Identification of atmospheric contamination source in an urban area by approximate bayesian computation methodology

NATIONAL CENTRE FOR NUCLEAR RESEARCH
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Motivation: historical events

- Accidental atmospheric releases of hazardous material:
- Release of ^{137}Cs in a steel mill in Algeciras, Spain, V.1998 r.
- Registered in Switzerland, France and Italy in June.

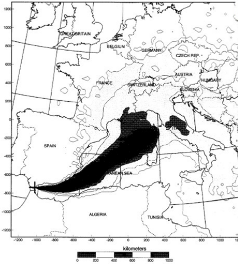

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Figure 2. Seven-day average air concentration at 1200 UTC on 5 June 1998. Contours >10 (outermost or lightest), >100, >500, and >1000 uBq/m3 (innermost or darkest).

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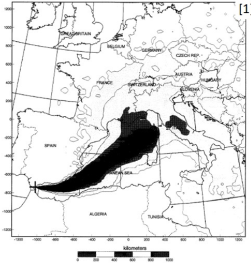
- Registered in Switzerland, France and Italy in June.
- ^{131}I - 2011,2012,2015,2017, ^{137}Cs-2015, ^{106}Ru - 2017.
- Source location was not known at the time when the first detections were reported.



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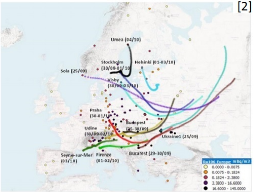

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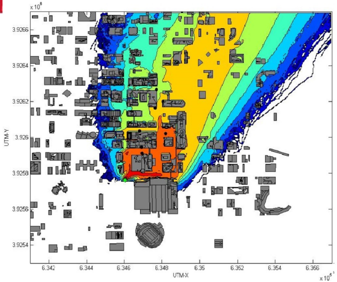
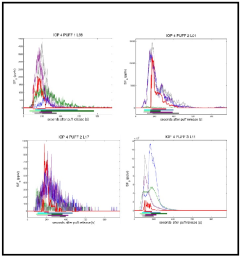
- The **most difficult** and requiring the **most resources** is the contamination in urbanized areas (micro-scale).
- Because, accurate modeling of atmospheric contaminant transportation in a dense urban area is not trivial.

Forward modeling: concentration point estimation



Forward



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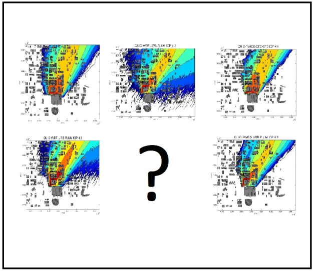
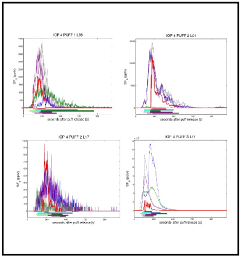
Inverse modeling: source terms estimation



Invers



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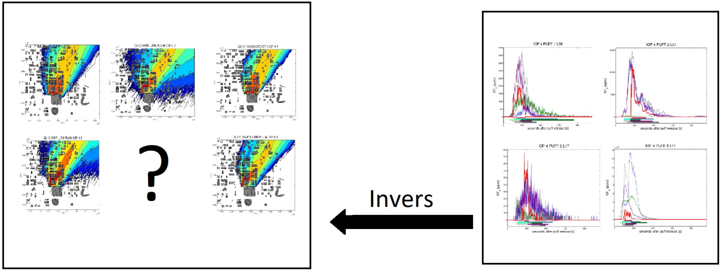

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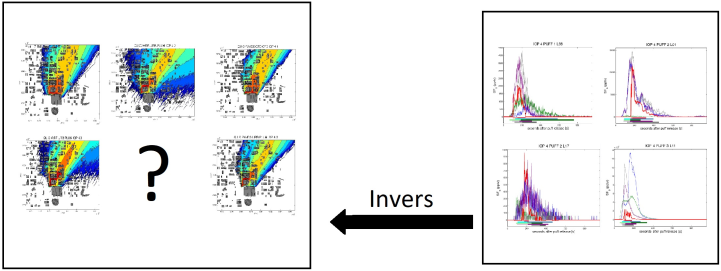

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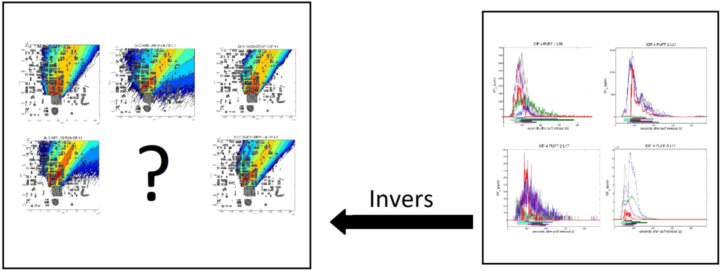

- *Questions*: How much material was released? When? Where? What are the potential consequences?
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- *Problem*: Find the values of the pollutant transport model parameters, for which outcome will be the best „fitted" to the observational data.

Bayesian inference

- In the framework of Bayesian statistics all quantities are modeled as random variables with joint probability distributions.
- This randomness can be interpreted as parameter variability.
- It is reflected in the uncertainty of the true values.
- So, in practice we can are looking for the values of parameters which are the most probable - **Posterior Probability Distribution**.

Bayes theorem

$$\underbrace{\pi(\theta|d_{obs}, I)}_{posterior} = \frac{\overbrace{L(d_{obs}|\theta, I)}^{likelihood}\,\overbrace{\pi(\theta|I)}^{prior}}{\underbrace{\pi(d_{obs}|I)}_{evidence}} \propto \pi(d_{obs}|\theta, I)\pi(\theta|I) \qquad (1)$$

- θ represents possible model configurations e.g $\theta \equiv (x, y, q, \ldots)$, d_{obs} are observed data e.g $d_{obs} \equiv C_t^{Sj}, ..., C_t^{SN}$, e.g I background information (e.g. meteorological measurements)
- Probability $\pi(\theta|d_{obs}, I)$ of certain model configuration given observed measurements (d_{obs}) (also known as the posterior distribution)
- $L(d_{obs}|\theta, I)$ - the probability of the data d_{obs} conforming a given model configuration θ
- $\pi(\theta|I)$ - the possible model configurations before taking into account the measurements

How to obtain posterior distribution of model parameters?

- Approximate Bayesian Computation with the sequential extension [5].
- *Idea*: Accept θ as an approximate posterior draw if its associate data d is close enough to the observed data d_{obs}.
- d - expected concentration in sensors locations with source θ_i setup: $MODEL(\theta_i) \rightarrow d$
- $\rho(d, d_{obs})$ - chosen measure of discrepancy between d and d_{obs},
- ϵ - threshold value.
- So, parameters are a sample from $\pi(\theta|\rho(d, d_{obs}|I) < \epsilon)$

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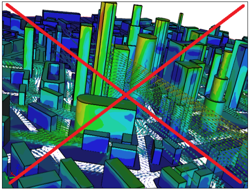

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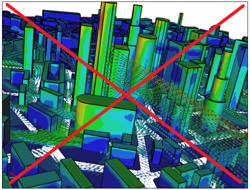

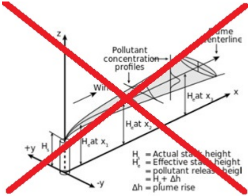

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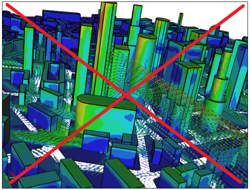
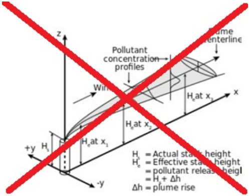
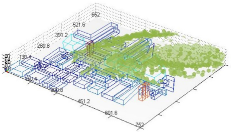
- A short (**QUIC**K!) computation time.

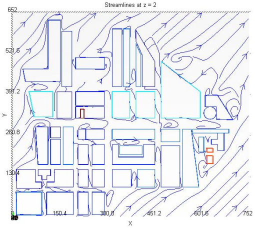






Quick Urban Industrial Complex (QUIC) Dispersion Modeling System Los Alamos

- QUIC-URB (originally developed by Rockle [6]) uses a 3D mass-consistent wind model to combine adequately resolved time-averaged wind fields around buildings



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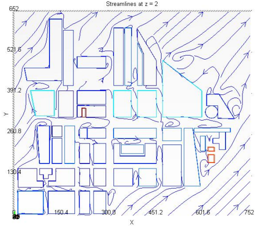

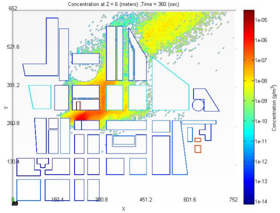

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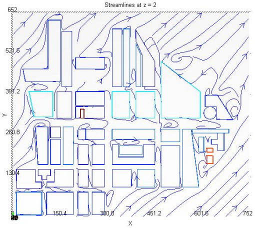
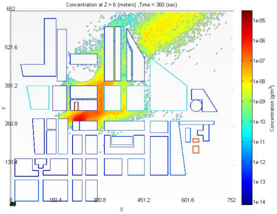
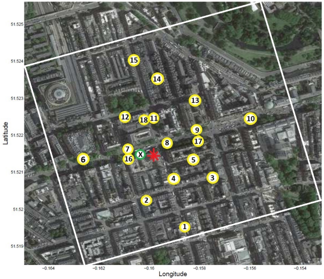
- Radioactive dispersion module is also supported





DAPPLE

- *Dispersion of Air Pollution and its Penetration into the Local Environment*
- *The building height* 10 *to* $64m$
- *Total mass emitted was* $323mg$ *of* $(PMCH, C7F14)$ *for 15 min*
- *10 samples taken over a 30 minute sampling period at 18 receptor*
- *The wind data sets take from rooftop Westminster City Council (WCC) (18 m)*
- *Funded by the Engineering for Health, Infrastructure and Environment Programme*



source position x=243.3m, y=282.8m, z=1.5m, mass q=323mg, duration and delay time l=900s, s = 0.0s

Final Bayesian STE framework setup

- Algorithm - ABC with Sequential Monte Carlo, Forward Model - QUIC , Data/Experiment: DAPPLE (28 Jun 07)
- Distance measure (Fractional Bias):

$$\rho(d^t, d^t_{obs}) = \frac{1}{18}\sum_{j=1}^{18}\left(\frac{1}{t}\sum_{i=1}^{t}\frac{|C_i^{Sj} - \hat{C}_i^{Sj}|}{C_i^{Sj} + \hat{C}_i^{Sj}}\right), \tag{2}$$

- Source parameters vector and prior definition:

$$\begin{aligned}
\pi(\theta^1) \equiv &(x, y) \sim U^{\Theta}([100, 600], [100, 500]) - (x = 243.3m, y = 282.8m)\\
&z \sim Gamma(3, 3) - z = 1.5m\\
&q \sim U(10, 500) - q = 323mg\\
&l \sim U(0, 1800) - l = 900s\\
&s \sim U(0, 180) - s = 0.0s
\end{aligned} \tag{3}$$

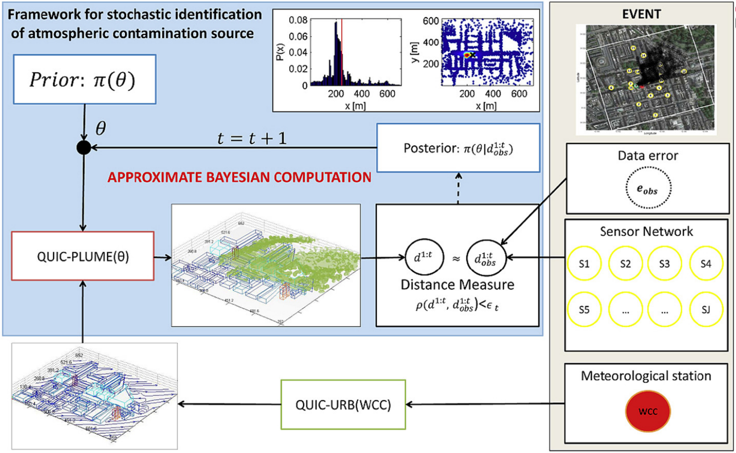


Figure 1: Framework for stochastic identification of atmospheric contamination source in an urban area

Results of reconstruction experiment

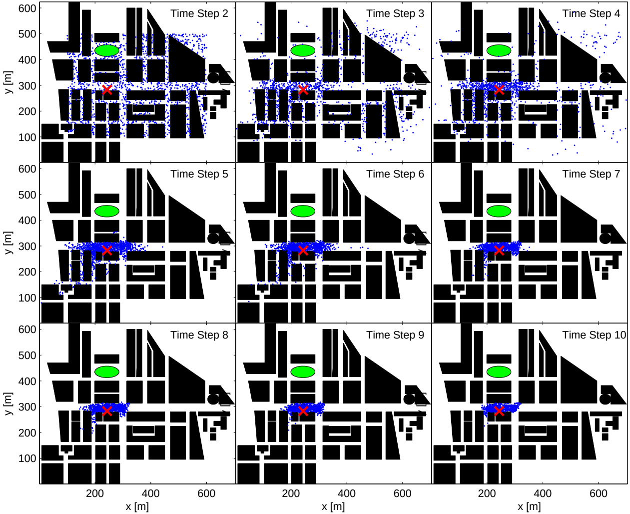


Figure 2: Scatter plot of all samples generate in the subsequent time steps $t = 2, 3, \ldots, 10$ in (x, y) space

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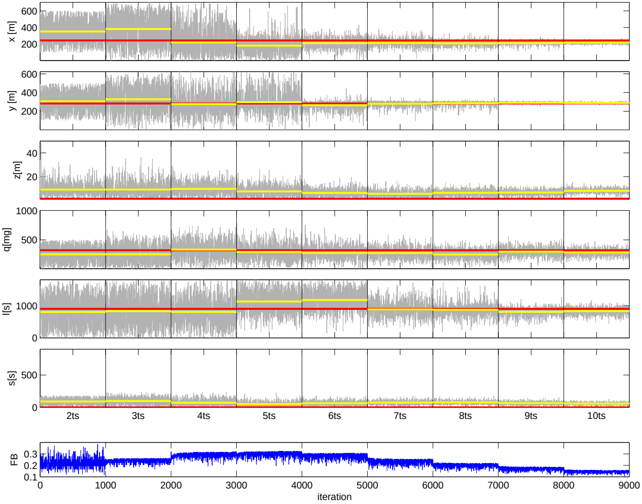

Figure 3: The trace plots for all searched parameters $\theta \equiv (x, y, z, q, l, s)$ in all time steps.

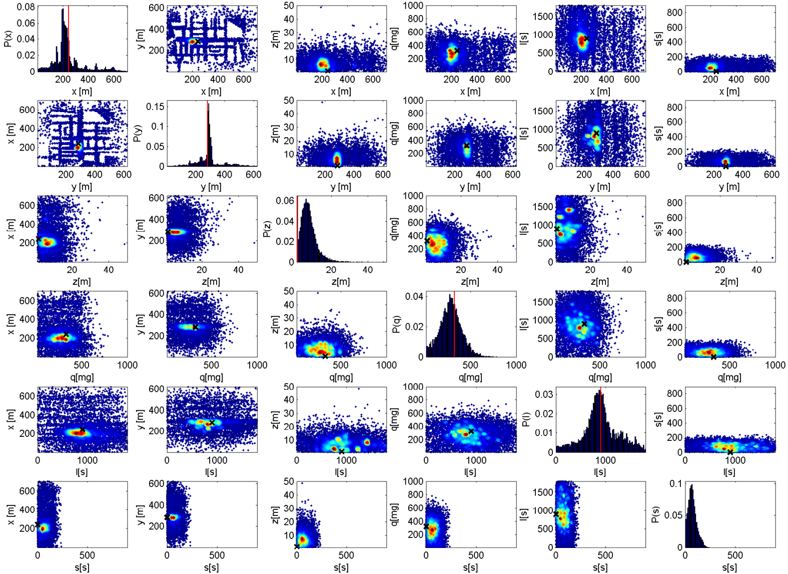

Figure 4: Bivariate and marginal posterior distributions for all parameters

Results of reconstruction experiment

Parameters	$x[m]$	$y[m]$	$z[m]$	$q[mg]$	$l[s]$	$s[s]$
θ^*	243.3	282.8	1.5	323.0	900.0	0.0
θ^{MAP}	203.5	291.8	5.4	265.7	881.0	71.0
$mean(\theta)$	243.9	290.9	7.6	280.0	903.3	72.4
$std(\theta)$	124.6	84.3	4.1	118.7	352.3	41.8
$CI_{LB}^{90\%}(\theta)$	35.0	150.0	1.1	59.1	359.7	0.7
$CI_{UB}^{90\%}(\theta)$	466.2	461.6	12.8	461.3	1624.0	130.9

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- One minute delay can be seen as important.

Conclusions

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- Published: *Framework for stochastic identification of atmospheric contamination source in an urban area P Kopka, A Wawrzynczak Atmospheric Environment 195, 63-77*

THANK YOU
FOR YOUR ATTENTION

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