Polynomial Chaos based Minimum Variance Approach for Characterization of Source Parameters

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Introduction

- Inverse Problem refers to problem of characterizing the system of interest by exploiting measurements resulting for the system (eg. source identification).
  - Source parameters, initial conditions, boundary conditions
  - Uncertainty in the identified source parameters, initial conditions, etc.

- Inverse problems are often ill-posed (eg. optical flow).
  - Tikhonov regularization

- For large scale systems (eg. volcanic plume source ID), the computational cost is significant.

PUFF simulation model

- PUFF is a *Lagrangian* Trajectory Volcanic Ash Tracking Model which initializes and transports a collection of discrete ash particles, representing a sample of the eruption cloud.

- Different types of transport include:
  - Advection: due to the wind field (W)
  - Diffusion: due to turbulent dispersion (Z)
  - Fallout: due to the gravity and Stoke's law (S)

- **Lagrangian Model:**

$$R_i(t+\Delta t) = R_i(t) + W(t)\Delta t + Z(t)\Delta t + S_i(t)\Delta t \qquad i = 1, \ldots \text{Number of particles}$$

where, $R_i(t)$ is position vector of i^{th} ash particle at time t.

PUFF simulation model

- **W(t)** is the local wind velocity which is calculated for each particle by interpolating four dimensional (longitude/latitude/height/time) wind data (obtained from forecast meteorological data) to the particle's position and time.

- Turbulent dispersion for each particle is modeled with a *random walk* process Z(t).
  - A random walk is a process where a particle takes a step at discrete time intervals in such a manner that each step is independent of the others.

- Turbulent dispersion $Z(t)\Delta t$ is a vector containing three dimensional Gaussian random numbers with zero mean and specific standard deviation $\sqrt{\frac{2K}{\Delta t}}$.
  - Diffusion coefficient **K** is independent of particle size and local wind dynamics.

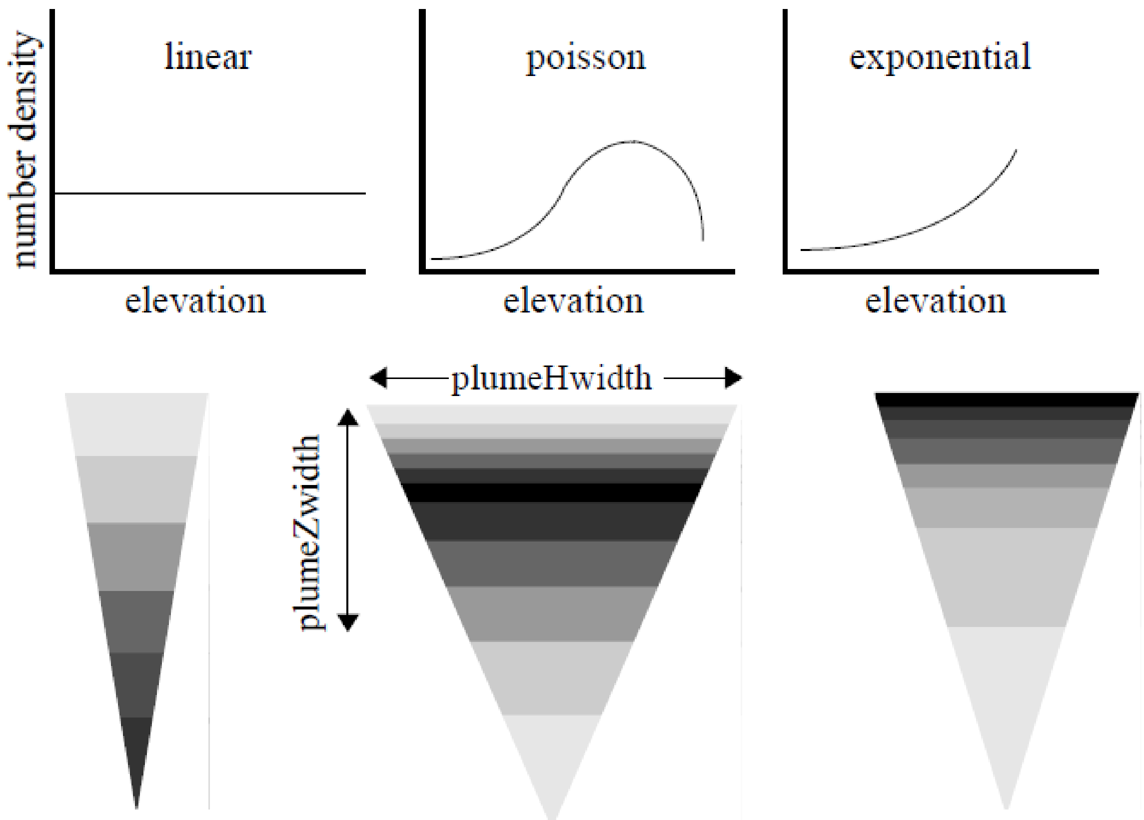
- Ash fallout $S_i(t)=[0\ \ 0\ \ s_i]^T$ is three dimensional vector where the terminal speed s_i is approximated by using Stoke's law and is a function of radius of the particle r_i, dynamic viscosity coefficient η, gravitational acceleration g, density of the particle ρ_{pi}, and density of the atmosphere ρ_f:

$$s_i = \frac{2}{9}\frac{\left(\rho_{p_i} - \rho_f\right)}{\eta} g R_i^2$$

PUFF simulation model

- Initialization

- To initialize the simulation, we need to specify initial location of ash *[lat, lon, z]*, time period of simulation t, and the number of particles N.
- Distribution of particles along elevation *z* direction can be defined in different ways:



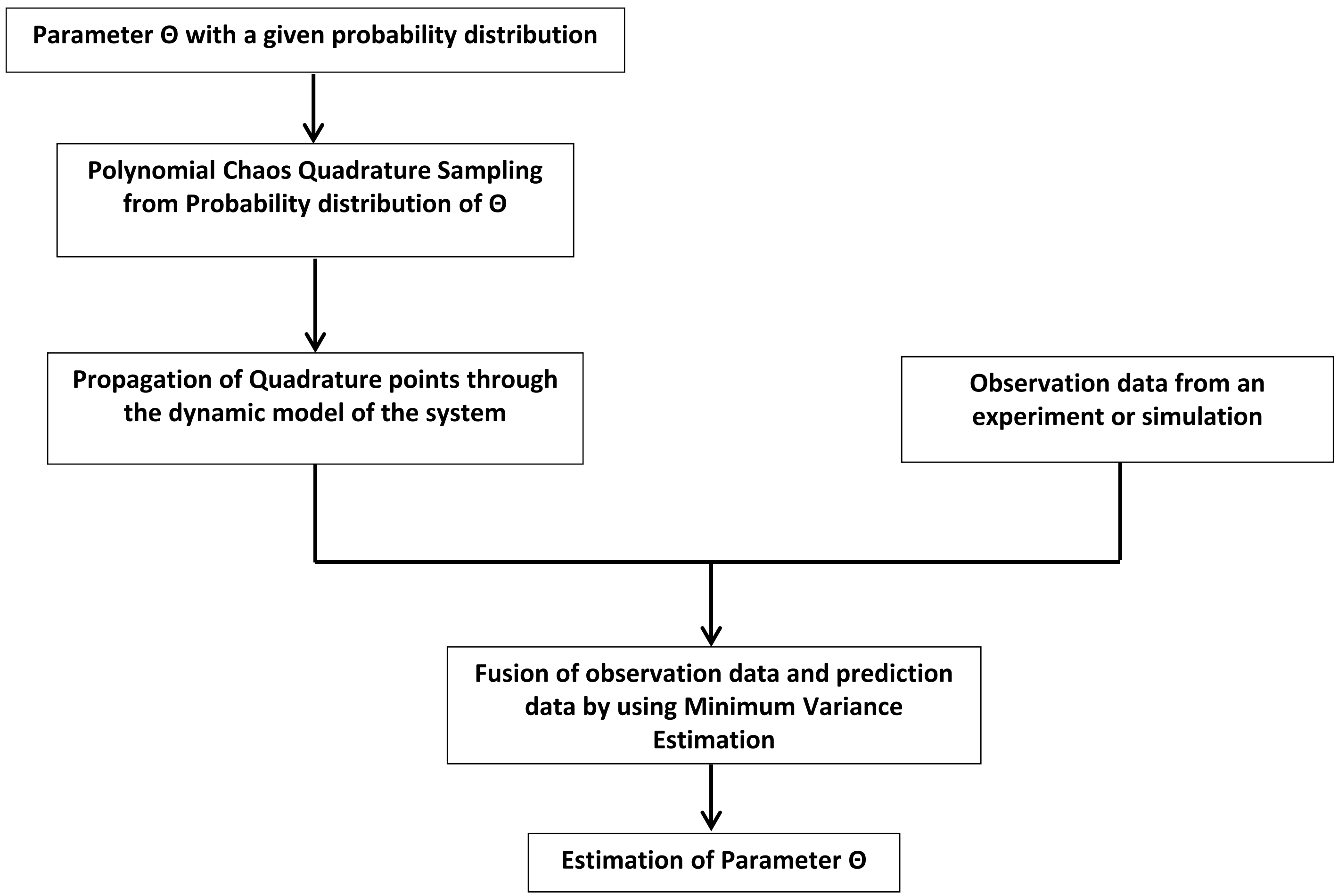
- Initialization
Bent model:

- In this simulation, Bent model has been used instead of mentioned methods for describing the initial distribution of particles along the height.
- BENT solves a cross-sectionally averaged system of equations for continuity, momentum and energy balance as a function of the eruption vent radius and speed of the ejecta.
- BENT assumes a distribution of pyroclasts of different sizes, and the model equations then predict the height distribution of the various sized clasts.
- For this research, the vent size, vent velocity, mean and deviation of particle size form the source parameters which drive the BENT/PUFF model.

Effect of wind on the rise height of volcanic plumes, M. Bursik,
Geophysical Research Letters, Vol. 28, No. 18, pp. 3621-3624, 2001

Inverse Problem

- The inverse problem requires a forward model and observations
  - The BENT/PUFF advection-diffusion model is used to represent the plume dynamics



Polynomial Chaos:

- Originally used by Norbert Wiener in 1938, to describe the members of the span of Hermite polynomial functionals of standard Gaussian random variables.

- The PC series representation of random variables is used (Ghanem & Spanos, 1991) to model uncertainty in dynamic systems.

- The Hermite polynomial chaos expansion :
  - A Gaussian random variable:
  - Basis: Hermite polynomials

$$\omega \in \mathcal{N}(\mu, \sigma^2) = a_0 H_0(\xi) + a_1 H_1(\xi)$$

$$H_0 = 1 \qquad H_1 = \xi \in \mathcal{N}(0, 1)$$

$$a_0 = \mu \qquad a_1 = \sigma$$

- Generalized (Xiu & Karniadakis, 2002) to use the orthogonal polynomials from the Askey-scheme to model various probability distributions in the scheme, with exponential convergence.

Probability Distribution	Polynomial basis
Gaussian	Hermite Polynomials
Gamma	Laguerre polynomials
Beta	Jacobi polynomials
Uniform	Legendre polynomials

Inverse Problem:

- Forward Propagation

- **Polynomial Chaos Quadrature:**

  The propagation of uncertainty due to time-invariant but uncertain input parameters can be approximated by a generalization of polynomial chaos.

$$\dot{\mathbf{x}}(t, \mathbf{\Theta}) = \mathbf{f}(t, \mathbf{\Theta}, \mathbf{x}, \mathbf{u}), \quad \mathbf{x}(t_0) = \mathbf{x}_0$$

  where, $X \in R^n$ and $\Theta \in R^m$ can be written in Polynomial Chaos Expansion as:

$$x_i(t, \mathbf{\Theta}) = \sum_{k=0}^{N} x_{i_k}(t)\phi_k(\boldsymbol{\xi}) = \mathbf{x}_i^T(t)\mathbf{\Phi}(\boldsymbol{\xi}) \Rightarrow \mathbf{x}(t, \boldsymbol{\xi}) = \mathbf{X}_{pc}(t)\Phi(\boldsymbol{\xi})$$

$$\theta_i(\boldsymbol{\xi}) = \sum_{k=0}^{N} \theta_{i_k}\phi_k(\boldsymbol{\xi}) = \mathbf{\Theta}_i^T \mathbf{\Phi}(\boldsymbol{\xi}) \Rightarrow \mathbf{\Theta}(t, \boldsymbol{\xi}) = \mathbf{\Theta}_{pc}\Phi(\boldsymbol{\xi}) \qquad \theta_{i_k} = \frac{\langle \theta_i(\boldsymbol{\xi}), \phi_k(\boldsymbol{\xi}) \rangle}{\langle \phi_k(\boldsymbol{\xi}), \phi_k(\boldsymbol{\xi}) \rangle}$$

- By substitution of these equations back into stochastic differential equation, we have

$$\mathbf{e}_i(\mathbf{X}_{pc}, \boldsymbol{\xi}) = \sum_{k=0}^{N} \dot{x}_{i_k}(t)\phi_k(\boldsymbol{\xi}) - \mathbf{f}_i(t, \mathbf{X}_{pc}(t)\Phi(\boldsymbol{\xi}), \mathbf{\Theta}_{pc}\Phi(\boldsymbol{\xi})), \quad i = 1, 2, \cdots, n$$

- To minimize this error, we use *Galerkin approach* to force its projections on basis functions $\boldsymbol{\varphi_i(\xi)}$s to be zero.

Inverse Problem:

- Forward Propagation

- Evaluation of projection integrals is not always easy!

$$\langle \mathbf{e}_i(\mathbf{X}_{pc}, \boldsymbol{\xi}), \phi_j(\boldsymbol{\xi})\rangle =$$

$$\sum_{k=0}^{N} \dot{x}_{i_k} \int_{\xi} \phi_k(\boldsymbol{\xi})\phi_j(\boldsymbol{\xi})d\boldsymbol{\xi} - \underbrace{\int_{\xi} \mathbf{f}_i(t, \mathbf{X}_{pc}(t)\Phi(\boldsymbol{\xi}), \boldsymbol{\Theta}_{pc}\Phi(\boldsymbol{\xi}))\phi_j(\boldsymbol{\xi})d\boldsymbol{\xi}}_{=\,?} = 0 \quad i = 1, \cdots, n, \quad j = 0, \cdots, N$$

- To simplify integration process, we use M *Quadrature Points*

$$\int \phi_i(\boldsymbol{\xi})\phi_j(\boldsymbol{\xi})p(\boldsymbol{\xi})d\boldsymbol{\xi} \simeq \sum_{q=1}^{M} w_q \phi_i(\boldsymbol{\xi}_q)\phi_j(\boldsymbol{\xi}_q)$$

$$\int \mathbf{f}_i(t, \mathbf{X}_{pc}(t)\Phi(\boldsymbol{\xi}), \boldsymbol{\Theta}_{pc}\Phi(\boldsymbol{\xi}))\phi_j(\boldsymbol{\xi})p(\boldsymbol{\xi})d\boldsymbol{\xi} \simeq \sum_{q=1}^{M} w_q \mathbf{f}_i(t, \mathbf{X}_{pc}(t)\Phi(\boldsymbol{\xi}_q), \boldsymbol{\Theta}_{pc}\Phi(\boldsymbol{\xi}_q))\phi_j(\boldsymbol{\xi}_q)$$

Inverse Problem:

- Data Assimilation

Minimum Variance Estimator:

$$
\begin{aligned}
\hat{\mathbf{z}}_k^+ &= \hat{\mathbf{z}}_k^- + \mathbf{K}_k[\tilde{\mathbf{y}}_k - \mathbf{E}^-[\mathbf{h}(\mathbf{x}_k)]] \\
\boldsymbol{\Sigma}_k^+ &= \boldsymbol{\Sigma}_k^- + \mathbf{K}_k \boldsymbol{\Sigma}_{zy} \\
\mathbf{K}_k &= -\boldsymbol{\Sigma}_{zy}^T \left(\boldsymbol{\Sigma}_{hh}^- + \mathbf{R}_k\right)^{-1}
\end{aligned}
$$

Where, z_k is the augmented state vector of states and parameters and prior and posterior mean and covariance matrices are equal to:

$$
\hat{\mathbf{z}}_k^- \triangleq \mathbf{E}^-[\mathbf{z}_k] = \begin{bmatrix} \mathbf{X}_{pc_1}^-(t) \\ \boldsymbol{\Theta}_{pc_1}^- \end{bmatrix} \quad \boldsymbol{\Sigma}_k{}^- \triangleq \mathbf{E}^-[(\mathbf{z}_k - \hat{\mathbf{z}}_k^-)(\mathbf{z}_k - \hat{\mathbf{z}}_k^-)^T] = \begin{pmatrix} \sum_{i=1}^N \mathbf{X}_{pc_i}^{-2} & \sum_{i=1}^N \mathbf{X}_{pc_i}^- \boldsymbol{\Theta}_{pc_i}^- \\ \sum_{i=1}^N \mathbf{X}_{pc_i}^- \boldsymbol{\Theta}_{pc_i}^- & \sum_{i=1}^N \boldsymbol{\Theta}_{pc_i}^{-2} \end{pmatrix}
$$

$$
\hat{\mathbf{z}}_k^+ \triangleq \mathbf{E}^+[\mathbf{z}_k] = \begin{bmatrix} \mathbf{X}_{pc_1}^+(t) \\ \boldsymbol{\Theta}_{pc_1}^+ \end{bmatrix} \quad \boldsymbol{\Sigma}_k^+ \triangleq \mathbf{E}^+[(\mathbf{z}_k - \hat{\mathbf{z}}_k^-)(\mathbf{z}_k - \hat{\mathbf{z}}_k^-)^T] = \begin{pmatrix} \sum_{i=1}^N \mathbf{X}_{pc_i}^{+2} & \sum_{i=1}^N \mathbf{X}_{pc_i}^+ \boldsymbol{\Theta}_{pc_i}^+ \\ \sum_{i=1}^N \mathbf{X}_{pc_i}^+ \boldsymbol{\Theta}_{pc_i}^+ & \sum_{i=1}^N \boldsymbol{\Theta}_{pc_i}^{+2} \end{pmatrix}
$$

Inverse Problem:

- Data Assimilation

- $\tilde{y}_k$ denotes the sensor output obtained from the following observation model:

$$\mathbf{y}_k \triangleq \mathbf{y}(t_k) = \mathbf{h}(\mathbf{x}_k, \boldsymbol{\Theta}) + \boldsymbol{\nu}_k$$

with known distribution for the noise v_k.

- As well, h_k, Σ_{zy} and Σ_{zz} are defined as:

$$\hat{\mathbf{h}}_k^- \triangleq \mathbf{E}^-[\mathbf{h}(\mathbf{x}_k, \boldsymbol{\Theta})] = \sum_{q=1}^{M} w_q \underbrace{\mathbf{h}(\mathbf{x}_k(\boldsymbol{\xi}_q))}$$

$$\boldsymbol{\Sigma}_{zy} \triangleq \mathbf{E}^-[(\mathbf{z}_k - \hat{\mathbf{z}}_k)(\mathbf{h}(\mathbf{x}_k) - \hat{\mathbf{h}}_k^-)^T] = \sum_{q=1}^{M} w_q(\mathbf{z}_k(\boldsymbol{\xi}_q) - \hat{\mathbf{z}}_k^-)(\mathbf{h}_q - \hat{\mathbf{h}}_k^-)^T$$

$$\boldsymbol{\Sigma}_{hh}^- \triangleq \mathbf{E}^-[(\mathbf{h}(\mathbf{x}_k) - \hat{\mathbf{h}}_k^-)(\mathbf{h}(\mathbf{x}_k) - \hat{\mathbf{h}}_k^-)^T] = \sum_{q=1}^{M} w_q(\mathbf{h}_q - \hat{\mathbf{h}}_k^-)(\mathbf{h}_q - \hat{\mathbf{h}}_k^-)^T$$

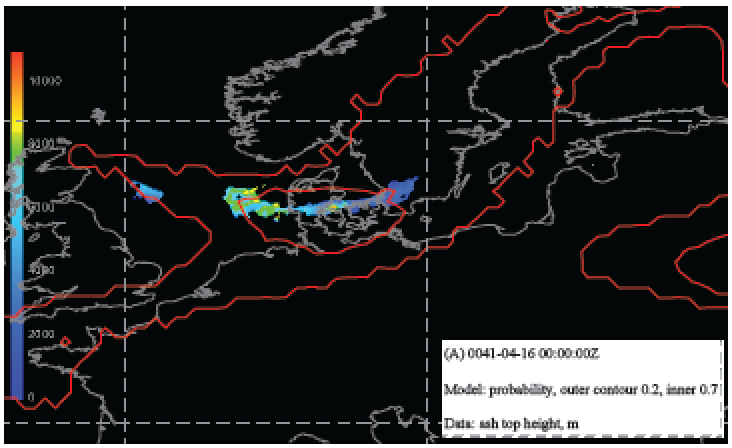
Simulation:

- For validation purposes, we consider the Eyjafjallajökull eruption scenario.
- PUFF model used to propagate ash parcels in a given wind field (NCEP Reanalysis) through time concentrating on the period 14–16 April 2010.
- Variability in the height and loading of the eruption is introduced through the volcano column model BENT.
- Table 1 lists all source variables together with their assumed uncertainties.

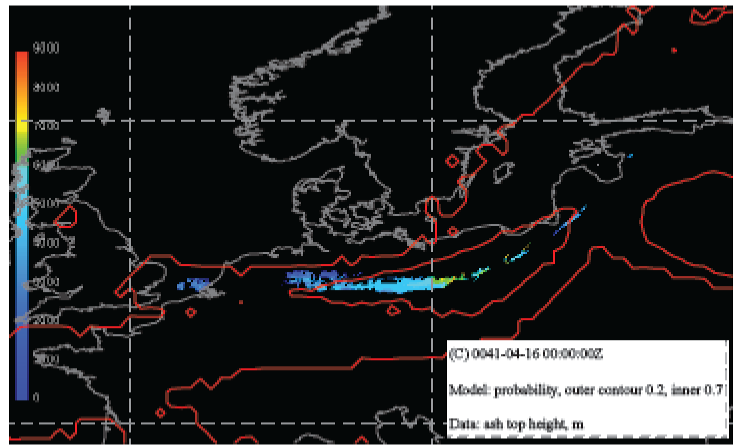
Parameter	Value Range	PDF
Vent Radius, b_0 (m)	65 – 150	Uniform, + definite
Vent Velocity, w_0 (m/s)	45 – 124	Uniform, + definite
Mean Grain Size, Md_ϕ, ϕ units	2 boxcars: 1.5 -2 and 3 – 5	Uniform ϵ R
σ_ϕ, ϕ units	2 - 6	Uniform ϵ R

Simulation

- Forward Propagation:



(a) April 16^{th}, 0000 hrs



(b) April 16^{th}, 1200 hrs

Probability distribution contours and satellite image

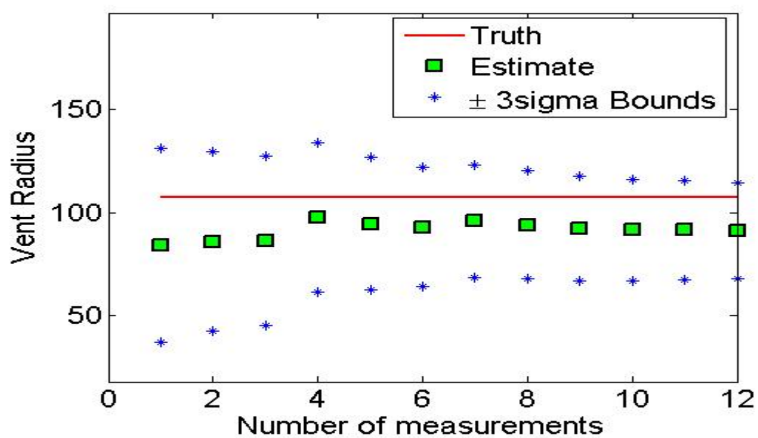
Outer Contour: 0.2 (probability of ash present in enclosed area is >=20%)

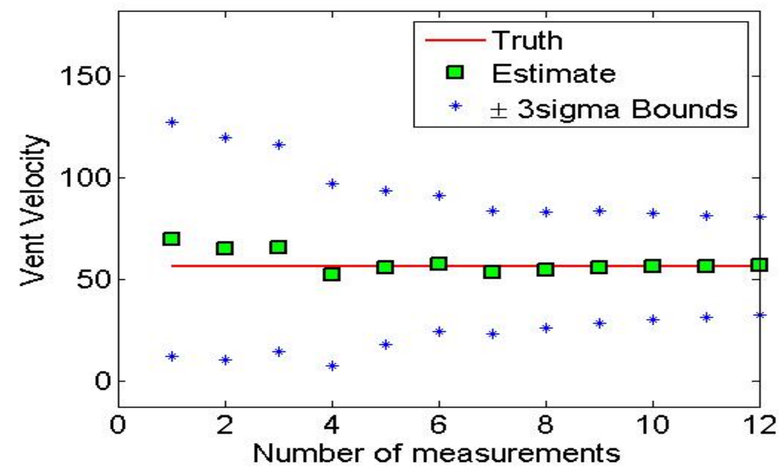
Inner Contour: 0.7 (probability of ash present in enclosed area is >=70%)

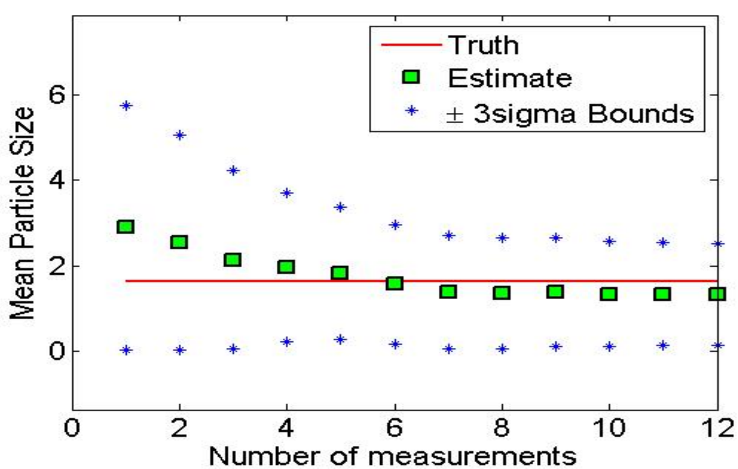
Colored plume: spatial variation of observed plume ash height

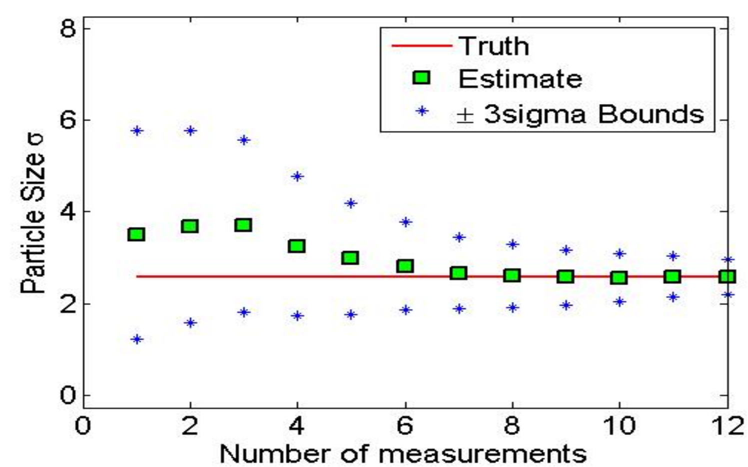
Simulation

- Inverse Problem:









SCIPUFF

SCIPUFF (**Second-order Closure Integrated PUFF**)

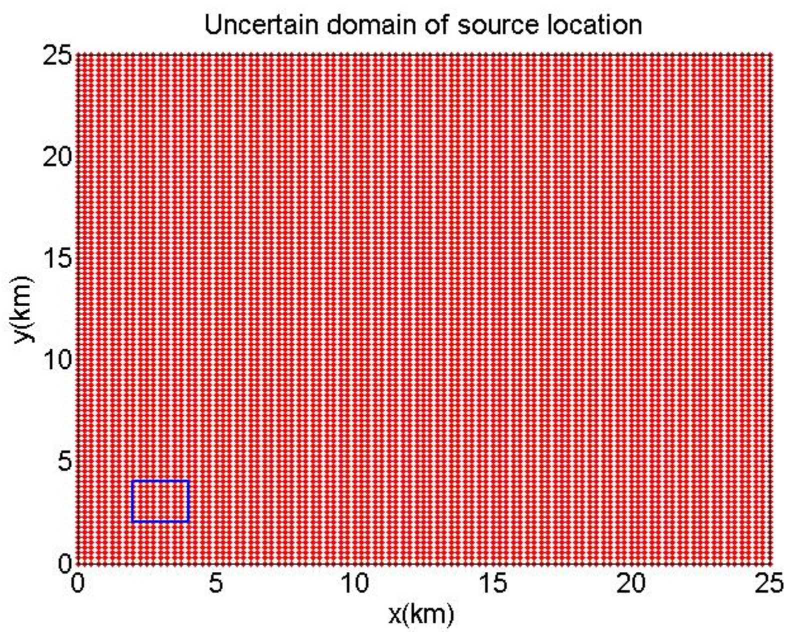
- Developed by Titan Corporation, Princeton, NJ under the sponsorship of U. S. Defense Special Weapons Agency (DSWA)
- a Lagrangian transport and diffusion model for atmospheric dispersion applications.
- uses three dimensional Gaussian puff representation for the concentration field of a dispersing contaminant to solve advection-diffusion equation.

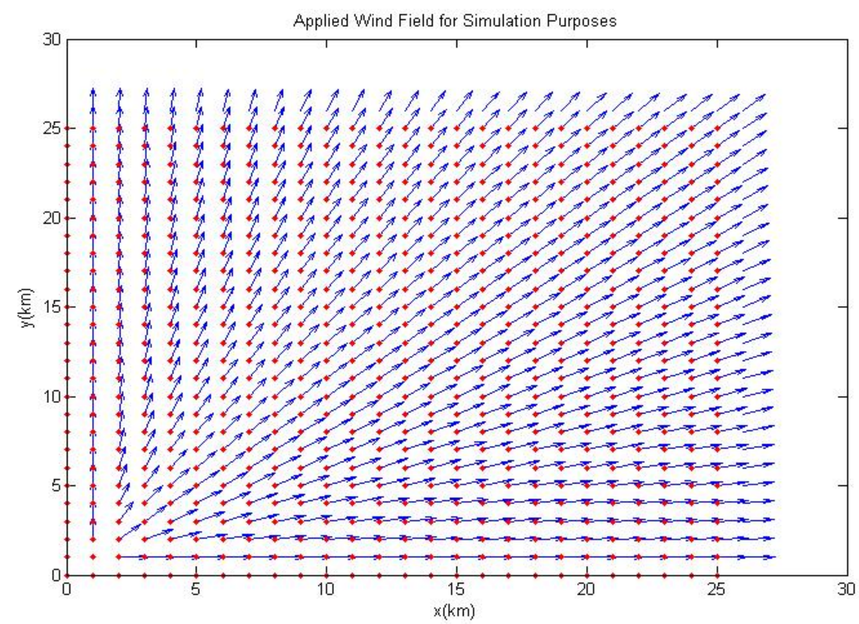
Location Uncertainty

• Source of the material is assumed to be uniformly distributed on a square of [2, 4] x [2, 4] km^2.

• Time period of simulation is considered to be 1 hour (3600 sec.)

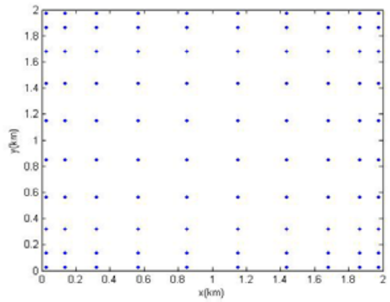
• 101 x 101 grid is used to record the concentration of Propane during the propagation time period.

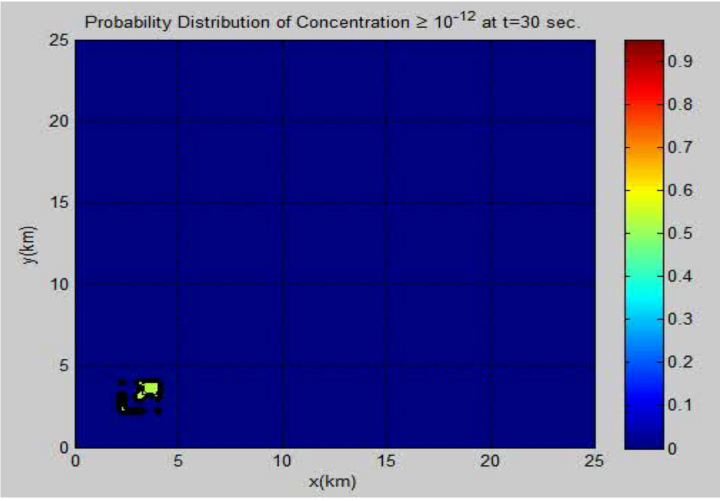




PCQ approach

- 10x 10 quadrature points are being used to cover the support of source location.
- These quadrature points are propagated by using SCIPUFF model during the time.
- Polynomial basis functions are constructed according to the applied distribution for the uncertain source location.
- Coefficients of PC expansions can be found using the Polynomial Chaos quadrature technique.
- After finding coefficients, PC expansion of the output of the SCIPUFF model is constructed acc. to distribution of uncertain source.
- Large number of realizations of PC expansion is generated.
- Probability Distribution of concentration > threshold is equal to the number of PC realizations which are greater than that threshold divided by the total number of realizations.



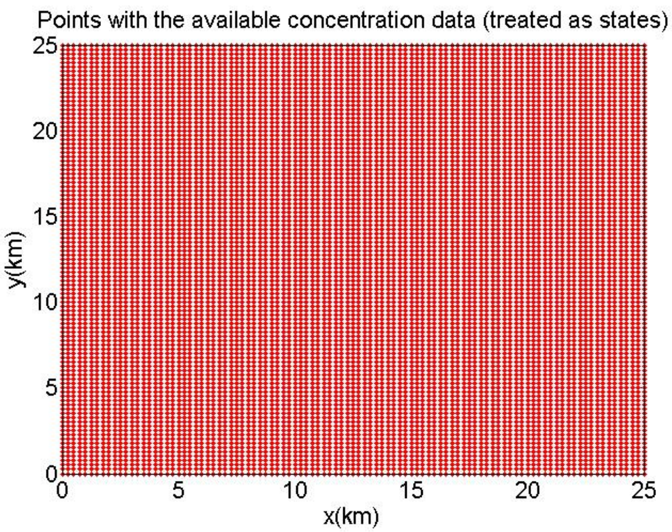


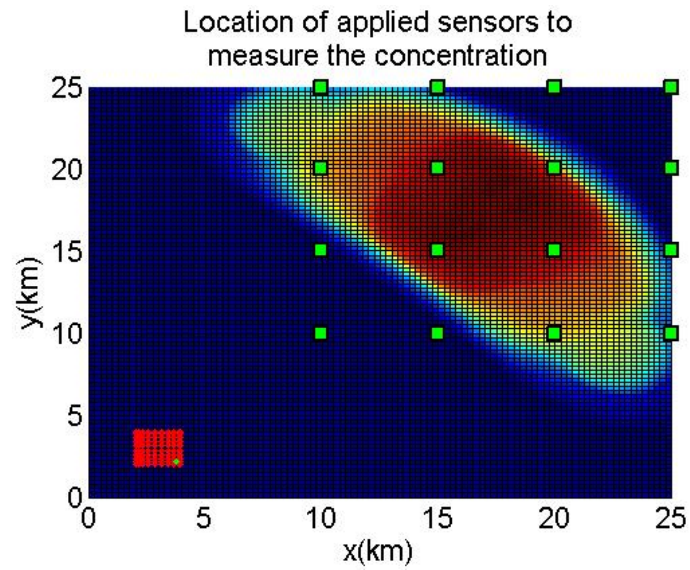
Inverse Problem:

- Given a *set of observation* data and a priori information about the source location, what is the best guess about the actual position of the source?

$$\tilde{y}_k = h(t_k, c_k(z)) + v_k$$
$$v = N(0, R)$$

where, $x \in R^n, \tilde{y} \in R^m, n >> m$ and $Z \in R^2$ represent states, observations, and coordination of source location, respectively.



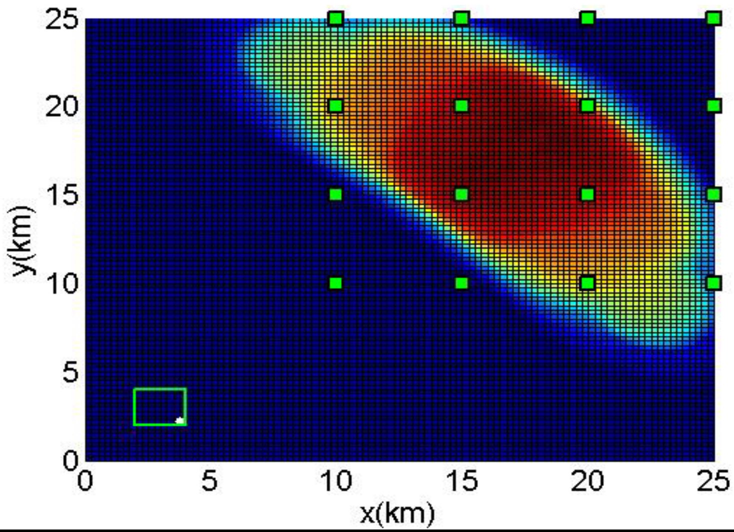


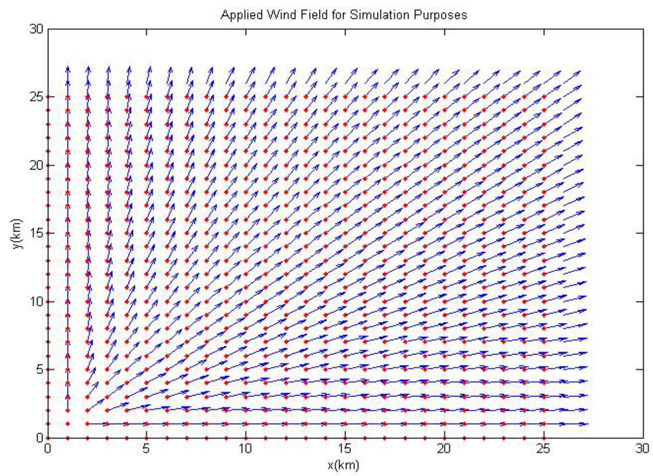
Source Identification

- Numerical Simulations

- 16 sparsely distributed sensors have been considered for observation purposes.
- Observation data are polluted with noise.
- Source location is assumed to be uniformly distributed over [2,4]x[2,4] km^2.
- Actual source location is at point (3.8 , 2.2).
- Source uncertainty is assumed to be the only uncertainty in the model dynamics.

- Polynomial Chaos Quadrature (PCQ) Points have been used during estimation.



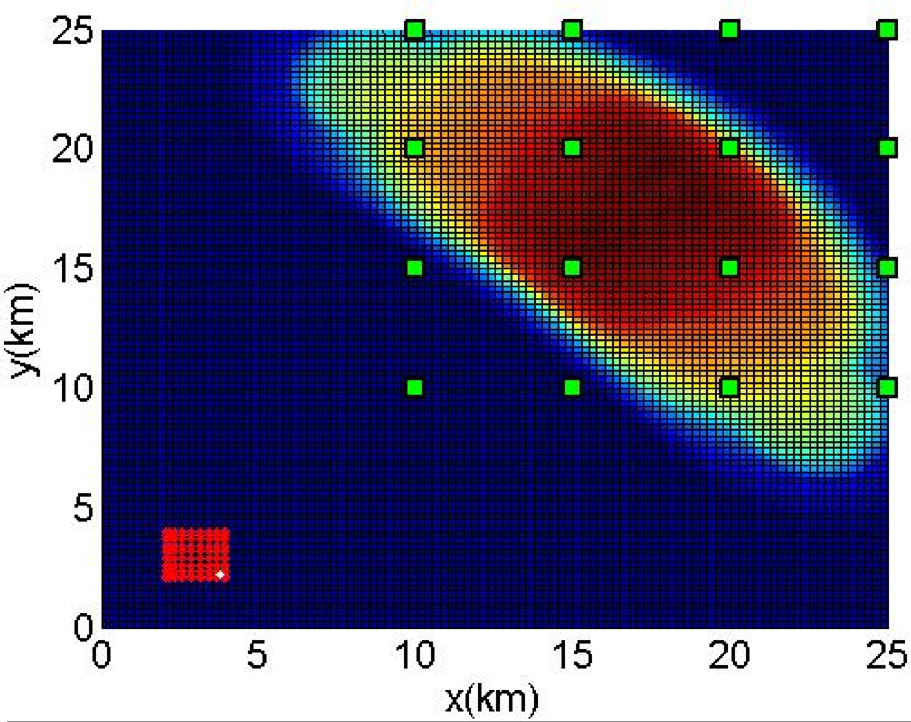


Source Identification using PCQ

-Green squares: Sensor location

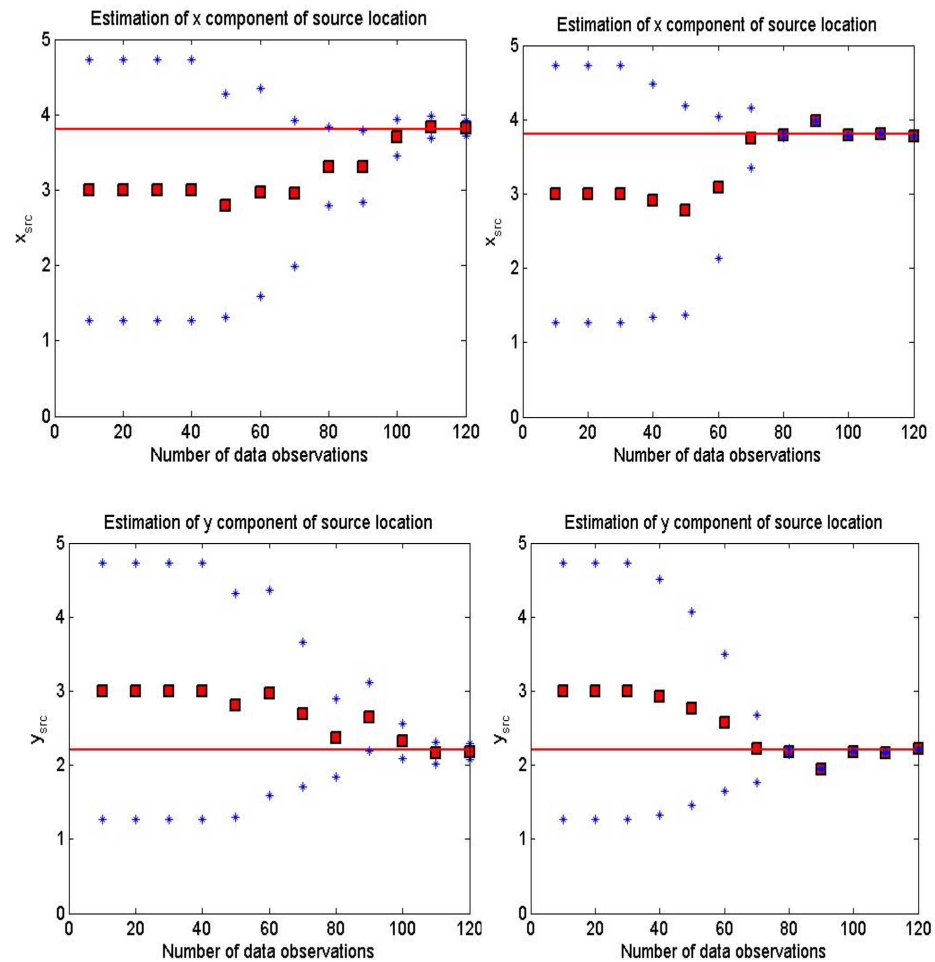
- Red points: Quadrature points applied to cover the domain of uncertain source

-White point: actual source location



Noisy Observations
R =6.25e-22

Pure Observations



Conclusion

Polynomial Chaos based minimum variance estimator

- Performs well in estimation of parameters of the system.
- Applicable to any type of probability distribution for the parameters (as opposed to Kalman Filter).
- Applicable to large scale systems (>18000 states in illustrated example, about 4000 grid locations with non-zero ash).
- Has been verified on other examples like source estimation of atmospheric releases by using SCIPUFF model.
- Can be applied as a batch or recursive estimation techniques.