Quantifying Initial Conditions Uncertainty in the Gulf of Mexico Using Polynomial Chaos Expansions
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Abstract. Polynomial Chaos (PC) methods are used to quantify initial conditions uncertainties in oceanic forecasts of the Gulf of Mexico circulation. Empirical Orthogonal Functions are used as initial conditions perturbations with their modal amplitudes considered as uniformly distributed uncertain random variables. These perturbations impact primarily the Loop Current system and several frontal eddies located in its vicinity. A small ensemble is used to sample the space of the modal amplitudes and to construct a surrogate for the evolution of the model predictions via a non-intrusive Galerkin projection. The analysis of the surrogate yields verification measures for the surrogate’s reliability and statistical information for the model output. A variance analysis indicates

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that the sea surface height predictability in the vicinity of the loop current is limited to 20 days.
1. Introduction

Material transport in the surface ocean is controlled by the combined action of ocean currents, waves and winds [Reed et al., 1999; Hénaff et al., 2012; Curcic and Chen, 2015; Judt et al., 2015]. Modeling material transport, for either risk management or for planning a response to an accidental oil spill, requires oceanic and atmospheric forecasts. The accuracy and usefulness of the transport model thus depends critically on the quality of these forecasts. Unfortunately, atmospheric and oceanic forecasts are inherently uncertain because of uncertainties in the models, and because of uncertainties in their input data such as the model’s initial and boundary conditions, forcing, empirical parameters in subgrid scale models, etc. Useful forecasts should thus include, in addition to the most likely estimates of the environmental conditions, a quantitative assessment of the uncertainties in these forecasts. Policy makers and emergency response managers are then able to consider a range of scenarios and outcomes that reflect the uncertainties in the environmental conditions.

The present article explores the use of Polynomial Chaos (PC) techniques [Ghanem and Spanos, 2002; Najm, 2009; Le Maître and Knio, 2010] to quantify the uncertainties in a HYCOM [Bleck, 2002] forecast of the circulation in the Gulf of Mexico stemming from uncertainties in the model’s initial conditions. The study period extends from May 1 2010 until Jun 30 2010 when the major concern was whether the oil spilled during the Deep Water Horizon accident would be entrained in the Loop Current. This period coincides with a presence of a frontal cyclone that influenced the shedding of Loop Current Eddy Franklin [Kantha, 2014]. The focus of the present article is thus on quantifying the uncertainties in the HYCOM forecast given the uncertainty in the strength and position of the frontal cyclone.
The major distinguishing feature of PC methods is the establishment of a functional relationship between the uncertain input data and the uncertain output. This functional relationship takes the form of a spectral series:

\[
M(x, t, \xi) \approx \sum_{n=0}^{P} \hat{M}_n(x, t) \Psi_n(\xi)
\]

(1)

where \(M(x, t, \xi)\) is a model output that depends on space \(x\), time \(t\) and the uncertain input variables \(\xi\), \(\hat{M}_n(x, t)\) are the series coefficients, and the \(\Psi_n(\xi)\) are suitably chosen basis functions. Different flavors of polynomial chaos methods can be derived depending on the choice of basis functions, and on the method used to determine the coefficients; an overview of these different techniques is presented in Iskandarani et al. [2015]. Here we rely on the Galerkin projection approach [Le Maître and Knio, 2010; Iskandarani et al., 2015]: the basis functions are orthogonal polynomials with respect to the probability density function (pdf) \(\rho(\xi)\) of the uncertain variable:

\[
\langle \Psi_m, \Psi_n \rangle = \int \Psi_m(\xi) \Psi_n(\xi) \rho(\xi) \, d\xi = \delta_{m,n} \|\Psi_m\|^2;
\]

(2)

and the series coefficients are determined by Galerkin projection with the integrals evaluated using numerical quadrature:

\[
\hat{M}_n(x, t) = \frac{\langle M, \Psi_n \rangle}{\|\Psi_n\|^2} \approx \frac{\langle M, \Psi_n \rangle_Q}{\|\Psi_n\|^2} = \frac{1}{\|\Psi_n\|^2} \sum_{q=1}^{Q} M(x, t, \xi_q) \omega_q.
\]

(3)

The \(\xi_q\) and \(\omega_q\) refer to multi-dimensional quadrature roots and weights such as tensorized Gauss quadrature. The evaluation of \(M(x, t, \xi_q)\) in equation 3 requires a model run with the uncertain variable set to specified values.
A PC series thus approximates the response of the model to changes in the uncertain variables $\xi$. The series can be used as a faithful surrogate for the model once the coefficients $M_k$ are known, and forms the basis for the statistical analysis of the model output. The orthogonality of the basis with respect to the probability density function of the input allows the statistical moments of $M$ to be calculated easily: the mean is simply the zero-th coefficient and the variance can be obtained by a weighed sum of the squared coefficients. Furthermore, the approximation properties of spectral series are well-understood: high accuracy can be achieved with few terms when $M$ varies smoothly with $\xi$, whereas the convergence is sub-optimal when $M$ exhibits large localized variations. The accuracy of the series can be monitored simply by inspecting the decay of the highest degree coefficients: power at the high end of the spectrum is indicative of low accuracy and missing variance.

PC methods for Uncertainty Quantification (UQ) present several advantages as their formulation combines probabilistic and approximations paradigms. First, PC methods can be implemented non-intrusively and in an ensemble fashion so that no modification of the forward model is needed. Second, the approximation error of the surrogate can be monitored to ascertain whether enough sampling has been performed to gain confidence in the results. Third, the PC approach does not impose restrictions on the output statistics or on the linearity of the forward model. It does, however, require the user to specify a distribution for the input uncertainties (the weight function appearing in the inner product 2) even though these pdfs are generally not well-known from observations; users must exercise judgement and use sensible distributions. It is worth noting that most traditional UQ in ocean and atmospheric models assume a representation for the output statistics (commonly Gaussian distributions), and are not really concerned
with representing the response surface itself (the problem of specifying the input uncertainty pdf is common to all UQ approaches whether based on PC polynomials or not.).

The functional nature of PC methods requires the association of an input uncertainty with a continuous random variable. This is easy enough to do with scalar quantities, but is more complicated for field quantities such as the model’s initial conditions. The initial conditions consist of the model state vector whose components can conceivably be varied independently. This would represent an uncertainty space with dimension in the millions for high resolution models; its exploration via quadrature sampling is computationally intractable and alternative approaches are required.

The state vector components are not independent and are linked by various dynamical relationships and constraints. This inter-dependency allows us to identify field uncertainties with variability modes. The uncertainties can then be decomposed into modes and the components of the uncertain variable $\xi$ can be associated with the amplitude of these modes. Furthermore, the Karahunen-Loève decomposition theorem provides the theoretical underpinnings for this modal decomposition; its discrete counterpart is the Empirical Orthogonal Function (EOF) decomposition. The modal decomposition provides a reasonable and practical pathway to “compress” uncertainties in a field to a few random variables.

In the following sections we illustrate the application of the PC approach to quantify the uncertainties in the HYCOM forecast caused by uncertainties in the initial conditions. We focus primarily on the implementation of the uncertainty analysis and refer the reader to Iskandarani et al. [2015] for the description of the PC methodology. Section 2 describes the construction of EOF perturbations designed to target uncertainties associated with Loop Current frontal dynamics; it also describes the PC-ensemble used to compute the series coefficients. Section 3 presents
the results of the forward propagation of the model uncertainty, and verifies the validity of the PC surrogate for various model outputs as they evolve in time. We conclude with a summary and a discussion section.

2. EOF analysis and PC perturbations

Our interest is focused primarily on uncertainties associated with the Loop Current (LC) and Loop Current Eddies (LCE) for short time-scale forecasts (2-3 weeks). The variability modes were thus obtained from a multivariate EOF analysis of a 14-day, data-assimilating HYCOM [Chassignet et al., 2007] time series. This relatively short series maximizes the probability of picking up spatially and temporally localized perturbations to the HYCOM initial conditions that can be associated with the dominant dynamical features in the basin, namely the Loop Current and its frontal eddies [Oey et al., 2005; Leben, 2005]. Furthermore, the small time window minimized the interference of basin-wide modes that could have leaked into the EOF analysis had a longer series been used. Figure 1 shows the SSH spatial patterns of the first two EOF modes. The first EOF mode is localized in the Loop Current region and seems to be associated with the presence of a frontal eddy. The second mode also has a signature in the same region and can be associated with variability emanating from a Loop Current Eddy (southwest of the Loop Current region). The first and second modes explain 35% and 15% of the variance, respectively. Figure 2 shows a vertical slice of the temperature perturbation one day after the start of the simulation. The perturbation exhibits a temperature anomaly of -2.5°C in the vicinity of the cyclone which extends to about 400 m depth. A separate warm anomaly on the western edge of the loop current at 100 m can also be discerned. Again, these anomalies seem to be localized in space and reflective of perturbations to Loop Current dynamics.
The two dominant EOF modes identified above were multiplied by two independent stochastic variables, $\xi_{1,2}$, and added to the mean fields to perturb the initial conditions. For example, the initial layer thicknesses are given by:

$$\delta p(x,0,\xi_1,\xi_2) = \delta p^{(0)} + \alpha \left[ \xi_1 \sqrt{\lambda_1} \delta p^{(1)} + \xi_2 \sqrt{\lambda_2} \delta p^{(2)} \right]$$

(4)

where $\delta p^{(i)}$ and $\lambda_i$ refer to the $i$-th EOF mode and corresponding eigenvalue for $i > 0$, and for $i = 0$ refers to the unperturbed layer thickness; $\alpha$ is a multiplicative factor introduced to control the size of the “kick” to the initial conditions (and set to 1 for the experiments shown in the following sections). The uncertain input variable consists of the two-dimensional vector $\xi = (\xi_1, \xi_2)^T$; additional variability modes could be added but at the expense of increasing the dimension of the uncertain parameter space. Here we limit ourselves to 2 modes to keep the computational load small for this exploratory study.

The uncertain modal amplitude are assumed to be uniformly distributed in the range $|\xi_i| \leq 1$; thus $\rho(\xi_1,\xi_2) = \left( \frac{1}{2} \right)^2$. The basis functions are then products of Legendre polynomials $\Psi_k(\xi) = P_m(\xi_1)P_n(\xi_2)$ [Le Maître and Knio, 2010]. The highest polynomial order is set to 6 and the series is truncated in a triangular fashion so that $\max(m + n) \leq 6$ as shown in the right panel of figure 3; a total of 28 coefficients needed to be determined. The integrals of the Galerkin projection in equation 3 are evaluated using tensorized Gauss-Legendre quadrature rules of order 7 in each dimension; they hence require a total of 49 realizations. The location of the quadrature roots in the uncertainty space is shown in figure 3; notice that these roots cluster near the end of the interval to maximize the accuracy of the approximation and integration.

3. Uncertainty analysis
The HYCOM configuration used to produce the PC quadrature ensemble is the US Navy operational configuration with its $1/25^{\circ}$ horizontal resolution and 20 vertical levels. The computational domain is open along portions of its southern, eastern and northern boundaries, where values are provided by a lower-resolution $1/12^{\circ}$ HYCOM configured for the Atlantic Ocean [Chassignet et al., 2007]. The model is forced at the surface by 3-hourly outputs from the Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMP Hodur [1997]), which has 27-km resolution. The output of the 49 HYCOM ensemble was saved daily and the uncertainty analysis is performed as a post-processing operation. Although the uncertainty analysis can be performed on any model output desired, here we focus on analysing the uncertainties in Sea Surface Heigh (SSH) and on temperature along a vertical section at $25^\circ$ N. This analysis consists of establishing the validity of the PC surrogates, and on calculating the mean and standard deviation of SSH and temperature.

### 3.1. The quadrature ensemble

Figure 4 shows the SSH evolution for the circled samples in figure 3, as well as the ensemble mean. The SSH contours support the association of the perturbations with the frontal eddy’s strength on day 1, where it is clearly suppressed in the negative perturbations (1,1) and strengthened in the positive perturbation (7,7). An eddy shedding event is recorded for all three realizations but with differing timing: the shedding occurs earlier for realizations associated with a stronger frontal eddy than for those associated with a weaker one. The ensemble mean of the SSH field reveal similar Loop Current dynamics: a northerly extended current cleaved by a frontal eddy, for the first 40 days; the 60-th day snapshot shows a diffused LC and LC eddy as a result of the algebraic averaging of differing LC states. Figure 5 shows the Loop Current edge for all 49 realizations superimposed on the PC-mean SSH. At day 20 all realizations show an
attached eddy, however, those with the strong frontal eddy show an imminent detachment about
to occur while the one with the weak frontal eddy exhibits only the onset of LC necking. The
day 40 snapshot show realizations where the LC has already shed its eddy and has moved to a
retracted position, while others are still in the middle of the shedding process. The mean SSH
on day 40 shows a large detached eddy and a retracted LC. All realizations exhibit a LC eddy
with the LC in retracted or retracting state. The diffused mean SSH in figure 4 is mostly due to
varying eddy location among the ensemble members.

In order to ascertain whether the PC ensemble reflects realistic estimates of the uncertainty in
SSH, we compare in figure 6 the uncertainty in the location of the Loop Current edge [Leben,
2005] to its observed location as estimated from AVISO altimeter data. The AVISO estimate
falls within the envelope of the possible states predicted by the PC ensemble throughout the
60 day period of the experiment. The EOF decomposition and the PC analysis seem to have
captured initial conditions perturbations that are consistent with observed oceanic states.

Figure 7 shows the temperature and salt profiles at the Deep Water Horizon (DWH) site for
the unperturbed solution as well as for the most extreme perturbations. Here the EOF based per-
turbations show only a very small impact on the local temperature at early times and a slightly
larger impact on the surface salt concentration. In both cases the perturbations impact is felt
only indirectly, when perturbations emanating from the LC region have had time to propagate
to the DWH site. This illustrates the large influence that the choice of initial perturbations plays
in determining the ensuing uncertainty, and that their design must be informed by the intended
objective of the uncertainty analysis. If the intended target is the to characterize the uncer-
tainty around the DWH site than either a localized EOF analysis needs to be undertaken and/or
additional sources of uncertainty must be included, such as wind stress forcing.
3.2. Verification of the Surrogate

We first attempt to establish the accuracy of the polynomial series before analyzing it for its statistical content. To this end we define the PC error as the difference between an actual model realization, $\eta(x, t, \xi_r)$, and its PC representation, $\eta_{PC}(x, t, \xi_r)$:

$$\epsilon(x, t, \xi_r) = M(x, t, \xi_q) - M_{PC}(x, t, \xi_r)$$  \hspace{1cm} (5)

Ideally one would used different realizations for the error verification than the ones used for quadrature. This is however expensive as it requires additional model realizations. Instead, we opt to re-use the quadrature runs for verification. This allows us to define an error metrics across all realizations:

$$\|\epsilon\|^2_2 = \int \epsilon^2 \, d\xi \approx \int [M(x, t, \xi_q) - M_{PC}(x, t, \xi_q)]^2 \omega_q$$  \hspace{1cm} (6)

Figure 8 illustrate the evolution of the PC-error for the SSH field. The errors remain below the level of 2 cm for the first twenty days over the entire Gulf of Mexico. At day 40 the PC-error exhibit local maxima of about 5-6 cm in the general vicinity of the LC region, and a global maximum of about 10 cm in the LC pinch-off region. By day 60 the PC-error in SSH has reached levels of about 15 cm in the LC region and the maximum error levels have spread to a wider area. A similar pattern can be discerned for a temperature section along 25N (which coincides with the general location of the frontal eddy). The errors are initially primarily located near the eastern and western edges of the Loop current. At day 10 the errors peak at less than 0.5°C, reach the 0.8°C range at day 20, and exceed the 2°C mark by day 60. The regions of high errors increase with time as well and end-up occupying the entire depth range between 200 and 400 m depth. The evaluation of whether the error levels are tolerable to perform an uncertainty
analysis will be deferred until section 3.3 when estimates of the variance in the model outputs are examined.

### 3.3. Statistical moments of PC-series

The mean of the model fields (w.r.t. the uncertain variables) can be obtained by evaluating the integral:

\[
E[M(x, t)] = \int M(x, t, \xi) \rho(\xi) d\xi = \left\langle \sum_{n=0}^{P} \hat{M}_n \psi_n, \psi_0 \right\rangle = \hat{M}_0 \|\psi_0\|^2\]

(7)

where the last equality follows from the orthogonality of the basis functions. If the basis functions are normalized so that \(\|\psi_0\| = 1\), the mean becomes simply the series zero-th coefficient.

The PC-mean SSH field is shown in the last column of figure 4.

The variance of the \(M\)-field can be shown to be:

\[
\text{var}[M(x, t)] = E\left[ (M - E[M])^2 \right] = \sum_{n=1}^{P} \hat{M}_n^2 \|\psi_n\|^2.
\]

(8)

Figure 8 presents the evolution of the PC-based standard deviation (among ensemble members) as a measure of the uncertainty in SSH. The initial uncertainty is of the order of a few centimeters and its maximum seems to be associated with the frontal eddy strength. This maximum grows to about 28 cm by day 20 when the frontal eddy is cleaving the LC. Multiple maxima appear in the day 40 snapshots reflecting that some realizations have already shed their eddies while others still exhibit an extended LC; interestingly the largest maximum occurs in the southwestern corner of the LC edge.

Figure 9 shows the evolution of the temperature standard deviation at a vertical section along 25N. The initial conditions perturbations exhibit peaks at a depth of 100 m in the vicinity of the frontal eddy (to the east) and near the western edge of the LC with amplitudes of about 1.2 and
2.4° C, respectively. The eastern peak grows rapidly to 4° C in the first 10 days and its depth
range at day 10 extends from the near surface down to about 400 m; at day 40 the uncertainty
spreads laterally to occupy a larger region (this large standard deviation of the temperature is
probably caused by the frontal eddy occupying different positions in each realization). By day
60 the peak of the temperature standard deviation exceeds 2.4° C, and the region of high standard
deviation has expanded to occupy the entire section between 90W and 85W from the surface
down to a depth of 400 meters. The western temperature uncertainty peak grows spatially at a
lower rate while maintaining an amplitude of about 1.4° C.

The variance calculation requires summing the square of the series of coefficients; hence
premature truncation of the PC-series will result in an underestimation of the variance. It is thus
essential that the PC-error remain small in order to gain confidence in the series estimates of the
statistical moments. In the case of the SSH field for example, the PC-error at day 60 reaches 15
cm whereas the estimated standard deviation is 40 cm; the PC-error is thus about 38% of the
standard deviation on that day. A similar trend can be seen for the temperature section where
the error estimate remain low (compared to the standard deviation for the first 40 days). By
day 60 however, the peak errors are about 50% of the estimated standard deviation and hence
there is little confidence in the day 60 results. Improvements in the surrogate’s approximation
properties requires a longer series than the one truncated at sixth degree polynomials, along
with an increase in the ensemble size in order to determine the additional coefficients.

The relatively long record of AVISO altimetry data allows us to calculate the standard devia-
tion of the SSH climatology, and subsequently to estimate the predictability limit of the present
ensemble since the predictability limit can be defined as the ratio of the forecast standard devi-
ation to that of the climatology’s. The AVISO standard deviation (figure 10) exhibits a broad
peak in the central portion of the region where the LC is active of about 35 cm. The right panels of figure 10) show regions where the ratio of the forecast standard deviation to that of the climatology for the different days. The magenta lines show areas where the ratio exceeds unity, and where the predictability limit has been lost. The predictability limit is reached fastest in the LC pinch-off area (day 20) and manifests itself later for the northern frontal LC region (between days 20 and 40).

The availability of the PC series permits the calculation of the covariance between different fields. Figures 11 shows the covariance between the SSH at the point marked by a white dot and the GOM SSH, and between that point SSH value and the temperature field along the vertical cross section. Note that the covariances peak in the neighborhood of the point SSH and decay fairly quickly away from it; furthermore the SSH-temperature covariance has a natural expression in the vertical. The covariance information can be useful for implementing PC-based data assimilation system where the ensemble covariance matrix is estimated via the PC-series.

Finally the orthogonality of the PC basis allows us to isolate the contribution of each term in the series to the total variance, and thus to assess the degree to which one uncertain variable contributes to the total variance, or whether the interaction of the two uncertainties leads to further growth in the model uncertainty. The left panel of figure 12 shows the SSH variance over the Deep Eastern part is dominated by the amplitude of the first modal perturbation which contributed about 3/4 and 2/3 of the total variance at day 20 and 40, respectively; the second perturbation mode contribution, on the other hand, starts very small, grows with time in tandem with that of the interaction terms and provides the remaining variance. The right panel of figure 12 shows the contributions of the different (total) polynomial degrees to the total variance; it is thus a measure of the magnitude of the PC coefficients and consequently of the accuracy of the
PC series. The figures show the magnitude of the highest (6-th degree) PC coefficients to be small but growing in time; by day 50 the 6-th degree polynomials produce a larger contribution to the variance than the other polynomial degrees except the first. This is another indication that the accuracy of the series has deteriorated and that statistics estimated beyond day 40 are not robust.

4. Discussion and Summary

The present article has presented a PC-based approach to quantify the uncertainties in a HYCOM forecast of the circulation in the Gulf of Mexico caused by uncertainties in the model’s initial conditions. The ingredients of this approach consist of first identifying variability modes of the system, second identifying the uncertain stochastic variables as the amplitudes of these modes and assigning them a probability density function, thirdly constructing surrogate series of specific model outputs using an ensemble of simulations, fourthly establishing the validity of the surrogate by monitoring its approximation errors, and finally analyzing the resulting surrogate series for statistical information.

In the present instance the variability modes were obtained through an EOF decomposition of a multi-variate 14-days time series that specifically targeted the LC frontal dynamics; only two variability modes were retained in the present experiment. Analysis of the evolution of the LC eddy reveals that the two modes identified perturb the strength of the frontal eddy and, consequently, the evolution of the LC system. Comparison of the ensemble estimates of the LC location to that obtained from altimetry indicate that the perturbation reflect “realistic” uncertainties and that the PC approach has produced reasonable forecasts for the future location of the LC. Comparison to additional observations should be performed to ascertain whether other model outputs behave similarly. Furthermore, the approximation errors for the PC series were
monitored: the 6-th degree polynomial series remained accurate for the first 20 days of the sim-
ulation for both SSH and temperature, remained acceptable between days 20 and 40 and started
to deteriorate quickly after that. The peak errors were located in dynamically active regions,
particularly in the vicinity of the LC detachment. Improvements to the series accuracy would
require a higher polynomial truncation than sixth and would demand a larger quadrature ensem-
ble. This extra cost however, has to be offset against the need to consider additional sources of
uncertainty, such as adding additional perturbations to the initial conditions or by considering
wind forcing uncertainties for example. The examination of the variance contributed by each
mode hints that adding higher EOFs modes to the initial condition perturbations would not alter
the variance estimates much, and that accounting for additional uncertainties would be more
useful.

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References
Bleck, R. (2002), An oceanic general circulation model framed in hybrid isopycnic cartesian
Chassignet, E. P., H. E. Hurlburt, O. M. Smedstad, G. R. Halliwell, P. J. Hogan, A. J. Wallcraft,
R. Baraille, and R. Bleck (2007), The HYCOM (HYbrid Coordinate Ocean Model) data


Figure 1. SSH patterns for mode 1 and 2 perturbations (left and center) along with the cumulative variance explained by the first 10 modes.

Figure 2. Vertical slice along 26.4N showing the temperature perturbations one day after the start of the simulation. The first mode shows a strong 2.5°C cooling in the vicinity of the frontal cyclones. The ”warm” perturbation around 90W is at the southern edge of a small anticyclone NW of the LC.
Figure 3. Left: Gauss Legendre quadrature (sample) points in the uncertain $\xi_1 - \xi_2$ space; the center red circle shows the unperturbed run, while the blue circles correspond to the largest negative and positive perturbations. Right: the polynomial degree in $\xi_1$ and $\xi_2$ retained in the series.
Figure 4. Time evolution of SSH realization (1,1) (first column) with weakest frontal eddy; of unperturbed realization (4,4) (second column) revealing a medium strength frontal eddy; and realization (7,7) (3rd column) with strongest frontal eddy. The 4th column shows the PC-ensemble mean of all 49 realizations, aka the 0-th mode of the PC-series. The times shown are in days since the start of the simulation, and SSH units are in cm.
Figure 5. Loop Current evolution for all realizations. The thin magenta contours are the PC-mean of the SSH field, while the thick lines indicate the LC edge as defined by the 17 cm contour. The blueish thick lines are associated with the strong frontal eddy realizations whereas the redish ones are associated with the weak frontal eddy.
Figure 6. Time evolution of the SSH anomaly showing Loop current edge, as defined by the 17 cm contour, in the PC ensemble (black lines) and in the AVISO altimeter (white line).

Figure 7. Temperature (left) and salt (right) profiles at the DWH for the reference and extreme perturbations.
Figure 8. Left panel: Temporal evolution and spatial distribution of the PC error, $\|\epsilon\|$ (shown in cm), associated with SSH. The errors grow in time with their maxima located primarily in the dynamically active LC region. Right panel: Evolution of SSH stddev (in cm) as estimated from the PC-series; the areas of largest uncertainties are located in the LC region.
Figure 9. The left panel shows the evolution of the PC-error associated with the temperature field along 25°N; the errors build up gradually with time and exceed 2°C by day 60 in the 200-400 m depth range. The right panel shows the evolution of the temperature standard deviation with the uncertainty manifesting itself primarily on the easter side of the loop current. On day 60 the PC-error is about 50% of standard deviation.
Figure 10. Predictability Limit: The left panel shows the climatological SSH standard deviation as inferred from AVISO. The right panel shows the evolution of the partial distribution of the ratio of the forecast standard deviation to climatology standard deviation for SSH (from AVISO).
Figure 11. Covariances between one value of SSH (white dot circled in black) and the GoM SSH, and between the same SSH value and the vertical temperature along the longitude line indicated on the left figure. The SSH point location is marked on the section with dashed line. The units are m$^2$ and m $^\circ$C.

Figure 12. Left: Evolution of the SSH variance over the Deep Eastern part of the GoM as contributed by the two modal perturbations and their interaction. Right contribution to the SSH variance over the deep Easter GoM by the different polynomial orders. The thick black lines shows the total variance whereas the thin black lines shows the contribution to the variance injected by the different polynomial orders.