Surrogate based approaches to parameter inference in ocean models*

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Outline

- Uncertainty quantification framework
  - Polynomial Chaos formalism
  - Surrogates via non-intrusive spectral projection, regression

- Bayesian inference of physical parameters
  - Markov-Chain Monte Carlo
  - Surrogate-based optimization

- Applications
  - Bottom friction
  - Internal friction
  - Initial conditions and wind forcing

- Concluding remarks
Outline

- **Uncertainty quantification framework**
  - Polynomial Chaos formalism
  - Surrogates via non-intrusive spectral projection, regression

- **Bayesian inference of physical parameters**
  - Markov-Chain Monte Carlo
  - Surrogate-based optimization

- **[real-world] Applications**
  - Bottom friction  [Coastal risk]
  - Internal friction  [Climate]
  - Initial conditions and wind forcing  [Assimilation, UAV]

- Concluding remarks
Spectral approach to UQ

Probabilistic approach to UQ

Stochastic solution is sought in a product space

- probability space (x axis)
- deterministic solution space (y axis)
- both are assumed to have Hilbert space structure, with a countable orthogonal basis
Spectral representation

- mean-square convergent expansion in the space of random variables:

\[ u(x, t; \xi) = \sum_k u_k(x, t) \Psi_k(\xi) \]

- solution mode
- vector of canonical random variables that are suitably used to parametrize the uncertain inputs
- orthogonal basis in the space of square integrable random functions
- solution mode (coordinate in Hilbert space) is unknown to be determined
Non-Intrusive Spectral Projection (NISP)

- Alternative to Galerkin formalism in situations where modification of production or legacy codes is not feasible
- Essentially amounts to a collocation approach to the evaluation of probability integrals

\[
\langle \Psi_k^2 \rangle Q_k = \langle Q(\xi) \Psi_k(\xi) \rangle \approx \sum_{i=1}^{N} Q(x_i)w_i
\]
Sparse quadrature

- Smolyak/Gauss Patterson
  - non-adaptive
  - nested grid
  - level p resolution \(\sim\) yields order p PC

- Adaptive extension
  - variance-based error indicators
  - “optimal” pseudo-spectral construction

- Both approaches well suited to moderate dimensionality
Adaptive refinement

Greedy algorithm that seeks terms that contribute most to $\| \tilde{f} \|_2^2$

- pick index with highest indicator
- add all admissible forward neighbors
- repeat until stopping criterion is reached
Bayesian inference

- Application of Bayes rule

\[ p(H|T) \propto p(T|H) \ p(H) \]

using model surrogate.

- Enables straightforward implementation of MCMC algorithm
  - avoids tens of thousands of forward model runs needed for convergence

- Yields full posterior distribution of parameters
Adjoint based formalism

- Going back to Bayes rule

\[
p(\theta, \sigma^2|T) \propto \prod_{i=1}^{N} \left[ \frac{1}{\sqrt{2\pi v_i^2}} \exp \left( \frac{-(M_i - T_i)^2}{2v_i^2} \right) \right] p(\theta, \sigma^2)
\]

- Taking logarithm

\[
\mathcal{L}(\theta, \sigma^2) = \sum_{i=1}^{N} \left[ \frac{(M_i - T_i)^2}{2v_i^2} + \frac{1}{2} \ln(2\pi v_i^2) \right]
\]

\[
- \sum_{d=1}^{D} \ln(p(\sigma_d^2)) - \ln(p(\alpha)) - \ln(p(V_{\text{max}})) - \ln(p(m))
\]

- Both Adjoint and Hessian can be readily evaluated
Parameters and hyper parameters can be found by minimizing cost functional:

\[ \mathcal{J}(\theta, \sigma^2) = \frac{1}{2} (M - T)^T R^{-1} (M - T) + \frac{1}{2} \ln |R| + \ln |S| \]

where \(R\) is a diagonal observation error covariance matrix and \(S\) is a diagonal matrix with entries given by the variances.
Derivatives of the cost function take the form:

\[
\begin{align*}
\partial_\theta \mathcal{J}(\theta, \sigma^2) &= A^T R^{-1} (M - T) \\
\partial_{\sigma^2} \mathcal{J}(\theta, \sigma^2) &= \frac{1}{2} (M - T)^T \frac{\partial R^{-1}}{\partial \sigma^2} (M - T) + \frac{1}{2} \{\text{Tr}(R_d^{-1})\}_{d=1}^D + \sigma^{-2}
\end{align*}
\]

\[
H(\theta, \sigma^2) = \partial^2 \mathcal{J} = \begin{bmatrix}
\partial_{\theta,\theta}^2 \mathcal{J} & \partial_{\theta,\sigma^2}^2 \mathcal{J} \\
\partial_{\sigma^2,\theta}^2 \mathcal{J} & \partial_{\sigma^2,\sigma^2}^2 \mathcal{J}
\end{bmatrix}
\]

Solution can be readily found using line search algorithm

Assuming locally symmetric (Gaussian-like) distribution, Hessian at minimum provides estimate of the spread of optimal parameters
Application – I

- Inference of bottom friction coefficient based on Tsunami (Tōhoku) data
Goal

- **Geoclaw model:**
  - 2D shallow water equations
  - Bottom friction parametrized in terms of Manning coefficient
  - Three regions: (i) near shore region, (ii) near-shore region, and (iii) deepwater region
- Inference of bottom friction coefficient based on DART buoy data
Setup

- Bathymetry: combination of 4’ and 1’ ETOPO data
- Earthquake model from Ammon (2011)
- Initial comparison based on default values $n_i = 0.025$
- Reasonable agreement but somewhat large scatter

Scatter plot of surface elevation. Simulations are plotted against DART buoy observations. Standard deviations are shown in the legend.
Prior and Likelihood Model

- Uniform iid prior for Manning’s coefficients:
  
  \[ 0.005 = n_{\text{min}} \leq n_i \leq n_{\text{max}} = 0.2 \]

- Gaussian independent error model: \( \epsilon_i = \mathcal{N}(0, \sigma^2) \)

- Jeffrey’s prior for hyperparameter:
  
  \[ q(\sigma^2) = \begin{cases} \frac{1}{\sigma^2} & \text{for } \sigma > 0 \\ 0 & \text{otherwise} \end{cases} \]

- Likelihood:
  
  \[
  L(\eta^a | n) = \frac{1}{\sqrt{2\pi\sigma^2}} \prod_i \exp \left[ -\frac{(\eta_i^a - G_i(n))^2}{2\sigma^2} \right]
  \]

  \( \eta^a \): vector of observations; \( G(n) \): model runs
PC surrogate

- Fully tensorized Gauss quadrature (4th order; 5 points along each dimension; d=3)

Fig. 4. Relative normalized error between realizations and the corresponding PC surrogates at different gauge locations calculated using Eq.(19).

Fig. 5. pdf of water surface elevation at the different gauge locations at t=7200 s.
Field variability – I
Field variability – II

Note that the evolution shown starts at $t = 6000$ s when the uncertainty becomes significant. An interesting observation is that the standard deviation in water surface elevations waxes and wanes as the tsunami evolves. The narrowing of the variance at these instances is possibly associated with the waves that arrive due to reflections from a single source and then move away from the gauge location, and thus cause no variance in the water surface elevation.

The predicted mean water surface elevation and its standard deviation can be used for comparison with the (DART) buoy observations collected during the tsunami event. Fig. 6 plots the PC mean water surface elevation with the observed water surface elevation at different gauge locations.

Fig. 7. Comparison of PC mean and observed DART data of water surface elevation with time at the four gauges.
Total sensitivity

Fig. 9. PC mean (top row) and standard deviation (bottom row) of the water surface elevation at different times.

Fig. 10. Total sensitivity index of different input parameters.
Marginal posteriors - coefficients

Next, the computed MCMC chains are used to determine the marginalized posterior distributions using kernel density estimation (KDE) (Parzen et al., 1962; Silverman et al., 1986). The resulting marginalized posterior pdfs of the three Manning’s \( n \) coefficients \( n_1; n_2; n_3 \) are shown in Fig. 14 (top row). Note that the first 2/10^5 iterations, associated with the burn-in period, were discarded. As expected from the chains shown in Fig. 13, the marginalized posterior pdfs of \( n_1 \) appear to be fairly flat, and similar to the uniform prior; an indication that the observed data were not informative to refine our prior knowledge for \( n_1 \). In contrast, the posterior pdf of \( n_2 \) exhibits a well-defined peak, with a Maximum A Posteriori (MAP) estimate of around 0.011 and an extended tail towards the larger Manning’s \( n \) coefficient values.

For \( n_3 \), we observe a posterior that has a well defined peak of 0.18 but no clear pdf shape. The posterior distributions of the noise variances are also shown in Fig. 14 (bottom row) at selected

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Fig. 14. KDE of the marginalized posterior distributions for the three Manning’s \( n \) coefficients \( P(n_1); P(n_2) \) and \( P(n_3) \) (top row), and for the noise variance \( P(r_2^2); P(r_2^2); P(r_3^2) \) at gauges 21401, 21413 and 21418, respectively (bottom row).

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Fig. 15. Comparison of prior and posterior water surface elevation at different gauges.
Marginal posteriors – water elevation

Next, the computed MCMC chains are used to determine the marginalized posterior distributions using kernel density estimation (KDE) (Parzen et al., 1962; Silverman et al., 1986). The resulting marginalized posterior pdfs of the three Manning’s #1; #2; #3 are shown in Fig. 14 (top row). Note that the first 2/10 iterations, associated with the burn-in period, were discarded. As expected from the chains shown in Fig. 13, the marginalized posterior pdfs of #1 appear to be fairly flat, and similar to the uniform prior; an indication that the observed data were not informative to refine our prior knowledge for #1. In contrast, the posterior pdf of #2 exhibits a well-defined peak, with a Maximum A Posteriori (MAP) estimate of around 0.011 and an extended tail towards the larger Manning’s # coefficient values. For #3, we observe a posterior that has a well defined peak of 0.18 but no clear pdf shape. The posterior distributions of the noise variances are also shown in Fig. 14 (bottom row) at selected gauges. 

Fig. 14. KDE of the marginalized posterior distributions for the three Manning’s # coefficients # and # at gauges 21401, 21413 and 21418, respectively (bottom row). 

Fig. 15. Comparison of prior and posterior water surface elevation at different gauges.
Remarks – I

- Surface elevations are most sensitive to $n_2$ which has the most peaked MAP value. Although the MAP value was lower than expected, the tail includes the most commonly used values (0.022–0.025).

- The deep-water value $n_3$ has a peak that is much higher than expected but a tail that does not taper off particularly quickly. This is due to the low sensitivity of $\eta$ to this region’s friction.

- The simulations and observations are insensitive to $n_1$ in present setting.

- Use of DART buoy observations only (and relatively coarse bathymetry is not sufficiently informative to invert for the Manning’s $n$ values with strong confidence, outside of the near-shore region.
Remarks – II

Current focus:
- Real-time assimilation (source inversion) and risk forecast
- Emphasis on adaptive meshes (needed for efficiency)

Challenges:
- Mesh error – particularly as it relates to assimilation [in a context where data is scarce]
- UQ/inference on adaptive meshes
Application – II

- Focus: calibrate K-profile parametrization in MIT General Circulation Model of tropical Pacific
- KPP model relies on a number of parameters based on a combination of theory, lab experiments, and atmospheric/oceanic boundary layer observations
- Goal: to quantify impact of parametric uncertainties in a regime resolving the chaotic dynamics
- Challenge: definition of suitable QoIs in turbulent multi-scale flow
Setup and Data Source

TOGA mooring array:
- Temperature, salinity, and horizontal current components
- Data range: November 2003 – November 2007
Raw (top), and band pass filtered (bottom), 10-day time series of wind stress (red), and sea surface temperature (blue) observations (solid) and model output (dotted) at buoy 2°N 125°W.

Qol: correlation between stress and SST
## KPP – uncertain parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Parameter Name</th>
<th>Symbol</th>
<th>Default Value</th>
<th>Uniform Prior $[a,b]$</th>
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<tr>
<td>$p_1$</td>
<td>Critical Bulk Richardson number</td>
<td>$R_{ic}$</td>
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<td>[0.1, 1.0]</td>
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<tr>
<td>$p_2$</td>
<td>Critical gradient Richardson number</td>
<td>$R_{ig}$</td>
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<td>$\varphi_{m,unst}$</td>
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<td>[3.60, 331.06]</td>
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<tr>
<td>$p_4$</td>
<td>Structure function, unstable forcing, tracer</td>
<td>$\varphi_{s,unst}$</td>
<td>16</td>
<td>[7.77, 67.02]</td>
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<tr>
<td>$p_5$</td>
<td>Nonlocal transport</td>
<td>$C^*$</td>
<td>10.0</td>
<td>[5.0, 15.0]</td>
</tr>
</tbody>
</table>
Forward Model

- Simulations performed using MIT GCM:
  - 1/3° resolution; 1 day time step
  - Time period 2004 – 2007
  - 22 hours on a 256-node cluster for a single forward run

- Isotropic Smolyak grid in 5 dimensions:
  - Uncertain parameters are represented in terms of iid uniforms
  - Level 5 sparse grid
  - 903 independent realizations

- With direct quadrature approach, database supports determination of PC coefficients up to order $r = 5$
Direct projection

2D projection of Smolyak quadrature nodes

PC spectrum via “direct” spectral projection
QoI behavior

Test statistic from MITGCM model runs when varying $Ri_c$ only infinitesimally
$l_1$ regression

$$\mathcal{O}_{1,\text{delta}} \simeq \{ \arg \min_{\mathbf{e}} \| \mathbf{e} \|_1 : \| E - \Psi \mathbf{e} \|_2 \leq \delta \}$$

- Optimal regression problem
- CS approach that seeks to minimize non-zero entries of coefficient vector, $\mathbf{e}$
- $E : \text{QoI vector}$
- $\delta = 0 : \text{Basis Pursuit algorithm}$
- $\delta \neq 0 : \text{Basis Pursuit De-Noising (BPDN)}$.
  - $d$ is a reflection of noise level and is itself optimized
  - function of data noise and resolution
PC regression – I

- FIG. 7. PC expansion normalized coefficients $|e_k/e_0|$ for PC order up to $r=5$. The dashed vertical lines separate the PC expansion terms into degrees. The coefficients were calculated using BPDN.

- FIG. 8. pdfs of test statistic $E$ with increasing order of PC constructed using BPDN-estimated PC surrogate model.
FIG. 9. Comparing test statistic \((E)\) from MITGCM model runs with their PC surrogate counterparts (Left) Superimposed (Right) Scatter plot. The shown cases correspond to the sparse quadrature and PC is constructed using BPDN. The normalized relative error (NRE) is also indicated.

\[
\text{NRE} \equiv \frac{\left( \sum_{q=1}^{Q} \left| E(\xi_q) - \sum_{k=1}^{R} e_k \Psi_k(\xi_q) \right|^2 \right)^{1/2}}{\left( \sum_{q=1}^{Q} |E(\xi_q)|^2 \right)^{1/2}}
\]
FIG. 12. Comparing test statistic ($E$) from MITGCM model runs with their PC surrogate counterparts (Left) Superimposed (Right) Scatter plot. The shown cases correspond to the independent random sample and PC is constructed using BPDN. The relative normalized error (NRE) is also indicated.

regression performed on random sample
Nominal response and effect of resolution

Response curves of test statistic function of different parameters. For each curve, the other four parameters are set to $\xi_j = 0$. Normalized relative error using different number of nodes corresponding to different Smolyak levels of refinement.
Marginal posteriors – I

\[ T = 0.6907 \]

\[ T = 0.1405 \]
Marginal posteriors – II

\[ T = 0.2079 \]

\[ T = 0.0472 \]

\[ T = 0.0784 \]
Remarks

- Despite careful analysis in defining proper QoIs, complex model response precluded application of quadrature methods.
- Challenge effectively addressed through $l_1$-regularized CS approach.
- Current focus:
  - Inference of all 9 KPP parameters.
- Challenges:
  - Larger databases.
  - More efficient sampling strategies.
Goal: Quantifying initial condition and wind forcing uncertainty in the GOM

Setup:
- Hybrid Coordinate Ocean Model (HYCOM)
- 4-km resolution; 20 vertical levels
- 3-hourly surface forcing from Coupled Ocean/Atmosphere Mesoscale Prediction System (COAMP)
- 2-months simulation period, starting May 1, 2010
Uncertain initial conditions

- Dimensionality reduction through empirical orthogonal functions (KL decomposition)
- Covariance matrices configured to target local variability of frontal dynamics at the edge of the Loop Current (LC). Constructed from 14 daily samples of the near-real-time HYCOM simulation of the GoM (performed at the Naval Research Lab in Stennis)

- EOF decomposition was performed simultaneously over:
  - 3D hydrostatic pressure increment – incorporates variability in the model vertical structure, which is associated with changes in heat and salt content, as well as in the dynamics
  - sea surface height (SSH) – a good proxy for the model surface dynamics.

- Four dominant EOF modes were retained in the initial conditions as they accounted for most of the variability experienced by the model during this 14-day period.

- Amplitude of each EOF mode is a random variable defining a new dimension in the uncertain parameter space.
Uncertain Wind Forcing

- Similar procedure was followed to characterize the uncertainty in the wind forcing
- EOF analysis used the wind forcing fields from COAMP over a 60-day period May-June of 2010
- EOF decomposition was performed over the wind vector in horizontal directions, before being projected onto the wind amplitude and wind stress vectors, which are the variables used to actually force the model
- First four space and time dependent dominant (scaled) modes are retained
Representation of uncertain inputs

- **Uncertain initial condition:**
  \[ u(x, t = 0, \xi_a) = \bar{u}(x, \xi_a = 0) + \alpha_u [\sqrt{\lambda_1 U_1}, \sqrt{\lambda_2 U_2}, \sqrt{\lambda_3 U_3}, \sqrt{\lambda_4 U_4}] \xi_a^T \]

- **Uncertain wind forcing:**
  \[ f(x, t, \xi_b) = \bar{f}(x, t, \xi_b = 0) + \alpha_f [\sqrt{\eta_1 F_1}, \sqrt{\eta_2 F_2}, \sqrt{\eta_3 F_3}, \sqrt{\eta_4 F_4}] \xi_b^T \]

\[ \xi_a = [\xi_1, \xi_2, \xi_3, \xi_4] \quad \xi_b = [\xi_5, \xi_6, \xi_7, \xi_8] \quad \xi_i \sim U[-1, 1] \quad \alpha_u = 0.8 \quad \alpha_f = 0.04 \]
PC surrogate

- Initially relied on adaptive, pseudo-spectral projection (aPSP), with metrics based on QoIs
- Difficulties:
  - noise – mainly in MLD
  - code “failure” – unphysical predictions of MLD
- Also considered LHS in conjunction with BPDN formalism:
  - code “failure” also an issue
  - handled by dropping “problematic” realizations
- $l_1$- regularized CS regression performed on LHS and aPSP grids lead to surrogates that are in close agreement
- Results presented based on LHS grid with 798 members
Response surfaces and error estimates

Left: PC response surfaces in \((\xi_1, \xi_5)\) plane.

Right: Cumulative distribution functions of the relative local errors.
Variability in locally averaged quantities

Guotu Li et al.

SSH(m) PDF

HYCOM PCE

MLD(m) PDF

HYCOM PCE

Fig. 4: Comparison of the SSH (top) and MLD (bottom) density functions estimated by KDE method. Empirical estimations from HYCOM realizations on LHS (red curves) and PC model predictions (blue curves) obtained by evaluating PC surrogates over a fine sampling of X using 10^5 points. The first wind forcing mode appears to be the main contributor to the MLD uncertainty. Further, the comparison of the total and first order indices reveals significant interactions between random sources within initial condition and wind forcing respectively, as one could have anticipated from the non-linearities of the model.

To simplify the sensitivity analysis, we now set IC = \{1,...,4\} and WF = \{5,...,8\}, such that S_{IC} and T_{IC} (resp. S_{WF} and T_{WF}) are the first and total order sensitivity indices associated with the uncertain initial condition (resp. uncertain wind forcing). Since no other source of uncertainty is considered, we have

T_{IC} + S_{IC} = T_{WF} + S_{WF} = 1, \quad (19)

and

S_{IC} \cdot S_{WF} = I_{IC \times WF}. \quad (20)

In the previous equation, we have denoted I_{IC \times WF} the sensitivity index, which measures the fraction of the variance due to the interaction between the uncertainties in the initial conditions and in the wind forcing. An alternative expression for this additional index is

I_{IC \times WF} = 1 - S_{IC} - S_{WF}. \quad (21)
Sensitivity indices at day 30

The graphs show the sensitivity indices for SSH and MLD at day 30. The indices are plotted against the stochastic dimension index.

- **SSH**
  - The sensitivity indices are high for the first index, indicating a significant impact.
  - The indices for subsequent indices are negligible.

- **MLD**
  - Similar to SSH, the sensitivity indices are high for the first index.
  - The indices for other indices are also negligible.

The graphs help in understanding the relative importance of different sources of uncertainty on the SSH and MLD responses.
Evolution of sensitivity indices

**SSH**

- Red line: Initial Condition
- Blue line: Wind Forcing
- Green line: Interaction

**MLD**

- Red line: Initial Condition
- Blue line: Wind Forcing
- Green line: Interaction
EOF-PC representation – I

- Define empirical mean and covariance:

\[ \bar{U}(x) = \frac{1}{N_{LHS}} \sum_{j=1}^{N_{LHS}} U(x, \xi_j), \quad U_j'(x) = U(x, \xi_j) - \bar{U}(x), \quad [C]_{i,j} = (U_i', U_j')_\Omega \]

- Decompose [C] into proper elements

\[ [C] \Phi^k = \lambda^k \Phi^k, \quad (\Phi^k)^T (\Phi^k) = 1. \]

- Define empirical spatial modes:

\[ u^k(x) = \sum_{j=1}^{N_{LHS}} U_j'(x) \Phi^k_j. \]
EOF-PC representation – II

- Define empirical mean and covariance:
  \[ U(x, \xi) \approx \bar{U}(x) + \sum_{k=1}^{r} u^k(x) \phi^k(\xi), \]

- Set \( r \) such that
  \[ \sum_{k=1}^{r} \lambda_k \geq p \sum_{k=1}^{N_{LHS}} \lambda_k \]

- Use BPDN algorithm to represent
  \[ \phi^k(\xi) \approx \tilde{\phi}^k(\xi) = \sum_{\alpha=0}^{N_p} c^k_{\alpha} \Psi_{\alpha}(\xi) \]
Mean and spectral decay

SSH: p=0.8 -> r=10

SSH: p=0.8 -> r=27
SSH: leading modes at day 30

Fig. 8: SSH field at day 30. Top: empirical average using the LHS set of HYCOM realizations. Bottom: spectrum of the empirical spatial covariance.

Fig. 9: First five spatial modes $u_k/p_l$ in the expansion of the SSH field at day 30.

Fig. 10: Standard deviation of SSH fields at day 30. Left: empirical standard deviation calculated from the LHS set of HYCOM simulations. Right: standard deviation in the truncated expansion of the field using $r = 10$ modes.

5.2.2 MLD field

We now repeat the analysis of the EOF-PC approximation of the previous section, but for the MLD field at day 30. The empirical MLD average on day 30, seen on Figure 12 (top plot) shows that the MLD is deeper in the LC region than that in the rest of the GoM, and it tends to be shallower along the coast. As for the small-region average, it is found that the MLD field is significantly more complex and more demanding to approximate. Specifically, Figure 12 shows that though the empirical average of the MLD field (top plot) is relatively smooth, the decay rate of the perturbation spectrum is significantly slower than that of the SSH field.
MLD: leading modes at day 30

Specifically, \( r = 142 \) modes are necessary to retain 90% of the empirical variance. Because faithful PC recovery of higher-order modes would require a larger ensemble than is practical, in this analysis below the EOF expansion for MLD is limited to retain 80% of field variability, which corresponds to \( r = 27 \) modes.

The first five dominant modes of the MLD covariance are plotted in Figure 13. As for the SSH decomposition, Mode 1 is dominated by variability in the LC, which is also the case for Mode 4 to a large extent. Modes 2, 3, and 5 are mixed, with signals in the deep GoM as well as along the coasts. Compared with the dominant modes in SSH (Figure 9), the dominant MLD modes involve shorter scale features, and tend to be less spatially localized.

In Figure 14 we compare the empirical standard deviation of the MLD field (left plot) with the standard deviation of its EOF-PC approximation (right plot). As for the SSH, it is seen that the EOF-PC approximation is able to properly capture the main structures of the MLD uncertainty, in particular 1) near the LC region, 2) along the northern coastline and 3) around the LC Eddy at \((26^\circ N, 94^\circ W)\). However, we also observe that the differences between the two standard deviation fields are more significant than in the case of SSH (Figure 10). In fact, the EOF-PC approximation contains only 80% of the fluctuating energy in the set of HYCOM realizations. It is noted that inclusion of additional modes in the EOF-PC approximation would slowly improve the capture of the remaining field variability; again, this can be explained by the complex response of the local MLD to random inputs, which makes it difficult to approximate the reduced random coordinates \( f_k(\cdot) \). Indeed, the PC approximation of the \( f_k \) yields an additional loss of variability, as some fluctuations are interpreted as realization noise by the PC construction procedure.

In Figure 14 we compare the empirical standard deviation of the MLD field (left plot) with the standard deviation of its EOF-PC approximation (right plot). As for the SSH, it is seen that the EOF-PC approximation is able to properly capture the main structures of the MLD uncertainty, in particular 1) near the LC region, 2) along the northern coastline and 3) around the LC Eddy at \((26^\circ N, 94^\circ W)\). However, we also observe that the differences between the two standard deviation fields are more significant than in the case of SSH (Figure 10). In fact, the EOF-PC approximation contains only 80% of the fluctuating energy in the set of HYCOM realizations. It is noted that inclusion of additional modes in the EOF-PC approximation would slowly improve the capture of the remaining field variability; again, this can be explained by the complex response of the local MLD to random inputs, which makes it difficult to approximate the reduced random coordinates \( f_k(\cdot) \). Indeed, the PC approximation of the \( f_k \) yields an additional loss of variability, as some fluctuations are interpreted as realization noise by the PC construction procedure.
Field sensitivities @ day 30

Left: SSH, Right: MLD
Top: 1st order sensitivity to initial condition
Mid: 1st order sensitivity to wind forcing
Bot: mixed effects
Effect of sample size

Do we need all samples? Address by subsampling full LHS grid

Subsampling aims at maintaining coverage
Normalized error behavior

Pointwise and mean-square errors can be large, especially for MLD
Field sensitivities: full and subsampled grids

SSH, IC

MLD, wind

Full grid, N=798
Subsampled grid, N=50
MLD standard deviation

Empirical – full grid

EOF/PC – full grid

EOF/PC – N=50
Remarks – I

- Ongoing work
  - Coupled atmosphere-wave-ocean (WRF/U. Miami wave model/HYCOM) model

- Challenges:
  - Simulation cost
  - Efficient sampling strategies
Remarks – II

➢ Ongoing work*
  ▪ Path planning for AUVs

➢ Challenges:
  ▪ Optimal planning under uncertainty
  ▪ Statistical downscaling [high-resolution regional forecasts]
  ▪ Multi-data assimilation
  ▪ Control algorithms

*Poster session