

Data assimilation in a coupled physical-biogeochemical
model of the California Current System using an
incremental lognormal 4-dimensional variational
approach: Part 3, Assimilation in a realistic context
using satellite and in situ observations

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Abstract

A fully coupled physical and biogeochemical ocean data assimilation system is tested in a realistic configuration of the California Current System using the Regional Ocean Modeling System. In situ measurements for sea surface temperature and salinity as well as satellite observations for temperature, sea level and chlorophyll are used for the year 2000. Initial conditions of the combined physical and biogeochemical state are adjusted at the start of each 3-day assimilation cycle. Data assimilation results in substantial reduction of root-mean-square error (RMSE) over unconstrained model output. RMSE for physical variables is slightly lower when assimilating only physical variables than when assimilating both physical variables and sur-

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face chlorophyll. Surface chlorophyll RMSE is lowest when assimilating both physical variables and surface chlorophyll. Estimates of subsurface, nitrate and chlorophyll show modest improvements over the unconstrained model run relative to independent, unassimilated in situ data. Assimilation adjustments to the biogeochemical initial conditions are investigated within different regions of the California Current System. The incremental, lognormal 4-dimensional data assimilation method tested here represents a viable approach to coupled physical biogeochemical state estimation at practical computational cost.

Keywords: Coupled Data assimilation, 4DVar, Biogeochemical model, California Current System, Coastal upwelling

1 **1. Introduction**

2 The study of marine ecosystems in regional environments is motivated by
3 a wide range of topics, spanning fundamental questions concerning controls
4 on primary production, community structure and carbon export to more ap-
5 plied problems in fisheries management, harmful algal blooms, and habitat
6 monitoring, to name but a few. Investigations generally require quantifica-
7 tion of various elements of the physical and/or biogeochemical constituents,
8 such as temperature, salinity, phytoplankton biomass, and processes such as
9 nutrient uptake or grazing. Short space and time scales of variability in the
10 coastal ocean present a challenge for direct and comprehensive observation
11 of key variables, though real progress in observing sensors and platforms has
12 been accomplished over the last decade.

13 Coupled physical and biogeochemical models provide a complementary

14 approach to direct observation for the study of marine ecosystems. World-
15 wide, a handful of advanced physical circulation models are widely used as
16 backbones for a much larger assortment of biogeochemical models that range
17 in complexity and purpose. Such coupled models show increasing skill in rep-
18 resenting marine ecosystems, but discrepancies between model predictions
19 and observations are inevitable. Such errors arise from multiple unavoid-
20 able issues such as uncertainty in model initialization and forcing as well as
21 incomplete or incorrect parameterization of basic model processes.

22 One approach to reduce discrepancies between ocean model output and
23 observations is through data assimilation, where observations are used to rig-
24 orously constrain ocean model trajectories. Data assimilation of the physical
25 circulation is well-established and carried out routinely on global and re-
26 gional scales. The assimilation of ecosystem variables into coupled physical-
27 biogeochemical models is less advanced, although considerable progress has
28 been made over the last two decades. Biogeochemical data assimilation has
29 been used to constrain model parameters, some of which are poorly known,
30 and to improve estimates of the biogeochemical state, and sometimes for both
31 purposes (See Gregg (2008) and Edwards et al. (2015) for recent reviews).

32 In two companion papers, we implemented a new formulation for biogeo-
33 chemical and coupled physical-biogeochemical data assimilation for ocean
34 state estimation (Song et al., 2016,). Our approach is an incremental form of
35 lognormal 4-dimensional variational assimilation (4DVar), first proposed by
36 Song et al. (2012) and described further by Fletcher and Jones (2014). We
37 choose a lognormal formulation because of the skewed statistical distributions
38 of biological variables that are clearly non-Gaussian and better represented

39 as lognormal (Campbell, 1995). We have implemented this capability within
40 the Regional Ocean Modeling System (ROMS; Shchepkin and McWilliams,
41 2004), building on its existing 4DVar capabilities developed for physical vari-
42 ables (Moore et al., 2011,).

43 In idealized model twin experiments, Song et al. (2016) show that the
44 lognormal form of 4DVar produces superior state estimates with lower root-
45 mean-square errors (RMSEs) for biological fields relative to those derived
46 assuming Gaussian error distributions. Song et al. (2016) implemented a
47 fully coupled physical and biogeochemical system allowing the simultaneous
48 assimilation of both Gaussian and lognormally distributed errors following
49 Fletcher (2010) and Fletcher and Jones (2014). Tests in an idealized model
50 twin experiment compared data assimilation of only physical variables, only
51 biological variables, and both physical and biological variables. The lowest
52 RMSE for both the physical and biogeochemical variables of the modeled
53 ocean state resulted from the assimilation of both physical and biological
54 observations.

55 Model twin experiment is a useful guide for understanding model perfor-
56 mance, but ultimately is limited because the assimilation model is identical
57 to that used as a surrogate for the true state. In a real application, the model
58 is imperfect and thus unable to exactly match nature. It is the purpose of
59 this paper to test the fully coupled 4DVar data assimilation system in a re-
60 alistic environment, and we choose the California Current System (CCS) as
61 our testbed.

62 The CCS refers to a collection of ocean currents and other circulation fea-
63 tures in the northeastern subtropical Pacific. As with other eastern bound-

64 ary regions, the CCS experiences seasonally vigorous upwelling driven by
65 equatorward wind stress near the coast. The wind-driven upwelling supplies
66 nutrients to the euphotic zone and drives substantial primary production,
67 ultimately supporting a disproportionately rich and complex ecosystem rel-
68 ative to its small area (Carr, 2002). The present investigation builds on
69 several previous modeling studies of the CCS, including efforts to describe
70 the physical circulation using forward, adjoint, and data assimilative models
71 (Veneziani et al., 2009,, Broquet et al., 2009, 2011), and various aspects of the
72 CCS ecosystem using non-data assimilative coupled physical-biogeochemical
73 models of varying complexity (Goebel et al., 2010, Fiechter et al., 2014).

74 Here we evaluate coupled physical-biogeochemical data assimilation us-
75 ing ROMS and a simple 4-component Nutrient-Phytoplankton-Zooplankton-
76 Detritus (NPZD) model (Powell et al., 2006) for one calendar year (2000).
77 Physical data assimilated includes sea surface height, sea surface temper-
78 ature, and in situ temperature and salinity. For biogeochemical data, we
79 assimilate satellite-derived sea surface chlorophyll. In situ nitrate and chloro-
80 phyll observations from two field programs are withheld for independent eval-
81 uation. Model initial conditions at the start of each assimilation cycle are
82 adjusted. We demonstrate both the utility of this approach in a realistic and
83 practical implementation and also investigate how the assimilation system
84 functions in different regions of the CCS for which different unconstrained
85 (prior) model deficiencies are identified with respect to the observations.

86 **2. Coupled data assimilation system**

87 Song et al. (2016) present a full description of the physical and biogeo-

88 chemical data assimilation (PBDA) procedure, and we include here only
 89 an abbreviated version. Using the 4-dimensional variational method, up-
 90 dates to a control vector are based on all available observations within an
 91 assimilation window. In general, the control vector can include multiple el-
 92 ements, such as model forcing fields and open boundary conditions (Moore
 93 et al., 2011), but for the present investigation, we consider for simplicity
 94 only a control vector consisting of model initial conditions. Describing the
 95 additional impact of adjustments to model forcing and lateral boundary con-
 96 ditions is left to future studies. The increment to the background initial
 97 state is denoted $\delta\mathbf{z}_0$ and consists of both physical and biological elements;
 98 more specifically, $\delta\mathbf{z}_0^T = [(\delta\mathbf{x}_0^{phy})^T (\delta\mathbf{x}_0^{bio})^T]$, where $\delta\mathbf{x}_0^{phy} = (\mathbf{x}_a^{phy} - \mathbf{x}_b^{phy})_0$ and
 99 $\delta\mathbf{x}_0^{bio} = (\mathbf{x}_a^{bio} - \mathbf{x}_b^{bio})_0$ are the $(n_g \times 1)$ and $(n_l \times 1)$ increment vectors of physical
 100 and biological variables at the initial time, respectively. The subscript a/b
 101 represents the posterior/prior solution.

102 Some biogeochemical variables are known to have non-Gaussian distribu-
 103 tions, with better consistency with lognormal distributions (Campbell, 1995,
 104 Campbell et al., 1995). As a result, the increments $\delta\mathbf{z}_0$ will not be Gaussian-
 105 distributed, and a solution assuming Gaussian errors for all variables will
 106 not be optimal. We proceed with the assumption that physical variables
 107 have Gaussian distributed errors while errors in biogeochemical variables are
 108 lognormally distributed. Though the lognormal assumption is likely also im-
 109 perfect, it allows a straightforward solution to the assimilation problem, and
 110 this solution has been shown in model twin experiments to be superior to
 111 the Gaussian assumption for biogeochemical variables (Song et al., 2016).

112 By definition, a logarithm transformation of lognormally distributed vari-

113 ables results in Gaussian distributed values, and the difference between Gaus-
 114 sian distributed variables also has a Gaussian distribution. As a result, we
 115 define $\delta \mathbf{g}_0^{bio} = (\ln \mathbf{x}_a^{bio} - \ln \mathbf{x}_b^{bio})_0$ whose distribution is Gaussian. In addition, if
 116 $\delta \mathbf{x}_0^{phy}$ is Gaussian distributed, the new control vector $\delta \mathbf{z}_0^T = [(\delta \mathbf{x}_0^{phy})^T (\delta \mathbf{g}_0^{bio})^T]$
 117 will also be drawn from a Gaussian distribution.

118 The optimal solution for $\delta \mathbf{z}_0$ minimizes the cost function J :

$$\begin{aligned}
 J(\delta \mathbf{z}_0) &= \frac{1}{2} \delta \mathbf{z}_0^T \mathbf{B}^{-1} \delta \mathbf{z}_0 \\
 &\quad + \frac{1}{2} \sum_{i=1}^{N_o} (\mathbf{d}_i - \mathbf{O}_i \mathbf{H}_i \mathbf{M}_{i,0} \mathbf{X} \delta \mathbf{z}_0)^T \mathbf{R}_i^{-1} \\
 &\quad (\mathbf{d}_i - \mathbf{O}_i \mathbf{H}_i \mathbf{M}_{i,0} \mathbf{X} \delta \mathbf{z}_0). \tag{1}
 \end{aligned}$$

119 Here, \mathbf{d}_i defines the innovations that can be partitioned into linear and log-
 120 space. More specifically, $\mathbf{d}_i = \mathbf{y}_i - \mathbf{x}_{b,i}^o$ for Gaussian distributed variables and
 121 $\mathbf{d}_i = \ln \mathbf{y}_i - \ln \mathbf{x}_{b,i}^o$ for lognormally distributed variables, where \mathbf{y}_i represents
 122 the i^{th} set of observations, and $\mathbf{x}_{b,i}^o$ indicates the corresponding background
 123 model estimates. \mathbf{d}_i can be a mixture of both Gaussian and lognormally dis-
 124 tributed variables. The matrices \mathbf{H}_i and $\mathbf{M}_{i,0}$ are tangent linear forms of the
 125 observation operator and nonlinear model, respectively. Diagonal matrices
 126 \mathbf{O}_i and \mathbf{X} have diagonal elements $[1, 1, \dots, 1, (\mathbf{x}_{b,i}^o)_1, (\mathbf{x}_{b,i}^o)_2, \dots, (\mathbf{x}_{b,i}^o)_{m_l}]^{-1}$
 127 and $[1, 1, \dots, 1, (\mathbf{x}_{b,0})_1, (\mathbf{x}_{b,0})_2, \dots, (\mathbf{x}_{b,0})_{m_l}]$, respectively, where m_l is the
 128 number of observations for lognormally distributed variables. Matrices \mathbf{B} and
 129 \mathbf{R} denote the background and observation error covariance matrices, respec-
 130 tively, and will be discussed further below. This cost function is quadratic,
 131 hence its optimal solution can be found using traditional methods such as
 132 conjugate gradient. The Jacobian and Hessian of this cost function can be
 133 found in a companion paper Song et al. (2016) along with more details.

134 **3. Observations**

135 Physical and biological observations were used to constrain the model
136 during the year 2000. More than 3 million physical observations including
137 sea surface height (SSH), sea surface temperature (SST), subsurface T and
138 S are used. In addition, more than a million surface chlorophyll data are
139 available for coupled physical and biological state estimation (Table 1).

140 *3.1. Physical observations*

141 A brief introduction to the physical observations is provided here, but
142 detailed descriptions about the data set and preprocessing can be found in
143 Moore et al. (2011) for the same collection of physical observations used
144 in this study. For SSH observations, we use the sum of the mapped sea
145 level anomaly product from Ssalto-Duacs system and the mean dynamic
146 topography estimated by Rio et al. (2004). Mean sea level is adjusted so
147 that the unconstrained model and data have the same spatio-temporal mean
148 value. Temporal and spatial resolution of the data are 7 days and $1/3^\circ$,
149 respectively, while the observation error is set to 0.02 m. Daily assimilated
150 SST data is from the Advanced Very High Resolution Radiometer (AVHRR)
151 with a horizontal resolution of approximately 0.04° (Kilpatrick et al., 2001).
152 The observation error assumed for SST is set to 0.4°C . In situ T and S
153 observations come from the quality controlled data prepared by the European
154 Union ENSEMBLES project (EN3) (Ingleby and Huddleston, 2007). This
155 data set includes CTD profiles sampled during the CalCOFI program from
156 the southern and central CCS, and GLOBEC-LTOP survey cruises from the
157 northern CCS. Observation errors for in situ T and S are assumed to be 0.1

158 °C and 0.01, respectively.

159 *3.2. Biological observations*

160 The biological model, NPZD (nutrients, phytoplankton, zooplankton and
161 detritus), solves for phytoplankton biomass, instead of chlorophyll. We first
162 import the SeaWiFS level 3 Standard Mapped Image (SMI) products with
163 roughly 9 km horizontal resolution and then convert chlorophyll observations
164 in units of mg m^{-3} to phytoplankton units of mmol N m^{-3} . The carbon
165 to nitrogen conversion is based on a Redfield ratio (C:N=106:16), and a
166 chlorophyll to carbon ratio of C:Chl=50:1, which is reasonable for diatoms
167 (i.e., the dominant phytoplankton species associated with coastal upwelling)
168 in the California Current System (Goebel et al., 2010). Although satellite
169 observations represent an integral over an optical depth, we choose for this
170 study the more simple approach of assimilating satellite-derived estimates of
171 phytoplankton biomass into the uppermost model level. The error level for
172 phytoplankton biomass data in log-transformed space is set to 0.3, which is
173 approximately 30 % of the observed value ($\pm 35\%$ for chlorophyll in Moore
174 et al. (2009)).

175 The SeaWiFS daily chlorophyll data does not provide good temporal cov-
176 erage in the coastal regions during 2000. Temporal data coverage in coastal
177 areas (which we define here as a nearshore strip approximately 100 km wide
178 and indicated by the blue line in Figures 1a and c) is in fact less than 30%. As
179 shown in Figure 1b, the temporal coverage for coastal chlorophyll is partic-
180 ularly low in winter at higher latitudes, which is most likely associated with
181 the passage of storm systems. NASA’s Ocean Biology Processing Group also
182 provides an 8-day composite product with close to 100% data coverage after

183 computing a temporal and spatial weighted mean (Campbell et al., 1995).
184 In this product, chlorophyll values are fixed for 8 days, whereas both physi-
185 cal and biological processes in coastal regions generally vary considerably on
186 shorter time-scales. Although the spatial coverage of the 8-day product is
187 good, the temporal variations captured are questionable. Therefore, we use
188 the daily chlorophyll data with low spatial coverage and with the expectation
189 that the data assimilation system will estimate missing observations using
190 model dynamics and error covariances. This interpolation capability is one
191 potential benefit of the 4DVar data assimilation.

192 For our investigation, we also consider subsurface biological data. Specifi-
193 cally, chlorophyll and nitrate (NO_3) from the CalCOFI and GLOBEC-LTOP
194 programs were available during the time-period of our experiment, and their
195 locations are shown in dots in Figure 1(a). These data are not assimilated
196 but used only for the evaluation of the coupled state estimates.

197 If more than one observation of a single type (e.g., temperature) is avail-
198 able in a model grid cell within one day, all observations of this type are
199 merged into a single value. This creation of “super observations” reduces
200 data redundancy, and an appropriate level of error for the merged data is
201 determined by the uncertainties of all observations within a model grid cell
202 (Moore et al., 2011).

203 *3.3. Observation filter*

204 Not all the biological observations were used in the system. As reported
205 in Song et al. (2016), our quadratic lognormal 4DVar formulation requires a

206 linear approximation to the logarithm transform as follows:

$$\begin{aligned} \ln(\mathbf{x}_{b,i}^o + \delta\mathbf{x}_i^o) &\approx \ln \mathbf{x}_{b,i}^o + \mathbf{L}_i \delta\mathbf{x}_i^o \\ &\approx \ln \mathbf{x}_{b,i}^o + \mathbf{L}_i \mathbf{H}_i \mathbf{M}_{i,0} \delta\mathbf{x}_0, \end{aligned} \quad (2)$$

207 where $\delta\mathbf{x}_i^o$ represents the increment for the i^{th} observation set, and

$$\begin{aligned} \mathbf{L}_i &\equiv \left. \frac{\partial \ln \mathbf{x}_i^o}{\partial \mathbf{x}_i^o} \right|_{\mathbf{x}_i^o = \mathbf{x}_{b,i}^o} \\ &= \begin{bmatrix} (\mathbf{x}_{b,i}^o)_1 & 0 & \cdots & 0 \\ 0 & (\mathbf{x}_{b,i}^o)_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & (\mathbf{x}_{b,i}^o)_{m_i} \end{bmatrix}^{-1}. \end{aligned} \quad (3)$$

208 Equation (2) results from a Taylor expansion of the logarithm function for
 209 \mathbf{x}_i^o . In the simplest case when there is only one observation, Song et al. (2016)
 210 suggest that the observation y should satisfy

$$(1 - \alpha)x_b^o < y < (1 + \alpha)x_b^o \quad (4)$$

211 for the Taylor series approximation to be valid, where α is a constant between
 212 0 and 1. In this experiment, we choose $\alpha = 0.5$ and discard observations
 213 outside the range in (4). This filtering reduces the number of observations
 214 that are used in the assimilation process, but helps to prevent the model
 215 from diverging due to violation of a linearity condition embedded in our
 216 formulation. It can also be thought of as a form of background quality
 217 control.

218 4. Model settings

219 Coupled PBDA for the year 2000 was performed with the NPZD model
220 coupled to ROMS. ROMS is a 3D ocean circulation regional model with
221 terrain following vertical coordinate (Haidvogel et al., 2000, Shchepkin and
222 McWilliams, 2004, Haidvogel et al., 2008). The model is configured for the
223 CCS with $1/10^\circ$ horizontal resolution and 42 vertical levels. This configura-
224 tion has been widely used in other studies and proven to reproduce the mean
225 CCS circulation as well as its seasonal variability (Veneziani et al., 2009,,
226 Moore et al., 2011). The model also captures the circulation by mesoscale ed-
227 dies with a length scale larger than 30 km, which imposes a greater challenge
228 for coupled state estimation at the same time because of highly nonlinear
229 features in the system. We note that this configuration has higher horizontal
230 resolution than the one used in the companion papers for the model twin
231 experiments ($1/3^\circ$ in Song et al. (2016,)).

232 The NPZD model has relatively simple dynamics linking the 4 compo-
233 nents (nutrient, phytoplankton, zooplankton and detritus) (Powell et al.,
234 2006). All components are budgeted in terms of nitrogen. Phytoplankton
235 grows with nutrient uptake using Michaelis-Menten kinetics and is consumed
236 by grazing and mortality. Zooplankton biomass increases by grazing phy-
237 toplankton (using an Ivlev formulation) and decreases through mortality.
238 Concentrations of detritus increase through phytoplankton and zooplankton
239 mortality as well as through unassimilated grazing. Remineralization reduces
240 detrital concentrations, returning nitrogen to its inorganic form. Table 2 lists
241 the parameter values tuned for the CCS region.

242 The NPZD model dynamics are critical for PBDA to determine the in-

243 crement to the biological initial condition from the misfit between observa-
244 tions and model estimates during the assimilation cycle. For example, if the
245 model prior has lower phytoplankton biomass than observed, the assimila-
246 tion procedure has several mechanisms by which it can increase the modeled
247 phytoplankton biomass. Model initial conditions can be adjusted to (a) in-
248 crease phytoplankton concentrations directly, (b) increase nutrient levels, (c)
249 decrease zooplankton biomass, or (d) because this is a fully coupled assimila-
250 tion system, alter flux divergences of phytoplankton, nutrients or zooplankton
251 via the velocity field resulting in the desired increase in phytoplankton at the
252 observation point. In practice, a combination of all these mechanisms occurs,
253 where the relative proportion of each is based on the model dynamics and
254 the prescribed uncertainties in the observations and model variables.

255 The target year for the PBDA experiment is the year 2000 during which
256 the CCS was close to the climatological norm despite La Niña conditions
257 (Durazo et al., 2001). The initial condition for physical variables was pre-
258 pared from the CCS 31-year historical reanalysis, CCSRA31 (Neveu et al.,
259 2015), a product using the ROMS-4DVar procedure on the same model grid
260 as this study. The initial condition for biological variables was derived from a
261 10-year spin-up of the coupled model. Physical boundary conditions and sur-
262 face forcing were taken from SODA (Carton and Giese, 2008) and COAMPS
263 (Hodur et al., 2002, Doyle et al., 2009), respectively. Biological boundary
264 conditions for nutrients are the nitrate field extracted from World Ocean At-
265 las 2009 climatology (Garcia et al., 2006). Other variables are set to a small,
266 constant value $C_0 = 0.1 \text{ mmol N m}^{-3}$.

267 The background error covariance matrix \mathbf{B} in (1) is a block matrix,

$$\mathbf{B} = \begin{bmatrix} \mathbf{B}_G & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_L \end{bmatrix}, \quad (5)$$

268 where \mathbf{B}_G and \mathbf{B}_L represent background error covariances for physical and
269 log-transformed biological variables, respectively. \mathbf{B}_G is adopted from the
270 error covariance matrix used in the CCSRA31. \mathbf{B}_L is estimated as $\mathbf{\Sigma}\mathbf{C}\mathbf{\Sigma}^T$
271 as in Broquet et al. (2009). The diagonal matrix of standard deviations, $\mathbf{\Sigma}$,
272 is computed using the log-transformed biological variables from the 10-year
273 spin-up run. The univariate correlation matrix \mathbf{C} is constructed with the
274 horizontal and vertical decorrelation length scale of 30 km and 7 m, respec-
275 tively. We assume that observation errors are independent and uncorrelated,
276 yielding an observational error covariance matrix \mathbf{R}_i in (1) that is diagonal
277 with error levels that appear in section 3.

278 We perform three experiments. The first simulation is a free run without
279 any constraints and is referred to here as FREE. The second experiment,
280 referred to as PDA, includes physical data assimilation only, and the model
281 solution is constrained by physical observations alone. The third integration
282 is called PBDA, assimilating both physical and biological observations in a
283 fully coupled sense. Comparison between these three simulations highlights
284 the impact of assimilating both physical and biological observations.

285 Each assimilation cycle spans 3 days. The chosen window length depends
286 on the time scale for which the tangent linear approximation is valid. In
287 the companion papers, the tangent linear approximation was found to be
288 valid for at least 5 days (Song et al., 2016,). Here, at higher horizontal
289 resolution and using realistic observations, we choose a more conservative

290 3-day window. Sensitivity experiments run with longer 4-day cycles achieved
291 comparable performance. Even 8-day cycles produce quite acceptable results
292 but are less favorable than 3- or 4-day cycles. Although the NPZD nonlinear
293 model conserves total nitrogen during forward integration, data assimilation
294 results in instantaneous adjustments to this quantity, as it does to physical
295 variables such as heat content and momentum.

296 The local minimum of the quadratic cost function J in (1) is found using
297 the Lanczos formulation (Fisher and Courtier, 1995, Tshimanga et al., 2008,
298 Moore et al., 2011). After the local minimum is identified using 10 inner
299 loops, the nonlinear coupled system is integrated forward with an updated
300 initial condition to start another optimization cycle (2 outer loops). There
301 is no model spin-up associated with each cycle, and no dynamical balance
302 of biological variables is imposed on that initial condition. The final model
303 trajectory is determined using the initial condition resulting from this second
304 optimization cycle.

305 **5. Evaluation**

306 Table 3 summarizes the RMSEs for the three experiments with respect to
307 assimilated observations (SSH, SST, $T_{in\ situ}$, $S_{in\ situ}$ and surface chlorophyll
308 (Schl)). In addition, the biological ocean states from each experiment are
309 evaluated against the independent observations of chlorophyll and NO_3 in the
310 upper 200 m from GLOBEC-LTOP and CalCOFI in Table 4. The RMSEs
311 for biological variables were computed without log-transformation.

312 *5.1. Physical variables*

313 For all physical variables, PDA yields the smallest RMSEs (Table 3).
314 PBDA also yields small RMSEs, with values comparable to but slightly larger
315 than those by PDA. This result differs from that of Song et al. (2016). In
316 that idealized model twin experiment, the smallest RMSE of physical vari-
317 ables occurred using PBDA. In both Song et al. (2016) and this study, the
318 quantitative differences between PDA and PBDA RMSEs were small relative
319 to their improvement over the FREE run. We note also that as should be
320 expected, the RMSE for physical variables can be reduced further in PBDA
321 with more iterations, and thus at somewhat higher computational cost (not
322 shown).

323 *5.2. Biological variables*

324 As in Song et al. (2016), PBDA results in the smallest RMSE for biologi-
325 cal variables (Table 3). The RMSE for surface chlorophyll is reduced by 40%
326 with respect to that of the FREE run. The observed annual mean surface
327 chlorophyll and Hovmöller diagram in Figure 1 present at least three charac-
328 teristics by which to evaluate assimilation performance: (1) high chlorophyll
329 biomass in coastal regions with an initially sharp and then much more grad-
330 ual decrease in the offshore direction (Figure 1(a,c)); (2) high chlorophyll
331 biomass near the northern Washington coast (46°N-48°N) throughout the
332 year (Figure 1(b,d)); and (3) episodic blooms of chlorophyll biomass along
333 the central California coast (34°N-46°N) that appear throughout spring and
334 summer, presumably responding to variable alongshore wind stress forcing
335 (Figure 2).

336 *5.2.1. Crossshore structure*

337 To some degree, all three model experiments capture the sharp, then more
338 gradual decrease of annual mean chlorophyll biomass in the offshore direc-
339 tion (Figure 3(a,c,e)). However, compared to observations, offshore concen-
340 trations of chlorophyll biomass are too low in the FREE run and too high in
341 PDA (Figure 3(a,c)). In this experiment, high chlorophyll biomass in PDA
342 must be driven by changes in physical properties alone, and two mechanisms
343 have been identified by Raghukumar et al. (2015). Because updated initial
344 conditions during each assimilation cycle are not required to be dynamically
345 balanced, assimilation cycles exhibit initialization shocks in which gravity
346 waves are released as part of their adjustment. These numerically-driven
347 waves transiently increase nutrient concentrations in the euphotic zone, lead-
348 ing to increased primary production and in turn phytoplankton biomass. The
349 second mechanism results from the update of subsurface physical tempera-
350 ture and/or salinity with no associated update to biological fields. Increased
351 nutrient variance on isopycnal surfaces results also in increased primary pro-
352 duction where density surfaces reach well-lit waters. Increased chlorophyll
353 biomass is most noticeable in regions of very low concentration (i.e., offshore),
354 though it is also visible in the coastal transition zone 100-200 km from shore.
355 In our experiment, PDA resulted in the highest RMSE against the surface
356 chlorophyll (Table 3). In contrast, the estimated offshore chlorophyll biomass
357 in the PBDA experiment is comparable to observations in both magnitude
358 and spatial distribution (Figure 3(e-f)). PBDA does not eliminate waves
359 produced through initialization shock, and it does impose changes in stratifi-
360 cation; however, PBDA also adjusts biogeochemical variables with the result

361 that systematically higher chlorophyll concentrations than observed do not
362 occur.

363 *5.2.2. Northern U.S. west coast (44°N-48°N)*

364 Along the U.S. west coast, like other eastern boundary upwelling systems,
365 equatorward wind stress brings nutrient-rich subsurface water to the surface,
366 supporting high chlorophyll biomass near coastal boundaries. Upwelling fa-
367 vorable wind stress is stronger along the central coast than the northern coast
368 (Figure 2). As a result, the FREE run (Figure 3(a,b)) shows lower simulated
369 chlorophyll biomass in the northern coastal region than along the central
370 coast because wind-driven upwelling is the main driver for nutrient supply
371 in the model. Indeed, wind-driven upwelling precedes high phytoplankton
372 biomass by about 1 week along the northern U.S. west coast in the FREE
373 run (Figure 4), offering support that the simulated chlorophyll biomass is
374 mainly associated with the nutrient supply due to wind-driven upwelling.
375 However, elevated levels of chlorophyll observed along the northern coast are
376 not well explained by Ekman transport alone (Figure 1(d) and 2), suggest-
377 ing that the current model configuration misses the key (either physical or
378 biological) mechanisms in that region. Similarly, low phytoplankton levels
379 in this northern coastal region have been noted in other forward modeling
380 studies (e.g., Goebel et al., 2010).

381 Hickey and Banas (2008) suggested several mechanisms that support a
382 highly productive north coast zone. Among them are a continuous nutrient
383 supply from the Strait of Juan de Fuca, localized canyon enhanced upwelling,
384 poleward coastally trapped wave and iron supply by the Columbia river. Re-
385 cently, Davis et al. (2014) have shown that the first of these is a major factor.

386 Tidal mixing within the Strait of Juan de Fuca and Puget Sound results in a
387 substantial nutrient flux to surface waters outside of the sound and ultimately
388 along the Washington coast. The present model configuration includes nei-
389 ther Puget Sound nor tidal forcing, and it uses climatological nutrient bound-
390 ary conditions along the northern boundary that are not especially elevated.
391 This deficiency suggests an erroneous representation of the ecosystem in this
392 region, including a systematically lower phytoplankton biomass. Since this
393 issue is locally the result of low nutrients and remote physical process that
394 occur outside of the model domain, it can not be improved by physical data
395 assimilation. Indeed PDA (Figure 3(c,d)) results in a quantitatively differ-
396 ent circulation in the region and an altered ecosystem response, including
397 somewhat higher phytoplankton levels in spring, fall and winter, and lower
398 levels in summer relative to the FREE run. But qualitatively, PDA is also
399 deficient in the northern coastal region.

400 On the other hand, PBDA allows for chlorophyll observations to con-
401 strain the model, and thus it can improve on low prior estimates. In this
402 system, model initial conditions are adjusted such that the misfit between
403 model chlorophyll estimates and those observed is reduced. Modeled PBDA
404 chlorophyll levels in the northern coastal region (Figure 3(e,f)) are mostly
405 higher than in either FREE or PDA simulations, and these higher levels are
406 relatively sustained through much of the year.

407 As mentioned above, PBDA can accomplish this adjustment through mul-
408 tiple mechanisms. The system can increase phytoplankton biomass directly,
409 increase nutrients (NO_3) to drive primary production, and decrease zooplank-
410 ton that grazes on phytoplankton. Figure 5 presents the PBDA increments to

411 phytoplankton, nutrient and zooplankton prior estimates. It reveals that all
412 three mechanisms occur in the northern coastal zone, which together elevate,
413 phytoplankton biomass in this region relative to the FREE run. It is also possible
414 that changes to physical properties alter transport and mixing and thus
415 overall phytoplankton levels. Although Raghukumar et al. (2015) showed
416 that adjustments to the physical circulation can improve spatial positioning
417 of features (e.g., a higher correlation coefficient), we find that spatially and
418 temporally averaged phytoplankton biomass is not substantially altered by
419 the physical adjustments.

420 It is important to note that the magnitude of each increment is quantitatively
421 determined by the prior model-data misfit, underlying model dynamics and prescribed
422 values of observation and model uncertainty. The quantitative contribution of each
423 increment can be assessed through analysis of source/sink terms in the phytoplankton
424 budget (e.g., primary production, grazing, and mortality) that contribute to changes
425 in phytoplankton biomass in the forward model. These changes can also be compared
426 to the direct adjustment of phytoplankton itself, and we present this information
427 averaged over the upwelling season (April to September) and nearshore 100
428 km in Figure 6 as a function of latitude. North of 44°N, direct phytoplankton
429 adjustments overwhelmingly dominate, with lesser contributions by productivity
430 (associated with changes to nutrients) and negligible contributions by grazing
431 (associated with changes to zooplankton). We note that increases in phytoplankton
432 biomass also result in non-negligible increases in mortality, which contribute
433 negatively to phytoplankton concentrations during each assimilation cycle.
434
435

436 *5.2.3. Central U.S. west coast (34°N-44°N)*

437 Along the central U.S. west coast, the FREE simulation overestimates
438 chlorophyll biomass from spring to early fall and underestimates it during
439 other times of the year (Figure 1). With upwelling favorable wind stress start-
440 ing in March (Figure 2), wind-driven phytoplankton blooms in the FREE run
441 occur regularly in this region (Figure 3b). The chlorophyll biomass responds
442 to wind-driven coastal upwelling after approximately 1 or 2 weeks (Figure
443 4). Assimilation of physical variables (PDA) does not change the simulated
444 nearshore chlorophyll biomass significantly (Figure 3d); better agreement
445 with the observation occurs in winter, but the timing and magnitude of phy-
446 toplankton blooms along the central coast disagree clearly with observed val-
447 ues. In contrast, PBDA successfully reduces the overall chlorophyll biomass
448 modeled during the upwelling season and increases the biomass during fall
449 and winter. Overall, PBDA alters the modeled structure of phytoplankton
450 stock substantially, both in space and in time, matching observations con-
451 siderably better than either FREE or PDA.

452 As in the northern region, multiple reasons may possibly exist for the dis-
453 crepancies in the FREE run. One simple explanation for the higher chloro-
454 phyll biomass in the model is the suboptimal choice for parameter values.
455 Another possible reason is the absence of iron limitation. In the central and
456 northern CCS, high macronutrient levels with intermediate or low chloro-
457 phyll concentrations have been shown to result from iron limitation (Hutchins
458 and Bruland, 1998, Hutchins et al., 1998, Bruland et al., 2001, Firme et al.,
459 2003, Chase et al., 2007). Our simple NPZD model, with only one nutri-
460 ent compartment arguably representing nitrate, neglects iron biochemistry

461 altogether. With no potential for iron limitation, our model may overesti-
462 mate phytoplankton growth, leading to higher chlorophyll biomass during
463 the upwelling season. Following the upwelling season, California central and
464 northern coast waters receive nutrients through riverine input (Chase et al.,
465 2007), and nearshore chlorophyll biomass is generally above 0.1 mg m^{-3}
466 (Figure 1(d)). Our model does not include riverine input, and this omission
467 may reduce nutrient supply in wintertime and early spring relative to nature,
468 resulting in lower levels of modeled chlorophyll biomass.

469 As discussed previously, changes in phytoplankton biomass can be influ-
470 enced by changes in multiple state vector components. We find that along
471 the central coast during the upwelling season, PBDA results in negative ad-
472 justments to phytoplankton and to nutrients, and more variable positive
473 or negative increments to zooplankton depending on latitude and specific
474 time-window (Figure 5). During fall and winter, changes to nutrients and
475 phytoplankton are reversed, and changes to zooplankton become exceedingly
476 small. As in the northern region, these increments are sensible considering
477 impacts to grazing and uptake.

478 Unlike the northern zone where phytoplankton increments dominate
479 changes to phytoplankton dynamics resulting from nutrient and zooplank-
480 ton increments, the central coast region during the upwelling season exhibits
481 changes in nearshore phytoplankton concentrations that are dominated by
482 primary production (Figure 6). Because uptake depends on both phyto-
483 plankton and nutrient levels, both the negative phytoplankton increment
484 and reduced nutrients resulting from PBDA contribute to lower uptake and
485 lower phytoplankton biomass.

486 5.2.4. Budget changes

487 Increments in initial conditions cause total nitrogen within the model
488 to be altered from cycle to cycle. As discussed, the coupled data assimilation
489 system removes phytoplankton and nutrients along the central coast
490 during the upwelling season (Figure 5). It is important to characterize the
491 magnitude of these changes with respect to changes resulting from modeled
492 biological dynamics. Here, we present terms in the budget for phytoplankton
493 and nutrients pools averaged along the U.S. west coast during the upwelling
494 season from April to September. The budget for phytoplankton, P , in the
495 absence of data assimilation can be written

$$\frac{\partial P}{\partial t} + \nabla \cdot (\mathbf{u}P) = \nabla \cdot (\mathbf{K}\nabla P) + \text{Production} + \text{Grazing} + \text{Mortality}, (6)$$

496 where the time-rate of change and advective flux divergences are bal-
497 anced by diffusive flux divergences and biological sources and sinks. For
498 phytoplankton, biological processes included in this model are phytoplankton
499 production, grazing by zooplankton and phytoplankton mortality. A simi-
500 lar equation applies to the nutrient budget, but biological sources consist of
501 unassimilated excretion and remineralization from detritus, phytoplankton
502 and zooplankton, and the nutrient sink is uptake by phytoplankton. ROMS
503 includes diagnostic tools to quantify each of these terms in a form consistent
504 with the discretization, and the budget for the time and space average is
505 shown in Figure 7. Time-mean increments for phytoplankton and nutrients,
506 δP and δN are also shown.

507 In the phytoplankton budget, the largest term is biological production,
508 and grazing has the next largest amplitude. The next most significant terms
509 in order of their magnitude are phytoplankton mortality, the vertical diffusive

510 flux, and the time-rate of change, ΔP . For comparison, we include the mean
 511 phytoplankton increment, denoted δP , produced by the assimilation, and
 512 observe that it is smaller than all the previously mentioned changes.

513 The nitrogen budget gives a similar impression. Although the
 514 assimilation-produced increment, δN is larger than the remineralization and
 515 excretion, it is smaller than the more dominant terms in the budget.

516 Finally, as a different measure of assimilation-induced budget changes,
 517 we calculate the time-mean of the absolute value of the ratio between the
 518 increment and the production in the phytoplankton budget and between the
 519 nutrient increment and uptake:

$$R_P = \frac{\overline{|\delta P|}}{\overline{|\text{Prod}|}} \quad (7)$$

$$R_N = \frac{\overline{|\delta N|}}{\overline{|\text{uptake}|}}. \quad (8)$$

520 We find $R_P = 6.4\%$ and $R_N = 7.4\%$ in our experiments. The assimilation
 521 procedure produces alterations to the state variables that are small compared
 522 to dominant biological processes in the respective biological budgets calcu-
 523 lated by the NPZD model.

524 5.2.5. *Subsurface, unassimilated data*

525 Finally, we note that the RMSE computed using unassimilated data
 526 (chlorophyll and NO_3 in the upper 200 m) is also smallest in the PBDA
 527 experiment (Table 4). The error reduction in PBDA is quite small relative
 528 to FREE, but it shows potential for the assimilation system to spread some
 529 information vertically. Satellite estimates of chlorophyll can differ from in

530 situ observations. Kahru et al. (2012) find that the chlorophyll estimation
531 algorithm for SeaWiFS underestimates chlorophyll biomass concentrations
532 in the California Current, indicating that assimilating SeaWiFS chlorophyll
533 observation may not ensure a good fit to in situ observations. We find that
534 the prior mean bias of chlorophyll for near-surface in situ observations is -0.37
535 mg m^{-3} , and it is reduced to -0.20 mg m^{-3} following assimilation. While this
536 bias reduction near the surface is substantial, it is possible that the bias in
537 satellite chlorophyll estimates limits the improvement in the posterior solu-
538 tion against in situ data.

539 As described in section 4, the background error covariance \mathbf{B} contains
540 the correlation matrix \mathbf{C} whose vertical length scale is 7 m. Hence, most
541 corrections for the initial biological conditions occur in the upper 20 m. Be-
542 low that level, chlorophyll RMSEs are not very different between the three
543 experiments. In deeper water, the background phytoplankton biomass is low,
544 particularly below the euphotic zone. In contrast, the RMSEs of NO_3 differ
545 from one another because of the different NO_3 fluxes associated with the
546 ocean circulation (not shown). Overall, the reduction of RMSEs by PBDA
547 is less than 13%, which is much smaller than the reduction for the surface
548 chlorophyll. We note that while it is reassuring that subsurface changes are
549 slightly improved by assimilation of surface information, subsurface RMSE
550 would most likely benefit much more substantially from the availability of
551 subsurface biogeochemical data.

552 **6. Summary and Discussion**

553 The theoretical development of the quadratic form for incremental, log-
554 normal biogeochemical ocean data assimilation and the coupled physical and
555 biogeochemical data assimilation (PBDA) approach are presented in compan-
556 ion papers (Song et al., 2016,), along with test cases using idealized model
557 twin experiments. In this study, we applied the PBDA approach to a real-
558 istic problem by assimilating actual observations from the California Cur-
559 rent System during the year 2000. PBDA was implemented using a simple
560 four-component NPZD ecosystem model coupled to ROMS. Both physical
561 observations from various platforms and SeaWiFS surface chlorophyll obser-
562 vations are used in PBDA to improve estimates of the physical and biological
563 ocean states. We compared model results for a free run of the model, a run
564 considering only physical data assimilation (PDA), and the PBDA solution.

565 Although PDA results in substantial improvements to the physical state,
566 this procedure also yields ecosystem fields that on average are not improved
567 over the free run. We find that PDA exhibits generally higher phytoplankton
568 stock than the free run, consistent with results of Raghukumar et al. (2015)
569 using a different biogeochemical model. In contrast, PBDA achieves dramat-
570 ically smaller RMSEs for assimilated biological variables (in this case surface
571 chlorophyll). PBDA also showed improvements in unassimilated subsurface
572 biogeochemical data, but the reduction in RMSE was small compared to the
573 free run (at most about 10-13%).

574 One intriguing result from Song et al. (2016) was that the lowest er-
575 rors for physical observations resulted from PBDA and not PDA, suggesting
576 that biological data can provide useful additional information to constrain

577 physical fields. Here we find lower RMSE in PDA than PBDA, though the
578 PBDA performance was only slightly worse than PDA relative to the im-
579 provement of both over the free run. In a model twin experiment of Song
580 et al. (2016), the same model was used to produce observations and test
581 the assimilation system. Thus in that configuration, the assimilation model
582 is capable of reproducing the truth exactly. In a realistic configuration, as
583 tested here, both physical and biological model components are inaccurate
584 representations of nature for many reasons (e.g., model resolution, repre-
585 sentation of subgridscale dynamics, parameterization of complex biological
586 processes, specification of model and/or observational error statistics) and
587 generally are not able to reproduce in a prognostic sense the natural envi-
588 ronment exactly. As a result, we speculate that physical and biogeochemical
589 model errors relative to nature are responsible for the slightly worse perfor-
590 mance in terms of physical RMSE in this realistic configuration compared
591 to the model twin experiment. Future studies will have to test whether im-
592 proved models (physical, biological or both) could yield greater improvement
593 in the physical variables through assimilation of biological information than
594 through physical assimilation alone.

595 Examination of the temporal and spatial structure of the surface chloro-
596 phyll fields indicates that PBDA successfully adjusted the amplitude and
597 timing of phytoplankton blooms in coastal waters to better match those
598 observed. Such a result is to be expected if the assimilation system is func-
599 tioning properly, but since this is the first demonstration of this technique
600 using real data, we explored how the system achieved these changes. The
601 assimilation model is free to adjust all elements of the control vector (in this

602 case, model initial conditions at the start of each assimilation cycle) and
603 the magnitude and relative proportion of those changes result from a com-
604 bination of model dynamics, embodied by the nonlinear, tangent linear, and
605 adjoint models, as well as prescribed observation and model uncertainties.

606 In regions where the free solution underestimated chlorophyll systemat-
607 ically (such as along the Pacific Northwest coast), the assimilation system
608 adjusted phytoplankton, nutrient, and zooplankton levels such that each in-
609 crement would contribute to an increase in phytoplankton stocks within the
610 nonlinear model. We found that during the upwelling season, increments to
611 the phytoplankton state variable contributed the most to the total change
612 in phytoplankton concentrations. In other regions (e.g., along the central
613 and northern California coast), the free solution overestimated chlorophyll
614 levels. Here, we found that a reduction in phytoplankton growth, resulting
615 from reductions in both phytoplankton stocks and nutrient levels by PBDA,
616 was responsible for the largest decrease in phytoplankton concentrations.

617 We also noted several deficiencies of the unconstrained model that po-
618 tentially limit agreement between the free run and observations. The model,
619 for example, does not include high nitrate levels near the northern boundary
620 that have been shown to result from tidal mixing within the Strait of Juan de
621 Fuca (Davis et al., 2014). It is possible, even likely, that different, or spatially
622 varying parameters for the NPZD model, different surface forcing or bound-
623 ary conditions, or alternate biogeochemical or physical models altogether,
624 may produce in a non-assimilative run ecosystem fields with greater fidelity
625 than the one used in this study. However, although an alternate model may
626 produce fields that are closer to the data available (and substantial effort

627 to improve forward model calculations should be made), differences between
628 observations and models are unavoidable. This study demonstrates that er-
629 rors present in unconstrained model calculations can be adjusted sensibly
630 through rigorous 4-dimensional data assimilation.

631 The improved spatial structure of surface chlorophyll produced by PBDA
632 over the free run identifies a possible application of these model results. As is
633 well known (and shown in Figure 1b), the coastal ocean undergoes frequent
634 cloud cover that prevents direct satellite assessment of surface chlorophyll.
635 We found that in the coastal strip defined here as the nearshore 100 km and
636 delineated approximately by the blue line in Figure 1a, daily satellite surface
637 chlorophyll estimates were unavailable about 70% of the year. More complete
638 coverage can be attained by using temporal composite estimates (such as the
639 8-day composite shown in Figure 1d). However, such composites necessar-
640 ily trade high frequency variability for temporal coverage. In contrast, the
641 assimilative model produces a complete 4-dimensional estimate of the ocean
642 state, regardless of cloud cover. It is data constrained during periods when
643 observations are available, but uses model dynamics to extend assimilated
644 fields through periods of low data availability. Hence, assimilative models
645 can be thought of as sensible dynamical interpolators of sparse data.

646 Sensitivity studies (not shown) revealed that the assimilation system is
647 quite robust, whereby small variations to a variety of assimilation-related pa-
648 rameters, such as assimilation window length and background error variances,
649 did not substantively change ocean state estimates. We did use a smaller
650 vertical decorrelation scale for phytoplankton (7 m) than for physical vari-
651 ables (30 m) because a larger vertical decorrelation scale in combination with

652 the logarithm transform resulted in unrealistic enhancement of sub- surface
653 mixed layer phytoplankton fields. The proposed data assimilation method
654 applied to a completely different biogeochemical model, NEMURO, is also
655 able to fit the satellite observations of surface chlorophyll well (Mattern et
656 al., in prep). NEMURO includes phytoplankton and zooplankton commu-
657 nity structure, and thus is arguably better suited to represent the different
658 nutrient zones of the California Current System than is the presently applied
659 NPZD model with single parameter values across the full domain.

660 Computational requirements for PBDA are increased over PDA by about
661 the same factor as running a coupled biogeochemical model over only physics
662 in a forward (nonlinear) run. In practice, 4-dimensional variational assimila-
663 tion costs $O(100)$ times the forward (nonlinear) model calculations because
664 multiple iterations of tangent linear and adjoint models are required to ap-
665 proach the cost function minimum. The added cost of PBDA over PDA is the
666 cost of running the biological tangent and adjoint models. For a 4-component
667 NPZD model, coupled calculations require approximately twice the memory
668 and processor time as a pure physics run. It is worth noting that ensemble
669 Kalman Filter calculations are similarly more expensive than forward model
670 calculations owing to the multiple runs of the forward model required to
671 estimate the background covariance matrix (Edwards et al., 2015).

672 As mentioned, the 4DVar approach uses model dynamics, embodied in
673 the tangent linear and adjoint models, to connect observations within each
674 assimilation cycle to the model initial conditions, and the magnitudes of
675 the initial condition increments are dependent on prescribed observation and
676 model error statistics. In this study, we assumed univariate model errors,

677 where the background error covariance matrix consists of variances on diag-
678 onal elements, and off-diagonal components are determined by the solution
679 of a diffusion equation. Thus connections between SSH and velocity or SSH
680 and phytoplankton, for example, are only attained through model dynamics.
681 SSH of course can be related dynamically to phytoplankton concentrations
682 through alterations of near surface velocity. Dynamics in this context dis-
683 tinguishes the 4DVar method from sequential methods, which rely purely on
684 statistics to distribute observational information both locally and nonlocally.
685 Multi-variate statistical approaches in sequential methods for coupled bio-
686 geochemical assimilation problems are beginning to emerge and have shown
687 great promise (e.g., Shulman et al., 2013). Such developments suggest that
688 4DVar solutions can be further improved through alterations of background
689 error covariances. For example, it may be possible to statistically relate lo-
690 cal changes in density below the euphotic zone to changes in nutrients that
691 should improve the nitrate density relationship relative to observations.

692 In addition, it has been demonstrated in physical systems that back-
693 ground error covariances can be partitioned into balanced and unbalanced
694 parts (Derber and Bouttier, 1999, Weaver et al., 2005, Moore et al., 2011).
695 This decomposition assumes that variables in the unbalanced part are un-
696 correlated. It is not clear how the imposition of a balance operator relat-
697 ing physical variables may impact coupled biogeochemical data assimilation.
698 Furthermore, it may be possible to find analogous first order balanced rela-
699 tionships in coupled dynamical problems that could be included in physical
700 and biogeochemical data assimilation. Investigating multivariate statistical
701 relationships and sensitivities to balance operators remain subjects for future

702 studies.

703 This investigation evaluates a fully coupled, physical and biogeochemical
704 4-dimensional variational data assimilation system in a realistic configuration
705 of the U.S. west coast at 1/10 degree resolution and spanning a 1-year du-
706 ration. We assimilate widely available physical and biological observations,
707 and substantially reduce errors in a biological variable over an unconstrained
708 model and a model that assimilates only physical observations. The approach
709 is model independent, although the coding of the tangent linear and adjoint
710 models is challenging and model-specific. While several improvements can
711 be made to both the forward models and assimilative procedures to further
712 improve estimates, this study demonstrates that implementation of 4DVar in
713 this context is practical and potentially useful. Such methods should be of
714 interest for historical reanalyses and regional ocean observing systems quite
715 generally.

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Table 1: Observations used in physical and biological coupled data assimilation. Their sources, frequencies and numbers are listed.

Variable	Source	Frequency	number
Sea surface height	AVISO gridded product	7-day	772,856
Sea surface temperature	AVHRR/PathFinder	Daily	3,026,628
Sea surface chlorophyll	SeaWiFS	Daily	1,029,735
in situ T	EN3 (Ingleby and Huddleston, 2007)		24,526
in situ S	EN3 (Ingleby and Huddleston, 2007)		9,669

Table 2: Parameter names, values and units for the NPZD model

Parameter name	Value	Units
Light		
Extinction coefficient for sea water (k_z)	0.067	m^{-1}
Photosynthetically active radiation	0.43	Dimensionless
Phytoplankton		
Self-shading coefficient (k_P)	0.02	$\text{m}^2 \text{mmol N}^{-1}$
Initial slope of P-I curve (α)	0.02	$\text{m}^2 \text{W}^{-1}$
Uptake rate for nitrate (V_m)	1.0	day^{-1}
Half-saturation constant for nitrate (k_N)	1.0	mmol N m^{-3}
Mortality rate (σ)	0.1	day^{-1}
Zooplankton		
Grazing rate (R_m)	0.65	day^{-1}
Ivlev constant (Λ)	1.4	Dimensionless
Excretion efficiency	0.3	Dimensionless
Mortality rate	0.145	day^{-1}
Detritus		
rem mineralization rate	0.1	day^{-1}
Sinking velocity	40	m day^{-1}

Table 3: The mean RMSEs for SSH, SST, $T_{in\ situ}$, $S_{in\ situ}$ and surface chlorophyll (SChl) are computed using assimilated observations. The chlorophyll RMSE was computed without logarithm transformation.

	SSH (cm)	SST ($^{\circ}$ C)	$T_{in\ situ}$ ($^{\circ}$ C)	$S_{in\ situ}$ (psu)	SChl (mg m^{-3})
Free	9.26	1.11	1.31	0.29	0.74
PDA	3.16	0.58	0.82	0.17	0.78
PBDA	3.94	0.59	0.89	0.20	0.45

Table 4: The mean RMSEs for subsurface chlorophyll (Chl) and NO_3 are also computed using the unassimilated in situ observations from the GLOBEC-LTOP and CalCOFI stations as marked in black and blue in Figure 1a, respectively.

	GLOBEC-LTOP		CalCOFI	
	Chl (mg m^{-3})	NO_3 (mmol N m^{-3})	Chl (mg m^{-3})	NO_3 (mmol N m^{-3})
Free	1.41	5.61	0.71	4.01
PDA	1.44	5.43	0.70	4.10
PBDA	1.39	4.88	0.65	3.96

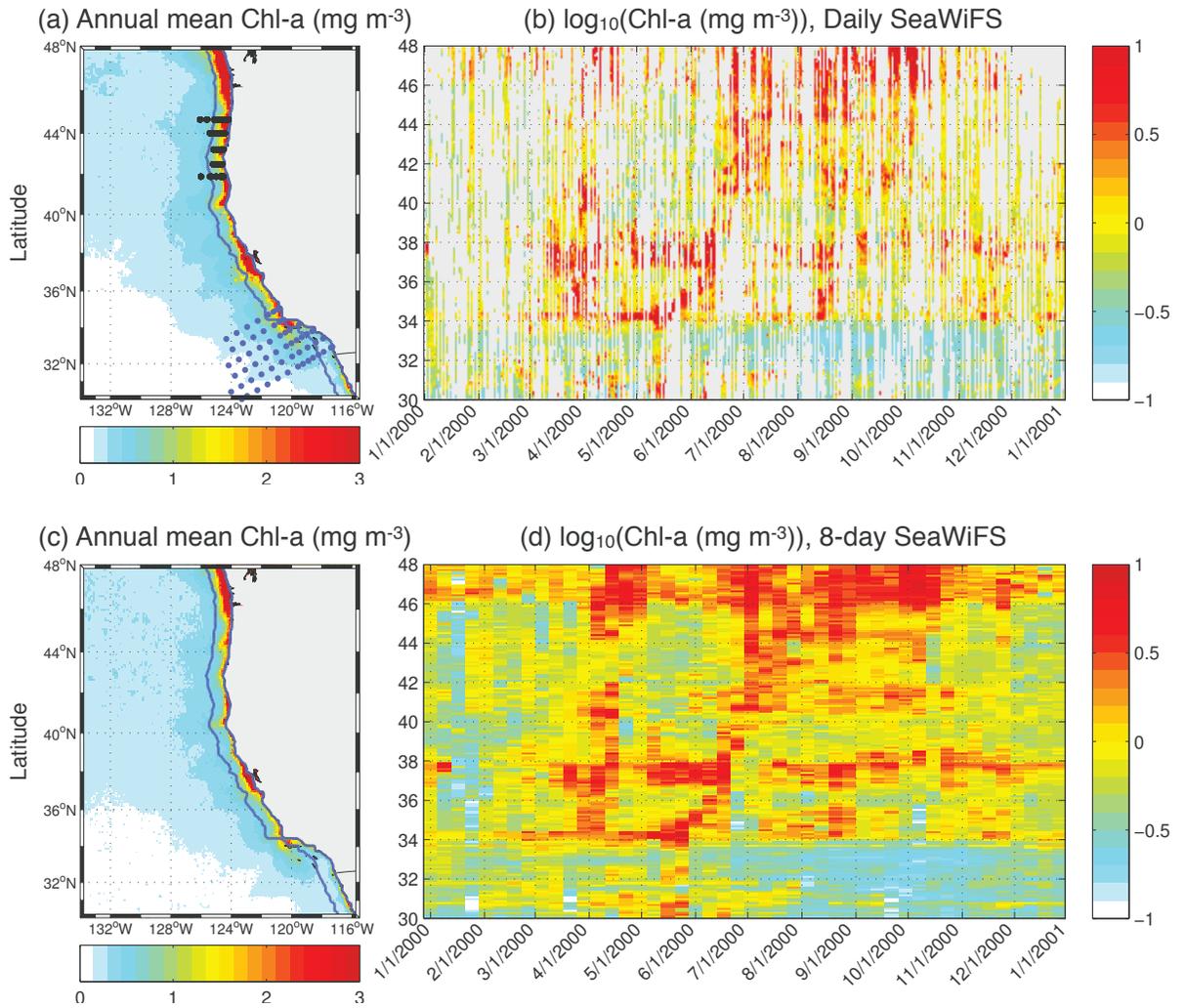


Figure 1: Annual mean surface chlorophyll (left) and Hovmöller diagrams of \log_{10} -transformed surface chlorophyll at the coast (right). (a,b) and (c,d) represent the daily and 8-day composite SeaWiFS chlorophyll data products, respectively. Surface chlorophyll within the blue contours (roughly 100 km wide) on the left column plots are averaged for the Hovmöller diagrams on the right column. Black and blue dots in (a) represent the GLOBEC-LTOP and CalCOFI stations, respectively.

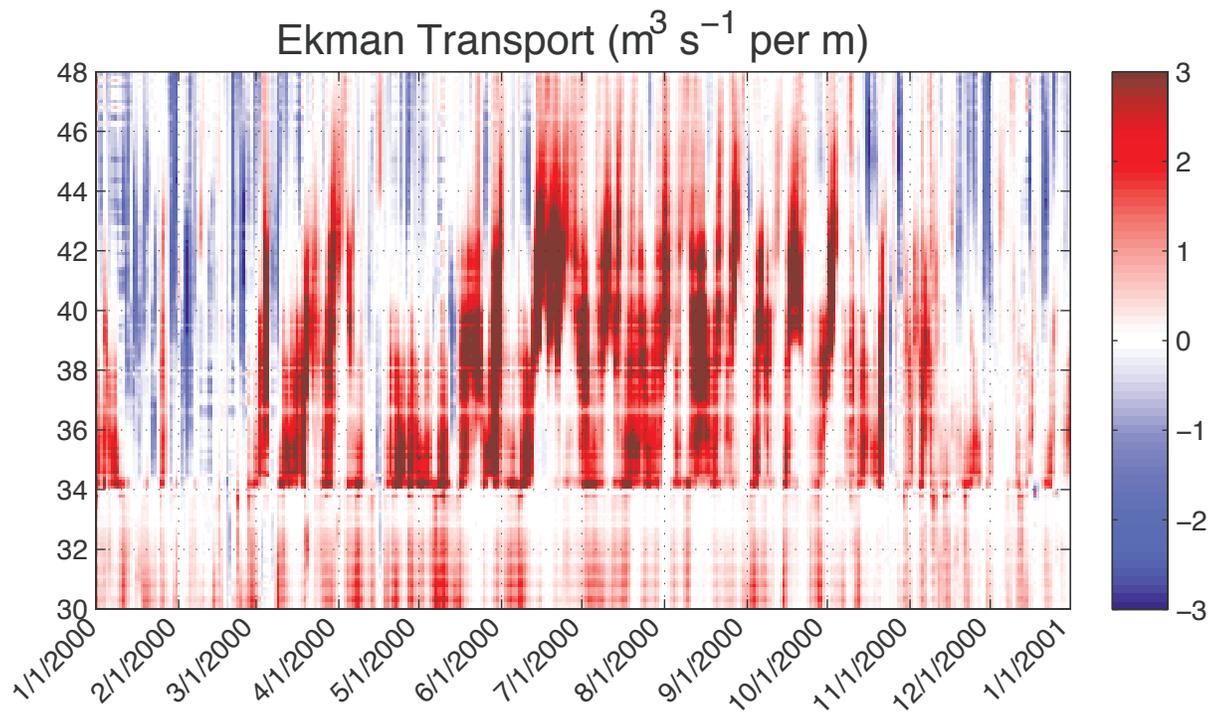


Figure 2: Hovmöller diagram of zonally averaged surface Ekman transport within 100 km of the coast (blue contour in Fig 1(a)).

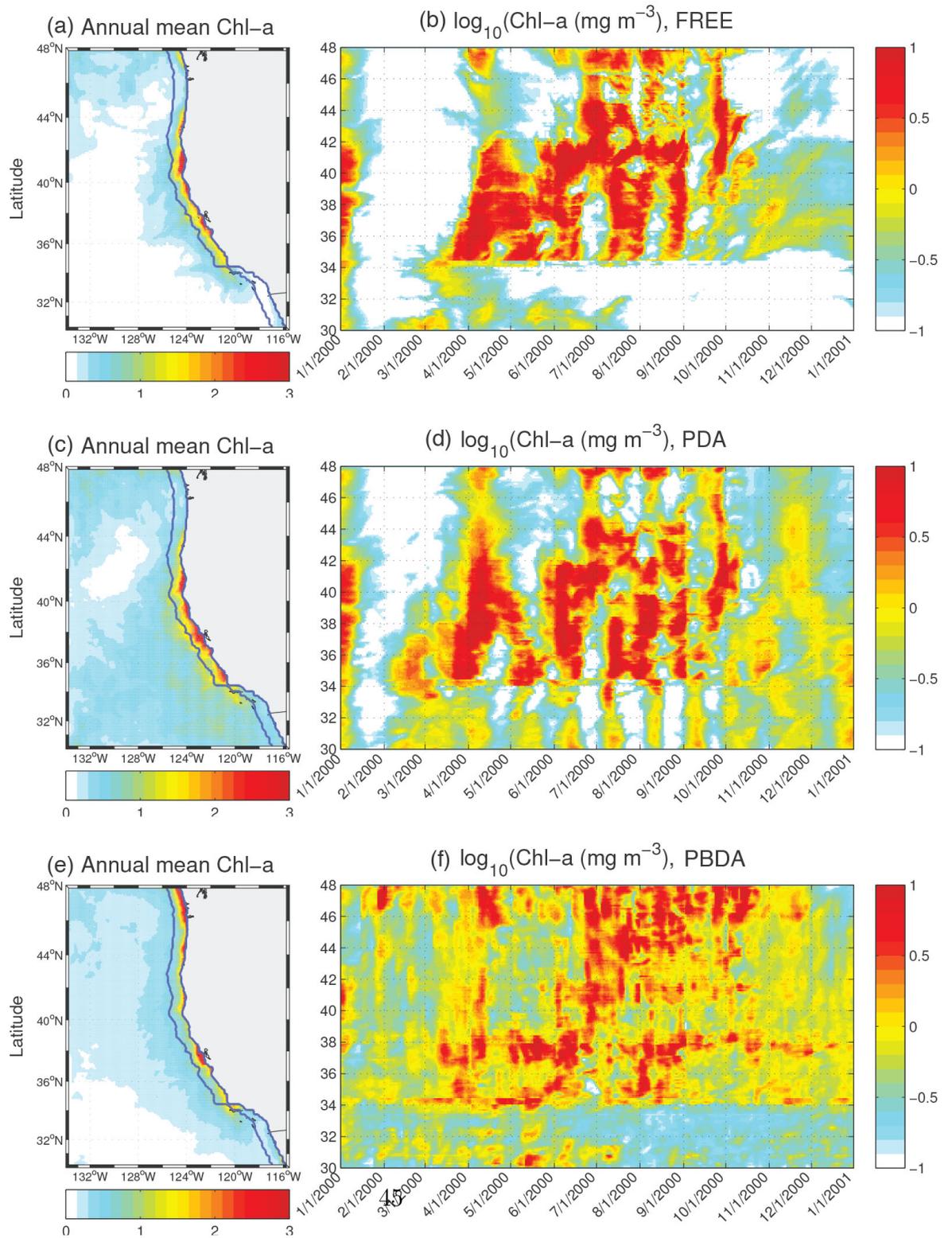


Figure 3: Same as Fig 1 with the data from (a, b) free forward simulation, (c, d) PDA and (e, f) PBDA state estimation.

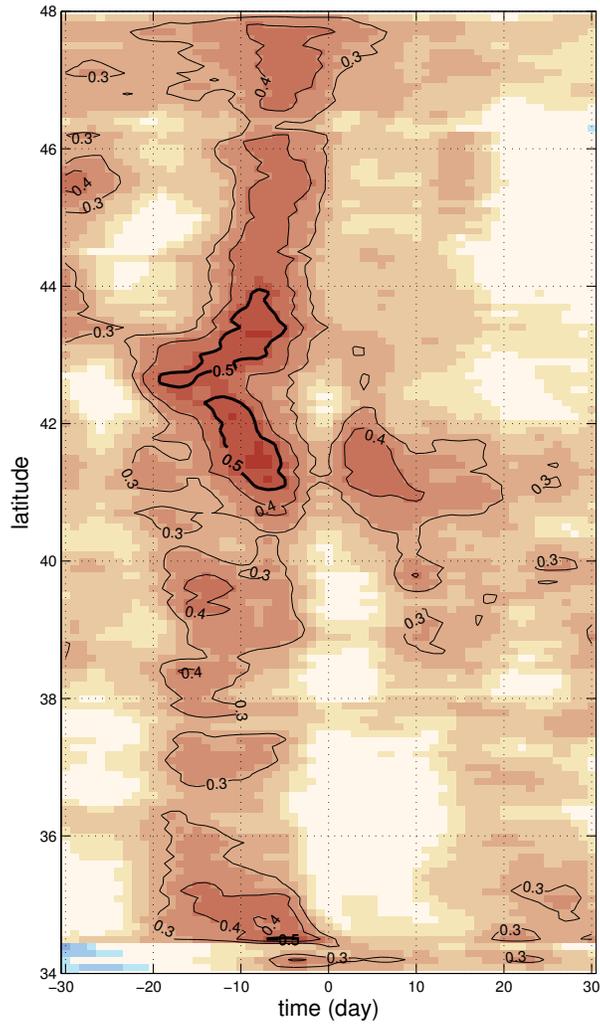


Figure 4: Lagged cross correlation between the Ekman transport (Figure 2) and phytoplankton biomass for the FREE run (Figure 3(b)). Negative time means that the Ekman transport precedes the growth of phytoplankton biomass.

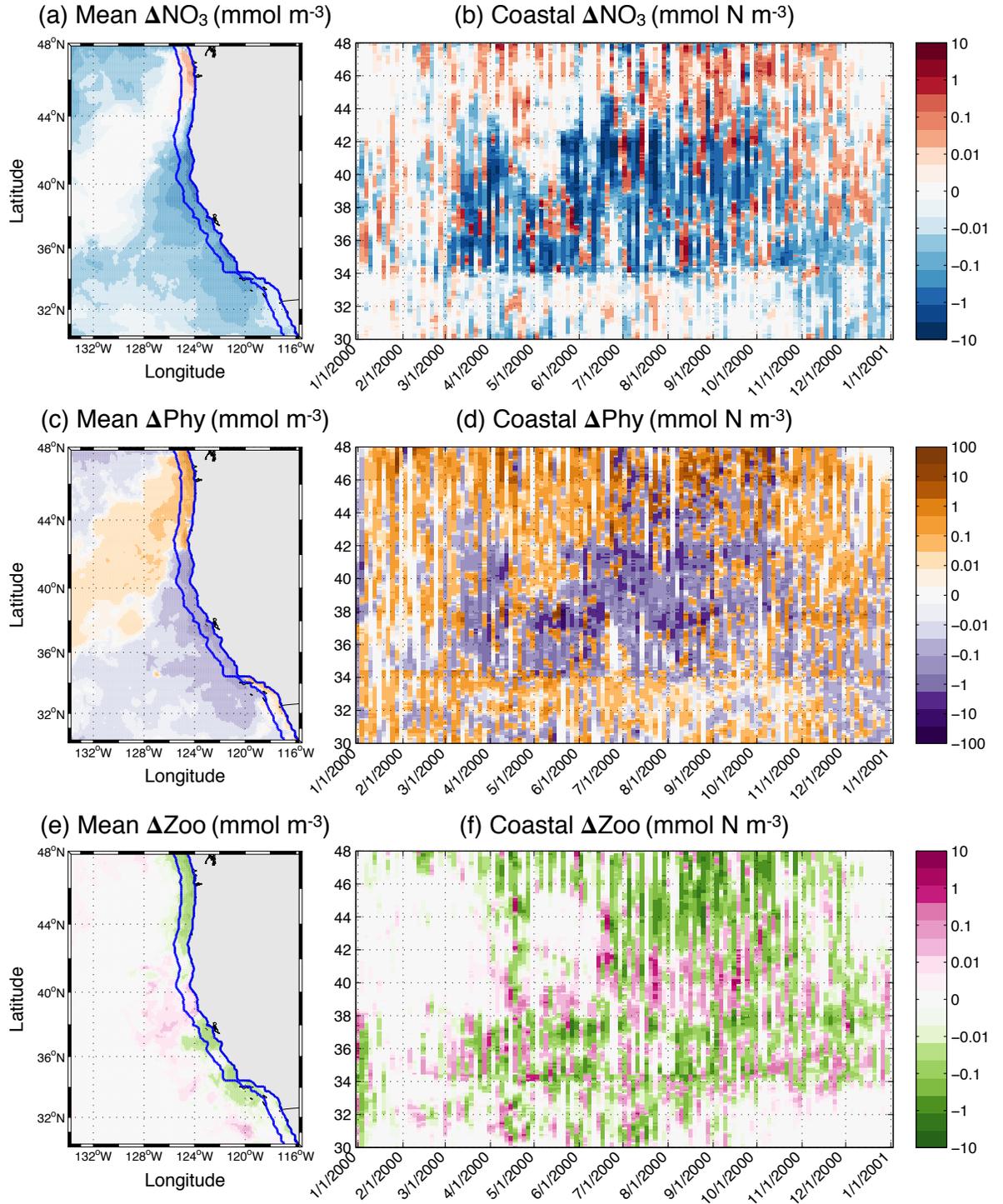


Figure 5: Spatial map and Hovmöller diagrams of initial increments by PBDA for (a,b) nitrate, (c,d) phytoplankton and (e,f) zooplankton. The increments are averaged in time (left column) or in space at the coastal regions (right column). It is noted that the scale for phytoplankton in (c,d) is greater than the other two variables.

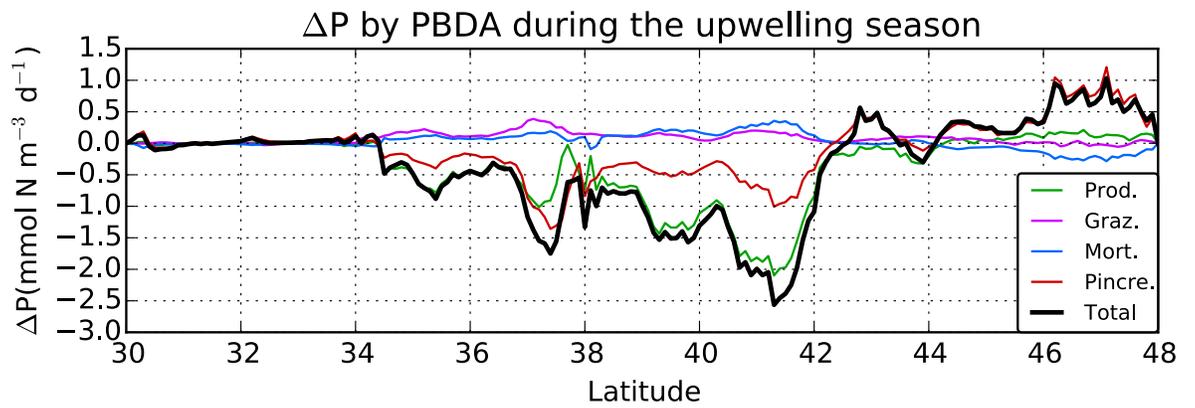


Figure 6: Changes in phytoplankton by assimilating physical and biological observations averaged over the upwelling season (from April to September). Total changes (black) are partitioned by the production (green), grazing (purple), mortality (blue) and increment in phytoplankton biomass (red).

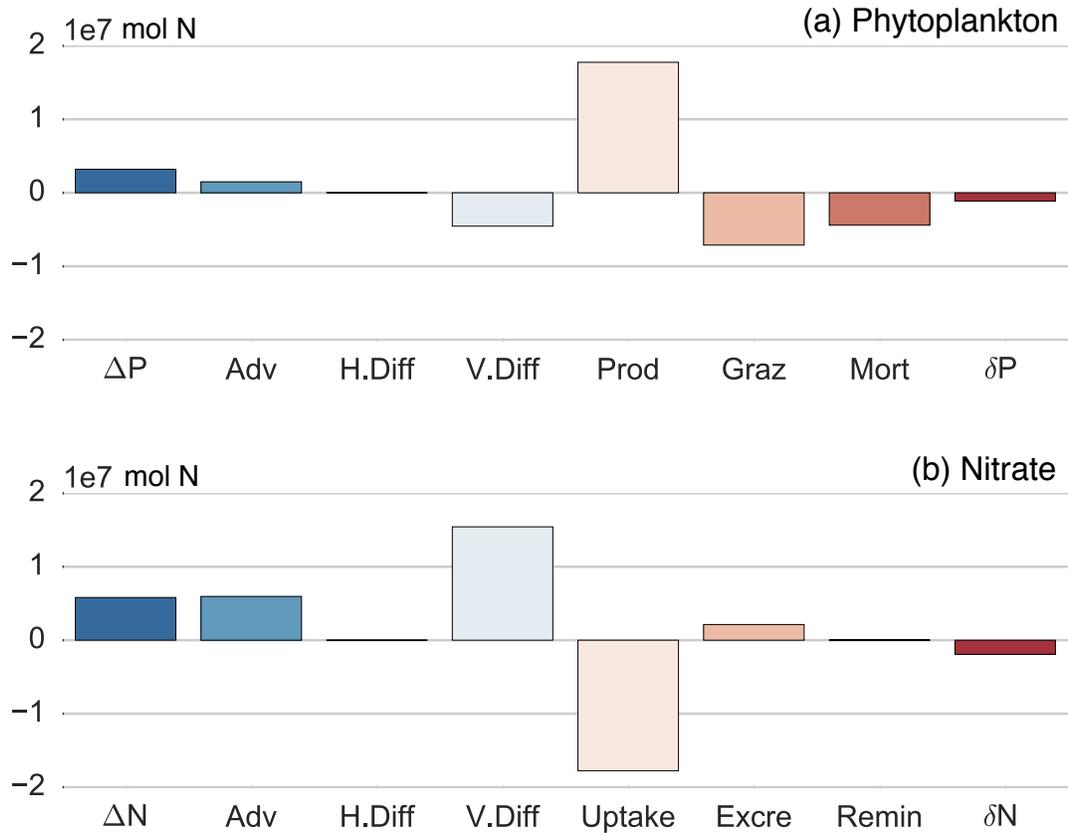


Figure 7: Terms in the phytoplankton (a) and nutrient (b) budgets averaged over the coastal area during the upwelling season (from April to September) from the posterior solution (after data assimilation). The time-rate of change in phytoplankton (ΔP) is partitioned into an advective flux divergence (Adv), horizontal diffusive (H.Diff) and vertical (V.Diff) flux divergence, primary productivity (Prod), grazing (Graz) and mortality (Mort). The phytoplankton increment produced by assimilation is denoted δP . In the NO_3 budget, biological sources consist of remineralization (Remin) and addition by excretion (Excre). Uptake is the sink, and the NO_3 increment is labeled δN .