (Gopalakrishnan et al. 2013b) between observed and model forecast subsurface temperature and salinity profiles were computed and labeled in Figure 7. A decrease (increase) in $rmsd_a$ (cc_a) indicates an improved model forecast. MIT-4DVAR, MIT-EnKF-Ens, and MIT-EnKF-Ave compare better with the glider data than MIT-C, with the MIT-EnKF-Ave providing the closest solution to the glider data. MIT-4DVAR exhibits a lower (higher) $rmsd_a$ for temperature (salinity) compared to MIT-EnKF-Ens. The results of the comparison differ for temperature and salinity and above and below 50 m depth. MIT-4DVAR, MIT-EnKF-Ens, and MIT-EnKF-Ave temperature forecasts show significant improvement at depth because the altimeter data can accurately constrain isopycnal displacements, while not improving the surface likely due to the large SST observation errors assumed and the dominance of atmospheric forcing over ocean dynamics in determining SST. The salinity shows similar improvements at depth, although the amplitude of the signal is smaller, reflecting the weaker vertical gradients of salinity. Irrespective of these two distinct approaches, both assimilation systems produced improved forecasts compared to MIT-C for SSH, as well as for subsurface temperature and salinity fields.

518 c. Ensemble Forecasts

519 Ensemble forecasting can boost forecast skill and provide an efficient model-based estimate of
520 uncertainties. The daily-averaged SSH fields from MITgcm-DART ensemble member forecasts,
521 along with MIT-4DVAR, MIT-C, MIT-EnKF-Ens, MIT-EnKF-Ave, and HYCOM-GLOBAL anal-
522 ysis, are differenced from the AVISO analysis SSH for the two month forecast period (May – June,
523 2010). The corresponding model-data *rmsd* is shown in Figure 8a. Please note that the y-axis of
524 this figure spans 5 cm to 20 cm to show the details. The MIT-4DVAR persistence (MIT-4DVAR-
525 P) forecast assumed the MIT-4DVAR forecast initial state fixed over the forecast period, while
526 the MIT-EnKF-Ens persistence (MIT-EnKF-Ens-P) forecast assumed the MIT-EnKF-Ens forecast
527 initial state fixed over the forecast period.

528 The MIT-4DVAR forecast has an overall *rmsd* of 9 cm, while the MIT-4DVAR-P *rmsd* increases
529 from 7 cm to 18 cm over the forecast period. The MIT-C *rmsd* is comparable to MIT-4DVAR
530 and HYCOM-GLOBAL during the first week of the forecast, but shows a slightly increased *rmsd*
531 compared to MIT-4DVAR after the third week. The MIT-EnKF-Ens and MIT-EnKF-Ave forecasts
532 remain closer to HYCOM-GLOBAL with an overall *rmsd* of 7 cm during the first two weeks, after
533 which MIT-EnKF-Ens performance degrades, reaching a *rmsd* of 15 cm by the end of the forecast
534 period. MIT-C forecast on the other hand shows an overall *rmsd* of 10 cm over the forecast period,
535 which is lower than MIT-EnKF-Ens forecast starting from the fifth week, but higher than MIT-
536 EnKF-Ave throughout the forecast period.

537 The range of SSH *rmsd* of the ensemble forecast members increases with time and shows a
538 larger *rmsd* ranging from 8 cm to 17 cm at the end of the forecast period, after starting from a
539 smaller *rmsd* ranging from 7 cm to 8 cm. The starting SSH forecast *rmsd* from ensemble members
540 shows a single outlier with higher (> 8.5 cm) *rmsd*, which is not a healthy behavior in an EnKF.

541 Sakov and Oke (2008) suggested that the use of mean-preserving random rotations in an ensemble
542 square root filter could help mitigate the buildup of ensemble outliers. The *rmsd* of this outlier
543 member did not however grow large enough over the 60-day forecast period to require introducing
544 a random rotation to the mean-preserving EAKF used here. Out of all forecasts, MIT-EnKF-
545 Ave shows comparable *rmsd* to that of HYCOM-GLOBAL, except during the last three weeks of
546 the forecast period. MIT-4DVAR-P and MIT-EnKF-Ens-P have the highest *rmsd* throughout the
547 forecast period.

548 MIT-EnKF-Ens provides a better forecast than MIT-C during the first five weeks of the forecast
549 period, whereas MIT-4DVAR shows a better forecast than MIT-C from the third week onward.
550 The MIT-EnKF-Ave forecast provides the best performance out of all solutions. As expected,
551 the mean of ensemble forecasts (MIT-EnKF-Ave) performs better than a single forecast from the
552 ensemble mean analysis (MIT-EnKF-Ens). Depending on the available computational resources,
553 an ensemble forecast might not be practical, especially with many ensemble members in high-
554 resolution ocean prediction systems. In that case, one might want to rely on a single forecast
555 starting from the ensemble mean analysis. Comparing the two assimilation systems, the MIT-
556 4DVAR performs better over long-range (about eight-weeks) SSH forecasts, and MIT-EnKF-Ens
557 performs better over short-range (up to about four-weeks) SSH forecasts, while both systems show
558 similar performance during the hindcast period.

559 In addition to the comparison of the model forecasts with AVISO analysis, a set of LC indices
560 (Leben 2005) were also computed by tracking a calibrated 17 cm SSH isoline in the various model
561 solutions and AVISO. The AVISO analysis SSH were interpolated to the model grid to provide
562 the reference for this comparison. Following the procedure reported by Leben (2005), the LC in-
563 dices, specifically the maximum western longitude, maximum northern latitude, and length of the
564 LC were computed from daily-averaged SSH fields during the forecast period, including ensem-

ble forecasts, although only the northward extent index is shown in Figure 8b. The MIT-4DVAR shows an LC eddy (Eddy-F) detachment at the same day (May 30, 2010) as the AVISO analysis, but does not show the LC eddy reattachment seen by AVISO analysis in late June 2010. Both MIT-EnKF-Ens and MIT-EnKF-Ave predict a LC eddy detachment around the last week of May, 2010, close to MIT-4DVAR and AVISO analysis, but the MIT-EnKF-Ens suggests an immediate reattachment of the LC eddy within two weeks, while MIT-EnKF-Ave shows a LC eddy reattachment at almost the same time as AVISO analysis. Even though all model forecasts used the same monthly climatological atmospheric forcings, open boundary conditions, and run-off fluxes, MIT-4DVAR seems to preserve the large-scale features of the LC but fails to reproduce the LC eddy reattachment shown by MIT-EnKF-Ave and AVISO analysis, suggesting that the initial conditions are important.

To further examine the evolution of the LC and eddy detachment/reattachment, the 17 cm SSH isoline from model forecasts, ensemble forecasts, and AVISO analysis are plotted for days 1, 14, 21, and 28 of the two-month forecast period (Figure 9). For the MIT-EnKF-Ave, the 17 cm SSH contour is computed from the mean of SSH forecasts from each ensemble member. On day 1, the LC shape from MIT-EnKF-Ens solutions stays closer to AVISO analysis than MIT-4DVAR, and the ensemble forecasts show very little spread (see Figure 10), reflecting the EnKF's expectation that it has a good nowcast of the field. As the time progresses to day 14, all model solutions estimate similar LC shape on the western side of LC, while exhibiting some differences on the eastern side, especially near the neck of the LC. On day 21, the LC features are more or less similar to that of day 14, with more pronounced formation of the LC eddy and differences on the eastern side near the neck of the LC, and larger ensemble spread (see Figure 10) in this region. On day 28, the MIT-EnKF-Ens and MIT-EnKF-Ave show an already detached LC eddy with a larger

ensemble spread near the region of LC eddy detachment, while both MIT-4DVAR and AVISO analysis suggest a LC eddy close to detachment from the LC.

The ensemble mean and spread of the MITgcm-DART SSH forecast are shown in Figure 10, for the same days as Figure 9. The ensemble spread starts with structures showing satellite tracks and increases as forecast time progresses, predominantly along the LC, showing higher values near the neck of the LC where the LC eddy detachment is thought to start, as shown in Figure 9. The SSH ensemble spread also increases near the cyclonic LCFE's on the eastern side of the LC, between the newly formed LC eddy and the LC, and also in the western GoM, where the previously shed LC eddy dissipates near the western boundary. The SSH ensemble mean shows a LC eddy just detached from the LC at the end of the first month of the two-month forecast as well as cyclonic small-scale LCFE's on the eastern side of the LC. The SSH ensemble mean and spread give information about the key regions that affect the LC forecasts in the GoM, especially during a LC eddy shedding event, and provide insight into the processes that drive the LC circulation and eddy shedding.

d. Sensitivity to Filter Parameters

A series of experiments were performed with the MITgcm-DART system using the same observations and forecast model but varying the ensemble size, covariance inflation parameter, localization length scale, and finally the number of assimilation cycles (hindcast period). The details of these experiments are listed in Table 4. As before, the SSH estimates from these experiments were compared to AVISO analysis during the hindcast and forecast periods, and the corresponding model-data *rmsd* were analyzed, focusing on the model performance during the two-month forecast period. In every experiment MIT-EnKF-Ave always led to a lower *rmsd* compared to a single forecast starting from the ensemble mean analysis (MIT-EnKF-Ens) at the end of the hindcast

period. Increasing the number of ensemble members from 25, to 50, and to 100, while using the
 same inflation factor of 1.2 and localization radius of 500 km, the MIT-EnKF-Ens forecast *rmsd*
 decreases from 18 cm for 25 members to 12 cm for 100 members (Figure 11a). Please note that
 the y-axis of all panels in Figure 11 spans 6 cm to 16 cm to show the details. Larger ensembles
 provide more degrees of freedom and spread, which allows a closer fit to observations and seem
 to result in better analysis state in these cases. Increasing the inflation factor from 1.2 to 1.3 while
 keeping the same ensemble size 50 and localization radius of 500 km is clearly worse with the
 MIT-EnKF-Ens forecast showing slightly increased *rmsd* for the experiment with inflation factor
 of 1.3, while both experiments show almost the same MIT-EnKF-Ens forecast *rmsd* at the end
 of the forecast period (Figure 11b). Two experiments were performed decreasing the localization
 radius from 500 km to 250 km, while keeping the same ensemble size and inflation of 1.2 for 25
 and 50 members. Both experiments resulted in markedly improved forecast *rmsd* during the first
 few weeks, with the 25 member experiments showing more improvement throughout the forecast
 period (Figure 11c). This is expected since the smaller ensemble has less freedom to fit the ob-
 servations and should benefit the most from localization. Although decreasing the localization
 length scale enables a better fit to the observations, it may degrade the dynamical balance of the
 estimates. Finally, we decreased the number of assimilation cycles (the length of the hindcast
 period) from two months to one month and then to two weeks, while keeping the same ensemble
 size of 25 members, inflation factor of 1.2, and localization radius of 250 km. The short-term
 forecast (one to two weeks) from the two week hindcast period improves, but the overall forecast
 performance degrades with the decreasing length of the assimilation (Figure 11d). With longer
 hindcast periods, the ensemble spread decreases with the number of assimilation cycles, and often
 results in unrealistically small spreads toward the end of the hindcast period, which limits the fit to
 the observations. Conversely, a shorter hindcast period maintains a better ensemble spread to the

635 end of the hindcast period, allowing a better fit to the observations and more spread to initialize
636 the ensemble forecasts. although the final state may be worse because fewer data were used.

637 *e. Other Assimilation Experiments*

638 The MITgcm-DART and MITgcm-ECCO were applied to three other periods to compute state
639 estimates and forecasts of the GoM circulation. The details of the three additional experiments
640 are as follows: 1) 2006: hindcast (July - August, 2006), forecast (September - October, 2006), 2)
641 2013: hindcast (January - February, 2013), forecast (March - April, 2013), and 3) 2014: hindcast
642 (February, 2014), forecast (March - April, 2014) are provided in Table 4 (MITgcm-DART exper-
643 iments) and Table 5 (MITgcm-ECCO experiments). Both MITgcm-DART and MITgcm-ECCO
644 followed the same settings as those of the 2010 experiment, but there were some changes in the
645 observations assimilated. The 2006 and 2010 experiments used SSH along-track data from satel-
646 lites J1, J2, and N1, and TMI/AMSR-E gridded SST data, whereas the 2013 and 2014 experiments
647 used SSH along-track data from J2, Saral AltiKa (Sa), and CryoSat-2 (C2) satellites. The results
648 were analyzed following a similar procedure to that used in the 2010 experiment. In particular,
649 we examined the model-data SSH *rmsd* with the AVISO analysis, focusing on the forecast perfor-
650 mance.

651 The 2006 experiment focused on the LC eddy Yankee (Eddy-Y), which showed initial detach-
652 ment in July 2006 and reattached and detached multiple times before it finally permanently sepa-
653 rated in January 2008 as per <http://www.horizonmarine.com/loop-current-eddies.html>.
654 The MITgcm-ECCO experiments were performed for July 1 - August 29, 2006, and MITgcm-
655 DART experiments were performed for the same period (60 days, with 20 assimilation cycles of
656 3-day assimilation window), using two ensemble sizes: 25 and 100, both with an inflation factor
657 of 1.2 and localization radius of 250 km. The MIT-4DVAR forecast shows better performance

658 compared to MIT-EnKF-Ens forecasts using 25 and 100 ensemble members, even with the shorter
659 localization radius, and MIT-C forecast initialized using HYCOM/NCODA 1/12° global daily
660 analysis (Figure 12a). Please note that the y-axis of all panels in Figure 12 spans 5 cm to 20
661 cm to show the details. The MIT-EnKF-Ens forecast performance improves when the ensemble
662 size is increased from 25 to 100. The hindcast period (July - August, 2006) exhibited a more
663 dynamically-active LC circulation, with Eddy-Y detaching/reattaching to the LC (not shown), and
664 the LC circulation is more complicated than in the 2010 experiment, where the LC was in the
665 slowly-evolving growth/extension phase. This may be why even 100 ensemble members were not
666 sufficient to match MIT-4DVAR forecast.

667 The 2013 and 2014 experiments focused on the formation of LC eddy Kraken (Eddy-K),
668 which first detached in April 2013 and finally permanently separated in October 2014 af-
669 ter multiple detachment/reattachment with the LC as per [http://www.horizonmarine.com/](http://www.horizonmarine.com/loop-current-eddies.html)
670 [loop-current-eddies.html](http://www.horizonmarine.com/loop-current-eddies.html). The assimilation experiments were performed during January 1
671 - March 1, and February 1 - 27, for 2013 and 2014, respectively. For 2013 and 2014, MITgcm-
672 DART was implemented with 25 ensemble members, inflation factor of 1.2, localization radius of
673 250 km, and a hindcast period of 60 days (20 assimilation cycles of 3-day assimilation window)
674 for 2013 and 27 days (9 assimilation cycles of 3-day assimilation window) for 2014. In 2013, the
675 MIT-C forecast is best beyond one month. The MIT-4DVAR forecast starts off with a large *rmsd*
676 compared to MIT-C and MIT-EnKF-Ens forecasts, but has slower *rmsd* growth toward the end of
677 the forecast period compared to MIT-EnKF-Ens. The MIT-EnKF-Ens provides comparable *rmsd*
678 to MIT-C during the first week of the forecast period and then diverges from MIT-C, showing
679 larger *rmsd* toward the end of the forecast period (Figure 12b). In 2014, MIT-C and MIT-EnKF-
680 Ens closely match during the early stage, but MIT-4DVAR provides a better solution at the end
681 of the forecast period (Figure 12c). Again, for all MITgcm-DART experiments the mean of the

ensemble forecasts (MIT-EnKF-Ave) showed lower *rmsd* compared to a single forecast starting from the ensemble mean analysis (MIT-EnKF-Ens).

Overall, both systems lead to mixed forecast performances, with generally better long-term forecasts by MITgcm-ECCO and more accurate short-term forecasts by MITgcm-DART. The forecast skill from both methods greatly depends on the background state of the LC and eddy circulation in the GoM. During slowly-evolving LC growth/extension phase, the LC system appears to be more linear and both methods produce reasonable, comparable forecasts, even with fewer ensemble members for MITgcm-DART. Whereas forecast skill from both methods degrades during dynamically-active LC eddy detachment/reattachment and permanent separation phases.

7. Summary and Conclusions

A comprehensive comparison of 4DVAR and EnKF ocean DA systems was conducted using a realistic application of the MITgcm to analyze and predict the LC circulation in the GoM. The ocean state estimates and forecasts from MITgcm-ECCO 4DVAR and MITgcm-DART EnKF systems and the contribution of ensemble prediction were evaluated by comparing with AVISO SSH analysis and TMI/AMSR-E gridded SST data for hindcasts and forecasts, and with Spray glider subsurface temperature and salinity observations for forecasts. The mean predicted state from ensemble forecasts was always seen to be superior to the predicted state from the ensemble mean analysis. The SSH and SST hindcasts from both systems were comparable and they follow closely the HYCOM/NCODA global daily analysis. The SSH forecasts from both systems, including ensemble forecasts, significantly outperformed their respective persistence forecasts (Figure 8a). The reference forecast initialized from assimilated HYCOM/NCODA daily global solutions were often as good as the forecasts from both systems, suggesting that HYCOM/NCODA provides another competitive model initialization. Additionally, while the MITgcm-ECCO 4DVAR results

presented in this work and in Gopalakrishnan et al. (2013b) are not exactly the same, they do appear very similar. This suggests that the inclusion of atmospheric forcing and open boundary controls had a small effect in this two-month short-term state estimate, at least with respect to this model, 4DVAR assimilation set up, parameters, background uncertainty covariances for model and observations, and times, which is an interesting result. Earlier, using Ensemble Optimal Interpolation (EnOI), Counillon and Bertino (2009) reported that changes in the lateral and surface boundary conditions appeared to control the propagation of LCFEs along the edge of the LC and contribute to the ensemble spread in the GoM.

The MITgcm-ECCO controls allow independent adjustment of the model initial conditions for temperature and salinity, while the MITgcm-DART builds in correlations between the fields. MITgcm-DART better deals with non-linearities and can propagate uncertainties forward. It however only provides limited degrees of freedom to fit the data depending on the ensemble size. Localization and inflation are then needed to obtain good performance. The MITgcm-DART estimates are generally closer to the observations, but typically require several assimilation cycles before reaching an acceptable solution, whereas MITgcm-ECCO estimates are dynamically-consistent over the whole hindcast period.

The MITgcm-DART experiments varying the ensemble size, covariance inflation, localization length scale, and number of assimilation cycles outlined the sensitivity of the ensemble forecasts to filter parameters. In general, MITgcm-DART predictions were enhanced by increasing the ensemble size. A larger ensemble provides more degrees of freedom and spread, which usually lead to a better analysis state. The MITgcm-DART predictability also improved with decreased localization length scale. A finer localization length scale enables a better fit with the observations, but may degrade the dynamical balance of the solutions (Houtekamer and Mitchell 2005). MITgcm-DART also showed better short-term predictability when using shorter hindcast periods (fewer

assimilation cycles) down to two weeks. This result is specific to the MITgcm-DART system and filter parameters used in this study, and cannot be generalized, but in this case, a shorter hindcast period might maintain a better ensemble spread toward the end of the hindcast period, leading to a better fit with observations, and more spread to initialize the ensemble forecasts. On the other hand, a properly tuned EnKF system is equally capable of maintaining ensemble spread over a longer hindcast period, and can efficiently fit the observations to provide good initializations for ensemble forecasting.

The MITgcm-DART ensemble forecasts provide enhanced predictions from the ensemble mean and an uncertainty estimate from the spread. The ensemble SSH spread increased with forecast time, as expected, and is largest in the regions of high SSH gradients such as the LC, the region of cyclonic LCFEs, and in the regions of LC eddy dissipation in the western GoM basin. The ensemble mean and spread highlight regions that affect the LC predictability and the spatial-temporal processes that might trigger LC eddy separation in the GoM.

The present work demonstrates a practical application of both assimilation methods for the GoM and performs a reasonable comparison between them. The overall conclusion is that, for the LC circulation in the GoM in these realizations, MITgcm-DART provided better short-term predictability (less than four weeks), while MITgcm-ECCO provided better long-term predictability (longer than four weeks). The conclusion from this study are however specific to a few 4DVAR and EnKF LC eddy separation experiments in the GoM and cannot be generalized to conclude the relative performances of both methods. The predictability results suggest the hypothesis that while the 4DVAR fit over a long time period and could not get as close to the observations as the sequential method, it is not limited to a reduced state space like ensemble methods and so can get closer to the true state which should lead to better long-term predictability. The MITgcm-ECCO and MITgcm-DART experiments in the GoM suggest that the performance of both systems critically depends

753 on the background state of the circulation in the GoM, which ranges from the slowly-evolving LC
754 growth/extension phase, to the dynamically-active LC eddy detachment/reattachment and perma-
755 nent separation phase. For this reason, among others, this study is only a start at understanding the
756 trade-offs between methods because of the many cases that could be tried and the large parameter
757 space to explore, including model resolution and mixing parameterizations.

758 *Acknowledgments.* We gratefully acknowledge the ECCO consortium, including MIT, JPL, and
759 the University of Hamburg and the NCAR Data Assimilation Research Section (DAReS). The
760 MITgcm code used in this study is checkpoint 64Y, and were obtained from [http://mitgcm.](http://mitgcm.org/)
761 [org/](http://mitgcm.org/). The Ssalto/Duacs altimeter product AVISO is produced and distributed by the Copernicus
762 Marine and Environment Monitoring Service (CMEMS) (<http://marine.copernicus.eu/>).
763 The HYCOM/NCODA 1/12° global analysis were obtained from the HYCOM consortium ([http:](http://hycom.org/dataserver/)
764 [//hycom.org/dataserver/](http://hycom.org/dataserver/)). The along-track altimetry data were obtained from the Radar Al-
765 timetry Database System (RADS), (<http://rads.tudelft.nl/rads/index.shtml>). The SST
766 data were obtained from the Remote Sensing Systems Inc. (<http://www.remss.com/>). The
767 NCEP/NCAR-Reanalysis-1 atmospheric forcings were obtained from the [http://www.esrl.](http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.html)
768 [noaa.gov/psd/data/gridded/data.ncep.reanalysis.html](http://www.esrl.noaa.gov/psd/data/gridded/data.ncep.reanalysis.html). The MITgcm-DART EnKF
769 and MITgcm-ECCO 4DVAR state estimates, input files including observations and error fields,
770 are available from the authors upon request (ggopalakrishnan@ucsd.edu). BDC is supported by
771 the Office of Naval Research Award Number: XXXX. GG is supported by the National Academy
772 of Sciences Award Number: XXXX

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TABLE 1: MITgcm-IAS Model Description

Description	Value/Source
Longitude	$98^{\circ} \text{ W} - 72.5^{\circ} \text{ W}$
Latitude	$8.5^{\circ} \text{ N} - 31^{\circ} \text{ N}$
Topography	Two-minute gridded global topography (ETOPO-2), with maximum depth of 6000 m.
Horizontal grid	$1/10^{\circ} \times 1/10^{\circ}$ ($\sim 11 \text{ km}$) spherical polar grid.
Vertical grid	40 vertical z - levels, with level spacing gradually increasing with depth from 5 m at the surface to a maximum of 500 m near the bottom.
Sub-grid scale parameterization	Vertical, second order diffusive operator.
Vertical diffusivity and viscosity parameterization	Laplacian mixing with a background value of $1 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ and $1 \times 10^{-4} \text{ m}^2 \text{ s}^{-1}$, respectively, and the K-profile parameterization (KPP) in the surface mixed layer (Large et al. 1994).
Horizontal diffusivity and viscosity (second order)	$1 \times 10^2 \text{ m}^2 \text{ s}^{-1}$
Horizontal diffusivity and viscosity (fourth order)	$1 \times 10^{11} \text{ m}^4 \text{ s}^{-1}$

TABLE 2: MITgcm-IAS Model Forcings

Description	Source
Initial conditions	The Hybrid Coordinate Ocean Model (HYCOM) global 1/12° daily analysis (http://hycom.org/dataserver/glb-analysis) using Navy Coupled Ocean Data Assimilation (NCODA) (Chassignet et al. 2007).
Open boundary (OB) conditions	HYCOM/NCODA global 1/12° estimates of T, S, and horizontal velocities (U: east - west and V: north - south components), sampled every 7 days.
OB sponge layer	Buffer zone of 1°, with restoring time scales varying linearly from 1 day at the boundary to 5 days at the inner edge of the sponge layers. HYCOM/NCODA normal velocity fields across the OB have been adjusted to have zero net volume flux into the model domain.
Atmospheric forcing	National Centers for Environmental Prediction (NCEP)/National Center for Atmospheric Research (NCAR) re-analysis (NCEP/NCAR-R1) project (Kalnay et al. 1996).
Atmospheric state	Bulk formulation (Large and Pond 1981) for the computation of the atmospheric fluxes. The atmospheric forcing includes 2° × 2° global gridded air temperature, specific humidity, zonal and meridional wind speed at 10 m from the ground, total precipitation, and short and long wave radiative fluxes, sampled every 6 hours.
Run-off fluxes	Monthly climatological freshwater fluxes from the ECCO global model (Stammer et al. 2002).

TABLE 3: Observations for 2010 experiment

Data type	Description	Source
Mean Dynamic Topography (MDT)	Danish National Space Center Mean Sea Surface 2008 (DNSCMSS08) minus Earth Gravity Model 2008 (EGM08): DNSCMSS08-EGM08.	(Andersen and Knudsen 2009; Pavlis et al. 2012)
Altimetry	Along-track Sea Surface Height (SSH) anomalies from three satellites: Jason-1 (J1), Jason-2 (J2), and Envisat (N1) with respect to DNSCMSS08-EGM08 MDT.	Radar Altimetry Database System (RADS), (http://rads.tudelft.nl/rads/index.shtml)
Sea-Surface Temperature (SST)	Daily, optimally interpolated product from the TMI/AMSR-E instruments on a $0.25^\circ \times 0.25^\circ$ grid.	Remote Sensing Systems Inc. (http://www.remss.com/)
Spray glider (Non-assimilated data, used only for model forecast validation)	Temperature and Salinity profiles.	SIO Spray glider (Sherman et al. 2001; Rudnick et al. 2004) data server (http://spraydata.ucsd.edu/projects/GoM)

TABLE 4: Details of the MITgcm-DART EnKF assimilation and forecast experiments

	Experiment	Ensemble size	Localization radius (km)	Inflation	Hindcast	Forecast
2010	EnKF2010-N50-I1.2-L250	50	250	1.2	2 months (03/01 - 04/29)	2 months (04/30 - 06/28)
	EnKF2010-N50-I1.2-L500	50	500	1.2	2 months (03/01 - 04/29)	2 months (04/30 - 06/28)
	EnKF2010-N50-I1.3-L500	50	500	1.3	2 months (03/01 - 04/29)	2 months (04/30 - 06/28)
	EnKF2010-N100-I1.2-L500	100	500	1.2	2 months (03/01 - 04/29)	2 months (04/30 - 06/28)
	EnKF2010-N25-I1.2-L250-2MN	25	250	1.2	2 months (03/01 - 04/29)	2 months (04/30 - 06/28)
	EnKF2010-N25-I1.2-L500	25	500	1.2	2 months (03/01 - 04/29)	2 months (04/30 - 06/28)
	EnKF2010-N25-I1.2-L250-1MN	25	250	1.2	1 month (03/31 - 04/29)	2 months (04/30 - 06/28)
2006	EnKF2010-N25-I1.2-L250-2WK	25	250	1.2	2 weeks (04/15 - 04/29)	2 months (04/30 - 06/28)
	EnKF2006-N25-I1.2-L125	25	250	1.2	2 months (07/01 - 08/29)	2 months (08/30 - 10/28)
2013	EnKF2006-N100-I1.2-L125	100	250	1.2	2 months (07/01 - 08/29)	2 months (08/30 - 10/28)
	EnKF2013-N25-I1.2-L125	25	250	1.2	2 months (01/01 - 03/01)	2 months (03/02 - 04/30)
2014	EnKF2014-N25-I1.2-L125	25	250	1.2	1 month (02/01 - 02/27)	2 months (02/28 - 04/28)

* The MITgcm-DART experiments are named as: EnKF<year> – <N: ensemble size> – <I: inflation factor> – <L: localization radius in km>

* Month is abbreviated as MN, and week is abbreviated as WK

TABLE 5: Details of the MITgcm-ECCO 4DVAR assimilation and forecast experiments

	Experiment	Hindcast	Forecast
2010	4DVAR-2010	2 months (03/01 - 04/29)	2 months (04/30 - 06/28)
2006	4DVAR-2006	2 months (07/01 - 08/29)	2 months (08/30 - 10/28)
2013	4DVAR-2013	2 months (01/01 - 03/01)	2 months (03/02 - 04/30)
2014	4DVAR-2014	1 month (02/01 - 02/27)	2 months (02/28 - 04/28)

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