

1 Detiding time series of dissolved oxygen for improved estimates 2 of ecosystem metabolism

3 Marcus W. Beck¹, Michael C. Murrell², James D. Hagy III²

¹ORISE Research Participation Program

USEPA National Health and Environmental Effects Research Laboratory

Gulf Ecology Division, 1 Sabine Island Drive, Gulf Breeze, FL 32561

Phone: 850-934-2480, Fax: 850-934-2401, Email: beck.marcus@epa.gov

²USEPA National Health and Environmental Effects Research Laboratory

Gulf Ecology Division, 1 Sabine Island Drive, Gulf Breeze, FL 32561

Phone: 850-934-2433, Fax: 850-934-2401, Email: murrell.michael@epa.gov

³USEPA National Health and Environmental Effects Research Laboratory

Gulf Ecology Division, 1 Sabine Island Drive, Gulf Breeze, FL 32561

Phone: 850-934-2455, Fax: 850-934-2401, Email: hagy.jim@epa.gov

- good start!
- pretty rough

- Long -

More comprehensive literature discussion to put related analysis in context.

See Scratches

Running head: Noise in Estuary Metabolism

Acknowledgments

Will add something here...

Abstract

Time series of dissolved oxygen (DO) can be used to estimate rates of primary production and respiration in aquatic ecosystems. However, continuous monitoring data at estuaries may reflect variation from both biological and physical processes, such that observed data may produce inaccurate or misleading estimates of metabolism. Statistical techniques that dynamically quantify variation in DO and tidal changes over time have the potential to isolate biological signals in DO variation to more accurately estimate metabolism. A weighted regression method was developed to normalize, or detide, the predicted DO signal to remove the influence of physical advection on metabolism estimates. The method was tested using a simulation approach to create multiple DO time series with known additive components of biological and physical variation on different periods. The method was further validated using one year of continuous monitoring data from four case studies. We provide a detailed discussion on use of the method for improving certainty in evaluation of DO measurements from sites with strong tidal influences. Moreover, we propose that the method could expand use of the open-water method for estimating ecosystem metabolism in estuaries given that the approach can produce robust estimates of DO that are independent of tidal advection. In particular, this could facilitate the use of shorter deployment periods for water quality monitors or incomplete time series given that known biases related to water movement could be removed.

~~Double~~ Double Splus
for subtidal zones?
NEPR Case Studies?

21 Introduction

22 Metabolism estimates from time series of dissolved oxygen provide integrated estimates
23 of production in aquatic ecosystems (Kemp and Testa 2012, Needoba et al. 2012). Autotrophic or
24 productive systems are characterized by high rates of energy transfer between trophic levels
25 leading to accumulation of organic matter, whereas heterotrophic systems are sinks of organic
26 matter that are supported by allochthonous sources of energy input. Integrated measures of
27 metabolism describe the balance between production and respiration that accounts for varying
28 rates in processes that create and consume organic matter. Although metabolic rates vary
29 naturally at multiple spatiotemporal scales (Ziegler and Benner 1998, Caffrey 2004, Russell and
30 Montagna 2007), anthropogenic stressors are often contributing factors that increase rates of
31 production (Diaz 2008). Inputs of limiting nutrients beyond background concentrations may
32 decrease the resilience of an ecosystem such that higher rates of production are coupled with
33 higher biological oxygen demand (Yin et al. 2004, Kemp et al. 2009). Cultural eutrophication is
34 frequently linked to declines in water quality through lower levels of dissolved oxygen,
35 degradation in aquatic vegetation habitat, and increased frequency of harmful algal blooms
36 (Cloern 1996, Short and Wyllie-Echeverria 1996, Rabalais et al. 2002). Reliable estimates of
37 ecosystem metabolism are critical for measuring both background rates of production and
38 potential impacts of human activities on ecosystem condition.

39 Ecosystem metabolism can be estimated using two basic techniques, each of which is
40 appropriate under different conditions or assumptions (Kemp and Testa 2012). Bottle-based
41 techniques rely on rate measurements from discrete water quality samples, whereas open-water
42 techniques infer metabolic rates using *in situ* measurements from continuous monitoring data.

It's not about "use", it's about the underlying theory

43 Bottle-based techniques are useful for partitioning metabolic contributions into discrete habitats,
44 such as pelagic production rates during specific time periods (Kemp and Testa 2012). However,
45 such measurements may be insufficient for evaluating whole ecosystem metabolism if significant
metabolism
46 production occurs in habitats that are not sampled, such as the benthos. As such, the open-water
metabolism
47 technique provides an integrative measure of metabolism by inferring process rates from *in situ*,
Fundamental?
concerned for stream environments
48 continuous monitoring data. Originally for use in streams (Odum 1956), the method has been
49 used with varying success in lakes (Staehr et al. 2010, Coloso et al. 2011, Batt and Carpenter
50 2012) and estuaries (Caffrey 2004, Hopkinson and Smith 2005, Caffrey et al. 2013). As with any
51 method, the ability of the open-water technique to accurately estimate whole system metabolism
the degree to which the theory met
52 depends on whether the assumptions for its use are not violated. Such assumptions are often only
53 implicitly verified in practice, leading to potential biases.

analysis *interpret*
54 The open-water method uses the diel fluctuation of dissolved oxygen to infer rates of
55 ecosystem metabolism, after correcting for losses or gains through air-water exchange (Kemp and
56 Testa 2012). Daily integrated measurements of metabolism represent the balance between
57 daytime *estimates* of gross production and nighttime *estimates* of respiration. The fundamental
58 assumption is that dissolved oxygen (DO) *measurements* describe the same water mass over time
yields series of
59 (Needoba et al. 2012). Estimates of metabolism from a single location may be inaccurate if
60 substantial variation in water column mixing occurs throughout the period of observation (Russell
61 and Montagna 2007). Application of the technique to estimate metabolism in streams requires the
62 comparison of data from an upstream and downstream station (Odum 1956). Application to lakes
63 or estuaries have often assumed that a single sampling station provides sufficient data for
64 estimating metabolism Staehr et al. (2010). While single stations may be valid under specific
65 conditions, numerous studies have shown that the open-water method may be inappropriate given

66 the effects of physical mixing in lakes or estuaries (Ziegler and Benner 1998, Caffrey 2003,
67 Coloso et al. 2011, Batt and Carpenter 2012, Nidzieko et al. 2014). An exhaustive analysis by
68 Caffrey (2003) applied the open-water method to estimate metabolism at 28 continuous
69 monitoring stations at 14 US estuaries. A non-trivial portion of the estimates were negative for X
70 production during the day and positive for respiration during the night. These 'anomalous' values
71 were attributed to the effects of tidal advection such that water masses with different metabolic
72 histories were sampled at multiple sites. *More importantly, they ignored!*

73 The effects of tidal advection on estimates of ecosystem metabolism have been a point of
74 *emphasis?* concern in numerous studies (Monbet 1992, Ziegler and Benner 1998, Caffrey 2003, Collins et al.
75 2013, Howarth et al. 2014), although systematic estimates of its effects have been minimal.

76 Analytical techniques to evaluate and correct for tidal advection could improve certainty in
77 metabolism estimates and increase the use of data from shorter deployment periods if sources of
78 bias are removed. This article describes the theory and application of a method for detiding an
79 observed DO time series to more accurately quantify estimates of ecosystem metabolism for

80 estuaries. Specifically, the method characterizes the effects of tidal advection on DO observations
81 to improve estimates of open-water metabolism with multi-year time series of high frequency (<

82 one hour) water quality data. The focus of our analysis is the use of a weighted regression method
83 previously developed for trend analysis of pollutant concentrations in streams and rivers (Hirsch
84 et al. 2010) and recently adapted for trend evaluation of water quality in estuaries (Beck and
85 Hagy, In review). The weighted regression approach creates dynamic predictions of DO as a

86 function of time and tidal height change, which are then used to normalize, or detide, the DO
87 signal. First, we use a simulation approach to create time series of DO observations with known
88 characteristics to evaluate ability of the weighted regression to remove the effects of tidal

Let's talk about
tell me what Monbet paper is about

advection. Second, four case studies from the National Estuarine Research Reserve System (NERRS, Wenner et al. 2004) are used to validate the method for improving estimates of ecosystem metabolism. Overall, the analysis is meant to improve the certainty of information obtained from monitoring data by evaluating the relative roles of biological and physical processes in estuarine systems. Applications are expected to have implications for ecosystem management by outlining strategies for interpreting water quality data with more accuracy.

Materials and Procedures

Weighted regression for modelling and detiding DO time series

The weighted regression model for detiding DO time series was adapted from the weighted regression on time, discharge, and season (WRTDS) method developed by Hirsch et al. (2010). The functional form of our model is a simple linear regression:

$$DO_{obs} = \beta_0 + \beta_1 t + \beta_2 H \quad (1)$$

where observed DO is a linear function of decimal time t and astronomical tidal height H .

Decimal time is a continuous variable for the day and time of each observation with time as a proportion of the number of total observations added to each day. The beginning of each day was considered the nearest thirty minute observation at which sunrise was expected for a given location and time of year. Days were centered on the diel cycle rather than conventional times (i.e., midnight) given that the objective was to develop a predictive model relevant for biological DO variation that follows solar and seasonal cycles. The functional form also differed from the original WRTDS method that included parameters to estimate variation of the response variable

Instead *based on water level*

108 on a sinusoidal period. DO variation was not modeled using this approach because rates of
109 change may be abrupt following diurnal variation in irradiance or daily DO variation may be
110 muted given the weather, as on cloudy days.

111 Weighted regression is implemented as a moving window that allows for estimation of DO
112 throughout the time series by adapting to variation through time as a function of tide. Regression
113 models are estimated sequentially for each observation in the time series using dynamic weight
114 vectors that change with the center of the window. Weight vectors quantify the relevance of
115 observations to the center of the window in respect to decimal time, hour of the day, and tidal
116 height. Specifically, weights are assigned to each variable using a tri-cube weighting function
PAST TENSE

117 (Tukey 1977, Hirsch et al. 2010):

$$w = \begin{cases} (1 - (d/h)^3)^3 & \text{if } |d| \leq h \\ 0 & \text{if } |d| > h \end{cases} \quad (2)$$

118 where the weight w of each observation is inversely proportional to the distance d from the center
119 of the window such that observations more similar to the point of reference are given higher
120 importance in the regression. Weights exceeding the maximum width of the window h are equal
121 to zero. The tri-cube weighting function is similar to a normal distribution such that weights
122 decrease gradually from the center until the maximum window width is reached. Observations
123 that are half the distance from the center of the window to the maximum window width are
124 weighted one third less than values at the center. Regressions that use simpler windows (e.g.,
125 boxcar approach) are more sensitive to influential observations as they enter or leave the window,
126 whereas the tri-cube function minimizes their effect through gradual weighting of observations

from the center (Hirsch et al. 2010). The final weight vector for each observation is the product of three separate weight vectors for decimal time (day), hour, and tidal height. Windows for decimal time and hour describe the the amount of time from the center of window, whereas the window for tidal height describes the distance as a proportion of the total range. A low weight is given to an observation if any of the three weighting values were not similar to the center of the window since the final weight vector is the product of three weight vectors for each variable (see the link in the multimedia section for graphical display of different weights).

A nontrivial issue with weighted regression is the choice of window width for each weight vector. Excessively large or small window widths may respectively under- or over-fit the data.

Additionally, optimal window widths may depend on the objective for using the model. The weighted regression approach can be used for predicting DO or normalizing to remove the variance from tidal changes. Optimal window widths that minimize prediction error or fit to the observed data are typically smaller than the optimum window widths for normalizing the time series. Similarly, window widths that more effectively detide the DO signal may produce predictions for the observed data that are not optimal. Evaluations of the weighted regression method with simulated DO time series, described below, used multiple window widths to identify an approximate optimal window width for detiding the DO signal. As such, the ability of the models to predict observed DO was not a primary concern given that the optimal window width for detiding likely corresponds to a model that predicts DO as a function of tide rather than observed DO as a function of both tide and biological variation.

How can you decide what is appropriate for the derivative of tidal height that we are using as a weighting variable ??

147 Detiding the DO signal using weighted regression

148 The primary objective of the weighted regression is to detide a DO signal to obtain more
149 accurate estimates of metabolism. Hirsch et al. (2010) developed the normalization approach for
150 the WRTDS method to remove the effects of stream discharge on estimates of pollutant
151 concentration using a two-dimensional interpolation grid of predicted pollutant concentrations
152 across the time series and the range of stream discharge values observed in the study system
153 (Hirsch et al. 2010). Normalized values for pollutant concentration are obtained by averaging the
154 model predictions across the discharge values that are likely to occur on a given day to provide an
155 estimate that is independent of flow variation. Similarly, predicted values of DO concentration
156 were normalized to remove variation from tidal height changes, although the approach differs
157 slightly from Hirsch et al. (2010). Only two time series are predicted from the observed time
158 series DO_{obs} , rather than creating an interpolation grid. The first time series is predicted values
159 from the model that represent DO as a function of time and observed tide. The second time series
160 are the same predictions conditional on time and constant tidal height set to the mean:

$$DO_{tid} = f(DO_{obs}|H, t) \quad (3)$$

$$DO_{nrm} = f(DO_{obs}|\bar{H}, t) \quad (4)$$

161
162 The first time series isolates variation in observed DO as a function of physical advection,
163 whereas the second represents variation related to biological processes (Fig. 1).

too much detail and redundant
Combine w/ previous

164 Assessment

165 Simulation of DO time series

166 The ability of the weighted regression to detide the DO signal was evaluated first using a
167 simulation approach. Observed DO time series were created to represent the sum of variation
168 from biological processes and physical effects related to tidal advection:

$$DO_{obs} = DO_{bio} + DO_{adv} \quad (5)$$

169 Biological DO signals are inherently noisy (Batt and Carpenter 2012) and can be further
170 described as:

$$DO_{bio} = DO_{die} + DO_{unc} \quad (6)$$

171

$$DO_{unc} = \epsilon_{obs} + \epsilon_{proc} \quad (7)$$

172 where the biological DO signal is the sum of diel variation plus uncertainty or noise. Total
173 uncertainty in the biological DO signal is described as variation from observation and process
174 uncertainty (Hilborn and Mangel 1997). Multiple time series at 30 minute time steps over 30 days
175 were created following eqs. (5) to (7) such that observed DO is generalized as the additive
176 combination of four time series (Fig. 2):

$$DO_{obs} = DO_{adv} + DO_{die} + \epsilon_{obs} + \epsilon_{proc} \quad (8)$$

Start off with something like:

To test our ability to model DO time series, we created
a simulated time series ¹⁰ ~~that has~~ thusly - - -

Moving

177 Time series were created by varying the relative magnitudes of each of the four components of

178 observed DO to test the effectiveness of weighted regression under different scenarios. The

179 effects of air-sea gas exchange were not considered in the simulation given that methods are

180 available for *in situ* data to correct observed DO for diffusion (i.e., Thébault et al. 2008).

181 Each component of the simulated time series was created as follows. First, the diel

182 component, DO_{die} , was estimated using a sine/cosine function (Cryer and Chan 2008):

$$DO_{die} = \alpha + \beta \cos(2\pi ft + \Phi) \quad (9)$$

183 such that the mean DO α was 8, amplitude β was 1, f was 1/48 to repeat on a 24 hour period

184 every 30 minutes, t was the time series vector and Φ was the x-axis origin set for an arbitrary

185 sunrise at 630am. The diel signal was increasing during the day and decreasing during the night

186 for each 24 hour period and ranged from 7 to 9 mg L⁻¹. Noise or uncertainty was added to the

187 diel DO signal to simulate natural variation in DO throughout the time series (Fig. 2). Total

188 uncertainty was the sum of observation and process uncertainty for $n = 1440$ (30 minutes by 30

189 days) observations (Hilborn and Mangel 1997), such that:

$$DO_{unc,n} = \epsilon_{obs,n} + \int_{t=1}^n \epsilon_{pro,t} \quad (10)$$

190 where observation and process uncertainty (ϵ_{obs} , ϵ_{pro}) were simulated as normally distributed

191 random variables with mean zero and standard deviation varying from zero to an upper limit,

192 described below. To induce auto-correlation, process uncertainty was estimated as the cumulative

193 sum of n observations where the noise at time $t + 1$ was equal to the noise at time t plus

too much drift

194 additional variation drawn from the normal distribution. The noise vector for process uncertainty
195 was rescaled to constrain the variation within the bounds for standard deviation defined by the
196 random variable. The total uncertainty, DO_{unc} , was added to the diel DO time series to create the
197 biological DO time series (eq. (6) and Fig. 2).

198 A semidiurnal tidal series was simulated as a sine wave with a period of 12.5 hours to

199 represent the principal lunar component (Foreman and Henry 1989). The amplitude was set to 1

200 meter and centered at 4 meters. Initial assessments indicated that tide type (i.e., diurnal,
201 semidiurnal, mixed) did not significantly affect the outcome of the results and a semidiurnal time
202 series was used to reduce the total number of simulations. The tidal time series was added to the
203 biological DO series to simulate DO changes with advection, DO_{adv} (eq. (8) and Fig. 2).

204 Conceptually, this vector represents the rate of change in DO as a function of horizontal water
205 movement from tidal advection such that:

$$\frac{\delta DO_{adv}}{\delta t} = \frac{\delta DO}{\delta x} \cdot \frac{\delta x}{\delta t} \quad (11)$$

$$\frac{\delta x}{\delta t} = k \cdot \frac{\delta H}{\delta t} \quad (12)$$

206 where the first derivative of the tidal time series, as change in height over time $\delta H/\delta t$, is
207 multiplied by a constant k , to estimate horizontal tidal excursion over time, $\delta x/\delta t$. The horizontal
208 excursion is assumed to be associated with a horizontal DO change, $\delta DO/\delta x$, such that the
209 product of the two estimates the DO change at each time step from advection, DO_{adv} . In practice,
210 the simulated tidal signal was used to estimate DO_{adv} :

$$DO_{adv} \propto H$$

*maybe summarize creation of
simulated time series
in a table - Table 10k*

Carefully state what purpose is being served by creating a simulated time series - it is far from clear ~~at this point~~ in the ms, and it should be,

$$DO_{adv} = 2 \cdot a + a \cdot \frac{H - \min H}{\max H - \min H} \quad (14)$$

where a is analogous to k in eq. (12) and is chosen as the transformation parameter to standardize change in DO from tidal height change to desired units. For example, $a = 1$ will convert H to a scale that simulates changes in DO from tidal advection that range from $\pm 1 \text{ mg L}^{-1}$. The final time series for observed DO was the sum of biological DO and advection DO (eq. (5) and Fig. 2).

Evaluation of weighted regression with simulated DO time series

Multiple time series were simulated by varying the conditions in eqs. (5) to (14). Specifically, the simulated data varied in the relative amount of noise in the measurement (e_{pro} , e_{obs}), relative amplitude of the diel DO component (DO_{die}), and degree of association of the tide with the DO signal (DO_{adv}). Three levels were evaluated for each variable: relative noise as 0, 1, and 2 standard deviations for both process and observation uncertainty, amplitude of diel biological DO as 0, 1, and 2 mg L^{-1} , and DO change from tidal advection as 0, 1, and 2 mg L^{-1} .

A total of 81 time series were created based on the unique combinations of parameters (Fig. 3). Three half window widths for each variable (day, hour of day, and tide height) were evaluated for each simulation: decimal time as 1, 3, and 6 days, time of day as 1, 3, and 6 hours, and tidal height as 0.25, 0.5, and 1 as a proportion of the total range given the height at the center of the window. The window widths were chosen based on preliminary assessments that suggested variation in model performance was adequately captured by these values. In total, 27 window width combinations were evaluated for each of 81 simulated time series, producing results for 2187 weighted regressions.

The detided or normalized values for each regression were compared to the simulated data to evaluate the ability of weighted regression to reproduce the biological DO signals. Results

were summarized using Pearson correlation coefficients and the root mean square error (RMSE) between the detided time series and the biological DO time series as a known component of the observed. Overall, the weighted regressions provided accurate results for the detided time series compared to the 'true' biological time series regardless of the simulation parameters (Table 1) or window widths (Table 2, results for each simulation can be viewed using the link in the multimedia section). Mean correlation for all time series and window widths between the detided and biological values was 0.60, with values ranging from -0.78 to 1.00. Mean error was 1.21, with values ranging from 0 to 2.40. Simulations with very poor performance (e.g., negative correlations) were those that had minimum widths for day windows and maximum widths for hour windows, or were those with the DO signal composed entirely of noise from observation uncertainty. Conversely, simulations with detided time series that were identical to the true time series (e.g., correlation of one, RMSE of zero) were those for which there was no biological or tidal influence. Although these examples do not represent real-world scenarios, they were included in the simulations to provide verification that the weighted regression provided reasonable results given extremes.

Characteristics of DO time series that contributed to improved model performance were increasing amplitude of the diel DO component (DO_{die}) and increasing process uncertainty (e_{pro}), whereas increasing observation uncertainty contributed to decreased performance (Table 1 and Fig. 4). Model performance was minimally influenced by magnitude of the tidal advection component (DO_{adv}), although performance decreased slightly with increasing tidal effects. Increasing widths for day and tidal proportion windows contributed to increasing model performance, whereas the opposite was true for increasing hour windows (Table 2 and Fig. 5). Graphical summaries of model performance by simulation parameters (Fig. 4) and half window

widths (Fig. 5) support the general trends described by Tables 1 and 2. Scale differences between Fig. 4 and Fig. 5 emphasize that model performance was more affected by characteristics of the DO time series rather than the selected window widths. For example, the range of correlation values comparing the effects of half window widths (averaged across all simulation parameters, Fig. 5) were approximately half the range of correlations for comparing the effects of simulation parameters (averaged across all half window widths, Fig. 4).

Validation of weighted regression with case studies

NERRS is a federally-funded network of 28 protected estuaries established for long-term research, water-quality monitoring, education, and coastal stewardship (Wenner et al. 2004).

Continuous water quality data have been collected at NERRS sites since 1994 through the System Wide Monitoring Program (SWMP). In addition to providing a basis for trend evaluation, data

from SWMP provides an ideal opportunity to evaluate long-term variation in water quality

parameters from biological and physical processes. Continuous SWMP data can be used to describe DO variation at sites with different characteristics, including variation from ranges in

tidal regime (Sanger et al. 2002) and rates of ecosystem production (Caffrey 2003, 2004).

Continuous DO time series and tidal height measurements at four sites from the SWMP database (CDMO 2014) were used to validate the detiding model with real data. Monitoring data

from January 1st to December 31st 2012 were obtained from a range of geographic locations

(Fig. 6 and Table 3). Astronomical tidal heights were predicted for each site using harmonic

regression applied to the sonde depth data (oce package in R, Foreman and Henry 1989, RDCT

2014). Although, the depth data represent tidal height variation from both astronomical (i.e.,

gravitational effects) and meteorological (e.g., wind, precipitation inflows) sources, we isolated

What datum? MSLW? MHW? Assumed?

DO time series

278 the former given that daily metabolism estimates were more likely to be affected by repeated diel
279 cycling from normal tidal changes. Each station was ~~also~~ chosen based on highly significant
280 correlations between DO and tidal changes. The four sites included the Vierra Mouth station at
281 Elkhorn Slough (California, 36.81°N, 121.78°W), Bayview Channel at Padilla Bay (Washington,
282 48.50°N 122.50°W), Middle Blackwater River station at Rookery Bay (Florida, 25.93°N
283 81.60°W), and Dean Creek station at Sapelo Island (Georgia, 31.39°N 81.28°W). The stations are
284 generally ~~macrotidal semidiurnal or mixed semidiurnal and net heterotrophic on an annual basis~~
285 (Table 3). Net heterotrophy (i.e., respiration exceeding production) is typical for shallow water
286 systems at temperate latitudes (Caffrey 2003), although values in Table 3 are from observed DO
287 time series that are strongly influenced by ~~we're correlated with water level height~~.
Filtering for apparent tidal effects

288 Estimates of ecosystem metabolism before and after detiding

289 The weighted regression method was applied to the time series for each station to obtain a
290 detided DO time series for estimating metabolism. Half window widths of six days, one hour, and
291 a tidal proportion of one half were chosen based on a balance between large and small window
292 widths, although the chosen window widths are arbitrary and a more exhaustive evaluation should
293 be conducted prior to using the results to inform management. Unlike the simulated data, the true
294 biological DO signal was unknown for the case studies. Accordingly, results were evaluated using
295 correlations of DO and metabolism estimates with tidal height before and after application of the
296 model. Daily metabolism estimates before and after detiding were compared to the mean rate of
297 tidal height change (i.e., first derivative of the predicted tidal height) for each day during separate
298 solar periods. Production rates were compared to mean rates of tidal height change during the
299 day, respiration rates were compared to mean rates of change during the night, and net

metabolism rates were compared to mean rates of change for the total 24 hour period each day.

Results were also evaluated based on the occurrence of ‘anomalous’ daily production or respiration estimates, where anomalous was defined as negative production during the day and positive respiration estimates during the night. Anomalous values have been previously attributed to the effects of physical processes on DO time series (Caffrey 2003). We hypothesized that metabolism estimates using the detided signal would contain less ‘anomalous’ values than those from the observed DO time series. Although anomalies could be caused by processes other than tidal advection, e.g., abiotic dark oxygen production (Pamatmat 1997), we assume that physical processes are the dominant sources of these values given the tidal characteristics at each site.

Finally, means and standard errors of metabolism estimates were evaluated before and after detiding to determine if annual aggregations were significantly different.

Ecosystem metabolism was estimated from the DO time series using the open-water technique (Odum 1956) as described in Caffrey et al. (2013). The method is used to infer net ecosystem metabolism using the mass balance equation:

$$\frac{\delta DO}{\delta t} = P - R + D \quad (15)$$

where the change in DO concentration (δDO , g O₂ m⁻³) over time (δt , hours) is equal to photosynthetic rate (P , g O₂ m⁻³ hr⁻¹) minus respiration rate (R , g O₂ m⁻³ hr⁻¹), corrected for air-sea gas exchange at the surface (D , g O₂ m⁻³ hr⁻¹) (Caffrey et al. 2013). D is estimated as the difference between the DO saturation concentration and observed DO, multiplied by a volumetric reaeration coefficient, k_a (Thébault et al. 2008). The diffusion-corrected DO flux estimates were averaged during day and night for each 24 hour period in the time series, where flux is an hourly

320 rate of DO change as the difference between observations at time t and $t + 1$ on an hourly scale.

321 Areal respiration rates were assumed constant during the night and subtracted from daily gross net

322 production estimates to yield net ecosystem metabolism (Table 3).

323 Detiding had significant effects on the correlations between tidal height changes, DO time with vertical

324 series, and metabolism estimates (Table 4, see the link in the multimedia section for graphical

325 results of each case study). Correlations of observed DO time series with predicted tidal height

326 were highly significant, with all sites indicating positive relationships, except Padilla Bay where

327 tidal increases were associated with declines in DO concentration. This suggests that seaward

328 water masses were less anoxic than landward masses, with the opposite being true for Padilla

329 Bay. The detided DO time series had greatly reduced correlations with tidal height, although

330 relationships were still significant after detiding likely because of the large sample size for each

331 site ($n \approx 17500$). Comparison of metabolic rates to tidal changes before and after detiding

332 produced inconsistent results (Table 4). Correlations for Elkhorn Slough and Sapelo Island

333 showed consistent reductions in all three metabolism estimates after detiding. Correlations for

334 Padilla Bay and Rookery Bay were of opposite sign and greater magnitude after detiding for

335 production and respiration, although net metabolism estimates had reduced correlations.

336 The proportion of daily integrated metabolism estimates that were anomalous (negative

337 production, positive respiration) were significantly reduced for most sites after detiding (Table 5).

338 Before detiding, anomalous values ranged from 0.09 (Rookery Bay) to 0.22 (Padilla Bay) for

339 production and 0.08 (Rookery Bay) to 0.21 (Elkhorn Slough) for respiration. Anomalous values

340 were reduced to near zero for Rookery Bay and Sapelo Island, by approximately half for Padilla

341 Bay (0.13 for production, 0.13 for respiration), and only slightly reduced for Elkhorn Slough

342 (0.17 for production, 0.17 for respiration). Metabolism estimates using detided DO time series

had decreased mean production and respiration for Elkhorn Slough, increased mean production
and respiration for Padilla Bay, and generally unchanged mean production and respiration for
Rookery Bay and Sapelo Island (Table 5). Mean net ecosystem metabolism was unchanged for all
sites. Decreases in the standard error for all metabolism estimates (production, respiration, and
net) were observed for all cases after detiding.

An example from Sapelo Island illustrates the effects of weighted regression on DO and
metabolism estimates (Figs. 7 to 9). A two-week period in February shows when the tidal
cycle changes were both in and out of phase with the diel cycling. Maximum tide heights were
generally out of phase with the diel cycle during the first week such that low tides were observed
during the middle of the night and the middle of the day (Fig. 8). The opposite scenario occurred
during the second week when the maximum tide height occurred during the day and night (Fig. 8).

The effects of tidal height change on the observed DO time series are visually apparent in the
plots. The first week illustrates a strong negative bias (less respiration, less production) in the
observed DO signal from low tides at mid-day and mid-night, whereas the second example
illustrates a strong positive bias (more respiration, more production) in the observed DO from
high tides. These biases are apparent in the metabolism estimates using the observed data (Fig. 9).

Anomalous estimates occur when low tides are in phase with the solar cycle, whereas metabolism
estimates are likely over-estimated when high tides are in phase with the solar cycle. The detided
time series shows noticeable changes given the direction of bias from the phasing between tidal
height and diel period. DO values were higher after detiding when low tides occurred during
night and day periods, whereas DO values were lower after detiding when high tides occurred
during day and night periods (Figs. 7 and 8). Changes in metabolism estimates after detiding
were also apparent, such that the anomalous values were removed during the first week and the

366 positive bias in the second week is decreased. Detiding had similar effects for the remaining sites,
367 particularly when tidal changes were strongly in or out of phase with diel periods.

368 Effects of aggregation and importance of detiding

369 A final point of concern is the period of observation within which observed DO is affected
370 by tidal height changes and the extent to which this affects the interpretation of ecosystem
371 metabolism. From a management or ecological perspective, the effects of tidal variation on daily
372 estimates may not be a primary concern given that seasonal or annual rates may be more relevant
373 for evaluating ecosystem dynamics with continuous monitoring data. The example from Sapelo
374 Island in the previous section highlights this point given that mean production and respiration
375 estimates before and after detiding were generally unchanged for the two-week period. Table 5
376 also indicated that mean annual estimates of production and respiration were unchanged for
377 Rookery Bay and Sapelo Island, whereas production and respiration estimates were significantly
378 different for Elkhorn Slough and Padilla Bay. Although we acknowledge that the specific results
379 may be related to the window widths, this suggests that tidal effects contribute to changes in
380 metabolic estimates from observed time series that are aggregated on longer time periods.
381 Therefore, an evaluation of the effects of tidal variation on ecosystem metabolism for different
382 periods of observation is critical for understanding practical implications of weighted regression.
383 Specifically, when should detiding be applied if aggregation of observed data on longer time
384 periods removes potential bias? A comparison of observed and detided estimates that are
385 aggregated over different periods of observation (e.g., annual, seasonal, monthly) could help
386 address this question.

387 The observed and detided daily estimates were averaged by month and season (Fall,

The weighted-regression analysis is a tool
for filtering DO time series to potentially
remove tidal anomalies.
Integrate this paper

388 Spring, Summer, and Winter) for each case study to evaluate effects of aggregation on mean
389 production and respiration estimates. Mean annual estimates in Table 5 also provided a basis of
390 comparison with monthly and seasonal aggregation. Significant variation in aggregated
391 production and respiration estimates for month and season was observed for each case study
392 (Figs. 10 and 11). Detided production and respiration estimates for Padilla Bay and Rookery Bay
393 exhibited seasonal and monthly variation that was more characteristic of expected trends with
394 increases in metabolism during warmer months. Specifically, production estimates based on
395 observed DO were substantially muted for both Padilla Bay (Fig. 10) and Rookery Bay (Fig. 11)
396 during summer months, whereas values were significantly higher based on the detided data.
397 Results for Sapelo Island suggested that winter and summer months were under- and
398 over-estimated, respectively, based on the observed data. Results for Elkhorn Slough varied
399 significantly such that production and respiration were significantly reduced after detiding
400 regardless of the aggregation period. Overall, these trends emphasize the importance of
401 considering different aggregation periods for interpreting metabolism estimates. Each case study
402 showed differences in observed and detided values at monthly and seasonal aggregations, whereas
403 only two of the four case studies had mean aggregated estimates that were substantially different
404 (Elkhorn Slough and Padilla Bay, Table 5). Periods of observation as long as one year may
405 include significant sources of bias from tidal advection, suggesting the need for applying
406 weighted regression given careful consideration of appropriate window widths.

407 Discussion

408 The primary objective for development and application of the weighted regression ~~use~~ ^{use} ~~applied~~
409 technique was to provide a method for more accurately estimating ecosystem metabolism by ~~improve~~ ^{of}

Review

removing variation associated with tidal change in observed DO time series. The application of weighted regression to simulated DO time series with known characteristics and extension to continuous monitoring data from selected NERRS sites provided a proof-of-concept that the method can isolate and remove variation in observed DO from tidal change. Further, aggregation of metabolism estimates using the detided DO time series were significantly different than those using the observed data, particularly for relatively long periods of observation. These results suggest that previous estimates of annual means may not accurately reflect true metabolic signals if the effects of tidal variation confound biological signals in observed DO time series. Additionally, variation of aggregated metabolism estimates were substantially reduced after detiding, suggesting greater confidence in interpreting detided estimates even if the mean values are similar. Monitoring data for periods of observation up to one year may also produce significantly different metabolism estimates if observed data are not detided.

Comparisons between detided and biological DO time series from the simulations indicated that adequate results can be obtained from weighted regressions for a range of characteristics of DO time series. An examination of scenarios that produced abnormal results can provide additional insight into factors that affect the performance of weighted regression. For example, poor performance was observed when the observation uncertainty (ϵ_{obs}) was high and both process uncertainty (ϵ_{pro}) and tidal advection (DO_{adv}) were low. These examples represent time series with excessive random variation, no auto-correlation, and no tidal influence. Poor performance is expected because the weighted regression models a non-existent tidal signal in a very noisy DO time series. These results were observed even for time series with a large diel component of the biological DO signal, suggesting that the model will produce random results in microtidal systems with high noise and no serial correlation. From a practical perspective,

433 weighted regression should not be applied to noisy time series if there is not sufficient evidence to
434 suggest the variation is related to tidal changes. Similarly, results with perfect or near-perfect
435 correlations between detided and biological DO time series were observed when observation
436 uncertainty and tidal effects were not components of the simulated time series. Although there is
437 no logical basis for applying weighted regression to time series with no apparent tidal influences,
438 the results will be as expected, as was true for cases with low tidal advection, high observation
439 uncertainty, and low process uncertainty. We emphasize that the weighted regression should only
440 be applied to time series for which specific conditions apply, as described below.

441 The performance metrics used to evaluate weighted regression with the case studies
442 suggested that detiding provided more accurate estimates of ecosystem metabolism. Correlations
443 of metabolism estimates with tidal height changes after detiding were generally reduced, although
444 trends were not always consistent as correlations were reduced in some cases (Sapelo Island) or
445 reversed in others (Padilla Bay). However, correlations of net metabolism estimates were reduced
446 in all cases. Tidal height change provided a proxy for horizontal advection that directly affects the
447 measured rate of change of oxygen. Further, changes in DO concentration represent integrated
448 measures of both production and respiration (eq. (15)). The inconsistent results in Table 4 are
449 potentially related to the effects of horizontal advection on the integrated DO signal, given that
450 production and respiration each represent a unique component of the diel DO variation that is
451 directly affected by tidal variation. Regardless, the proportion of anomalous metabolism estimates
452 was reduced by detiding for all case studies, although this measure may also be an incomplete
453 indication of the combined effects of tidal variation. Negative production and positive respiration
454 estimates suggest assumptions of the open-water method are violated (Needoba et al. 2012),
455 whereas ‘normal’ estimates (positive production and negative respiration) may still include a

Synchrony of Solar/Tidal cycles

456 significant source of bias from physical advection by providing over-estimates of true values. For
457 example, Nidzieko et al. (2014) observed that net metabolism at Elkhorn Slough was more often
458 heterotrophic during maximum spring tides that occurred at nighttime, as a substantially larger
459 area of salt marsh was inundated leading to higher respiration estimates. Although this result
460 supports our general conclusions, a broader discussion regarding whether or not this represents an
461 actual bias in metabolism from physical advection may be needed.

462 A strength of the weighted regression approach is a lack of assumptions describing the
463 relationships between DO and tidal variation over time. Although the functional form of the
464 model is a simple linear regression with only two explanatory variables (eq. (1)), the moving
465 window approach combined with the adaptive weighting scheme allows for quantification of
466 complex tidal effects that may not be possible using alternative approaches. For example, Batt
467 and Carpenter (2012) described the use of a moving window or Kalman filter (Harvey 1989) to
468 improve estimates of ecosystem metabolism in lakes. The approach minimizes the influences of
469 process and observation uncertainty on observed DO time series, which is attributed to the effects
470 of water movement on metabolic signals. Although a similar approach may be useful for estuaries
471 if process and observation uncertainty are the only sources of variation in the DO series, the
472 weighted regression approach is more appropriate if periodic tidal advection is the primary
473 confounding factor. Additionally, results from the case studies illustrated the ability of the
474 weighted regression approach to model changes over time in the relationships between tidal
475 change and DO. Results for Padilla Bay and Rookery Bay suggested that detiding had the largest
476 effect during the summer, whereas the results for cooler months were not significantly different
477 from the observed. The weighted regression method produced detided time series that
478 accommodated seasonal variation in DO conditional on tidal height change, whereas moving

This literature needs to
be cited/introduced in the
Introduction

479 window filters or standard regression techniques would likely not have characterized these
480 dynamic relationships.

481 **Comments and recommendations**

482 Results from the simulations and case studies suggested that weighted regression can be a
483 practical approach for detiding DO time series to remove the effects of physical advection on
484 estimates of ecosystem metabolism. However, application of the method may only be appropriate
485 under specific situations. The case studies were chosen based on the relatively high proportion of
486 metabolism estimates that were anomalous and the strength of correlation between the observed
487 DO time series and tidal height. Despite these similarities among the case studies, detiding had
488 variable effects on metabolism estimates. The results for Elkhorn Slough and Padilla Bay are of
489 particular concern given that mean annual estimates were substantially different compared to
490 those from the observed DO time series. Although the correlation of DO and tidal height was
491 reduced for both cases, in addition to a reduction of anomalous estimates, the relative change in
492 mean metabolism before and after detiding suggests a more careful evaluation of the method is
493 needed. In particular, alternative window widths should be evaluated for the ability to remove tidal
494 effects while preserving the biological signal. The window widths in the above analysis may have
495 removed variation in the DO signal from both of these sources.

496 Although the above analyses suggest the approach has merit, the case studies emphasize a
497 critical challenge in applying weighted regression to monitoring data. Specifically, the true
498 biological signal is not known and the relative contribution of horizontal advection to bias is not
499 accurately quantified with the available data. Comparative analyses between systems with varying
500 tidal influence or within-system evaluations of multiple sites at fixed distances are necessary to

501 further validate the performance of weighted regression. In the absence of additional validation,
502 we propose a precautionary approach for application of the weighted regression to monitoring
503 data. Weighted regression may be most effective at macrotidal sites with strong evidence of the
504 effects of tidal advection on biological signals. A weight-of-evidence approach should be used
505 such that the occurrence of anomalous metabolism estimates, strong correlations between
506 observed DO and tide height, and clear visual patterns of tide change on DO would suggest
507 detiding is appropriate. The choice of window widths may also produce varying results. Window
508 widths that produce large changes in mean annual estimates should be interpreted with caution. In
509 general, a pragmatic approach is emphasized such that results should be evaluated based on the
510 preservation of diel variation from production while exhibiting minimal changes with the tide.
511 Such an approach, combined with further validation, will support informed management
512 decisions through more accurate estimates of ecosystem metabolism.

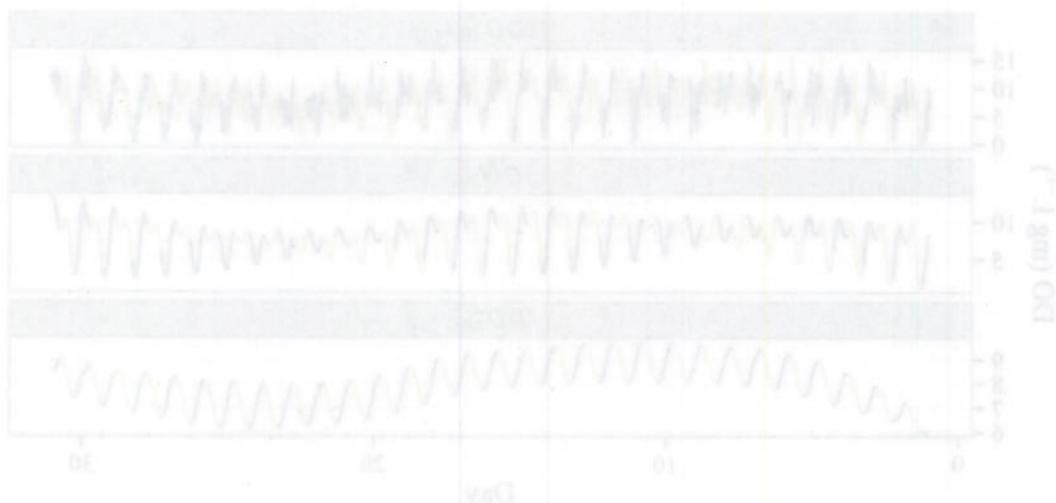
513 *References*

- 514 Batt RD, Carpenter SR. 2012. Free-water lake metabolism: Addressing noisy time series with a
515 Kalman filter. Limnology and Oceanography: Methods, 10:20–30.
- 516 Beck MW, Hagy III JD. In review. Adaptation of a weighted regression approach to evaluate
517 water quality trends in an estuary. Environmental Modeling and Assessment.
- 518 Caffrey JM. 2003. Production, respiration and net ecosystem metabolism in U.S. estuaries.
519 Environmental Monitoring and Assessment, 81(1-3):207–219.
- 520 Caffrey JM. 2004. Factors controlling net ecosystem metabolism in U.S. estuaries. Estuaries,
521 27(1):90–101.
- 522 Caffrey JM, Murrell MC, Amacker KS, Harper J, Phipps S, Woodrey M. 2013. Seasonal and
523 inter-annual patterns in primary production, respiration and net ecosystem metabolism in 3
524 estuaries in the northeast Gulf of Mexico. Estuaries and Coasts.
- 525 CDMO (Centralized Data Management Office). 2014. National Estuarine Research Reserve
526 System. <http://cdmo.baruch.sc.edu/>. (Accessed January, 2014).

- 527 Cloern JE. 1996. Phytoplankton bloom dynamics in coastal ecosystems: A review with some
528 general lessons from sustained investigation of San Francisco Bay, California. *Review of*
529 *Geophysics*, 34(2):127–168.
- 530 Collins JR, Raymond PA, Bohlen WF, Howard-Strobel MM. 2013. Estimates of new and total
531 productivity in Central Long Island Sound from in situ measurements of nitrate and dissolved
532 oxygen. *Estuaries and Coasts*, 36(1):74–97.
- 533 Coloso JJ, Cole JJ, Pace ML. 2011. Difficulty in discerning drivers of lake ecosystem metabolism
534 with high-frequency data. *Ecosystems*, 14(6):935–948.
- 535 Cryer JD, Chan KS. 2008. *Time Series Analysis with Applications in R*. Springer, New York,
536 New York, second edition.
- 537 Diaz RJ. 2008. Spreading dead zones and consequences for marine ecosystems. *Science*,
538 321:926–929.
- 539 Foreman MGG, Henry RF. 1989. The harmonic analysis of tidal model time series. *Advances in*
540 *Water Resources*, 12(3):109–120.
- 541 Harvey AC. 1989. *Forecasting, Structural Time Series Models and the Kalman Filter*.
542 Cambridge University Press, Cambridge, United Kingdom.
- 543 Hilborn R, Mangel M. 1997. *The Ecological Detective: Confronting Models with Data*.
544 Princeton University Press, Princeton, New Jersey.
- 545 Hirsch RM, Moyer DL, Archfield SA. 2010. Weighted regressions on time, discharge, and season
546 (WRTDS), with an application to Chesapeake Bay river inputs. *Journal of the American Water*
547 *Resources Association*, 46(5):857–880.
- 548 Hopkinson CS, Smith EM. 2005. Estuarine respiration: an overview of benthic, pelagic, and
549 whole system respiration. In: Giorgio PAD, Williams P, editors, *Respiration in Aquatic*
550 *Ecosystems*, pages 122–146. Oxford Press, Oxford, United Kingdom.
- 551 Howarth RW, Hayn M, Marino RM, Ganju N, Foreman K, McGlathery K, Giblin AE, Berg P,
552 Walker JD. 2014. Metabolism of a nitrogen-enriched coastal marine lagoon during the
553 summertime. *Biogeochemistry*, 118(1-3):1–20.
- 554 Kemp WM, Testa JM. 2012. Metabolic balance between ecosystem production and consumption.
555 In: Wolanski E, McLusky DS, editors, *Treatise on Estuarine and Coastal Science*, pages
556 83–118. Academic Press, New York.
- 557 Kemp WM, Testa JM, Conley DJ, Gilbert D, Hagy JD. 2009. Temporal responses of coastal
558 hypoxia to nutrient loading and physical controls. *Biogeosciences*, 6(12):2985–3008.
- 559 Monbet Y. 1992. Control of phytoplankton biomass in estuaries: A comparative analysis of
560 microtidal and macrotidal estuaries. *Estuaries*, 15(4):563–571.

- 561 Needoba JA, Peterson TD, Johnson KS. 2012. Method for the quantification of aquatic primary
562 production and net ecosystem metabolism using in situ dissolved oxygen sensors. In:
563 Tiquia-Arashiro SM, editor, Molecular Biological Technologies for Ocean Sensing, pages
564 73–101. Springer, New York.
- 565 Nidzieko NJ, Needoba JA, Monismith SG, Johnson KS. 2014. Fortnightly tidal modulations
566 affect net community production in a mesotidal estuary. *Estuaries and Coasts*.
- 567 Odum HT. 1956. Primary production in flowing waters. *Limnology and Oceanography*,
568 1(2):102–117.
- 569 Pamatmat MM. 1997. Non-photosynthetic oxygen production and non-respiratory oxygen uptake
570 in the dark: A theory of oxygen dynamics in plankton communities. *Marine Biology*,
571 129(4):735–746.
- 572 Rabalais NN, Turner RE, Scavia D. 2002. Beyond science into policy: Gulf of Mexico hypoxia
573 and the Mississippi river. *BioScience*, 52(2):129–142.
- 574 RDCT (R Development Core Team). 2014. R: A language and environment for statistical
575 computing, v3.1.0. R Foundation for Statistical Computing, Vienna, Austria.
576 <http://www.R-project.org>.
- 577 Russell MJ, Montagna PA. 2007. Spatial and temporal variability and drivers of net ecosystem
578 metabolism in western Gulf of Mexico estuaries. *Estuaries and Coasts*, 30(1):137–153.
- 579 Sanger DM, Arendt MD, Chen Y, Wenner EL, Holland AF, Edwards D, Caffrey J. 2002. A
580 synthesis of water quality data: National estuarine research reserve system-wide monitoring
581 program (1995–2000). Technical report, National Estuarine Research Reserve Technical Report
582 Series 2002:3. South Carolina Department of Natural Resources, Marine Resources Division
583 Contribution No. 500, Charleston, South Carolina.
- 584 Short FT, Wyllie-Echeverria S. 1996. Natural and human-induced disturbance of seagrasses.
585 *Environmental Conservation*, 23(1):17–27.
- 586 Staehr PA, Bade D, de Bogert MCV, Koch GR, Williamson C, Hanson P, Cole JJ, Kratz T. 2010.
587 Lake metabolism and the diel oxygen technique: State of the science. *Limnology and
588 Oceanography: Methods*, 8:628–644.
- 589 Thébault J, Schraga TS, Cloern JE, Dunlavey EG. 2008. Primary production and carrying
590 capacity of former salt ponds after reconnection to San Francisco Bay. *Wetlands*,
591 28(3):841–851.
- 592 Tukey JW. 1977. Exploratory Data Analysis. Addison-Wesley, Reading, Massachusetts.
- 593 Wenner E, Sanger D, Arendt M, Holland AF, Chen Y. 2004. Variability in dissolved oxygen and
594 other water-quality variables within the National Estuarine Research Reserve System. *Journal
595 of Coastal Research*, 45(SI):17–38.

- 596 Yin KD, Lin ZF, Ke ZY. 2004. Temporal and spatial distribution of dissolved oxygen in the Pearl
597 River Estuary and adjacent coastal waters. Continental Shelf Research, 24(16):1935–1948.
- 598 Ziegler S, Benner R. 1998. Ecosystem metabolism in a subtropical, seagrass-dominated lagoon.
599 Marine Ecology Progress Series, 173:1–12.



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600 **Figures**

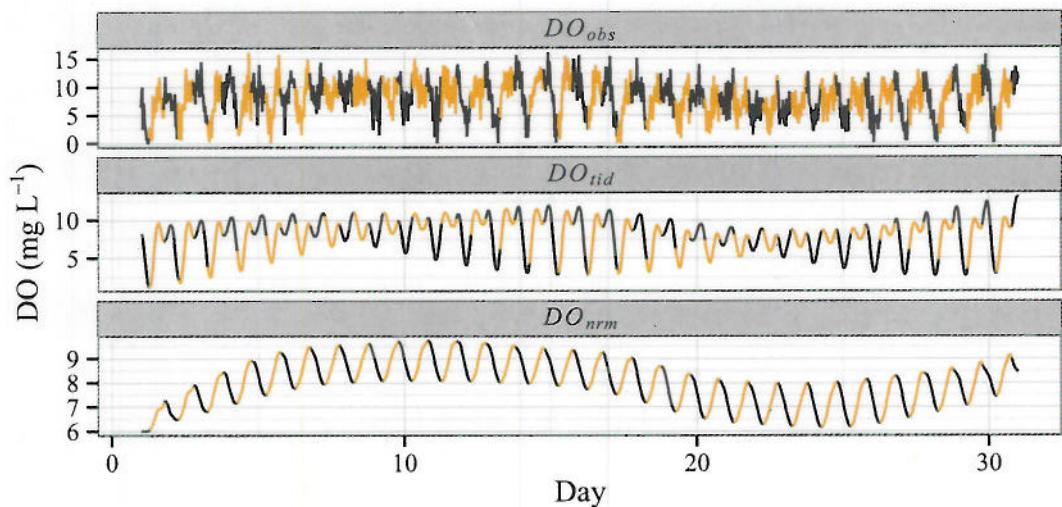


Fig. 1: Example of detiding a simulated DO time series. DO_{obs} represents an additive time series as in eq. (8), DO_{tid} represents the predicted values of DO conditional on tidal height and time (eq. (3)), and DO_{nrm} represents the detided values of DO conditional on constant tidal height and time (eq. (4)). Yellow indicates daylight periods.

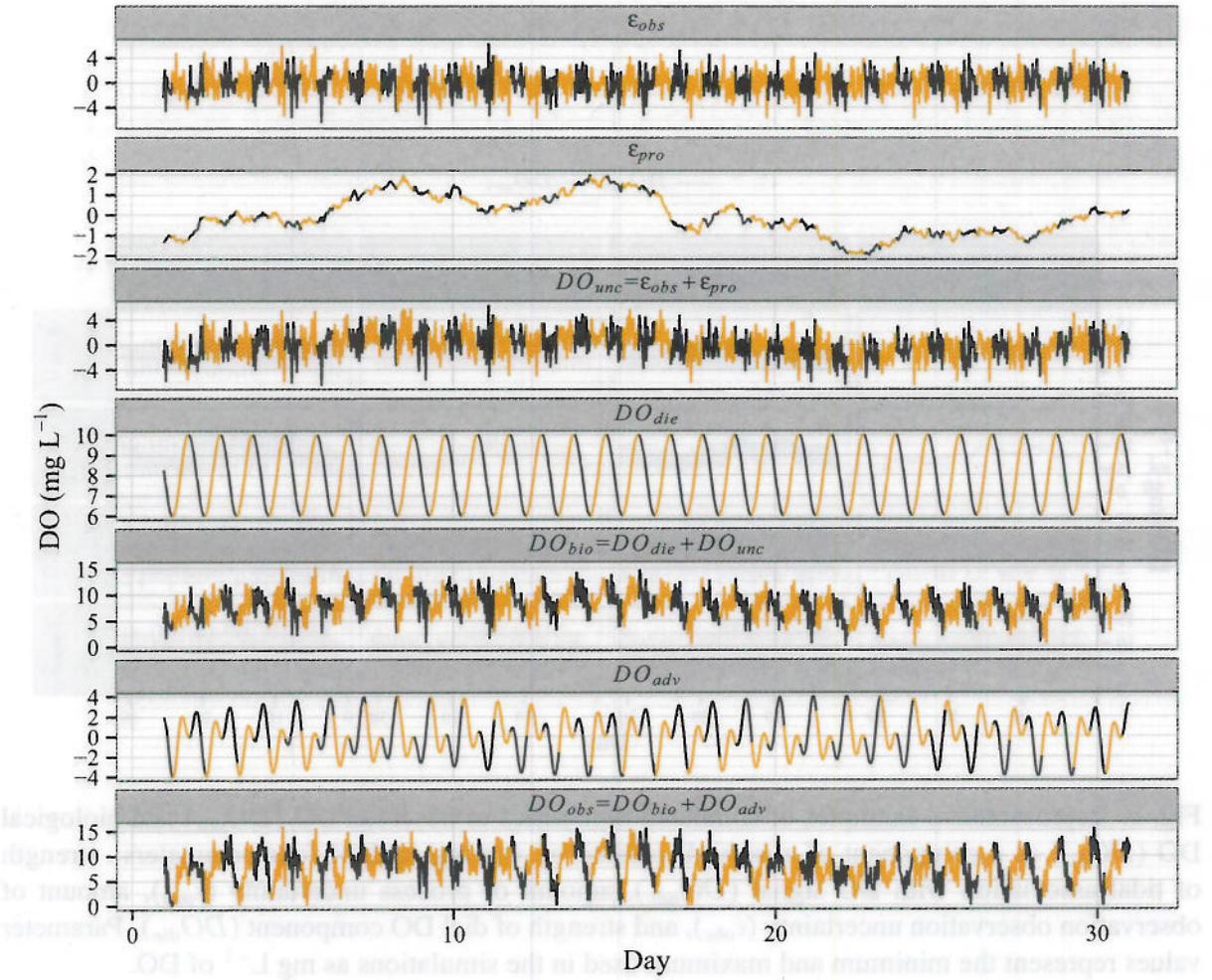


Fig. 2: Example of each component of a simulated DO time series for testing weighted regression. The time series were created using eqs. (5) to (14). Yellow indicates daylight periods.

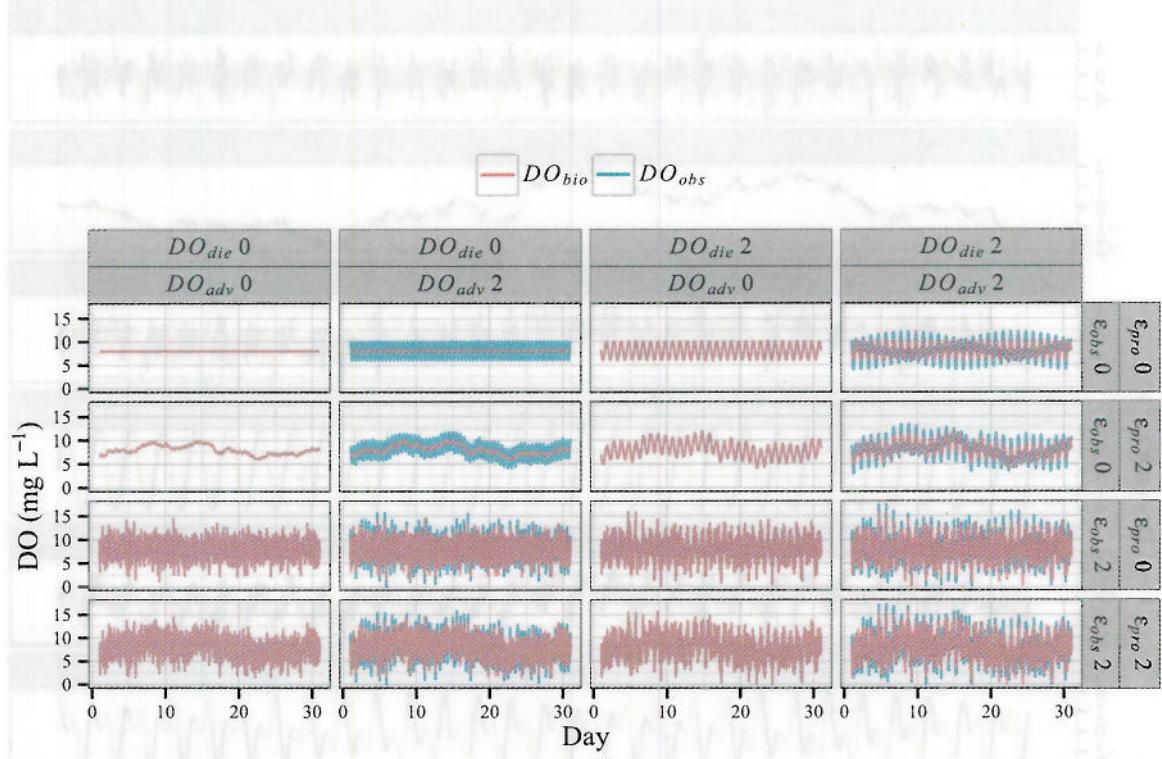


Fig. 3: Representative examples of simulated time series of observed DO (DO_{obs}) and biological DO (DO_{bio} , as a component of observed) created by varying each of four parameters: strength of tidal association with DO signal (DO_{adv}), amount of process uncertainty (ϵ_{pro}), amount of observation observation uncertainty (ϵ_{obs}), and strength of diel DO component (DO_{die}). Parameter values represent the minimum and maximum used in the simulations as mg L⁻¹ of DO.

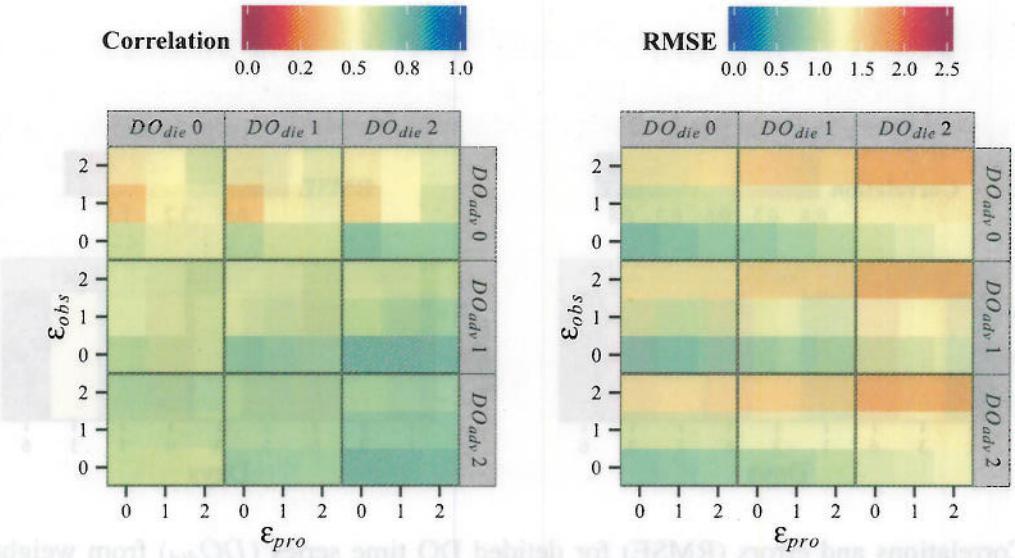


Fig. 4: Correlations and errors (RMSE) for detided DO time series (DO_{dt_d}) from weighted regression with ‘true’ biological DO (DO_{bio}) for varying simulation parameters: strength of tidal association with DO signal (DO_{adv}), amount of process uncertainty (ϵ_{pro}), amount of observation observation uncertainty (ϵ_{obs}), and strength of diel DO component (DO_{die}). Each tile represents the correlation or error from results for a given combination of simulation parameters averaged for all window widths (Fig. 5).

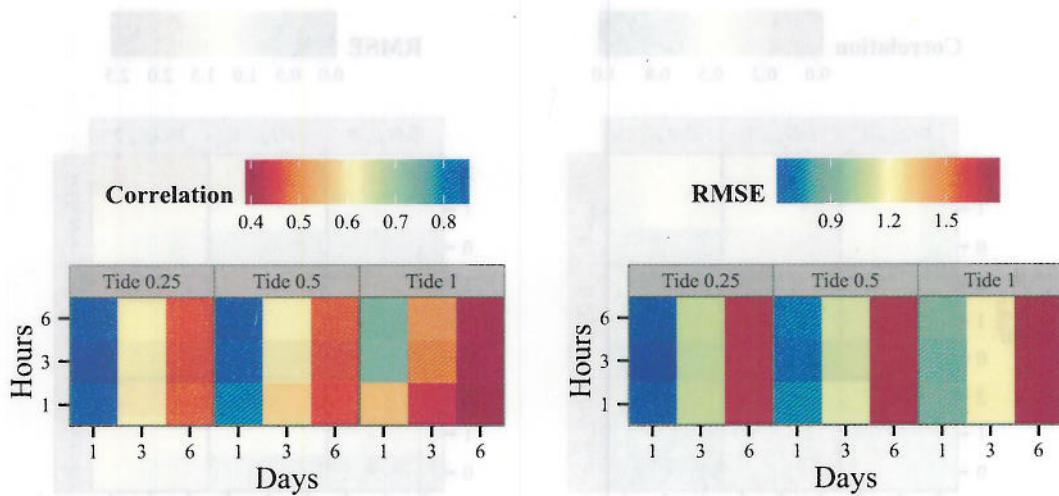


Fig. 5: Correlations and errors (RMSE) for detided DO time series (DO_{dtt}) from weighted regression with ‘true’ biological DO (DO_{bio}) for varying half window widths: days, hour of day, and proportion of tidal range. Each tile represents the correlation or error from results for a given combination of window widths averaged for all simulation parameters (Fig. 5).

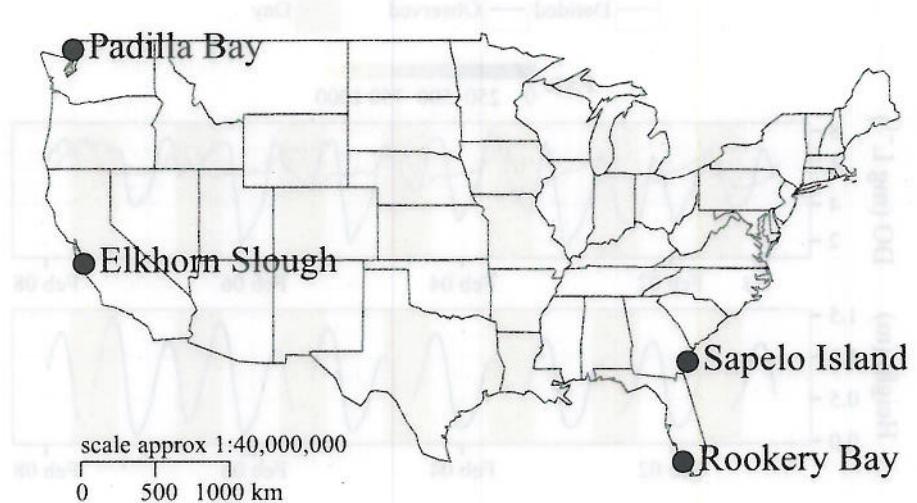


Fig. 6: Locations of NERRS sites used as case studies to validate weighted regression. Stations at each reserve are ELKVM (Vierra Mouth at Elkhorn Slough), PDBBY (Bayview Channel at Padilla Bay), RKBMB (Middle Blackwater River at Rookery Bay), and SAPDC (Dean Creek at Sapelo Island).

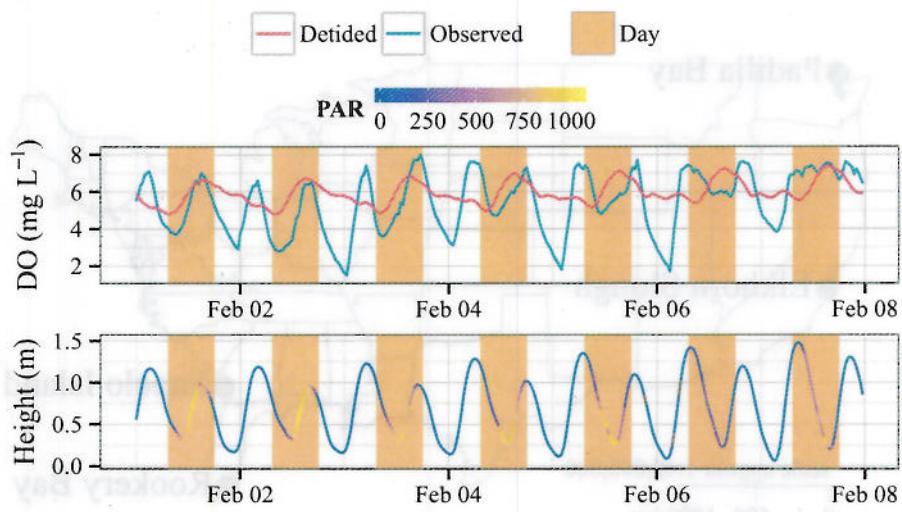


Fig. 7: Continuous DO time series before (observed) and after (detided) detiding with weighted regression (top) and tidal height colored by total photosynthetically active radiation (bottom, mmol m⁻²). Results are for the Sapelo Island station for a seven day period when high tide events were out of phase with diel periods, creating lower than expected observed DO during night and day periods. Detided values are based on a weighted regression with half window widths of six days, one hour within each day, and tidal height proportion of one half.

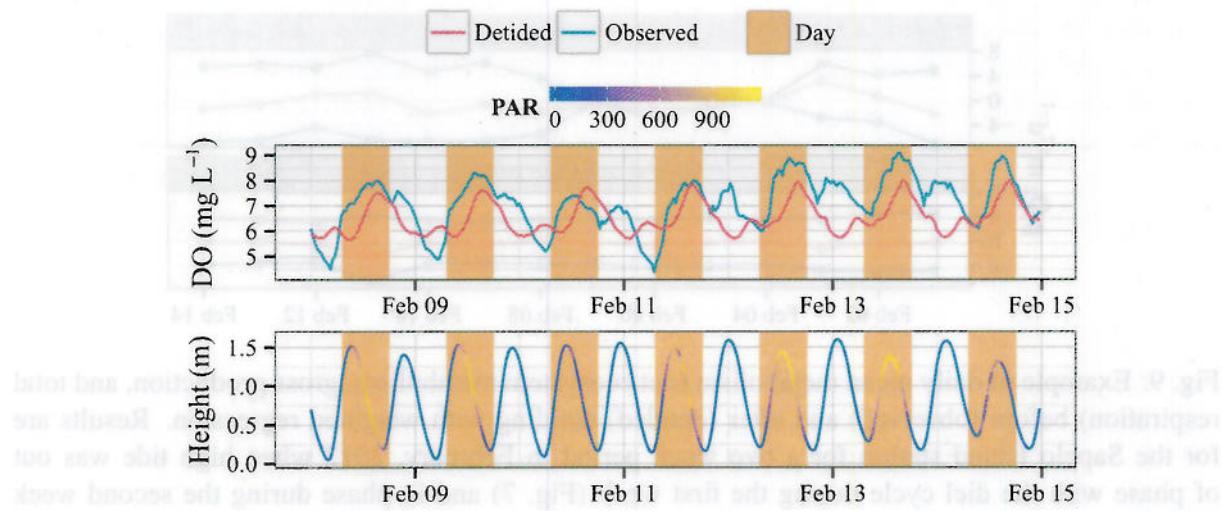


Fig. 8: Continuous DO time series before (observed) and after (detided) detiding with weighted regression (top) and tidal height colored by total photosynthetically active radiation (bottom, mmol m⁻²). Results are for the Sapelo Island station for a seven day period when high tide events were in phase with diel periods, creating higher than expected observed DO during night and day periods. Detided values are based on a weighted regression with half window widths of six days, one hour within each day, and tidal height proportion of one half.

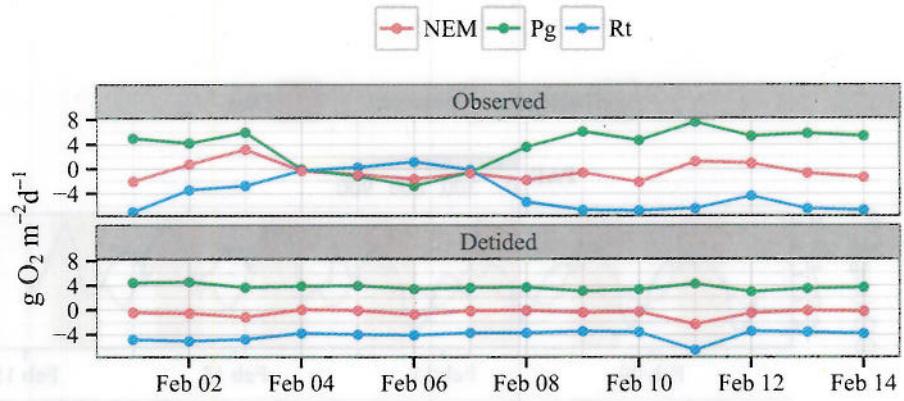


Fig. 9: Example of daily mean metabolism (net ecosystem metabolism, gross production, and total respiration) before (observed) and after (detided) detiding with weighted regression. Results are for the Sapelo Island station for a two week period in February, 2012 when high tide was out of phase with the diel cycle during the first week (Fig. 7) and in phase during the second week (Fig. 8).

longer than the tidal range (high tide) with low (low tide) water levels. The results show that the net ecosystem metabolism (Pg) and total respiration (Rt) are significantly affected by the tidal cycle. The Pg values are higher during high tide (positive correlation) and lower during low tide (negative correlation). The Rt values are also affected by the tidal cycle, with higher values during high tide and lower values during low tide. The NEM values are relatively stable throughout the entire period.

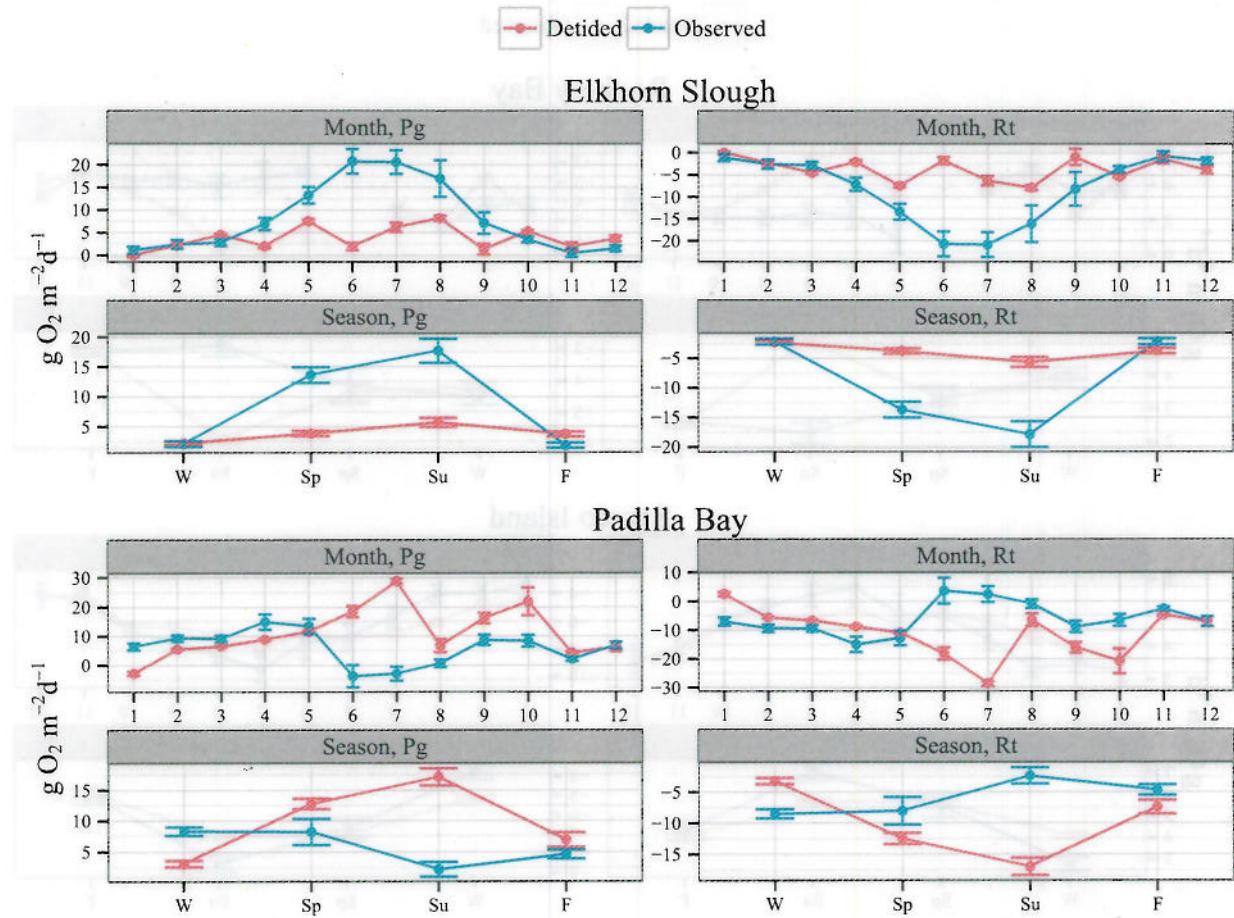


Fig. 10: Means and standard errors of daily metabolism estimates (gross production, total respiration) aggregated by month and season. Aggregated estimates are for Elkhorn Slough and Padilla Bay from observed and detided DO time series.

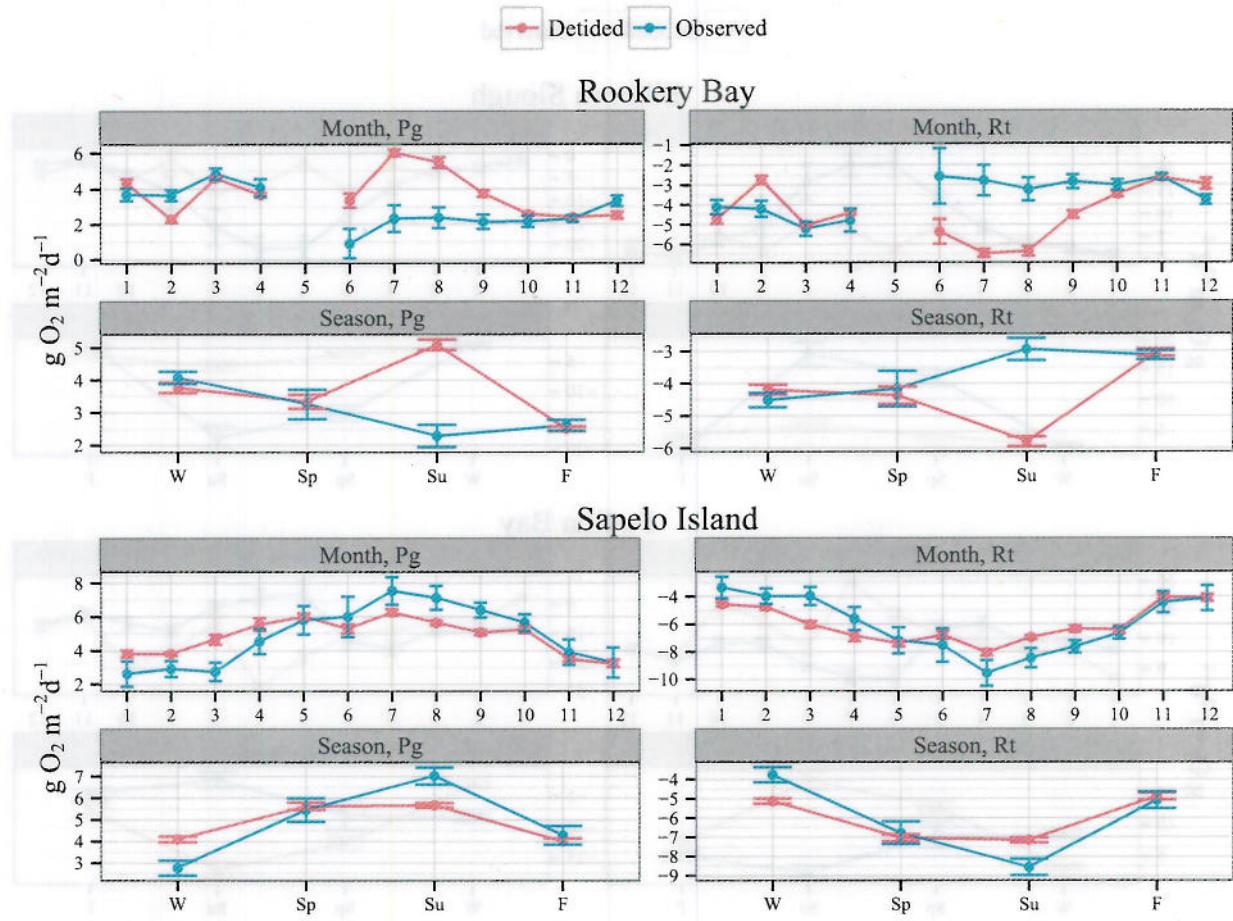


Fig. 11: Means and standard errors of daily metabolism estimates (gross production, total respiration) aggregated by month and season. Aggregated estimates are for Rookery Bay and Sapelo Island from observed and detided DO time series. May was removed from Rookery Bay because of incomplete data.

601 *Tables*

quartiles

Table 1: Summary (range, mean, percentiles) of correlations and error estimates comparing detided and biological DO time series for different simulation parameters (DO_{die} , DO_{adv} , ϵ_{pro} , ϵ_{obs}). Values represent averages from multiple simulations with common parameters (e.g., row one is a summary of all simulations for which diel DO component was zero).

Parameter	Correlation					RMSE				
	Min	25 th	Mean	75 th	Max	Min	25 th	Mean	75 th	Max
DO_{die}										
0	-0.78	0.30	0.53	0.82	1.00	0.00	0.68	1.22	1.97	2.39
1	-0.28	0.38	0.61	0.88	1.00	0.00	0.59	1.20	1.96	2.40
2	-0.39	0.46	0.65	0.90	1.00	0.00	0.62	1.22	1.97	2.40
DO_{adv}										
0	0.00	0.27	0.57	0.93	1.00	0.00	0.34	1.07	1.96	2.12
1	-0.78	0.37	0.59	0.83	1.00	0.00	0.63	1.18	1.98	2.12
2	-0.78	0.47	0.63	0.82	1.00	0.00	0.98	1.38	1.99	2.40
ϵ_{pro}										
0	-0.78	0.34	0.58	0.86	1.00	0.00	0.63	1.19	1.96	2.40
1	-0.78	0.37	0.59	0.85	1.00	0.00	0.63	1.21	1.97	2.40
2	-0.78	0.41	0.61	0.85	1.00	0.00	0.63	1.24	1.98	2.40
ϵ_{obs}										
0	-0.78	0.31	0.65	0.98	1.00	0.00	0.29	0.92	1.50	2.40
1	0.05	0.37	0.57	0.81	0.99	0.07	0.98	1.18	1.49	2.39
2	0.05	0.40	0.57	0.70	0.99	0.15	1.06	1.54	2.01	2.40

Mix & match punctuation &

Non parametric

Nonparametric methods

Use medicine instead!

Table 2: Summary (range, mean, percentiles) of correlations and error estimates comparing detided and biological DO time series for simulations using different half window widths in the weighted regressions (days, hours, and proportion of tidal range). Values represent averages from multiple simulations with common window values (e.g., row one is a summary of all simulations for which the half window width was one day).

Window	Correlation					RMSE				
	Min	25 th	Mean	75 th	Max	Min	25 th	Mean	75 th	Max
Days										
1	-0.78	0.63	0.78	0.97	1.00	0.00	0.28	0.74	1.04	2.12
3	-0.07	0.40	0.56	0.75	1.00	0.00	0.99	1.15	1.28	2.08
6	0.00	0.26	0.45	0.58	1.00	0.00	1.95	1.75	2.05	2.40
Hours										
1	-0.78	0.36	0.57	0.82	1.00	0.00	0.63	1.22	1.96	2.40
3	0.00	0.40	0.61	0.87	1.00	0.00	0.58	1.20	1.97	2.36
6	0.03	0.37	0.61	0.85	1.00	0.00	0.64	1.22	1.98	2.40
Tide										
0.25	0.00	0.42	0.64	0.91	1.00	0.00	0.51	1.14	1.97	2.21
0.5	0.06	0.43	0.63	0.88	1.00	0.00	0.61	1.20	1.97	2.27
1	-0.78	0.30	0.52	0.79	1.00	0.00	0.73	1.30	1.97	2.40

Table 3: Summary statistics of tidal component amplitudes (m), selected water quality parameters (DO mg L⁻¹, chlorophyll-a µg L⁻¹, salinity psu, water temperature °C) and metabolism estimates (gross production, respiration, and net ecosystem metabolism as g m⁻² d⁻¹) for each case study. Tidal components are principal lunar semidiurnal (O1, frequency 25.82 hours), solar diurnal (P1, 24.07 hours), lunar semidiurnal (M2, 12.42 hours), and solar semidiurnal (S2, 12 hours) estimated from harmonic regressions of tidal height (`oce` package in R, [Foreman and Henry 1989](#), [RDCT 2014](#)). Water quality data are averages for the entire period of record (30 minute observations) for each site. Metabolism estimates are means of daily integrated values.

Site	Tidal amplitude				Water quality				Metabolism ^a		
	O1	P1	M2	S2	DO	Chl	Sal	Temp	Pg	Rt	NEM
ELKVM	0.24	0.12	0.48	0.13	7.87	3.87	32.43	13.78	8.14	-8.19	-0.05
PDBBY	0.46	0.23	0.63	0.15	8.97	2.24	29.17	10.44	5.95	-5.90	0.05
RKBMB	0.13	0.04	0.36	0.10	4.48	4.50	30.53	25.85	3.02	-3.62	-0.60
SAPDC	0.10	0.02	0.54	0.07	4.96	5.98	27.30	21.77	4.89	-6.04	-1.16

^aPg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 4: Correlations of tidal changes at each site with continuous DO observations and metabolism estimates (gross production, respiration, and net metabolism) before (observed) and after (detided) detiding with weighted regression. DO values are correlated with predicted tidal height at each observation, whereas metabolism estimates are correlated with mean tidal height change between observations during day, night, or total day periods for production, respiration, and net metabolism, respectively.

	Site	DO	Pg ^a	Rt	NEM
ELKVM					
01.0	Observed	0.47***	0.60***	0.73***	0.35***
20.0	Detided	0.02*	0.19***	0.13*	0.06
PDBBY					
00.0	Observed	-0.45***	-0.33***	-0.46***	-0.25***
20.0	Detided	0.07***	0.48***	0.47***	-0.21***
RKBMB					
00.0	Observed	0.28***	0.34***	0.39***	0.24***
20.0	Detided	-0.02**	-0.31***	-0.36***	0.12*
SAPDC					
00.0	Observed	0.48***	0.54***	0.71***	0.41***
20.0	Detided	-0.03***	0.16**	0.18***	-0.05

* $p < 0.05$; ** $p < 0.01$; *** $p < 0.001$

^aPg: gross production, Rt: respiration, NEM: net ecosystem metabolism

Table 5: Summary of metabolism estimates (gross production, respiration, and net metabolism) for case studies using DO time series before (observed) and after (detided) detiding with weighted regression. Means and standard errors are based on daily integrated metabolism estimates. Anomalous values are the proportion of metabolism estimates that were negative for gross production and positive for respiration. Results are for weighted regressions with half window widths of six days, one hour within each day, and a tidal height proportion of one half.

Site	Pg ^a			Rt			NEM		
	Mean	Std. Err.	Anom	Mean	Std. Err.	Anom	Mean	Std. Err.	
ELKVM									
Observed	8.14	0.67	0.19	-8.19	0.69	0.21	-0.05	0.16	
Detided	3.63	0.23	0.17	-3.67	0.24	0.17	-0.04	0.05	
PDDBY									
Observed	5.95	0.69	0.22	-5.90	0.74	0.19	0.05	0.22	
Detided	10.36	0.63	0.13	-10.32	0.63	0.13	0.04	0.08	
RKBMB									
Observed	3.02	0.14	0.09	-3.62	0.15	0.08	-0.60	0.06	
Detided	3.73	0.09	0.01	-4.35	0.10	0.00	-0.62	0.04	
SAPDC									
Observed	4.89	0.23	0.13	-6.04	0.25	0.11	-1.16	0.09	
Detided	4.85	0.08	0.00	-6.04	0.10	0.00	-1.19	0.05	

^aPg: gross production, Rt: respiration, NEM: net ecosystem metabolism

602 **Multimedia**

603 The supporting information for this manuscript includes a graphical illustration of the
604 weighting scheme described in the material and procedures section
605 (http://spark.rstudio.com/beckmw/weights_widget), results for each simulation
606 (http://spark.rstudio.com/beckmw/detiding_sims), and results for each case study
607 (http://spark.rstudio.com/beckmw/detiding_cases). Each link is a graphical summary of data
608 based on interactive inputs to support the results in the manuscript.

Marcus

~~Assume have had~~

This is a good start to describe a method to analyze time series data

We should discuss several things

- 1) Relevance of in-depth description of simulated data Beyond the ~~purpose~~ of convincing yourself that the analysis is working, it serves no other purpose therefore, should be more in the background ~~background~~
- 2) Add to discussion of relevant literature of people who have done similar things
Kalman filter?
- 3) Use of word "de-tide"