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Quantifying Prediction Fidelity in Ocean CirculationModels

Mohamed Iskandarani
Rosenstiel School of Marine and Atmoshperic Science
University of Miami
4600 Rickenbacker Causeway, Miami, FL 33149
phone: (305) 421-4045 fax: (305) 421-4696 email:miskandarani@rsmas.miami.edu

Omar Knio
Department of Mechanical Engineering and Materials Science
Duke University
144 Hudson Hall, Box 90300, Durham, NC 27708
phone: (919) 660 5344 fax: (919) 660-8963 email:omar.knio@duke.edu

Ashwanth Srinivasan
Rosenstiel School of Marine and Atmoshperic Science
University of Miami
4600 Rickenbacker Causeway, Miami, FL 33149
phone: (305) 421-4763 fax: (305) 421-4696 email:asrinivasan@rsmas.miami.edu

William C. Thacker
Cooperative Institute for Marine and Atmospheric Studies University of Miami
4600 Rickenbacker Causeway, Miami, FL 33149
phone: (305) 361-4323 fax: (305) 421-4696 email:carlisle.thacker@noaa.gov

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LONG-TERM GOALS

The development, validation and application of robust uncertainty quantification methods to ocean modeling and forecasting.

OBJECTIVES

This project explores the use of Polynomial Chaos (PC) expansions for improving our understanding of uncertainties in Ocean General Circulation Models (OGCM). Given adequate initial and boundary conditions, most OGCMs can be used to forecast the evolution of the oceanic state consistent with known physical laws. Reliable ocean forecasts, however, require an objective, practical and accurate methodology to assess the inherent uncertainties associated with the model *and* data used to produce these forecasts. OGCMs uncertainties stem from several sources that include: physical approximation

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of the equations of oceanic motion; discretization and modeling errors; an incomplete set of sparse (and often noisy) observations to constrain the initial and boundary conditions of the model; and uncertainties in surface momentum and buoyancy fluxes.

Our objective is the development of an uncertainty quantification methodology that is efficient in representing the solutions dependence on the stochastic data, that is robust even when the solution depends discontinuously on the stochastic inputs, that can handle non-linear processes, that propagates the full probability density functions without apriori assumption of Gaussianity, and that can be applied adaptively to probe regions of steep variations and/or bifurcation in a high-dimensional parametric space. In addition we are interested in developing utilities for decision support analysis; specifically, we plan to demonstrate how PC representations can be used effectively to determine the non-linear sensitivity of the solution to particular components of the random data, identify dominant contributors to solution uncertainty, as well as guide and prioritize the gathering of additional data through experiments or field observations.

APPROACH

Our approach to uncertainty quantification (UQ) is built on applying PC expansions (Le Maître and Knio, 2010) to investigate uncertainties in simulating the oceanic circulation in the Gulf of Mexico. We have opted to use the HYbrid Coordinate Ocean Model (HYCOM) as our simulation engine because it has been developed as the next generation model for the US Navy and has been adopted by NOAAs National Center for Environmental Prediction. HYCOM is also equipped with a suite of sequential assimilation schemes that will be used to investigate how UQ may be beneficial to data assimilation. Details about the model, its validation, and sample applications can be found in Bleck (2002); Halliwell (2004); Chassignet et al. (2003, 2006) as by visiting http://www.hycom.org. We have chosen the Gulf of Mexico for our experimentation because of the pre-existing HYCOM configurations for that basin and the wealth of experience accumulated in simulating its circulation, the availability of observations for model validation, and for the importance of that region to the social and economic prosperity of the South East United States. In the following subsections we present the main ideas of the PC expansion before we summarize our efforts to date.

PC expansions express the dependency of the solution on the uncertain parameter as a series expansion of the form:

$$u(\boldsymbol{x},t,\boldsymbol{\xi}) = \sum_{k=0}^{P} \hat{u}_k(\boldsymbol{x},t)\Psi_k(\boldsymbol{\xi}). \tag{1}$$

Here $u(\boldsymbol{x},t,\boldsymbol{\xi})$ is a model solution that depends on space $\boldsymbol{x}$, time t and the uncertain parameters $\boldsymbol{\xi}$; $\Psi_k(\boldsymbol{\xi})$ is a suitably chosen orthogonal basis; and $\hat{u}_k(\boldsymbol{x},t)$ are the expansion coefficients. In our approach to UQ, u can represent a variable expressed directly in the model such as sea surface temperature or velocity at a specified point, or a derived quantity such as the mean surface cooling under a hurricane track. In the jargon of UQ the quantity of interest u is often referred to as an observable.

The choice of basis function is dictated primarily by the probability density function of the uncertain input data, $p(\boldsymbol{\xi})$, which enters all aspects of the UQ computations. These can be made much more efficiently if the basis vectors are orthonormal with respect to $p(\boldsymbol{\xi})$. Hence the basis functions are Legendre, Hermite, or Laguerre polynomials when the input uncertainty is described by uniform, Gaussian, or Gamma distributions, respectively.

The computation of the stochastic modes is best achieved by the so-called Non-Intrusive Spectral Projection (NISP) method since we would like to avoid modifying the original OGCM code. Taking advantage of the orthonormality of the basis, NISP works by projecting the solution u on the basis function Ψ_k via inner products, and by replacing the integrals with quadrature formula. The coefficients can then be computed simply by running the model at specified values of the uncertain parameters, storing the desired observable, and post-processing via a simple matrix-vector multiplication. No modification to the OGCM need be performed.

The investigative team at Johns Hopkins University consisted of Dr. Omar M. Knio (now at Duke University), and his post-doctoral associates, Dr. Alen Alexanderian and Ihab Sraj, and graduate student, Justin Winokur; they have concentrated on advancing the technical aspects and theoretical aspects of the Uncertainty Quantification efforts. Dr. Mohamed Iskandarani, Ashwanth Srinivasan and William C. Thacker (University of Miami) have focused on formulating the oceanographic uncertainty problems, the modification to the HYCOM code and its actual execution, and the preparation of the necessary data to carry out the research agenda. Dr. Matthieu Le Henaff assisted us with the Gulf of Mexico configuration, and we have held discussions with Dr. François Counillon as to the applicability of PCs in Ensemble Kalman Filters based data assimilation.

WORK COMPLETED

Our work proceeded along several parallel tracks: studying the uncertainty stemming from nesting boundary conditions, investigating parametric uncertainty in HYCOM mixed-layer model and wind-drag bulk formula, assessment of uncertainties in an oil spill model, and developing an efficient procedure to handle stochastic dynamical systems with multiple time scales.

Our initial experimentation with UQ revolved around the impact of nesting boundary conditions uncertainty on the ocean circulation forecasts in the Gulf of Mexico. In addition to the development of the non-intrusive HYCOM and UQ machinery to carry out this task, we proposed an original approach to cast the problem within a PC-framework so that only two stochastic parameters are needed. The nesting data was decomposed into space-time Empirical Orthogonal Functions and the two dominant modes were perturbed. An ensemble of 49 simulations were needed to characterize the entire uncertainty space. Figure 1 shows the evolution of the 17 cm surface height field for these 49 runs, and figure 2 shows PC-estimates of the standard deviation at various times. An article describing this work has been submitted for publication (Thacker et al., 2011).

The Deep Water Horizon oil spill afforded us the opportunity to use UQ for a pressing environmental problem, and to help understand the fate and potential impact of the discharged oil. The simulation combined two nested HYCOM models (at 2 km and 900 m resolutions) and a 3D oil spill model that included the effects of advections by ocean currents and waves, and the effects of various physical, chemical and biological processes. The uncertainty in the initial distribution of oil droplet size and compositions were propagated through the model using the UQ machinery and the results are illustrated in figure 3. It should be noted that this work required a herculian effort to marshal and synchronize a set of heterogeneous and distributed high performance computing resources to carry out the simulations; this accomplishment has been recognized in a talk and a publication in a prestigious journal Srinivasan et al. (2010).

The parametric study focused on quantifying ocean model uncertainties, associated with mixed layer and air-sea momentum exchange parametrizations, when the ocean is forced by hurricane-strength winds. The wind-stress and the mixed layer parameterization modulate the ocean Sea Surface Temperature (SST) response to hurricane forcing, a key parameter in determining the exchanges of energy and momentum between the ocean and atmosphere, and in impacting hurricane intensity forecast. The setting chosen for our experiments is the circulation in the Gulf of Mexico during the passage of hurricane Ivan from Sep 9–16 2004. We used PC expansions to systematically characterize the entire response surface of the ocean model to parametric uncertainties in its subgrid parameterizations. Four parameters were perturbed in this study: three KPP parameters (The critical Richardson number controlling the definition of the ocean mixed layer, and the background viscosity and diffusion), along with the wind-drag coefficient. A total of 385 simulations were necessary to explore the entire uncertainty space and determine all the stochastic modes; various consistency checks were done to confirm that the PC representation remained accurate. Figures 4-6 illustrate the statistical output that can be mined from these simulations. Figure 4 shows the mean mixed-layer depth as estimated by the PC expansions. Figure 5 shows the evolution of the SST probability density function at a NOAA buoy (located at 85.1 W and 26.1 N); the latter shifts to cooler temperature, as expected in the hurricane wake, and broadens with time. Figure 6 illustrates how sensitivity analysis metrics can be used to identify the main contributors to SST uncertainty throughout the Gulf of Mexico.

A preconditioning approach was developed to improve the efficiency of representing uncertainty in dynamical systems with PC expansions. The approach is based on the definition of an appropriate multiscale stretching of the individual components of the dynamical system, and which can robustly recovery the unscaled transient dynamics. The stochastic modes are then obtained through non-intrusive spectral projections of the stretched measures. Implementation of the present approach was illustrated through application to a chemical system with large uncertainties in the reaction rate constants. Computational experiments showed that, despite the large stochastic variability of the stochastic solution, the resulting dynamics can be efficiently represented using sparse low-order PC expansions of the stochastic multiscale preconditioner and of stretched variables. We will explore extending these preconditioning ideas to oceanic simulations in the near future.

The work associated with this project has been publicized at several conferences, workshops, seminars and invited talks, including:

- the workshop on Uncertainty Quantification for Multiscale Systems, Baltimore MD, July 20 2010;
- the workshop on Mathematical Theory and Modelling in Atmosphere-Ocean-Science, Oberwolfach Germany 08/08/2010–08/14/2010;
- "Many Task Computing for Modeling the Fate of Oil Discharged from the Deep Water Horizon Well Blowout", MTAGS 2010, 3rd IEEE Workshop on Many-Task Computing on Grids and Supercomputers, New Orleans LA, 11/15/2010;
- the Layered Ocean Model workshop, Miami FL, 02/07/2011-02/09/2011;
- the SIAM Conference on Computational Science and Engineering, Reno NV, 02/28/2011–03/04/2011;
- the SIAM Conference on Mathematical and Computational Issues in the Geosciences, Long Beach CA, 03/21/2011–03/24/2011.
- "Probabilistic Methods for Uncertainty Quantification: Recent Developments and Implications to Extreme Scale Computing," DOE-SCGF Annual Meeting, July 18, 2011.
- "Stochastic Multiscale Approaches in Fluid and Thermal Systems, KAUST, May 22, 2011.
- "Stochastic Multiscale Approaches in Fluid and Thermal Systems," Masdar Institute, May 8, 2011.
- "Multiscale Simulations, Uncertainty Quantification and Data Challenges," University of Lugano,

March 28, 2011.

- "Multiscale Paradigms in Reactive Solids and in Fluids," Duke University, March 22, 2011.
- "Spectral Approaches of Uncertainty Quantification in Complex Dynamical Systems," UC Berkeley, February 16, 2011.
- "Spectral Approach to Uncertainty Quantification in Complex Dynamical Systems," plenary lecture, 2010 MetStroem Program Meeting, FU Berlin, October 28, 2010.

RESULTS

The Empirical Orthogonal Function decomposition proved to be an effective method to recast the uncertainty quantification problem into a PC-based practical framework. A similar decomposition can be envisioned for perturbations to initial conditions. This is an on-going investigation.

A number of scripts have been developed to coordinate the launching of the HYCOM ensemble and the collection of the output for UQ post-processing. In addition, Smolyak nested integration rules were coded to mitigate the growth in the size of the ensemble as the number of stochastic variables increases. This nested quadrature is a good basis upon which to build adaptive sampling techniques.

The PC-premise of casting the probabilistic uncertainty as an approximation/interpolation problem is paying off in a couple of ways. First it allows for self-consistency checks as to the error committed in the approximation, and second it allows the expansions to act as a cheap emulator for the model. Thus, histograms of output uncertainties can be built cheaply. More importantly various variance and sensitivity analysis metrics can be devised to assess which of the uncertain input parameters have the greatest impact on the output uncertainties. This is illustrated in figure 6 which shows how the fraction of variance in SST that can be attributed to the uncertain input parameters; here the background diffuvisity is the dominant factor in the absence of strong wind forcing whereas the drag coefficient takes over in the hurricane track region.

IMPACT/APPLICATIONS

The present project presents an approach to characterize the entire response surface of an ocean model to uncertainties in its input data. This has implications for the field of data assimilation, particularly for ensemble Kalman filter based approaches. The methodology developed here will be of use either for the efficient update of the covariance matrices and/or quantifying the errors incurred by small size ensembles. We plan to explore these ideas in the near future.

TRANSITIONS

RELATED PROJECTS

Dr. Ashwanth Srinivasan was partially supported by an NSF-RAPID grant (NSF OCE-1048697) for his work on the oil-fate model.

PUBLICATIONS

A. Alexanderian, O. Le Maître, H. Najm, M. Iskandarani, and O. Knio. Multiscale stochastic preconditioners in non-intrusive spectral projection. *Journal of Scientific Computing*, pages 1–35, 2011.

A. Srinivasan, J. Helgers, C. B. Paris, M. LeHenaff, H. Kang, V. Kourafalou, M. Iskandarani, W. C. Thacker, J. P. Zysman, N. F. Tsinoremas, and O. M. Knio. Many task computing for modeling the fate of oil discharged from the deep water horizon well blowout. *Many-Task Computing on Grids and Supercomputers (MTAGS), 2010 IEEE Workshop on*, pages 1–7, November, 2010. IEEE.

W. C. Thacker, A. Srinivasan, M. Iskandarani, O. M. Knio, and M. L. Henaff. Propagating oceanographic uncertainties using the method of polynomial chao expansion. *Ocean Modelling*, 2011. submitted.

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A. Alexanderian, O. Le Maître, H. Najm, M. Iskandarani, and O. Knio. Multiscale stochastic preconditioners in non-intrusive spectral projection. *Journal of Scientific Computing*, pages 1–35, 2011. ISSN 0885-7474. doi: 10.1007/s10915-011-9486-2. URL http://dx.doi.org/10.1007/s10915-011-9486-2.

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O. P. Le Maître and O. M. Knio. *Spectral Methods for Uncertainty Quantification*. Springer-Verlag, 2010.

A. Srinivasan, J. Helgers, C. B. Paris, M. LeHenaff, H. Kang, V. Kourafalou, M. Iskandarani, W. C. Thacker, J. P. Zysman, N. F. Tsinoremas, and O. M. Knio. Many task computing for modeling the fate of oil discharged from the deep water horizon well blowout. In *Many-Task Computing on Grids and Supercomputers (MTAGS), 2010 IEEE Workshop on*, pages 1–7, November, 2010. IEEE. doi: 10.1109/MTAGS.2010.5699424. URL http://dx.doi.org/10.1109/MTAGS.2010.5699424.

W. C. Thacker, A. Srinivasan, M. Iskandarani, O. M. Knio, and M. L. Henaff. Propagating oceanographic uncertainties using the method of polynomial chao expansion. *Ocean Modelling*, 2011. submitted.

Listing of publications produced during this effort. If you use BibTEX, you can use e.g., bibunits or multibib to insert a second set of references, or just copy the contents of a .bbl file here.

PATENTS

HONORS/AWARDS/PRIZES

O. Knio named Director of Uncertainty and Risk Assessment Thrust, Pratt School of Engineering, Duke University.

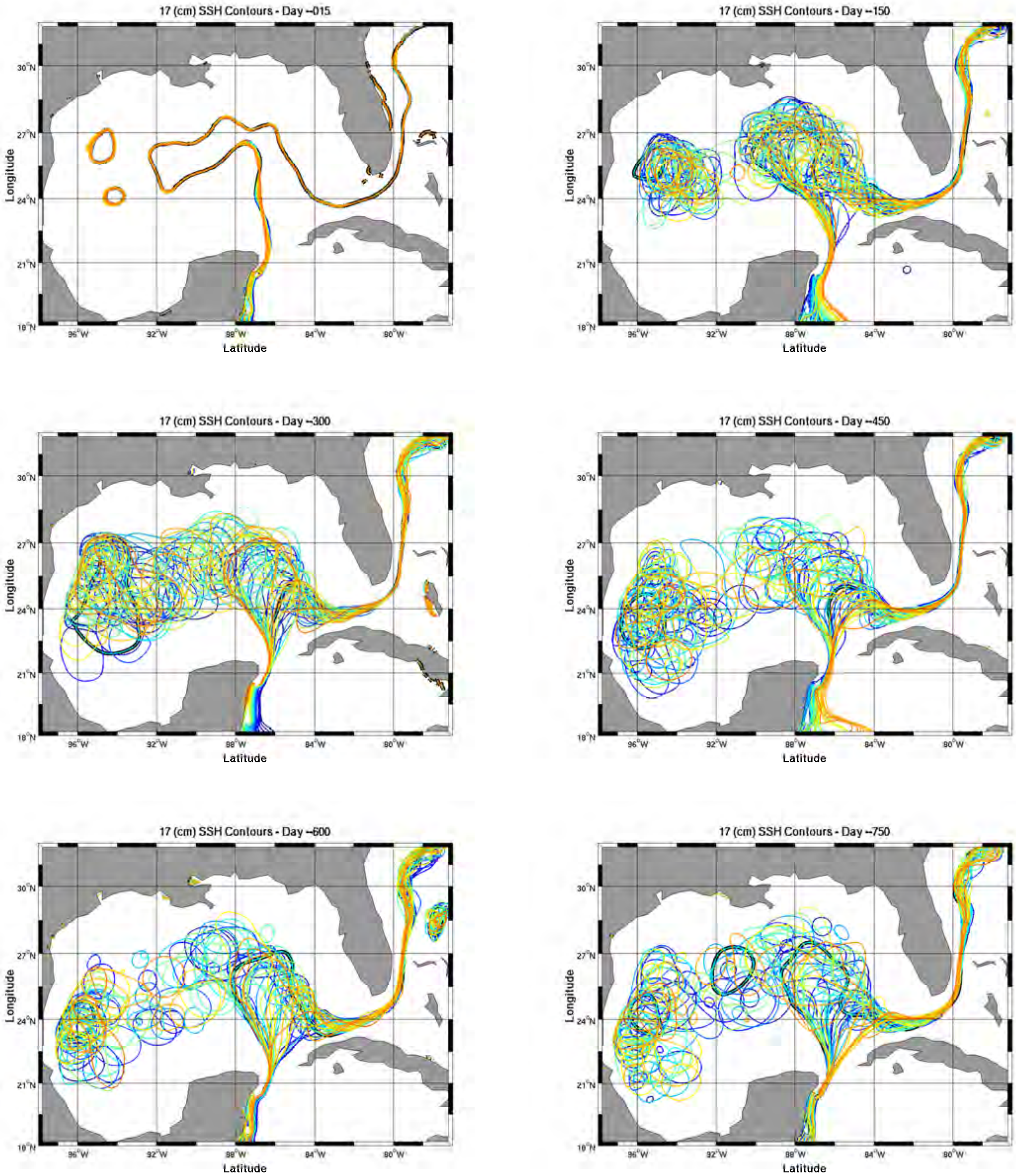

Figure 1: Sea Surface Height contours from the ensemble HYCOM runs at the quadrature points. The panels show the state of the 17 ***cm contour, used as a proxy for the Loop Current, at different times. The contour from each deterministic run of HYCOM (realization) is plotted using a unique color***

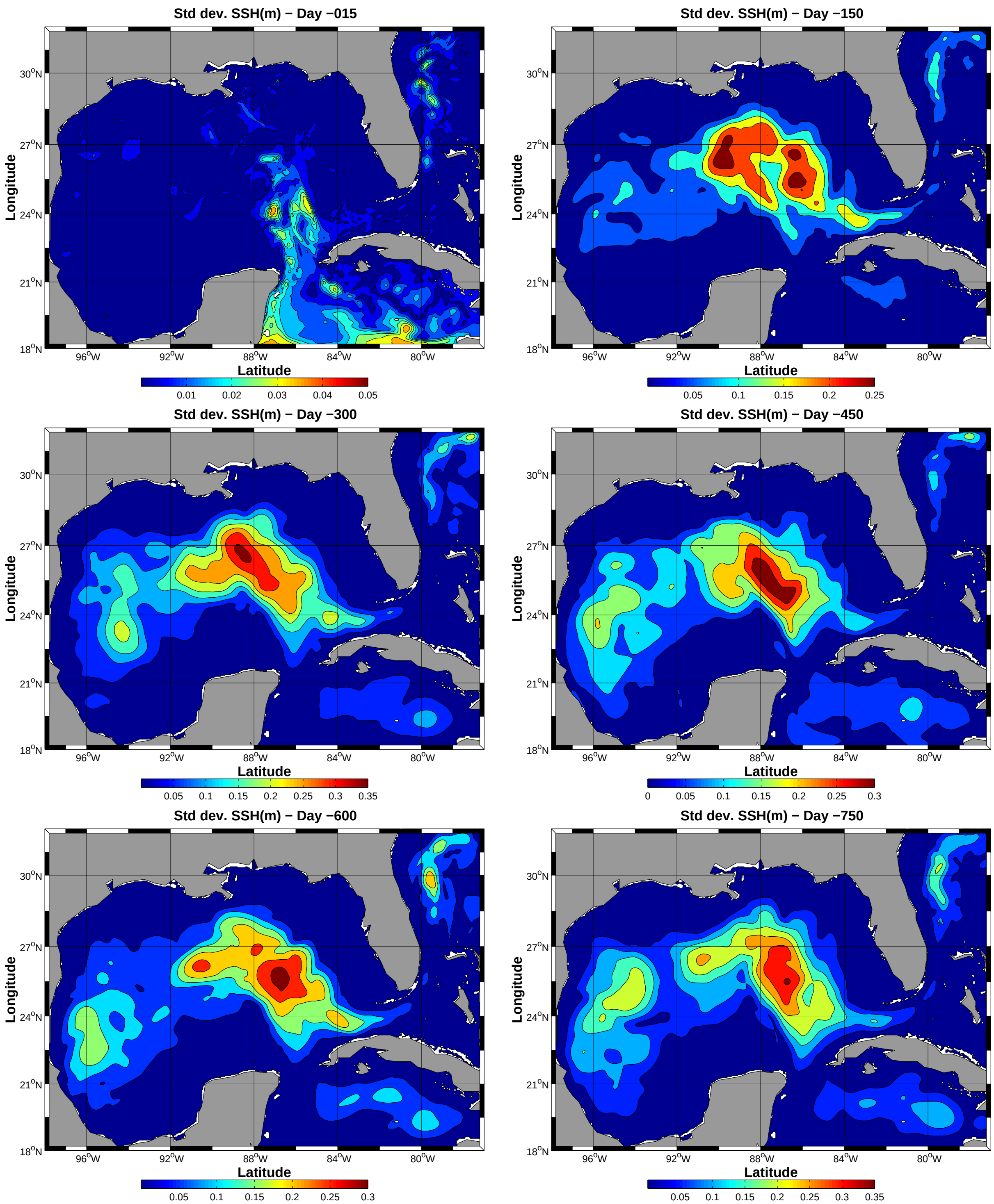

Figure 2: Standard Deviation of the Surface Height field obtained from the Polynomial Chaos Expansions. The panels show the evolution of the uncertainty every 150 days. The standard deviation is computed using a 6 order polynomial expansion.

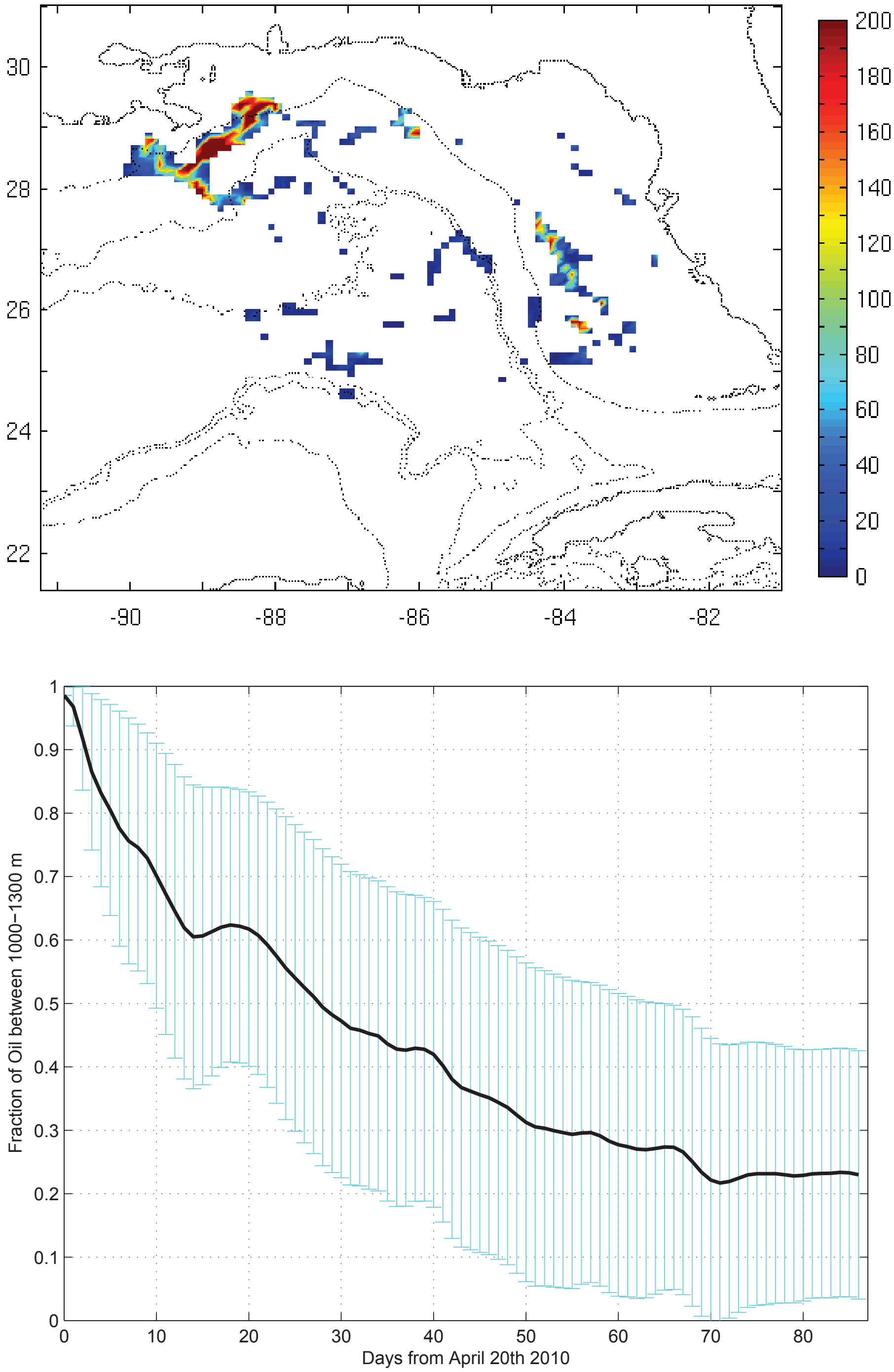

Figure 3: The upper figure shows the surface slick simulated by the oil model for June 11, and compares well with satellite based composites. The lower figure shows the subsurface fraction of oil between 1000-1400 m as a function of time. The error bars are based on input uncertainties on the oil droplet size and the oil composition. The results suggest that about 80 % of the oil has been removed from the water column by evaporation and degradation and the uncertainty analysis assigned a 20% uncertainty to this estimate.

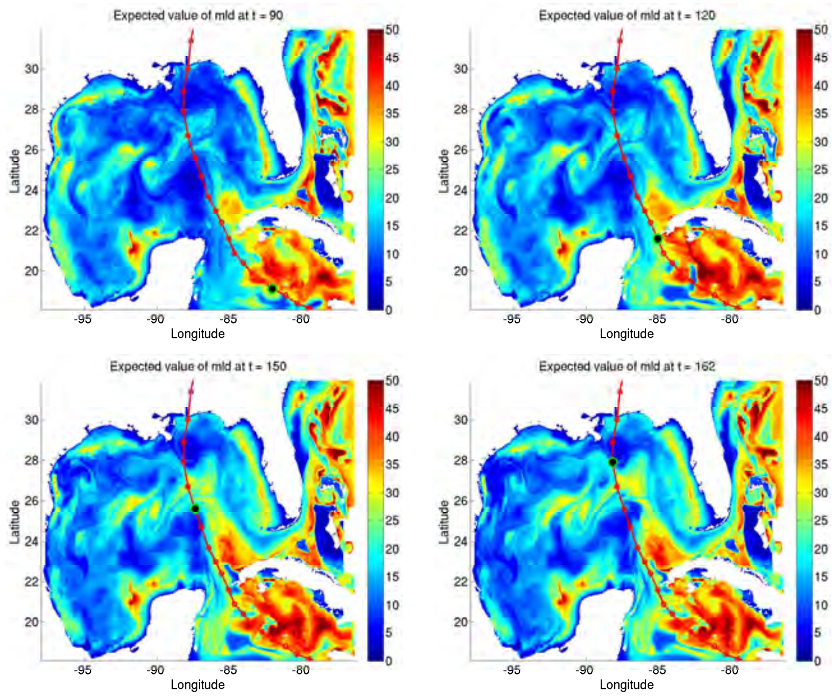

Figure 4: Time evolution of the expected Mixed Layer Depth. The red curve and the black dot refer to Ivan's obeserved track and to its center, respectively.

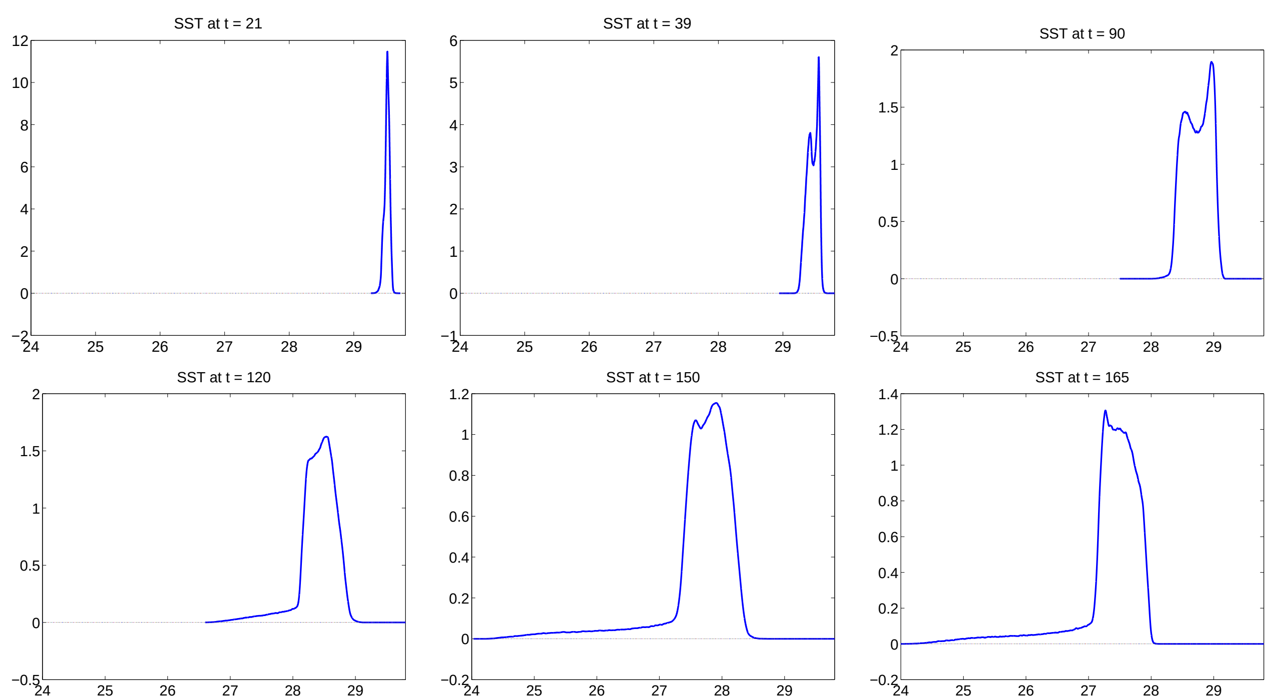

Figure 5: Distribution of SST at the buoy location over time (generated by sampling the PC expansions with sample size of 10^6.) Note that as the hurricane nears the Gulf ($t \approx 90$), enters the Gulf ($t \approx 120$) and gets close to the buoy ($t \approx 150$) we see the cooling of water through the shift of the distribution to left. Also, note the emergence of long tails for the distributions stretching toward cooler temperatures.

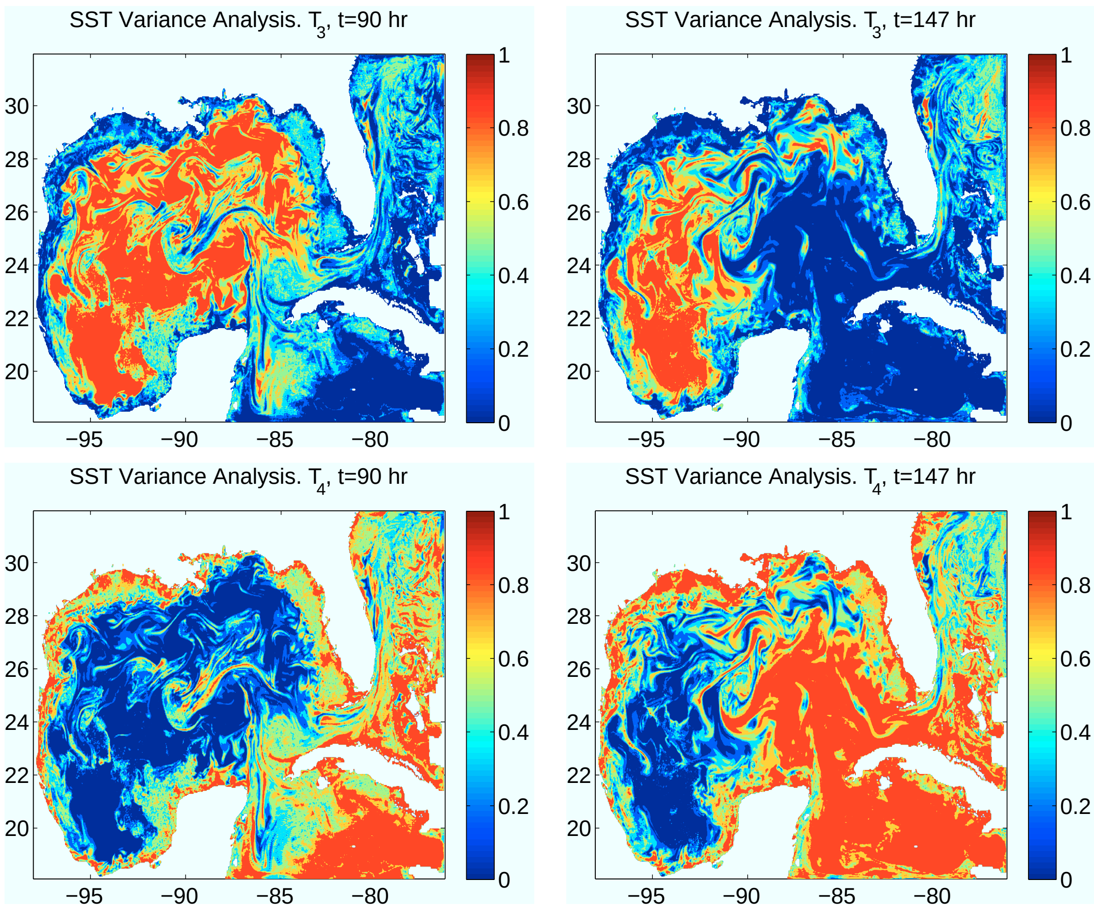

Figure 6: SST sensitivity analysis with Hurricane Ivan, before (t=90 hr) and after (t=147 hr) the hurricane enters the Gulf. Here we look at T_3 ***(sensitivity due to background diffusivity) and*** T_4 ***(sensitivity due to stochastic wind drag coefficient). Background diffusivity accounts for most of the variance in the absence of the hurricane while the drag coefficients has the most influence in the region of strong wind forcing (right column).***