EOF-based constrained sensor placement and field reconstruction from noisy ocean measurements: Application to Nantucket Sound

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[1] Sensor placement at the extrema of empirical orthogonal functions (EOFs) is efficient and leads to accurate reconstruction of the ocean state from a limited number of measurements. In this paper, we develop important new extensions of this approach that optimize sensor placement to avoid redundant measurements, employ imperfect EOF modes, and take into account measurement errors. We use the simulation outputs of the Finite Volume Community Ocean Model applied to the Nantucket Sound region to evaluate the performances of the new approach and compare it against other similar techniques. Specifically, we find that there exists a critical size of exclusion volume (whose value is unknown a priori) surrounding each sensor that prevents clustering of sensors while minimizing the reconstruction error. In addition, we propose a new algorithm that can be effective in incorporating gappy data in assimilation schemes. We also derive analytical formulas of the uncertainty in the reconstructed field given any inaccuracies in the measurements. Taken together these developments will aid further in the development of truly real-time adaptive sampling for ocean forecasting.


1. Introduction

[2] A progress report from a joint NSF-ONR workshop [Lermusiaux et al., 2006] on data assimilation (DA) identified the need for improving "real-time" adaptive sampling and recommended the development of new economical DA approaches without loss of accuracy based on reduced dimension schemes that will complement adjoint- and ensemble-based methods. In light of the ocean complexities over a wide range of scales (see the “multiscale ocean” from Dickey [2003]) extracting the proper hierarchy can be both valuable in physical understanding but also in developing such new economic ways of modeling and forecasting ocean processes. Indeed, there has been a lot of interest recently in developing efficient methods for sensor placement and ocean state reconstruction based on limited measurements that can be used to improve ocean forecasting at least for regional modeling. A relatively simple method for dimension reduction is Proper Orthogonal Decomposition (POD) [see Venturi, 2006; Rempfer, 2003; Bekooz et al., 1993; Aubry et al., 1991; Sirovich, 1987a, 1987b, 1987c], also known as the method of empirical orthogonal functions (EOFs), and oceanographers have used it to both analyze their data and to develop reconstruction procedures for gappy data sets [see Zhang and Bellingham, 2008; Venturi and Karniadakis, 2004; Alvera-Azcarate et al., 2005; Beckers and Rixen, 2003; D’Andrea and Vautard, 2001; Hendrick et al., 1996; Everson et al., 1995; Wilkin and Zhang, 2006; Pedder and Gomis, 1998; Houseago-Stokes, 2000; Preisendorfer and Mobley, 1988].

[3] The success of EOFs approaches depends critically on the fundamental question of such possible low-dimensional representation of the ocean processes, given the wide spatiotemporal scales, from 1 mm for molecular processes to more than 10 km for fronts, eddies and filaments, and corresponding characteristic times from 1 second to several months [Dickey, 2003]. However, in the context of the DA problem, the proper question to pose is what range of such scales is captured in simulations using some representative regional ocean models, and what is the corresponding energy hierarchy. In previous work [Yildirim et al., 2009] we analyzed simulation results from three different regional ocean models (HOPS, ROMS, and Finite Volume Community Ocean Model (FVCOM)) and we showed that only a few spatiotemporal EOF modes are sufficient to describe the most energetic ocean dynamics. In particular, we demonstrated...
that the extrema of the EOF spatial modes are very good locations for sensor placement and accurate field reconstruction given a limited number of observing stations and assuming perfect measurements.

There are several other possible optimization approaches, e.g., using the reconstruction error directly as a cost function or set up different minimization procedures using other sets of sampling points [e.g., see Nguyen et al., 2008]. For adaptive sampling in forecasting the ocean state, the simplest and most efficient approach may be the "optimum" one.

1.1. A Review of Gappy EOF and EOF-Based Sensor Placement Strategies

The key idea of the EOF method is to expand a state variable \( u(x, t) \) in a spatiotemporal domain \( X \times T \) as a biorthogonal series

\[
 u(x, t) = \sum_{k=1}^{\infty} a_k(t) \Phi_k(x),
\]

where \( \Phi_k(x) \) and \( a_k(t) \) are orthonormal spatial modes and orthogonal temporal modes, respectively. Orthogonality of \( a_k \) and \( \Phi_k \) here is considered with respect to the standard inner products in the Lebesgue spaces \( L^2(T) \) and \( L^2(X) \), respectively. The expansion (1) is normally truncated after \( K \) terms, which represents the dimensionality of the system. In order to reconstruct gappy flow fields from a limited number of measurements, a technique that employs EOF modes has been recently proposed by Venturi and Karniadakis [2004], based on the original ideas of Everson and Sirovich [1995] [see also Beckers and Rixen, 2003; Alvera-Azcârate et al., 2005; Gunes et al., 2006].

This technique is known as gappy EOF and here we briefly review its basic formulation. To this end, let us consider a scalar gappy field \( \tilde{u}(x, t) \) as a point-wise product of an indicator function \( \delta(x, t) \) and a complete field \( u(x, t) \), i.e.,

\[
 \tilde{u}(x, t) \overset{\text{def}}{=} \delta(x, t) u(x, t).
\]

The indicator function \( \delta(x, t) \) has values 0 or 1 depending on whether we have data at the corresponding space-time location or not. Our goal is to construct a reliable estimator \( \tilde{u}(x, t) \) of \( u(x, t) \) in the space-time regions where \( \delta(x, t) = 0 \). In the gappy EOF framework this is done iteratively by filling in missing data until the approximation error in the so-called gappy norm reaches a minimum value.

The zero-order estimator \( \tilde{u}^{(0)} \) is usually constructed by filling in missing data at a specific spatial location with the time average of the available data at that location. Higher-order estimators \( \tilde{u}^{(k)} \) are computed iteratively from \( \tilde{u}^{(0)} \) through the following procedure. We first look for a representation of \( \tilde{u}^{(i+1)} \) in the form

\[
 \tilde{u}^{(i+1)}(x, t) = \sum_{k=1}^{K} b_k^{(i+1)}(t) \Phi_k(x),
\]

where \( \Phi_k \) are normalized EOF spatial modes of \( \tilde{u}^{(0)} \) and \( b_k^{(i+1)} \) are unknown time coefficients. Then we minimize the approximation error between \( u \) and \( \tilde{u}^{(i+1)} \) in the gappy norm

\[
 \| u - \tilde{u}^{(i+1)} \|_m^2 \overset{\text{def}}{=} \sum_{k=1}^{K} \left( b_k^{(i+1)}(t) \Phi_k(x) \right)_m^2 + \sum_{k=1}^{K} \left( \Phi_k(x) \right)_m^2 \rightarrow \min,
\]

where \( (a, b) \) denotes the (gappy) inner product \( (a, b) \) and \( \| \cdot \| \) is the gappy norm.

**Minimization of (4) with respect to \( b_k^{(i+1)} \) yields the linear system**

\[
 \mathbf{M}_i b^{(i+1)} = \mathbf{f}^{(i)},
\]

where \( \mathbf{M}_i \) is obviously time dependent and it reduces to a \( K \times K \) identity matrix in case of complete data. The new time coefficient vector \( b^{(i+1)} = [b_1^{(i+1)}(t), \ldots, b_K^{(i+1)}(t)] \) can be easily obtained from (6), provided the matrix \( \mathbf{M}_i \) is invertible.

A very similar algorithm has been found effective in the context of sensor placement strategies based on EOF modes [Willcox, 2005; Mokhadi and Rempfer, 2004]. In this case the indicator function \( m \) is defined in terms of sensor locations, i.e., \( m(x, t) = 1 \) if there is a (working) sensor at position \( x \); zero otherwise. The key idea of gappy EOF for data assimilation is to estimate new time coefficients \( b_k(t) \) based on a limited number of measurements, enabling one to reconstruct a close approximation to the entire flow which is optimal in a certain sense. To this end, a set of previously computed, numerical, EOF spatial modes is combined with experimental data following an assimilation scheme that closely resembles iterative gappy EOF. The only difference is that the complete field \( u \) is now substituted by sensor measurements \( \delta(I, j) \) of \( u \), where \( I \) denotes the position of the \( j \)th sensor and \( N \) is the total number of sensors. Only one iteration is required to assimilate sensor data in the new time coefficients \( b_k(t) \) and therefore, with some abuse of notation, the linear system (6) will be written as

\[
 \mathbf{M} b = \mathbf{f},
\]

where \( \mathbf{M}_i = (\Phi_k, \Phi_j)_m \) and \( f_j = (u, \Phi_j)_m \). Critical to the success of this data assimilation procedure is the generation of ensembles of EOF modes that manage to capture a wide range of system behaviors. In many data assimilation schemes, however, new measurements will be provided from outside the available flow ensemble and therefore the EOF basis needs to be updated properly in order to reduce the approximation error. This question will be discussed further in section 3.2.

1.2. Current Objectives

The objective of this paper is to extend the method developed by Yildirim et al. [2009] by further optimizing both sensor network selection and field reconstruction. Specifically, in our previous work we assumed that the condition number of the matrix \( \mathbf{M} \) [see also Willcox, 2005]
is an indicator of optimality, an assumption which we will reexamine here. Furthermore, we will impose “declustering” constraints on the sensors as we have observed that there may be some redundancy in the required measurements at near-by points. Finally, we will consider more realistic scenarios by taking into account “imperfect” EOF modes and also by incorporating the measurement uncertainty. In order to demonstrate the new ideas we will test our method with simulation data for the Nantucket Sound, a region close to Cape Cod (Massachusetts, USA).

2. Simulation Data and EOF Analysis

We will use simulation data from the regional ocean model (FVCOM, http://fvcom.smast.umassd.edu). The specific site we target is the Nantucket Sound (NS) region, just across from the Woods Hole Oceanographic Institute (WHOI) (see Figure 1), a relatively small but well-defined domain due to the limited inlets and outlets. The geographical coordinates of this area are 41°6′–41°42′N, 69°45′–71°15′W. The data set we consider includes 720 flow snapshots within an area of about 110 km × 60 km, starting from 1 September 2006 at 0000 LT. The time difference between two successive snapshots is 1 h, namely, snapshot 1 corresponds to data at 0000 LT 1 September 2006, snapshot 2 corresponds to the data at 0100 LT 1 September 2006, etc., covering the entire month of September 2006. By cross-correlating different snapshots we easily construct the covariance matrix and its eigen decomposition, which yields the EOF eigenvalues and corresponding hierarchical modes. In order to deal with large matrices we have implemented a parallel version of the EOF algorithm based on ScaLAPACK.

In Table 1 we list the relative energy of the first nine EOF modes for the temperature field and the total velocity $U$ and $T$ fields, where $u$ and $v$ denote Cartesian velocity components along $x$ and $y$ directions, respectively. Clearly, the sum of the normalized EOF eigenvalues is representative of the relative energy captured by the superimposition of the corresponding modes. From Table 1 we see that the first mode, approximating the time-average flow, is responsible for nearly 100% of temperature and nearly 90% of total velocity.

In order to determine characteristic features of the ocean dynamics in the Nantucket Sound region we have computed EOF decompositions over different time periods: 12 h, 10 days, and 30 days. In Figure 2 we show the normalized EOF eigenvalue spectra of total velocity and temperature for the three different cases examined. We note that the first nine eigenvalues of total velocity are very similar while the eigenvalues of temperature for the short-time case (12 h) are quite different from those of long-term cases (10 days and 30 days). The reason is that there exists a tide that dictates a time periodicity of approximately 12 h for the velocity field but not for the temperature. For illustration purposes, in Figure 3 we show the contour plots of the normalized first (dominant) EOF mode at the

Table 1. Relative Energy of EOF Eigenmodes for Total Velocity $U$ and Temperature $T$ Fields

<table>
<thead>
<tr>
<th>Mode</th>
<th>30 Days</th>
<th>10 Days</th>
<th>12 Hours</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$U$</td>
<td>$T$</td>
<td>$U$</td>
</tr>
<tr>
<td>First</td>
<td>88.37%</td>
<td>99.93%</td>
<td>88.37%</td>
</tr>
<tr>
<td>Second</td>
<td>5.41%</td>
<td>0.03%</td>
<td>5.49%</td>
</tr>
<tr>
<td>Third</td>
<td>2.64%</td>
<td>0.01%</td>
<td>2.76%</td>
</tr>
<tr>
<td>Fourth</td>
<td>1.65%</td>
<td>&lt;0.01%</td>
<td>1.59%</td>
</tr>
<tr>
<td>Fifth</td>
<td>0.65%</td>
<td>&lt;0.01%</td>
<td>0.63%</td>
</tr>
<tr>
<td>Sixth</td>
<td>0.26%</td>
<td>&lt;0.01%</td>
<td>0.24%</td>
</tr>
<tr>
<td>Seventh</td>
<td>0.19%</td>
<td>&lt;0.01%</td>
<td>0.18%</td>
</tr>
<tr>
<td>Eighth</td>
<td>0.13%</td>
<td>&lt;0.01%</td>
<td>0.14%</td>
</tr>
<tr>
<td>Ninth</td>
<td>0.12%</td>
<td>&lt;0.01%</td>
<td>0.11%</td>
</tr>
</tbody>
</table>

*Results for 30 days, 10 days, and 12 h dynamics are shown.
surface of the ocean for the total velocity and the temperature (12 h case).

3. Constrained Sensor Placement

[13] In view of the periodicity of the velocity data we will consider the short-time ocean dynamics (12 h) and form an ensemble of 13 snapshots for the EOF analysis as shown in Figure 4 (left), essentially setting up an “interpolation”, i.e., we assume that all EOF modes $\Phi_k(x)$ are known within the tide interval. Using these data we first consider the problem of finding the best possible locations where to deploy a limited number of sensors.

[14] Cohen et al. [2003] considered this problem for unsteady flow past a cylinder and the sensors were placed at the extrema of the EOF modes. Yildirim et al. [2009] presented results of reconstructing several 3D ocean fields with this method and concluded that the extrema of EOF modes are very good locations, if not optimum, to place the sensors for regional ocean forecasting. They also showed that given a fixed number of sensors, it is more effective to distribute them at the extrema of more EOF modes rather than to put them at more extrema of fewer EOF modes.

For example, in the Nantucket Sound we find that using 24 sensors, the error for 4 modes sampled using 6 sensors for each mode is 9% whereas for 6 modes sampled using 4 sensors for each mode is 6%.

[15] In general, sampling fields in the modal space may result in lowering the dimensionality. However, there may be cases where the location of the extrema of different order modes may be very close to each other or even coincide. This is indeed the case for our region of interest, i.e., Nantucket Sound, where we found that some sensors distributed according to the method by Yildirim et al. [2009] (we will call it original method) cluster together. This leads to significant inefficiencies in reconstructing a close approximation to the flow field. In this section we will improve this sensor placement strategy by imposing certain positional constraints in order to decluster the sensors. To this end, let us associate with every sensor a cylinder of radius $R$ and height $2H$, as shown in Figure 5a. The criterion for sensor declustering then is formulated in terms of this exclusion cylinder as follows. If we place a sensor

\[ u_1, u_2, \ldots, u_{13}, \tilde{v}_{14}, \tilde{v}_{15}, \ldots \]

interpolation \hspace{2cm} extrapolation

Figure 4. Simulation data sets used for (left) interpolation and (right) extrapolation. $U_i$ denotes the $i$th snapshot of the total velocity.
connection with the first six (most energetic) EOF modes. Note that in Case 1 higher-order modes are sampled more; in Case 2 all modes are equally sampled; in Case 3 lower-order modes are sampled more.

[17] Next we fix the number of sensors to be 24 and use 6 modes with configuration Case 1 and to see the effect of the exclusion volume cylinder size in reconstructing the total velocity. For each flow snapshot we define the reconstruction error as

\[ e_i^2 \overset{\text{def}}{=} \frac{1}{X} \int \frac{(\hat{U}_i - U_i)^2}{U_i^2} \, dX, \]

where \( \hat{U}_i \) denotes the estimator of the \( i \)th flow snapshot \( U_i \) obtained by solving equation (7). In order to measure the reconstruction error within the whole period of interest we also define the time-averaged error as

\[ e^2 = \frac{1}{S} \sum_{i=1}^{S} e_i^2, \]

where \( S \) denotes the total number of available snapshots within the considered time interval. In Figure 5 we show that for a fixed cylinder radius \( R \) the averaged error decreases as \( H \) increases while for a fixed \( H \) a larger cylinder radius leads to a nonmonotonic error decrease. Hence, there is an optimum size of the cylinder to exclude sensor placement that affects the reconstruction error.

[18] In Figure 6 we show two different sensor networks obtained by using the method of Yildirim et al. [2009] (original method) and our modified method. In both cases we consider 4 EOF modes, 12 sensors and configuration Case 1. For illustration purposes the sensor locations are superimposed on the contour plots of the normalized second EOF mode evaluated at the ocean surface (layer \( H = 0 \)). In general, the critical points of the EOF modes are obviously not necessarily located on the ocean surface; however, for the total velocity we have found that they do lie on (or nearby) the ocean surface. Results of Figure 6 show that the sensor networks predicted by the original method and the modified method are different. This is clearly due to the exclusion volume cylinder constraint implemented in the modified method. Specifically, according to the original strategy, sensor 5 should be placed at layer 0 (ocean surface) while sensor 6 at layer 1, i.e., they should be at two successive layers. The same phenomenon is observed for sensors 7 and 8, which correspond to the minima of mode 3. Moreover, according to the original method, sen-

**Table 2. Sensor Network Configurations in Modal Space**

<table>
<thead>
<tr>
<th>Sensor Network Configurations in Modal Space(^a)</th>
<th>4 Modes</th>
<th>6 Modes</th>
<th>8 Modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case 1</td>
<td>2-2-4-4</td>
<td>2-2-4-4-6-6</td>
<td>2-2-4-4-6-6-8-8</td>
</tr>
<tr>
<td>Case 2</td>
<td>3-3-3-3</td>
<td>4-4-4-4-4</td>
<td>5-5-5-5-5-5-5-5-5</td>
</tr>
<tr>
<td>Case 3</td>
<td>4-4-2-2</td>
<td>6-6-4-4-2-2</td>
<td>8-8-6-6-4-4-2-2</td>
</tr>
</tbody>
</table>

\(^a\) A configuration denoted as “2-2-4-4” means that 2, 2, 4, and 4 sensors are used in connection with the EOF modes 1, 2, 3, and 4, respectively. Similarly, a configuration denoted as “4-4-8-8-12-12” means that we are using a total number of 48 sensors in connection with the first six (most energetic) EOF modes.

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**Figure 5.** Comparison between time-averaged errors for different sizes of the exclusion volume cylinder defined in the legend.

at the point \((x_1, y_1, z_1)\), then any other sensor located at \((x_2, y_2, z_2)\) should satisfy

\[ |z_1 - z_2| > H ~ \text{or} ~ \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2} > R. \]  

The FVCOM ocean model of the Nantucket Sound region consists of 30 layers in the depth direction \( z \), the ocean surface being defined as layer 0. Therefore, in order to characterize the volume of the exclusion cylinder it is convenient to use a discrete dimensionless vertical coordinate label \( H \) ranging within layer numbers, while the cylinder radius \( R \) will be expressed in meters.

[16] In order to investigate the effectiveness of the constrained sensor placement strategy (we will call it modified method) against the original one, we have considered several different cases. In Table 2 we summarize three relevant sensor networks among many others we have tested. In terms of the notation we adopt here, a configuration denoted as “2-2-4-4” means that 2, 2, 4, and 4 sensors are used in connection with the EOF modes 1, 2, 3, and 4, respectively. Similarly, a configuration denoted as “4-4-8-8-12-12” means that we are using a total number of 48 sensors in connection with the first six (most energetic) EOF modes.
sors 7 and 8 are too close to sensor 1, which is already in place. Hence, the modified strategy (Figure 6b) keeps sensor 5 unchanged while redistributes sensor 6. Similarly, sensors 7–12 are redistributed in the modified method. Correspondingly, the time-averaged error (11) reduces from 11.3% to 10.0% while the truncation errors 8.98%. The truncation error is obtained by truncating the EOF representation of the complete FVCOM data after a selected number of EOF modes. It clearly represents a lower bound for all errors achievable with reconstruction/estimation procedures employing the same number of modes. More detailed tests performed with the modified (declustered) sensor placement strategy confirm the conclusion of Yildirim et al. [2009], i.e., the smallest reconstruction error is obtained if more EOF modes are sampled rather than.

Figure 6. Sensor networks for total velocity obtained from (a) the original method and (b) the modified method. The sensor locations are superimposed on the contour plot of the normalized second EOF mode, configuration Case 1 (2-2-4-4), based on snapshots 696–708. Squares denote maxima while circles denote minima of different modes. In Figure 6a, sensors 1 and 2 are located at extrema of mode 1, sensors 3 and 4 are located at extrema of mode 2, sensors 5–8 are located at extrema of mode 3, and sensors 9–12 at extrema of mode 4.
Figure 7. Comparison between time-averaged errors for sensor networks identified by the modified method with (a) 4 modes and (b) 6 modes. The exclusion cylinder size is kept fixed at $H = 28$, $R = 3000$ m.

We notice that the relative energies of the EOF eigenvalues for the velocity and temperature fields show strong dominance of the first mode. This mode represents an approximation of the mean flow (temporal average) and sometimes it is useful to subtract it before decomposing the ocean dynamics into orthogonal functions. In the present application, however, there is no need to perform such a subtraction because all the orthogonal modes can be employed in the construction of the sensor network, including the first one, which represents the time-average flow. In order to quantify the difference between sensor networks based on full EOF decompositions and mean-subtracted EOF decompositions we fix the number of sensors to be 12 and we consider configuration Case 2. The results of this comparison are shown in Figure 9.

3.1. Comparison With Other Methods

[21] In a recent paper, Zhang and Bellingham [2008] developed another criterion for sensor placement, by minimizing the normalized sum of the cross products of the EOF modes. Specifically, the following minimum principle was considered for the identification of an optimal sensor network ($\{I_1, \ldots I_n\}$ identifies the selected location for the $i$th sensor)

$$\{I_1, \ldots I_n\} = \min_{\{x_1, \ldots x_N\}} \mathcal{F}[x_1, \ldots x_N],$$

where

$$\mathcal{F}[x_1, \ldots x_N] \equiv \sum_{i=1}^{K} \lambda_i \sum_{n=1}^{N_i} \phi_i(x_n)\phi_j(x_n)^2.$$

They defined $\mathcal{F}[\cdot]$ as total ratio ($\lambda_i$ are EOF eigenvalues). It is interesting to compare sensor networks obtained by our modified method and the Zhang and Bellingham’s minimization approach. This is done in Figure 10 for configuration Case 1 (2-2-4-4). Four EOF modes are used in Zhang and Bellingham’s method. The sensor locations are superimposed on the contour plot of the normalized first empirical orthogonal function of total velocity. We can see that the sensor locations predicted by the two approaches are totally different. In particular, the locations selected by Zhang and Bellingham’s method have a much wider distribution along the depth direction while those selected by our method are mostly located near the sea surface. For the case shown in Figure 10, our method identifies 12 sensor locations within the first 10 layers (layer 0 corresponding to the sea surface) while Zhang and Bellingham’s method selects only 4 sensors within the same layers. Also, unlike the original method of Yildirim et al., the locations predicted by the Zhang and Bellingham method are distinct, perhaps due to the orthogonality condition involved in their selection criterion that may prevent clustering. In Table 3 we compare the reconstruction errors based on the original and the modified methods and also based on the Zhang and Bellingham’s method. We see that the modified method is the best among the three with reconstruction errors only slightly above the truncation error which, we recall, is a lower bound. The original method has the largest error for 4 modes (12 sensors) but as the number of modes is increased to 6 (24 sensors) it performs better than the...
Zhang and Bellingham’s method. For the modified method we use the optimum exclusion volume cylinder corresponding to $H = 28$ and $R = 3000$ m; however, even for other values of $H$ and $R$ we have found that the error with this method is minimum with respect to the other two methods. We have also included the values of the total ratio that is used as a criterion in the Zhang and Bellingham’s method. Obviously, these values are minimal for the sensor networks selected by the Zhang and Bellingham’s method compared with any other method. While the differences listed in Table 3 may be small, their relative magnitude compared to the truncation error are up to 20%. [22] A drawback of our modified method is that we cannot determine a priori the size of the optimum exclusion cylinder that sets the constraints in the sensor placement strategy. To this end, we have investigated if the minimization criterion proposed by Zhang and Bellingham [2008] can be used to tackle this problem. Hence, in order to

Figure 8. Sensor networks for temperature field obtained from (a) the original method and (b) the modified method. The sensor locations are superimposed on the contour plot of the normalized first temperature EOF mode, configuration Case 1 (2-2-4-4), based on snapshots 696–708. Squares denote maxima while circles denote minima of different modes. In Figure 8a sensors 1 and 2 are located at extrema of mode 1, sensors 3 and 4 are located at extrema of mode 2, sensors 5–8 are located at extrema of mode 3, and sensors are located 9–12 at extrema of mode 4.
identify any relationships between the exclusion volume and the corresponding total ratio, in Figure 11 we plot the total ratio as a function of the cylinder size corresponding to the same cases studied in Figure 5. These results show that the values of total ratio decrease monotonically and therefore it seems that there is no optimum point identified by this criterion for selecting the critical cylinder size.

We conclude this section by emphasizing two interesting connections between the constrained sensor placement algorithm (modified method) and the method of Zhang and Bellingham [2008]. Indeed, the denominator appearing in the objective function (13) dictates that the EOFs should have large magnitudes at the selected locations, which share the same attribute with the “POD extrema” criterion proposed by Yildirim et al. [2009]; similarly, the numerator dictates that the cross product between the EOFs should be small at the selected locations, which appears to have some effect of preventing clustering of sensors.

3.2. Extrapolation-Based Reconstruction

In section 3.1, we have considered reconstruction of the velocity and temperature fields assuming perfect EOF

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**Figure 9.** Comparison between sensor networks based on full EOF decompositions (circles) and mean-subtracted EOF decompositions (triangles). The sensor locations are superimposed on the contour plot of the first normalized EOF mode for the total velocity.

**Figure 10.** Sensor networks for total velocity as selected by Zhang and Bellingham's [2008] method (diamonds) and our modified method (circles) of Case 1. The sensor locations are superimposed on the contour plot of the normalized first EOF mode for total velocity.
Table 3. Comparison Between Time-Averaged Reconstruction Errors \( e_{\text{avg}} \) and Total Ratios \( F \) Obtained With Different Sensor Placement Strategies

<table>
<thead>
<tr>
<th>Truncation</th>
<th>Original Method</th>
<th>Modified Method</th>
<th>Zhang and Bellingham [2008]</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>( e_{\text{avg}} )</td>
<td>( F )</td>
<td>( e_{\text{avg}} )</td>
</tr>
<tr>
<td>4 modes 12 sensors</td>
<td>8.98%</td>
<td>11.32%</td>
<td>397,914</td>
</tr>
<tr>
<td>4 modes 24 sensors</td>
<td>8.98%</td>
<td>11.35%</td>
<td>398,480</td>
</tr>
<tr>
<td>6 modes 24 sensors</td>
<td>5.51%</td>
<td>8.27%</td>
<td>443,833</td>
</tr>
</tbody>
</table>

*For Case 1.

modes and a limited number of “synthetic” flow measurements. More specifically, we have extracted the EOF modes \( \Phi_1, \Phi_2, \ldots, \Phi_{13} \) from full FVCOM data \( U_1, U_2, \ldots, U_{13} \) and we have used the gappy data (i.e., measurements at few sensor locations) \( \bar{U}_1, \bar{U}_2, \ldots, \bar{U}_{13} \) to construct \( f \) in equation (7). However, in any data assimilation procedure, new measurements will be provided from outside the ensemble, while the EOF basis is obtained from snapshots corresponding to previous time steps. In this case we can still determine reliable time coefficients by solving equation (7) provided the modes \( \Phi_k \) manage to capture a wide range of flow behaviors. In general, however, a data assimilation scheme for measurements outside the flow ensemble could yield to a mismatch between modes and data.

In order to carefully examine this important point we have computed the time-averaged error for reconstructing field snapshots within a 12 h period outside the available ensemble, i.e., reconstruct \( U_{14}, U_{15}, \ldots, U_{25} \) based on \( U_{14}, U_{15}, \ldots, U_{25} \) (see Figure 4). A summary of our results is shown in Figure 12 where we also include the truncation error plot, which is the lower bound for all the results, i.e., for all reconstruction errors based either on interpolation (within the ensemble) or on extrapolation (outside the ensemble). Clearly, the interpolation error is lower than that of extrapolation. The number of sensors we employ in the interpolation-based reconstruction is 24 and does not improve with more sensors. We also include in the plot the lower bound of extrapolation achieved by using the full data set (i.e., complete snapshots) \( U_{14}, U_{15}, \ldots, U_{25} \). We see that increasing the number of sensors leads to errors that are of the same level as for the full data curve.

[26] Next, we address the question if we can reduce the extrapolation error further by minimizing the effect of mismatch between EOF modes and measurements. To this end, we propose to correct the EOF modes by extracting a new basis that takes into account the new measurements. Let us assume that we have full data for the snapshots \( U_1, U_2, \ldots, U_{13} \) and gappy data, measurements at few locations, for \( U_{14} \). We start the correction procedure by extracting the EOF modes of the full data \( \Phi_1^{(0)}, \Phi_2^{(0)}, \ldots, \Phi_{13}^{(0)} \) and then reconstruct a provisional field \( U_{14}^{(1)} \) by extrapolation using the EOF expansion. Subsequently, we construct a new flow ensemble by combining \( U_1, U_2, \ldots, U_{13} \) with the estimated \( U_{14}^{(1)} \) and extract new EOF modes \( \Phi_1^{(1)}, \Phi_2^{(1)}, \ldots, \Phi_{13}^{(1)} \). Based on these new modes we obtain new \( \mathbf{M}^{(1)} \) and \( \mathbf{f}^{(1)} \) in equation (7). Then we can solve the linear system for new time coefficients \( \mathbf{b}^{(1)} \) and hence obtain the new (and final) \( U_{14}^{(2)} \). In summary, the data assimilation algorithm we propose is as follows: (1) Solve \( \mathbf{M}^{(0)} \mathbf{b}^{(0)} = \mathbf{f}^{(0)} \) to obtain \( U_{14}^{(1)} \) to fill the missing data. (2) Extract new EOF modes \( \Phi_1^{(1)}, \Phi_2^{(1)}, \ldots, \Phi_{13}^{(1)} \) from \( U_1, U_2, \ldots, U_{13}, U_{14}^{(1)} \). (3) Construct new \( \mathbf{M}^{(1)} \) and \( \mathbf{f}^{(1)} \) with \( \Phi_1^{(1)}, \Phi_2^{(1)}, \ldots, \Phi_{13}^{(1)} \) to obtain the final field \( U_{14}^{(2)} \).

[27] The reconstruction procedure is obviously applied only to the missing points, since it is unnecessary to estimate the field where we already have observation data. We remark that sometimes the changes in the EOFs before and after the application of the extrapolation procedure are not significant, especially when there are only few measurement locations.

Figure 11. Total ratio used in the Zhang and Bellingham [2008] method versus the radius of the exclusion volume cylinder.

Figure 12. Comparison of time-averaged error for interpolation-based (squares) and extrapolation-based (pentagons) reconstruction for the sensor configuration of Case 2.
that the sensor signals are affected by random noise while the EOF modes are deterministic, i.e., we consider the case where the right hand side in equation (7) contains uncertainty while the matrix \( \mathbf{M} \) is constructed according to full deterministic EOF modes obtained from FVCOM simulation outputs. Specifically, we assume that the total velocity detected by the sensors has the form

\[ d(l, t; \xi) = U(l, t) + \xi(l, t), \tag{14} \]

where \( \{l_1, \ldots, l_{N_s}\} \) are sensor locations, \( U \) is total velocity and \( \xi(l, t) (i = 1, \ldots, N_s) \) are \( N_s \) zero-mean uncorrelated Gaussian processes with standard deviation \( \sigma_\xi(l, t) \). In order to include the measurement uncertainty in the field reconstruction process we look for a representation of the total velocity in terms of random temporal modes and deterministic spatial modes [Mathelin and Le Maitre, 2009; Venturi et al., 2008] as

\[ U_r(x, t; \xi) = \sum_{k=1}^{K} \eta_k(t; \xi) \Phi_k(x), \tag{15} \]

where \( \Phi_k \) are based on full FVCOM data. The notation \( U_r(x, t; \xi) \) emphasizes that the stochastic total velocity (15) depends on the random vector

\[ \xi \overset{\text{def}}{=} [\xi(l_1, t_1), \ldots, \xi(l_{N_s}, t_5)], \tag{16} \]

characterizing the measurement errors. Next we consider the following functional:

\[ \mathcal{J}[\eta_k] = \int_{T} \left( \sum_{i=1}^{N_s} \left[ \sum_{j=1}^{K} d(l_i, t; \xi) - \sum_{j=1}^{K} \eta_j(t; \xi) \Phi_j(l_i) \right]^2 \right) dt, \tag{17} \]

where \( \langle \cdot \rangle \) denotes an average with respect to the joint probability density of the random vector (16). More general data assimilation schemes based on quadratic regularization functionals can be considered. Minimization of (17) with respect to \( \eta_k \) yields the following Euler-Lagrange equations:

\[ \sum_{j=1}^{K} \eta_j(t; \xi) \sum_{i=1}^{N_s} \Phi_j(l_i) \Phi_m(l_i) = \sum_{i=1}^{N_s} d(l_i, t; \xi^w) \Phi_m(l_i). \tag{18} \]

This system can be rewritten in the same form as equation (7), i.e.,

\[ \sum_{j=1}^{K} \langle \Phi_j, \Phi_j \rangle_{\omega \eta} = \langle d, \Phi_j \rangle_{\omega}, \tag{19} \]

provided the gappy inner product (5) is defined in terms of the sensor locations, that is \( m(x, t) = 1 \) if \( x = l_i \); zero otherwise. If the matrix \( M_{ij} = \langle \Phi_i, \Phi_j \rangle_{\omega} \) is not singular, then we obtain a unique solution to (19) in the form

\[ \eta_j(t; \xi) = \sum_{j=1}^{K} M_{ij}^{-1}(d, \Phi_j)_{\omega}. \tag{20} \]

Now we can easily calculate the standard deviation of the estimate (15) based statistical assumption of the measurements errors. Specifically, by using the independence

![Figure 13. Reconstruction error in snapshot 14th as a function of the number of sensors deployed by using the EOF-based extrapolation procedure. The sensor network is constructed according to the original method, i.e., no constraints are imposed (Case 2).](image)

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hypothesis of the measurement errors we obtain (repeated indices are summed unless otherwise stated)

\[
\sigma_{U_e}(x, t) \equiv \sqrt{\langle \eta \eta \rangle - \langle \eta \rangle \langle \eta \rangle} \Phi_i(x) \Phi_k(x),
\]

where

\[
\langle \eta \rangle = M_{ij}^{-1}(d(l_j, t; \xi)) \Phi_i(l_j),
\]

\[
\langle \eta \eta \rangle = M_{im}^{-1}M_{nk}^{-1}(d(l_j, t; \xi)d(l_p, t; \xi)) \Phi_m(l_j) \Phi_n(l_p).
\]

A substitution of (22) and (23) into (21) yields the following formula

\[
\sigma_{U_e}(x, t) = \sigma_\xi(l_j, t) \sqrt{M_{im}^{-1}M_{nk}^{-1}(\Phi_m(l_j))\Phi_n(l_j)\Phi_i(x)\Phi_k(x)},
\]

where \(\sigma_\xi(l_j, t)\) denotes the standard deviation of the measurement errors at location \(l_j\).

Figure 14. Standard deviation of total velocity at the surface of the ocean for noisy sensors networks of configuration Case 1. The measurement standard deviation is uniform and equal to \(\sigma_\xi = 0.2\). (a–c) Original sensor placement strategy. (d–f) Modified sensor placement strategy. It is seen that sensor networks obtained from the modified procedure with exclusion cylinder radius \(R = 3000\) m significantly reduce the standard deviation of the estimate \(U_e\).
4.1. Results for Uniform Measurement Errors

Let us assume that the standard deviation of the measurement errors is a constant, i.e., \( \sigma(z, t) = \sigma_z \). In this case equation (24) simplifies to

\[
\sigma_e(x) = \sigma_z \sqrt{M^{-1}_{ik} \phi_i(x) \phi_k(x)},
\]

yielding to a time-independent standard deviation of the estimate (15). This implies that even for a time-dependent flow we have a simple time-independent indicator field (25) that can be used to measure the quality of the sensor network. More specifically, formula (25) implies that the spectral radius of the matrix \( M^{-1} \) affects the standard deviation of the estimate (15), in the sense that if \( M^{-1} \) has a small spectral radius then we can use a more noisy sensor network and obtain the same level of global uncertainty for the reconstructed field. Hence, the spectral radius of the matrix \( M^{-1} \) depends on the sensor location and it is related to an upper bound for the uncertainty level of the estimate (15).

Figure 14 shows results of standard deviation calculations for different sensor placement strategies. In particular, we compare the original method (Figures 14a–14c) and the modified method (Figures 14d–14f) that imposes the exclusion volume constraint on the sensor placement. We use different numbers of EOF modes, i.e., 4, 6 and 8 modes in both approaches. Our first finding is that the modified method indeed leads to smaller standard deviations. For instance, by comparing the plots in Figures 14a and 14b we notice that the maximum of the standard deviation reduces from 0.19 to 0.16 while its spatial average reduces from

<table>
<thead>
<tr>
<th>Method</th>
<th>4 Modes</th>
<th>6 Modes</th>
<th>8 Modes</th>
</tr>
</thead>
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<tr>
<td>Original method</td>
<td>12.9901</td>
<td>237.1705</td>
<td>1.2059e5</td>
</tr>
<tr>
<td>Modified method</td>
<td>6.6399</td>
<td>19.4194</td>
<td>27.0716</td>
</tr>
</tbody>
</table>

*Results are for total velocity field.

![Figure 15](image_url)

**Figure 15.** Standard deviation of total velocity at the surface of the ocean for noisy sensor networks of configuration Case 1. The measurement standard deviation is in the form \( \sigma_z = \alpha U \), i.e., it is locally dependent on the total velocity. (a and b) Original sensor placement strategy. (c and d) Modified sensor placement strategy. It is seen that sensor networks obtained from the modified procedure with exclusion cylinder radius \( R = 3000 \text{ m} \) significantly reduce the standard deviation of the estimate \( U_e \).
Our second finding shows that the condition number and also the spectral radius of $M^{-1}$ can be used to indicate small or large levels of uncertainty. Table 4 lists the condition number and spectral radius of $M^{-1}$ for the original and the modified methods. In this case, a smaller condition number or smaller spectral radius both lead to smaller standard deviations. We have obtained similar results for the temperature field (not shown here).

### 4.2. Results for Nonuniform Measurement Errors

Next we study a more realistic case where the standard deviation of $\xi(x, t)$ is functionally dependent on the total velocity $U(x, t)$. The simplest case is $\sigma_\xi(x, t) = \alpha U(x, t)$, where $\alpha$ is a positive constant ($U \geq 0$ by construction, see equation (8)). From equation (24) we easily obtain the following analytical expression for the standard deviation of $U_e$:

$$\sigma_{U_e}(x, t) = \alpha U(1, t) \sqrt{M^{-1}_{m,n} \Phi_m(\ell) \Phi_n(\ell) \Phi_f(x) \Phi_k(x)}.$$  \hspace{1cm} (26)

Comparing equation (25) with equation (26) we notice that now the standard deviation of the improved estimate depends on time. We can obtain numerical results by assigning a typical value $\alpha = 0.1$ corresponding to 10% errors in measuring velocity. We can then compute the average and maximum standard deviation of the estimate $U_e$. The results of these calculations are summarized in Figure 15. A comparison between Figures 15a and 15b shows that the maximum standard deviation reduces from 0.11 (original method) to 0.09 (modified method), while the average standard deviation reduces from 0.0219 to 0.0202. Similar conclusions can be drawn by comparing Figures 15c and 15d. In Figure 16 we show the standard deviation obtained by using a different number of sensors and 4 modes; here we consider all three cases reported in the first column of Table 2.

Table 5 reports on the condition number and on the spectral radius of $M^{-1}$ for different sensor networks reported in Table 2.

### 4.3. Point Versus Line Measurements

So far we have used measurements at specific points to reconstruct the velocity and temperature fields instead of measurements in an entire vertical line that can be provided by oceanographic instruments, such as CDT. We have conducted several tests using outputs of FVCOM for the Nantucket Sound and we found that at least for the “mean”
predictions the improvement with the line measurements is less than 1%. Typical results are shown in Figure 17 for 4 and 6 modes reconstruction. However, line measurements help in reducing greatly the uncertainty as shown in the corresponding plots in Figure 18. These results were obtained using 4 modes for reconstruction and 12 sensors while the noise level was at 10% of the local velocity (nonuniform $\sigma_x$).

5. Summary

[35] Proper orthogonal decomposition can be used to analyze the scale hierarchy of the ocean state dynamics but it can also provide good, if not optimum, locations for placing sensors in adaptive sampling. This was demonstrated in previous work of Zhang and Bellingham [2008] and Yildirim et al. [2009], where different optimization criteria were employed. Specifically, the approach of Zhang and Bellingham employs a minimization principle based on the normalized sum of the cross products of the EOF modes while the approach of Yildirim et al. identifies the sensor locations simply as the extrema of the spatial EOF modes.

The simplicity of the latter technique, however, comes at a price since the corresponding sensor network often suffers from redundant information due to the fact that multiple extrema may coexist in a local region, hence creating an oversampling in that region while neglecting equally important dynamics elsewhere in the domain.

[36] In order to make EOF-based sensor placement approaches more effective, we have modified the technique of Yildirim et al. [2009] by imposing a constraint that excludes other sensors to collocate in a cylindrical region surrounding a certain sensor. (Other types of exclusion volumes such as spheres or cubes may be more appropriate for sensor placement in simulations of ocean regions with multiphysics dynamics. In this paper we have chosen the cylindrical exclusion volume because the Nantucket Sound exhibits a negligible vertical stratification due to its rather small depth.)

[37] Our numerical tests suggest that there is an optimum size of volume exclusion but we could not establish a rigorous criterion to determine it a priori as it may be problem dependent. It may be possible that such an optimum size of the exclusion volume is related to an “effective wavelength” of the EOF modes but further work is required to document this hypothesis. In particular, due to the fact that the EOF modes are multidimensional and cannot easily expressed in tensor product form, especially for complex geometry domains, it is not clear how to determine such an effective wavelength. Nevertheless, we found that in all cases we tested any reasonable size of the cylindrical exclusion volume (e.g., a few kilometers) leads to more accurate reconstruction than the original method which does not employ any constraints. For instance, in one particular case we have studied for the Nantucket Sound region, we have found that in order to reduce the reconstruction error to about 4% we would need 48 sensors with the constrained sensor placement algorithm but more than 10,000 sensors with the unconstrained approach of Yildirim et al. [2009].

[38] Another modification, particularly important in data assimilation, is the use of “imperfect” EOF modes. In previous work, we assumed that reconstruction of the field takes place within the time interval for which we have complete knowledge of the EOF modes. In practice, however, in assimilating data we have available EOF modes from previous time steps and new measurements at later times, i.e., outside the interval employed for the computation of the EOF base. Hence, the reconstruction error is much larger due to extrapolation, and in our case it is almost doubled compared with the interpolation error. To this end, we proposed a correction procedure that reduces this error by recalculating the EOF modes and accounting for the new information both on the right- and left-hand side of equation (7). The computational complexity of solving this equation is very low as the rank of the matrix $\mathbf{M}$ is equal to the number of sensors, which is typically small.

[39] Finally, we addressed the issue of uncertainty in the measurements by adding Gaussian noise in the simulation outputs of FVCOM. In particular, we considered two cases: first we assumed that the uncertainty in the measurements is constant everywhere in the domain (i.e., $\sigma_z$ is constant), and secondly we allowed the uncertainty to vary in space and time. In both cases, we derived analytically expressions for the standard deviation of the reconstructed field in terms of the EOF modes and the matrix $\mathbf{M}$. We demonstrated that the
levels of uncertainty in the reconstructed field are lower compared to the reconstruction based on the original method. Lastly, we compared the effect of point measurements versus line measurements (e.g., in a water column using CDT) and we found that there is no much difference in the mean of the reconstructed field but the standard deviation is reduced substantially by performing line measurements.

[40] Taken together the above developments will improve the effectiveness of EOF-based sampling and reconstruction of the ocean state toward the ultimate goal of truly real-time adaptive sampling. However, further testing of this approach is required in regions with diverse dynamics in order to diagnose any limitations and possibly rectify them.

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References


