Overview of Polynomial Chaos Methods for Uncertainty Quantification

with Application to HYCOM

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Outline

1. Background.
   - What is polynomial chaos?
   - How does polynomial chaos work?
2. Uncertain inflow through Yucatan Straits.
   - Setup.
   - Results.
3. Omar: advanced techniques.

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What is polynomial chaos?

- Idea of polynomial chaos originated with Norbert Wiener in 1938 — before computers.
- It is being used by engineers to assess how uncertainties in a model's inputs manifest in its outputs.
- It can be much more efficient than Monte Carlo methods.
- Can it be useful to oceanographers?

Why “polynomial”? Why “chaos”?

- “Chaos” simply refers to uncertainty. Nothing to do with strange attractors?
- Want to compute how uncertainties of a dynamical system’s inputs manifest in its outputs.
- “Polynomial” refers to use of polynomial expansions to propagate uncertainties.
- Idea is to exploit orthogonality of the polynomials.

HYCOM: uncertain inputs.

- Initial conditions.
- Boundary conditions.
- Forcing.
- Parameters.

- Polynomial Chaos can handle only a limited number of uncertain inputs.
- But it focuses on *all* likely values of those few uncertain inputs.

HYCOM: uncertain outputs.

- Every field at every time.
- Value of a particular field at a particular point and a particular time.
- Derived quantities,
  e.g. maximum of the Meridional overturning stream function.

- Polynomial Chaos allows focus to be on points of interest.
- Not necessary to explore all uncertainties simultaneously.

Simplest case: one uncertain input, one output of interest.

- Call the uncertain input ξ and the output ϕ.
- Uncertainty of ξ is specified via its pdf $\rho(\xi)$.
- Want pdf of ϕ or at least information about how it varies as ξ varies.
- Basic Idea: Express output as a polynomial series.

$$\phi(\xi) = \phi_0 + \phi_1 P_1(\xi) + \phi_2 P_2(\xi) + \ldots$$

- Orthogonal polynomials P_k are related to pdf ρ.

$$\int P_j(\xi) P_k(\xi) \rho(\xi) d\xi = \delta_{j,k}$$

Simplest case, continued: one uncertain input, one output of interest

$$\phi(\xi) = \phi_0 + \phi_1 P_1(\xi) + \phi_2 P_2(\xi) + \dots$$

$$\int P_j(\xi) P_k(\xi) \rho(\xi) d\xi = \delta_{j,k}$$

- Is the series guaranteed to converge?
- In practice, it must be truncated.
- How to compute the coefficients $\phi_0, \phi_1, \phi_2, \dots$?

$$\phi_k = \frac{1}{N_k} \int \phi(\xi) P_k(\xi) \rho(\xi) d\xi$$

$$N_k = \int P_k^2(\xi) \rho(\xi) d\xi$$

- Use Gaussian quadrature to evaluate the integrals.

Simplest case, continued: one uncertain input, one output of interest

- Coefficients:

$$\phi_k = \frac{1}{N_k} \int \phi(\xi) P_k(\xi) \rho(\xi) d\xi$$

- Gaussian Quadrature:

$$\int \phi(\xi) P_k(\xi) \rho(\xi) d\xi \approx \sum_p \phi(\xi_p) P_k(\xi_p) w_p$$

- Quadrature points: ξ_p
- Quadrature weights: w_p
- Computing outputs $\phi(\xi_p)$ for inputs at quadrature points ξ_p requires multiple model runs.
- How many quadrature points (runs) are needed?

Several outputs of interest, one uncertain input.

- Two outputs:

$$\phi(\xi) = \phi_0 + \phi_1 P_1(\xi) + \phi_2 P_2(\xi) + \dots$$
$$\psi(\xi) = \psi_0 + \psi_1 P_1(\xi) + \psi_2 P_2(\xi) + \dots$$

- Two or more outputs require no more runs than does one output.
- Just save values for all outputs of interest, $\phi, \psi, \dots$.
- More coefficients, so more quadrature integrals are needed.
- Quadrature integrals are computationally cheap.
- Can examine uncertainty of an entire field.

How to use expansion coefficients?

- mean:

$$\langle \phi \rangle = \int \phi(\xi)\rho(\xi)d\xi = \phi_0$$

- variance:

$$\langle (\phi - \phi_0 \rangle)^2 = \sum_{k=1}^{k\max} \phi_k^2$$

- covariance:

$$\langle (\phi - \phi_0 \rangle)(\psi - \psi_0)\rangle = \sum_{k=1}^{k\max} \phi_k \psi_k$$

- Generate a cheap ensemble.

$$\phi(\xi) = \phi_0 + \phi_1 P_1(\xi) + \phi_2 P_2(\xi) + \dots$$

Two uncertain inputs, one output of interest

- Call the uncertain inputs ξ and χ.
- Uncertainties of are specified via joint pdf $\rho(\xi, \chi)$.
- Now have polynomial series in two variables:

$$\phi(\xi, \chi) = \phi_0 + \phi_1 P_1(\xi, \chi) + \phi_2 P_2(\xi, \chi) + \dots$$

- If uncertain inputs are independent, pdf factors:

$$\rho(\xi, \chi) = \rho_\xi(\xi)\rho_\chi(\chi)$$

- Then 2D quadrature reduces to two 1D quadratures.
- Number of quadrature points (runs) is squared.
- Curse of dimensionality.
- Sparse cubature might provide economy when exploring consequences of several uncertain inputs.

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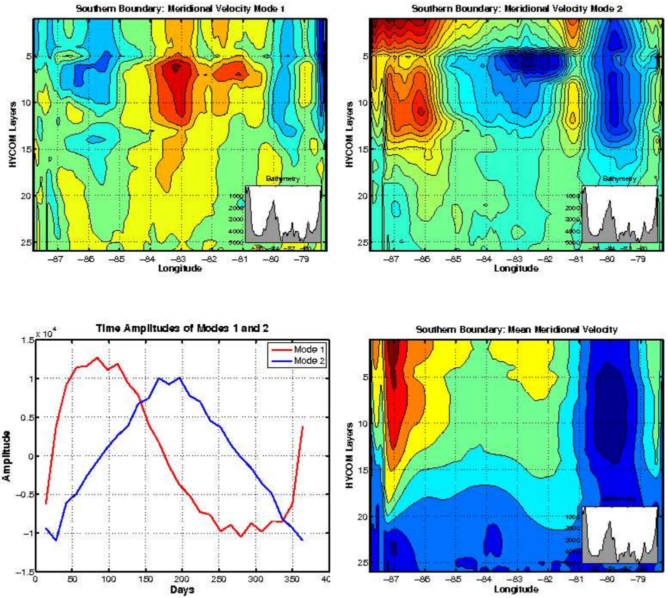
Problem: How do uncertainties of the Yucatan inflow manifest within the Gulf of Mexico?

- Need to quantify inflow uncertainties.
- Inflow is characterized by several 2D time-varying fields.
- Computational cost increases dramatically with number of uncertain parameters.
- How to characterize uncertainties of inflow with only a few parameters?

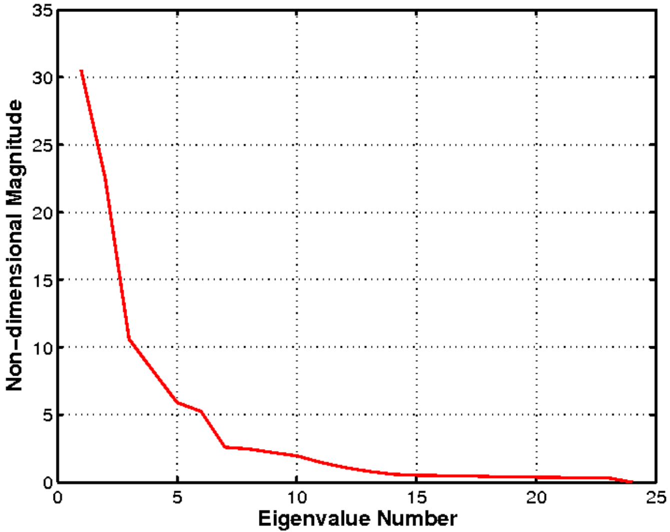
How to characterize uncertainties of inflow with only a few *independent* parameters?

- Use multivariate EOFs to characterize 2D spatial patterns of inflow uncertainty.
- Use corresponding principal components to characterize their temporal variability.
- Each mode's amplitude is assumed to have a Gaussian pdf.
- Hermite polynomials — Gauss-Hermite quadrature.
- Quadrature points dictate the required HYCOM runs.
- Each run is the sum of a "favorite" inflow and its particular EOF contributions.

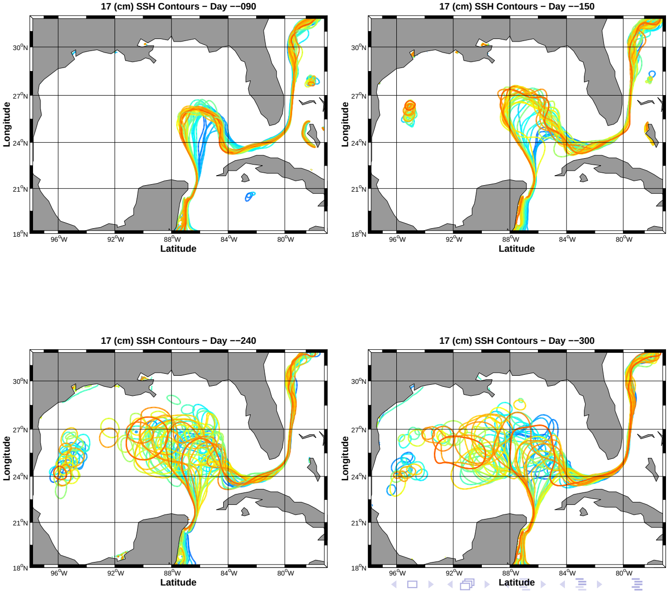
Meridional velocity component of EOF.



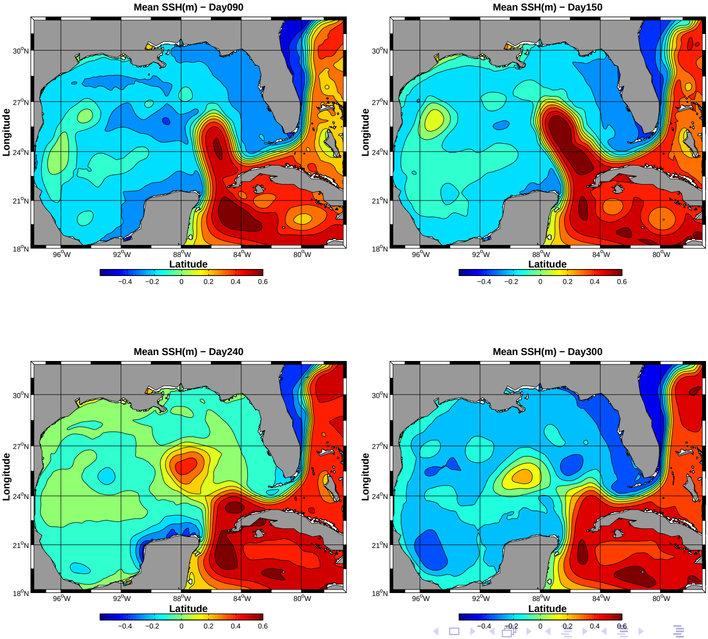
Eigenvalue spectrum.



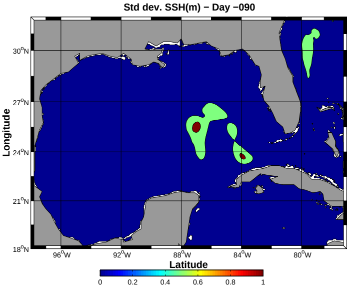
Contours of 17 cm SSH from quadrature ensemble of 17 cm runs.

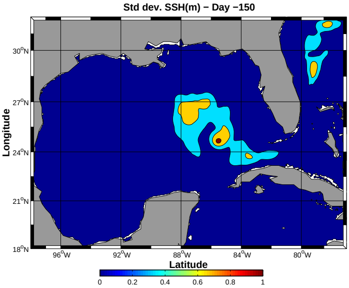


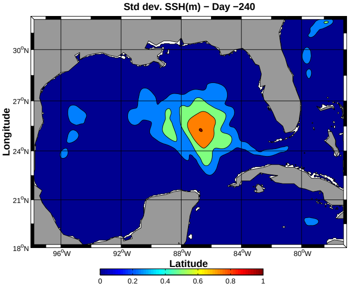
Mean sea-surface height.

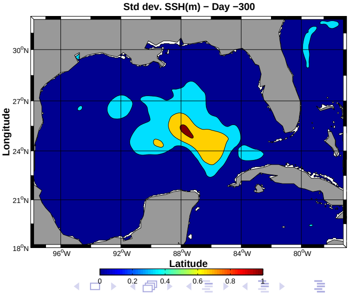


Standard deviation of sea-surface height.

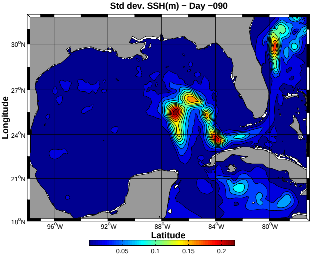


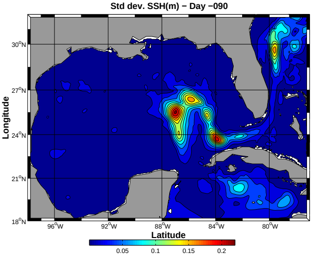


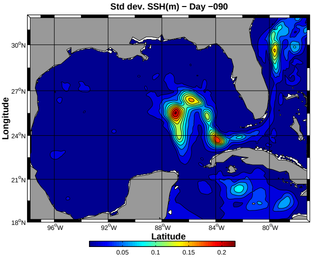


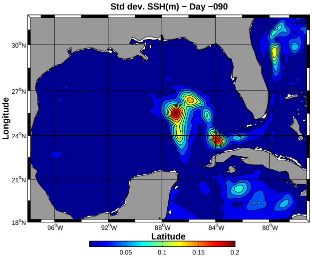


Convergence of series for SSH standard deviation for day 90.









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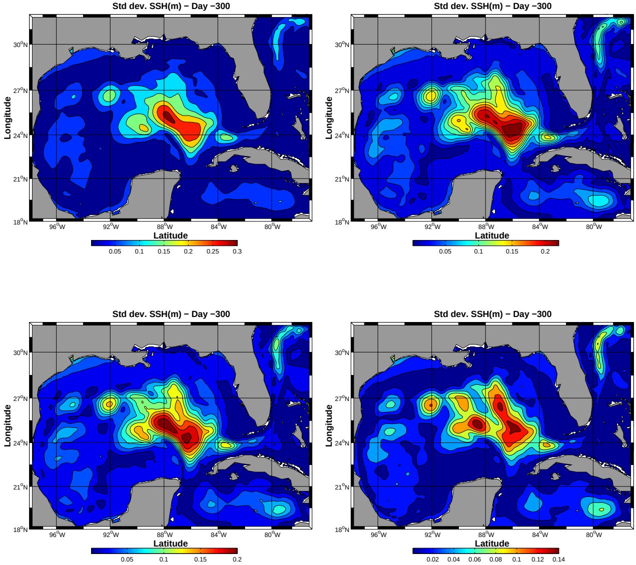
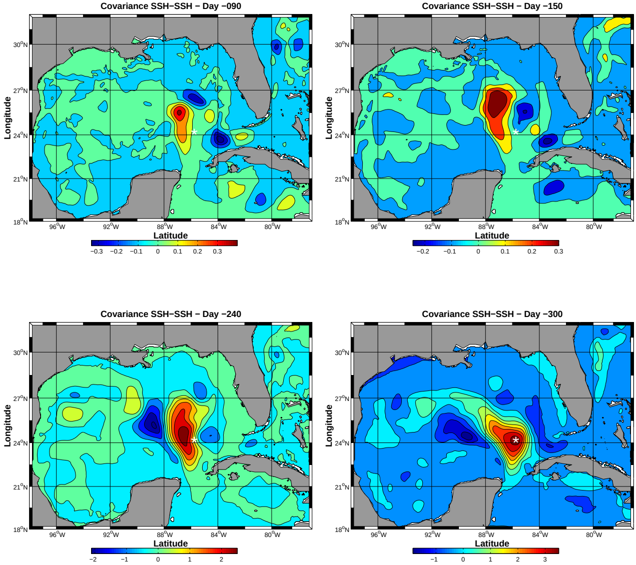
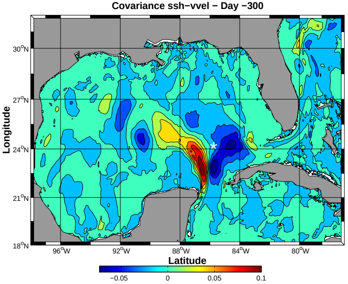
Convergence of series for SSH standard deviation for day 300.

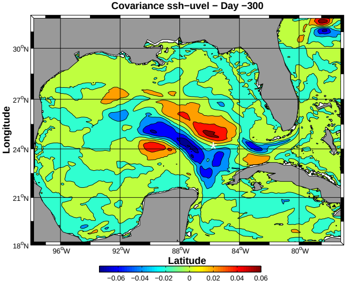


Covariance of SSH with SSH at one point for days 90, 150, 240, and 300.

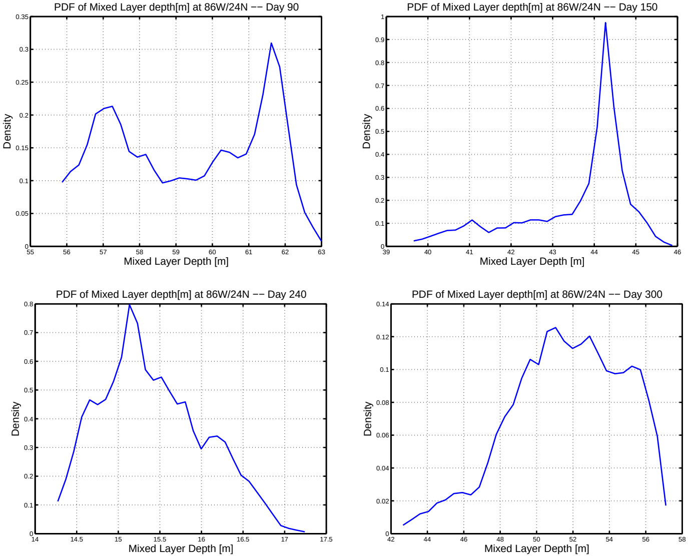


Covariance of u,v-velocity with SSH at one point for day 90.





Kernel density estimates for mixed-layer depth at day 90 from *artificial ensemble*.



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