Quantifying uncertainty in the fate of oil discharged from the Deep Water Horizon accident using Polynomial Chaos expansions and HYCOM outputs

A. Srinivasan[1], M. Iskandarani[1], W. C. Thacker[1] and O. M. Knio[2]

[1]University of Miami
Miami, Florida, USA

[2]Johns Hopkins University
Baltimore, Maryland, USA

07 Feb, 2011

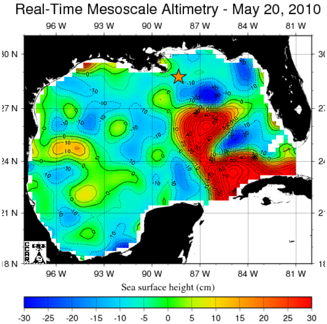
The Deep Water Horizon Well Blowout

- On April 20th 2010 the Deep Water Horizon Rig exploded due to a well blowout. Between April 20th and July 15th 2010, an unknown quantity of crude was discharged into the Gulf of Mexico

- Simulations are used to evaluate various scenarios and provide guidance for field measurements.
- Many sources of uncertainty; need to estimate confidence in simulation results for such problems

Questions:

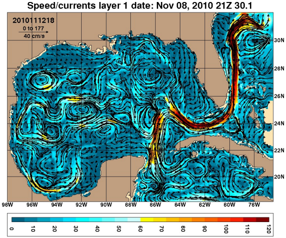
- What is the fate of discharged oil?
- What fraction of oil trapped below the surface?
- Where might the subsurface oil end up? Will it affect the Florida Keys?



- How to assign error bars to the model based answers to the above questions ?

The Oil Fate Modeling Appilcation

- Combine information from ocean circulation models with a 3D oil model which simulates time history of the oil
- We use the the 1/25 ° NRL GOM-HYCOM ocean prediction system outputs



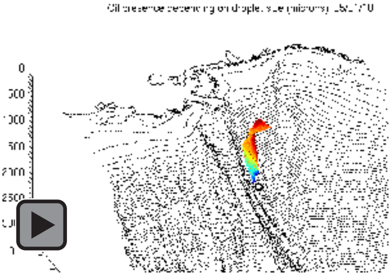
- Data assimilative GOM-HYCOM ocean state estimates generated using the NCODA system
- We use hourly surface data and daily 3D U,V, W, T, S data interpolated to z levels
- Available via the HYCOM THREDDS server http://tds.hycom.org/thredds/dodsC/GOM2010

The Oil Model

The Oil model is a re-implementation of the model described by Korotenko et al (2003) and (2010) with modificatios to include Zheng and Yapa (2003) size and density dependent parameterizations for vertical motion and windage at the surface

- Discharged oil modeled as particles - each representing an aggregation of oil droplets
- Number of particles released is such that each particle represents an oil mass of approximately 1kg
- Particles released 300 m above the well depth of approximately 1500 m
- Particles represent three hydrocarbon fractions - light, medium, heavy
- 3D spreading due to buoyancy, currents and wind
- Weathering, biodegradation, evaporation filters to simulate physical and chemical processes affecting oil.

The Oil Model-2



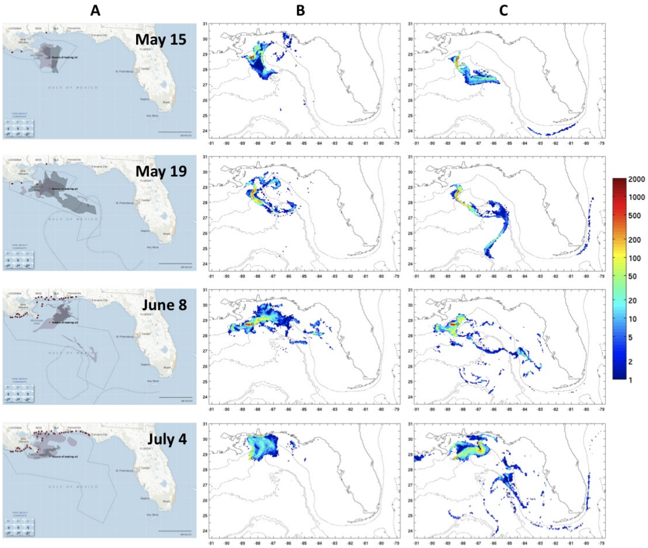
- Particles released every time step
- Particle size is log-normally distributed around a randomly generated modal radius within a specified range.
- The three fractions add up to match the density of the discharged sweet crude oil
- Up to 10 million particles used in simulation

Results:

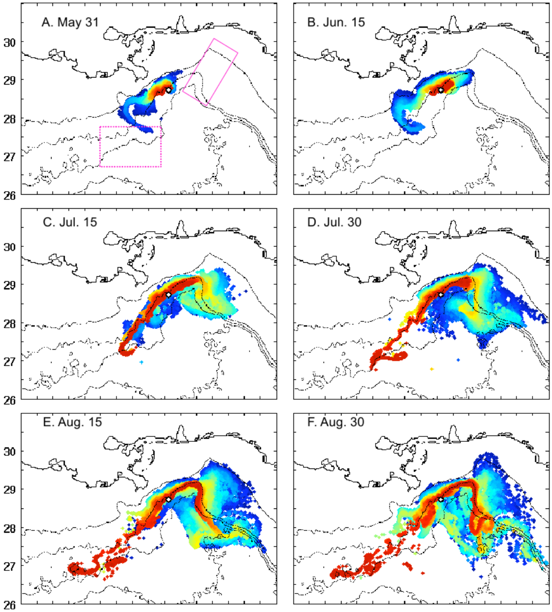
Detailed results are presented in three papers (two submitted to Nature Geoscience and 1 in press in Science)

- Paris et al., Three dimensional simulations of the fate of oil - Part I: Trapped in the deep
- LeHenaff et al.,Three dimensional simulations of the fate of oil -Part II: Gone with the wind
- deGouw et al., 2011 Organic Aerosol Formation Downwind From the Deepwater Horizon Oil Spill

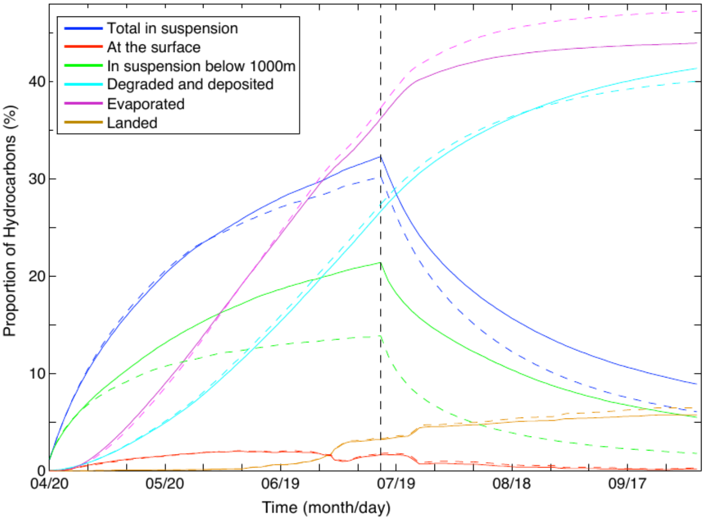
Surface Slick: LeHenaff et al. 2011 submitted



Deep Plumes: Paris et al., 2011 submitted



Oil Inventory: Paris et al. 2011 submitted



Uncertainty Estimation

Two sources of errors or uncertainty in numerical simulations:

- Model Structural deficiency or Model error
- Parametric Uncertainty arising due to errors in parameters such as empirical constants, model inputs etc.
- Usually both types of errors are present
- Here we only consider errors in model parameters
- In this case most of the uncertainty is due to conflicting reports on chemical composition, dispersant use etc.

Propagating and quantifying uncertainty

We would like to propagate uncertainty in oil droplet size and chemical composition and quantify the uncertainty in the solutions and assign error bars

- traditionally Monte Carlo type of analysis is used - straightforward but slow convergence and does not give a response surface

We want to explore the use of stochastic spectral expansion based on Wieners Polynomial Chaos expansions

- model outputs quantified as a function of input uncertainties
- once the functional approximation of the solution is available it is possible to generate pdf's of the solution without re-running the model
- allows us to refine results based on new measurements and transfer uncertainties through the application

Uncertainty Quantification using Stochastic Spectral Expansions

The model solution can be represented as a spectral expansion in terms of suitable orthogonal polynomial basis functions associated with random variables of a given probability density as:

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

- 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. Each uncertain parameter adds a dimension to the probability space that must be explored

Uncertainty Quantification using Stochastic Spectral Expansions

We apply the Non-Intrusive Spectral Projection (NISP) approach to obtain the PC coefficients of the spectral expansion. In this case the orthogonal modes are obtained as:

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

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

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

using quadrature rules: e. g., Gauss-Hermite quadrature; Lengendre quadrature etc.

Uncertainty Quantification using Stochastic Spectral Expansions

Once we have the PC coefficients we can compute approximate statistics of the solution with the following formulas:

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

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

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

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

Uncertain Dimensions and the Number of Model Runs

For a 5th order polynomial, using full tensor products for evaluating stochastic cubatures:

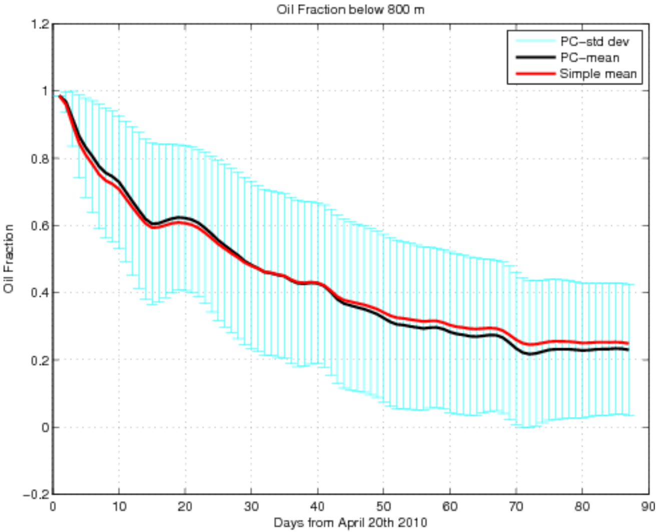
- 2 uncertain parameters - 36 runs
- 3 uncertain parameters - 216 runs
- 4 uncertain parameters - 1024 runs

Leads to "the curse of dimensionality". Also leads to a big data processing problem!!! We consider two random dimensions for this problem

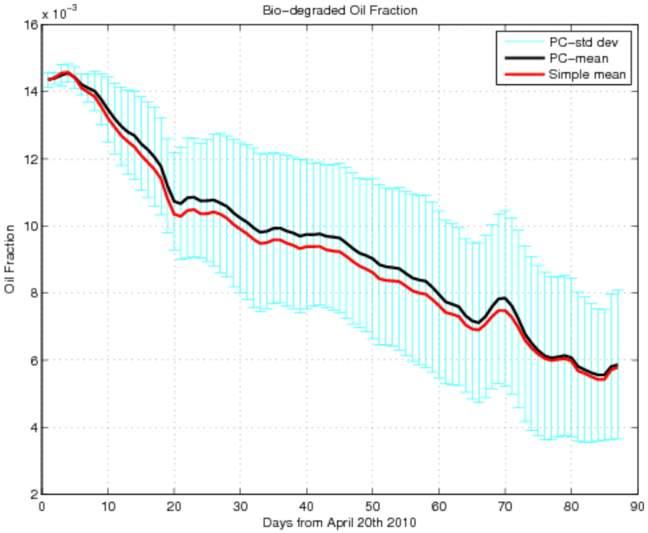
- radius of the oil drops uniformly distributed between 1-300 microns.
- chemical composition of the oil uniformly distributed between 0-1.

We can also propagate errors in HYCOM outputs but it will require at least two additional random dimensions

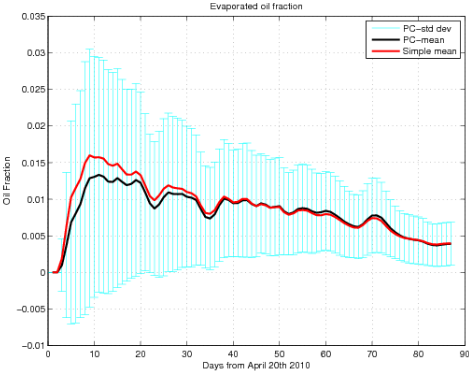
Sample Results:



Sample Results:



Sample Results:



Summary:

- We have tested a Polynomial Chaos based methodology for quantifying uncertainties in the fate of oil discharged in the DWH incident
- The method is seen to be a viable alternative to monte-carlo type methods to quantify uncertainties arising due to a relatively small number of inputs
- We are extending the analysis to acccount for uncertainties in HYCOM outputs.