# Inferring Release Characteristics From an Atmospheric Dispersion Model

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#### The Cast

#### The work presented in this talk was done in collaboration with



Devin Francom, LANL



#### Vera Bulaevskaya, TCC

#### Matthew Simpson, LLNL



Donald Lucas, LLNL

## Diablo Canyon Nuclear Power Plant





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Air samples were obtained from 7:00 to 18:00 at 150 sites. 24% are missing.



## FLEXPART Simulations



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18,000 different combinations of the 11 input parameters of FLEXPART are sampled from a latin hypercube. These result in 18,000 plumes varying in space and time.

#### Input Parameters

#### Continuous Input Parameters

Input	Lower Bound	Upper Bound	True Value
Latitude	35.1977	35.2250	35.2111
Longitude	-120.87	-120.83	-120.8543
Altitude	1	10	2
Start Time	7:00	9:00	8:00
Duration	6	10	8
Amount	10	1000	146.016

#### Categorical Inputs

Input	Number of values
Pre-release Initialization time	2
Boundary Layer Model	3
Nudging	3
Reanalysis	3
Land Model	3

There are five nested domains for WRF models. Each combination of the five categorical variables produces a different wind field at 300 meters resolution.

#### Emulator

We build an emulator for the computer output corresponding to location s, time t and input values x, by using the representation on empirical orthogonal functions

$$y^{c}(s,t,x) = \sum_{i=1}^{k} K_{i}(s,t)w_{i}(x) + u(s,t)$$

The EOFs are calculated from the model runs

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For the truncation we take a non-Gaussian error

$$u(s,t) \sim Unif[y^c(s,t,x_j) - \sum_{i=1}^k K_i(s,t)w_i(x_j),$$
$$j = 1, \dots, n_x]$$

This is important in order to propagate truncation uncertainty

#### Estimating the EOF coefficients

To estimate the coefficients in the EOF we set:

$$w_i(x) = \eta_i(x) + \epsilon_i$$

where

$$\eta(x) = a_0 + \sum_{m=1}^{M} a_m B_m(x)$$

is a representation on adaptive spline basis composed of M (unknown) terms, that uses products of hockey sticks with varying signs, number of interactions, and unknown knots.



0.4

0.6

08

1.0

0.0

0.2

Spline Fit

## Categorical an Continuous Inputs

Our application requires the emulator to handle continuous and categorical inputs. Assume that  $x_1$  and  $x_2$  are continuous, and  $x_3$  and  $x_4$  are categorical, then

$$B(x) = [s_1(x_1 - t_1)]^{\alpha}_+ [s_2(x_2 - t_2)]^{\alpha}_+ \mathbf{1}_{x_3 \in C_3} \mathbf{1}_{x_4 \in C_4}$$

where t1 and t2 are the knots and

 $s_i = \pm 1$ 

and Ci corresponds to one or more categories of the i-th variable.

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- Allows for basis functions specific to some categories
- Allows for basis functions common to all categories
- Learn from the data the categorical variables in each basis function, if any

## **Emulation Performance**



Predictions at 15 of the of the 137 locations considered for a held out configuration of the input parameters.

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Predictions at 15 of the of the 137 locations considered for another held out configuration of the input parameters.

## Global Sensitivity



Analytic expressions are available for the time and spacevarying Sobol coefficients for the different inputs and interactions.

**Calibration:**  $p(\theta|Y^F, Y^C)$ 

Observation Equation with Gaussian error



System Equation with additive discrepancy with U[0,2] multiplication factor

Discrepancy  $\zeta(s,t) = \underbrace{y^P(s,t,\theta)}_{+} + \gamma \delta(s,t)$ 

Best Estimate

**Calibration:**  $p(\theta|Y^F, Y^C)$ 

Observation Equation with Gaussian error



System Equation with additive discrepancy with U[0,2] multiplication factor

$$\zeta(s,t) = \underbrace{y^P(s,t,\theta)}_{\nabla \delta(s,t)} + \underbrace{\gamma \delta(s,t)}_{\nabla \delta(s,t)}$$

Best Estimate

We estimate the discrepancy by fitting the emulator at the prior mean of the inputs. We then fit the discrepancy using adaptive splines (BASS).  $\gamma$  provides information about the relevance of the discrepancy.

# Posteriors for Continuous Inputs



Discrepancy

No discrepancy

# Posteriors for Categorical Inputs



No discrepancy



Discrepancy

#### Calibrated Predictions



## Calibrated Release Location



The release location was originally misreported. Our posterior distribution reveals that a second source of information corresponds to a much more probable location

# Analysis of Discrepancies



Clusters of discrepancy curves identifying clear location patterns.

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- Our method can handle continuous and categorical inputs.
- We able to perform a time and space-varying sensitivity analysis of the inputs based on accurate analytic expressions for the global sensitivity coefficients.
- The method uses a fully probabilistic approach that allows to account for all sources of variability and provides a coherent quantification of the uncertainty.

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