Polynomial Chaos based uncertainty propagation and quantification in oil drift simulations

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What are Polynomial Chaos Expansions?

- Polynomial Chaos expansions are a form of stochastic spectral expansions that can be used to approximate the probability density of a dynamical system.
- Some desirable aspects of polynomial chaos based probability density estimates include:
  - faster convergence than the standard Monte Carlo type sampling in some cases
  - can provide us with an efficient emulator/surrogate model for use in Bayesian Inference problems
  - model outputs are a function of input uncertainties - allows transfer of uncertainties through complex multi-model applications

Technical Details

- Series expansions using orthogonal polynomial basis functions. Model inputs/parameters are random processes - approximated by a finite dimensional series expansion in input random variables ξ: characterized by its PDF $\rho(\xi)$

$$\mathbf{u}(x,t,\xi_1,\xi_2,\ldots,\xi_N) = \sum_{k=0}^{P} \mathbf{u}(x,t)_k \mathbf{\Psi}_k(\xi_1,\xi_2,\ldots,\xi_N)$$

- $u(x,t,\xi)$: a model output (aka observable)
- $u_k(x,t)$: series coefficients
- $\psi_k(\xi)$: basis functions
- ξ: input characterized by its PDF $\rho(\xi)$

Problem is to determine the P expansion coefficients where:

$$P = \frac{(N+K)!}{(N!K!)} - 1$$

N is the number of uncertain parameters and K is the order of polynomial used.

Non Intrusive Spectral Projections

The orthogonal modes are obtained as:

$$\mathbf{u}(x,t)_k = \langle \frac{\mathbf{u}(x,t,\xi_1,\xi_2,\ldots,\xi_N)\mathbf{\Psi}_k}{\mathbf{\Psi}_k^2} \rangle \quad k = 0,1\ldots.P$$

where the expectations are found by evaluating the equivalent stochastic integrals over ξ-space, e.g.,

$$\langle \mathbf{u}(x,t,\xi_1,\xi_2,\ldots,\xi_N)\psi_k \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathbf{u}(x,t,\xi_1,\xi_2,\ldots,\xi_N)\mathbf{\Psi}_k e^{\frac{-\xi^2}{2}} d\xi$$

using numerical quadrature rules: e. g., Gauss-Hermite quadrature; Lengendre quadrature etc. Once we have the PC coefficients we can compute approximate statistics of the solution with the following formulas:

$$E[u] = E\left[\sum_{k=0}^{P} \mathbf{u}(x,t)_k \mathbf{\Psi}_k\right] = u_0 E[\mathbf{\Psi}_0] + \textstyle\sum_{k=0}^{P} u_0 E[\mathbf{\Psi}_0] = u_0$$

$$Var[u] = E[(u - E[u])^2] = E[((\sum_{k=0}^{P} \mathbf{u}(x,t)_k \mathbf{\Psi}_k) - u_0)^2]$$

$$= E[(\sum_{k=1}^{P} \mathbf{u}(x,t)_k \mathbf{\Psi}_k) - u_0)^2] = \sum_{k=1}^{P} \mathbf{u}(x,t)_k{}^2 E[\mathbf{\Psi}_k{}^2]$$

We can also approximate the PDF of U by sampling from the distribution of ξ and plugging them into the PCE.

Uncertainty in Oil Drift Simulations

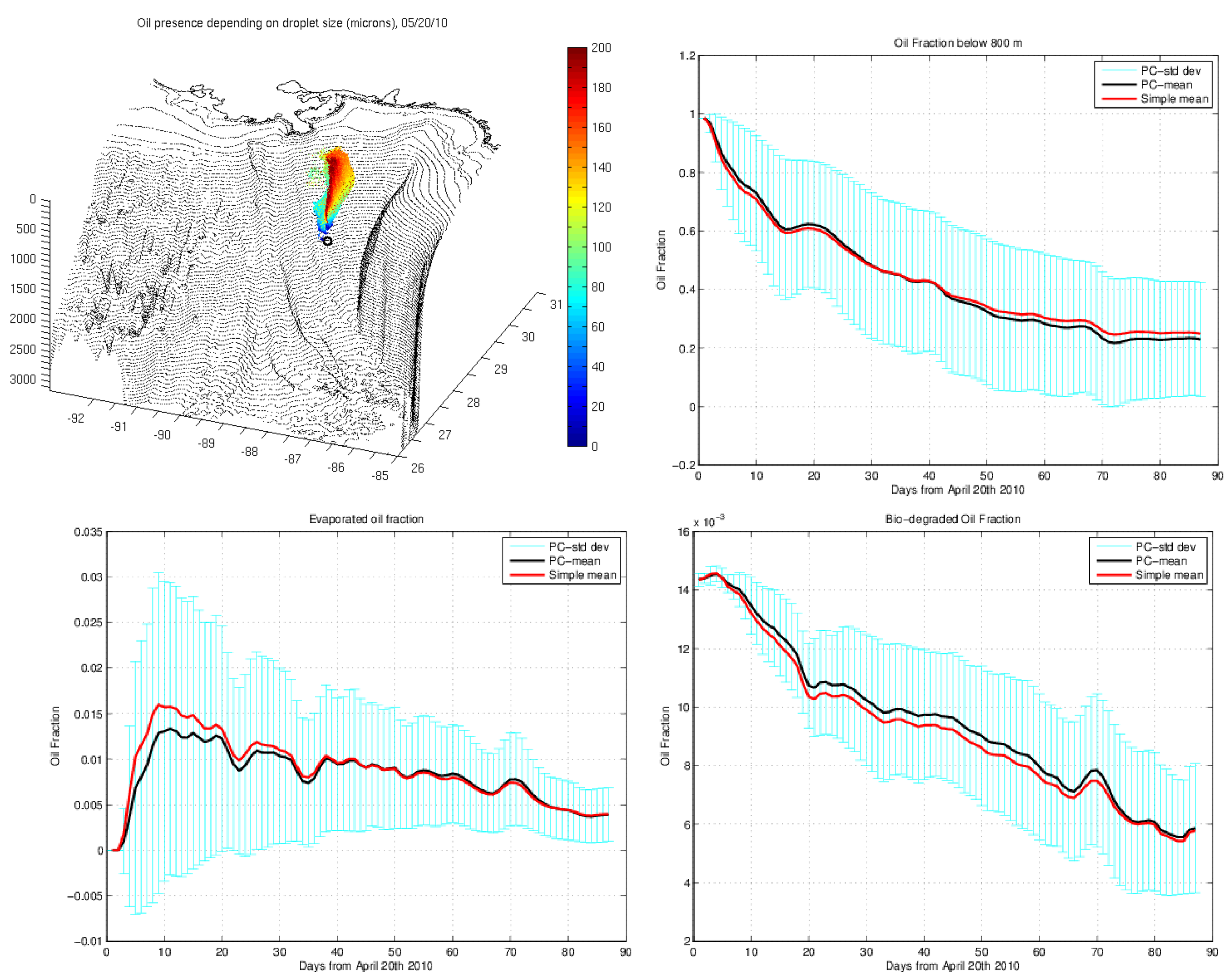
Uncertainty in oil drift simulations arise from:

- model structural deficiency or model error due to simplified representation of real world phenomena
- parametric uncertainty arising due to errors in parameters such as:
  - external inputs such as winds, waves and currents
  - oil chemcial composition, evaporation rates, initial droplet size distribution etc.

Whatever the source, uncertainty is present in every component of an oil drift model and ultimately imposes limitations on the accuracy of the model's output.

A simple test problem applied to the Deep Water Horizon Case

The oil chemical composition and initial droplet size distribution are major sources of uncertainties in the Deep Water Horizon incident. Here we use the polynomial chaos technique to propagate uncertainties in these quantities and assign error bars to computed quantities. We verify the method by comparing it with the traditional Monte Carlo method of estimating uncertainty



Summary

- Polynomial chaos approach looks promising for quantifying uncertainties in oil drift simulations
- The expansions can be mined a posteriori for valuable statistical information at little extra cost to generate PDF's
- The method works well when we have a good understanding of the input uncertainties. These can be sharpened with Bayesian inference when observations are available
- The method is limited by the curse of dimensionality for problems with more than a few uncertain parameters.
- Sparse quadratures might help to extend the method to a larger set of uncertain parameters

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