APPLICATION OF THE BAYESIAN APPROACH AND INVERSE DISPERSION MODELLING TO SOURCE TERM ESTIMATES IN BUILT-UP ENVIRONMENTS

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INTRODUCTION AND RATIONALE (1)

- This work is a contribution to the preparedness and response to CBRN threats (CBRN = Chemical, Biological, Radiological, Nuclear)
- The identification of a possible CBRN source is important in order to evaluate the consequences of such an event and support the first-response teams
- The goal of the source term estimation (STE) is to detect the source and assess the parameters of the CBRN release
  - ✓ With sufficient accuracy
  - ✓ With a quantification of the uncertainty
  - ✓ Within a reasonable amount of time

INTRODUCTION AND RATIONALE (2)

- There are several approaches for the same objective in the field of STE

1) Adjoint transport modelling and retro-transport
    - Pudykiewicz (1998)
    - Issartel and Baverel (2003)
2) Optimization of a cost function using least square or genetic algorithms
    - Issartel (2005), Winiarek et al. (2012)
    - Haupt (2005), Rodriguez et al. (2011)
3) Bayesian inference coupled with stochastic sampling
    - Delle Monache et al. (2008)
    - Chow et al. (2008)
    - Keats et al. (2007)
    - Yee (2008)
    - Rajaona et al. (2015) → Adaptive Multiple Importance Sampling (AMIS)

All these authors use Monte Carlo Markov Chain (MCMC) methods

- The Bayesian framework allows:
  - ✓ Taking into account errors from the model and from the observations
  - ✓ Dealing with the possible presence of prior knowledge
  - ✓ Estimating the uncertainty of the results

- In our case, we consider the vector of observations $\boldsymbol{y}$ given by Nc sensors each one collecting Tc time samples: $\boldsymbol{y} = [\ y_{1,1} \dots y_{1,Tc} \dots y_{Nc,1} \dots y_{Nc,Tc}\ ]^T$

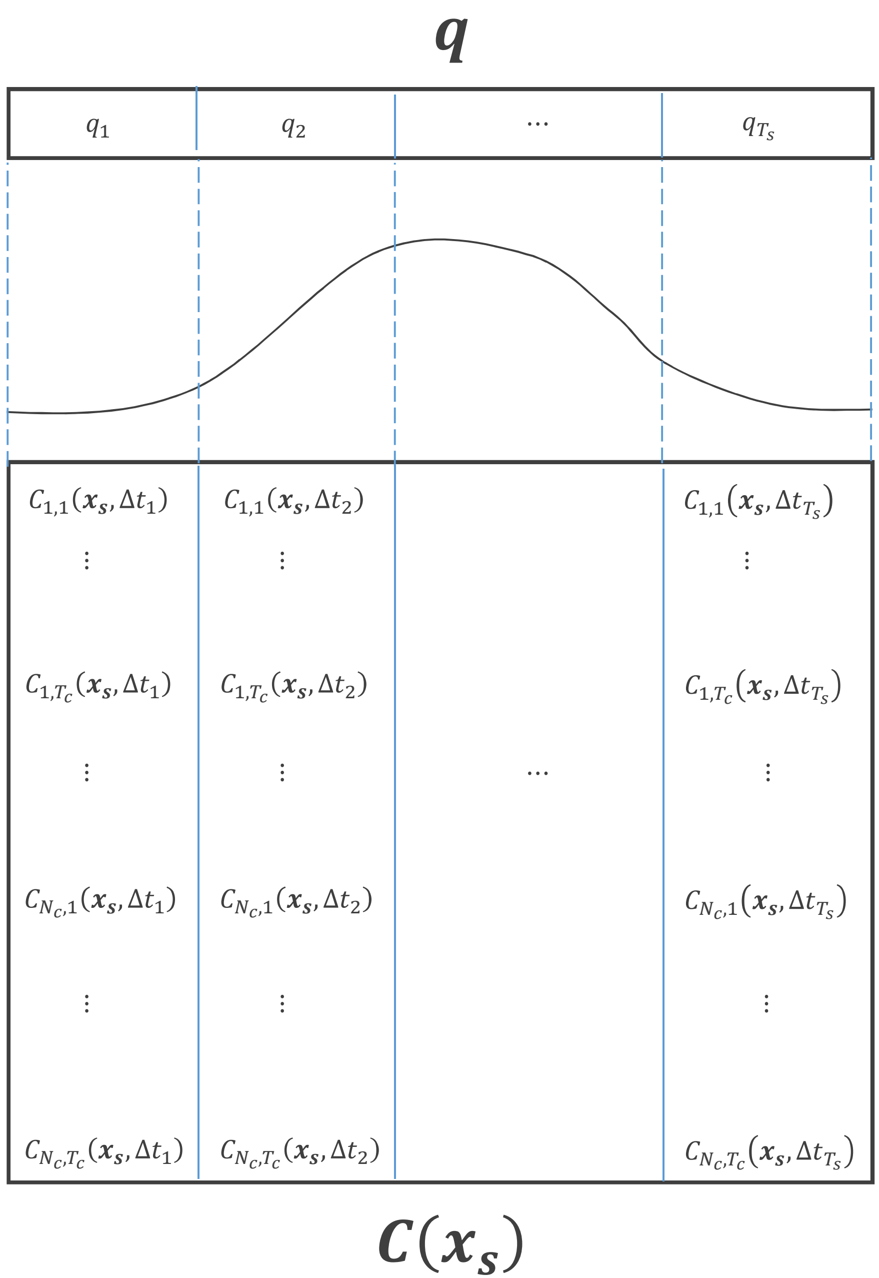
- The parameters of the source $\boldsymbol{\theta} = (\boldsymbol{x}_s, \boldsymbol{q})$ are the position $\boldsymbol{x}_s = (x_s, y_s)$ and the release rate vector $\boldsymbol{q}$ which is discretized into T_s time steps

- The data model can be written as follows: $\boldsymbol{y} = \boldsymbol{C}(\boldsymbol{x}_s)\ \boldsymbol{q} + \boldsymbol{\epsilon}$

  - $\boldsymbol{y}$: Observations
  - $\boldsymbol{C}(\boldsymbol{x}_s)$: Source-receptor matrix
  - $\boldsymbol{\epsilon}$: Noise vector assumed to be Gaussian with zero mean vector and covariance matrix $\sigma_\epsilon^2 \mathbf{I}_{N_c T_c}$

THE BAYESIAN FRAMEWORK (2)

- The vector $\boldsymbol{q}$ is a discretization in time of the emitted quantity during the release
- Each element of the source-receptor matrix $\boldsymbol{C}(\boldsymbol{x}_s)$ is the concentration obtained for a unitary release of the source $\boldsymbol{\theta}$
- Each column n can be seen as the result of a quasi-instantaneous release q_n
- As in Winiarek et al. (2011), a multivariate Gaussian distribution is considered as prior knowledge on the emission rate vector, i.e. $p(\boldsymbol{q}) = \mathcal{N}(\boldsymbol{q} ; \boldsymbol{\mu}_q, \boldsymbol{\Sigma}_q)$



- Instead of just a point-wise estimation of the source characteristics, the Bayesian solution allows to obtain the full posterior distribution of the parameters $p(\boldsymbol{\theta}|\boldsymbol{y})$
- The joint posterior distribution can be expanded as follows:

$$p(\boldsymbol{\theta} \mid \boldsymbol{y}) = p(\boldsymbol{x}_s, \boldsymbol{q} \mid \boldsymbol{y}) = \boldsymbol{p}(\boldsymbol{q} \mid \boldsymbol{y}, \boldsymbol{x}_s)\, p(\boldsymbol{x}_s \mid \boldsymbol{y})$$

- Owing to the Gaussian assumption of the observation errors (likelihood) and the prior distribution of $\boldsymbol{q}$, the rule of conjugate priors states that $\boldsymbol{p}(\boldsymbol{q} \mid \boldsymbol{y}, \boldsymbol{x}_s)$ is therefore Gaussian
- Unfortunately, $p(\boldsymbol{x}_s \mid \boldsymbol{y})$ is analytically intractable due to the highly non-linear dependence of the source position and the measurements reflected by the complex structure of the source-receptor matrix $\boldsymbol{C}(\boldsymbol{x}_s)$
- Our proposition is to use sampling technique to efficiently approximate $p(\boldsymbol{x}_s \mid \boldsymbol{y})$

SAMPLING AND THE AMIS ALGORITHM (1)

- Monte Carlo draws are powerful numerical methods to approximate distributions
- One of the most popular algorithms of stochastic sampling is the Monte Carlo Markov Chain (MCMC) algorithm, widely used in many domains including STE…
- In this study, we focus on another branch of Monte Carlo methods, based on the principle of Importance Sampling (IS) as developed originally in Cornuet et al. (2012) and in Rajaona et al. (2015) for an application to STE

	MCMC	IS
Convergence	**Require a burn-in period** • Difficult to assess when the chain has reached the stationary regime • Samples from this burn-in period are unusable	**Direct**
Adaptive sampling	**Yes but very constraint** to ensure that the Markov chain will reach a stationary regime	**Yes**

- Our proposition is to enhance this original IS-based STE by utilizing results of the dispersion model in backward mode at several crucial steps of the algorithm

- IS consists in drawing a set of samples (particles) from a proposal distribution ϕ

$$\{\boldsymbol{x}^1, \dots, \boldsymbol{x}^{N_p}\} \sim \phi(\boldsymbol{x})$$

and compute their associated importance weights

$$w^i = \pi(\boldsymbol{x}^i) \,/\, \phi(\boldsymbol{x}^i) \quad \text{for } i = 1, \dots, N_p$$

in order to approximate the target distribution π as $\pi(\boldsymbol{x}) \approx \sum_{i=1}^{N_p} \overline{w}^i \delta_{\boldsymbol{x}^i}(\boldsymbol{x})$

with $\overline{w}^i = w^i \left[\sum_{j=1}^{N_p} w^j\right]^{-1}$ the normalized weights

- Iterative schemes of IS have been designed, among them the Population Monte Carlo (PMC) algorithm allows to tune adaptively the proposal at each iteration

- The Adaptive Multiple Importance Sampling (AMIS) algorithm enhances the PMC by adding a recycling scheme of all the particles previously generated to improve the learning of the proposal and the accuracy of the approximation of the target distribution

SAMPLING AND THE AMIS ALGORITHM (3)

- AMIS algorithm in Rajaona et al. (2015)

  1) Draw a population of N_p samples, $\left\{\boldsymbol{x}_{s,t}^1, \dots, \boldsymbol{x}_{s,t}^{N_p}\right\}$, from a proposal distribution $\phi(\boldsymbol{x}_s\,;\,\varphi_t)$

  2) Compute the importance weights $\left\{w_t^1, \dots, w_t^{N_p}\right\}$
     [involves computing $\boldsymbol{C}(\boldsymbol{x}_{s,t}^j)$ with the dispersion model for each particle ⇢ Time consuming !]

  3) Update all the previously computed weights $w_{1:t-1}$ [recycling step]

  4) Adapt the parameters φ of the proposal distribution $\phi(\boldsymbol{x}_s\,;\,\varphi_t)$ using all the generated random weighted samples $\{\boldsymbol{x}_{s,1:t}^i, w_{1:t}^i\}_{i=1}^{N_p}$ so that it tends to fit $p(\boldsymbol{x}_s\,|\,\boldsymbol{y})$

- Final empirical approximation of the full posterior distribution:

$$p(\boldsymbol{x}_s, \boldsymbol{q}|\boldsymbol{y}) \approx \sum_{t=1}^{T}\sum_{i=1}^{N_p} \overline{w}_t^i \boldsymbol{p}(\boldsymbol{q}|\boldsymbol{y}, \boldsymbol{x}_{s,t}^i)\delta_{\boldsymbol{x}_{s,t}^i}(\boldsymbol{x}_s)$$

- In this paper, we propose to use a mixture of D normal distributions and an additional "defensive" component which will remain unchanged through adaptive procedure:

$$\phi(\boldsymbol{x}_s; \varphi_t) = \alpha^{(0)}\phi^{(0)}(\boldsymbol{x}_s) + (1-\alpha^{(0)})\sum_{d=1}^{D}\alpha_t^{(d)}\boldsymbol{\mathcal{N}}(\boldsymbol{x}_s; \boldsymbol{\mu}_t^{(d)}, \boldsymbol{\Sigma}_t^{(d)})$$

ENHANCEMENT OF THE AMIS USING BACKWARD LPDM

Our proposition is to run the Lagrangian dispersion model in backward mode

- Use the forward/backward dispersion duality relationship as Keats et al. (2007) to obtain $C(x_s)$ by running a backward LPDM before starting AMIS iterations

$N_c \times T_c$ instead of $\underbrace{T \times N_p}$ $\times T_s$ runs of LPDM

Number of generated samples → Candidates for the possible source location

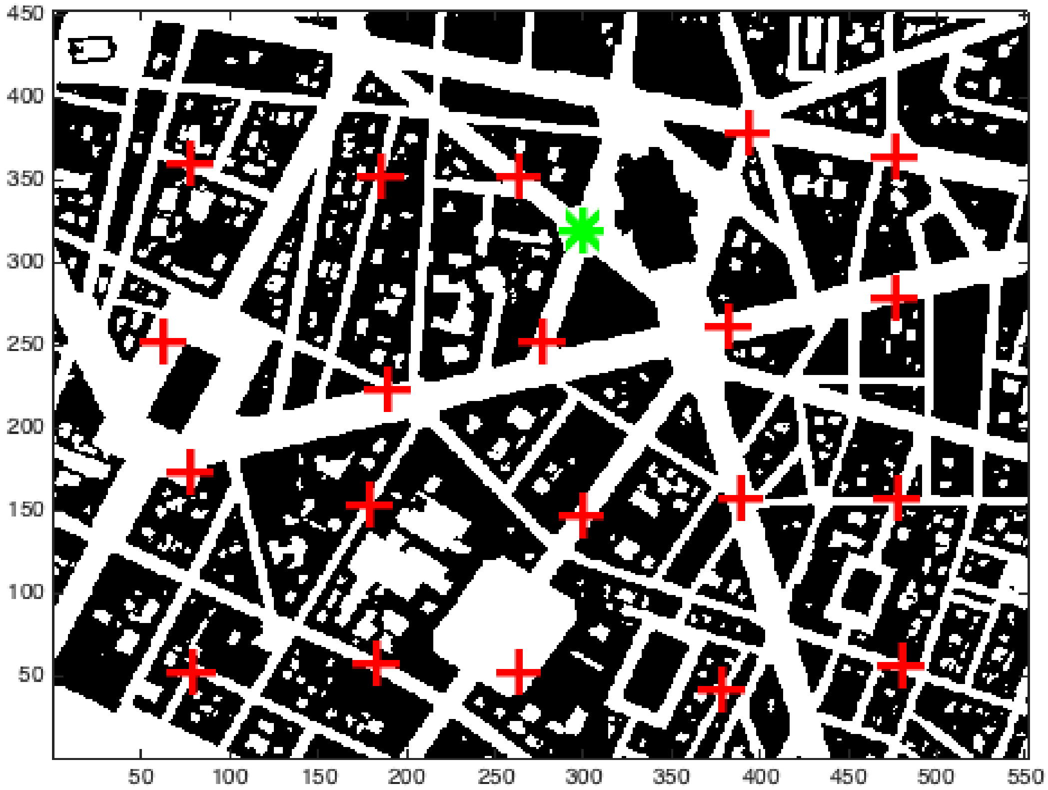
$T \times N_p \times T_s \gg N_c \times T_c$

- Use the outputs of these backward LPDM runs to design an efficient procedure to automatically set the initial parameters, φ_0, of the adaptive proposal distribution of the AMIS

- Starting distribution has clearly a major impact on the resulting performances
  → It is quite difficult to recover from a poor starting sample

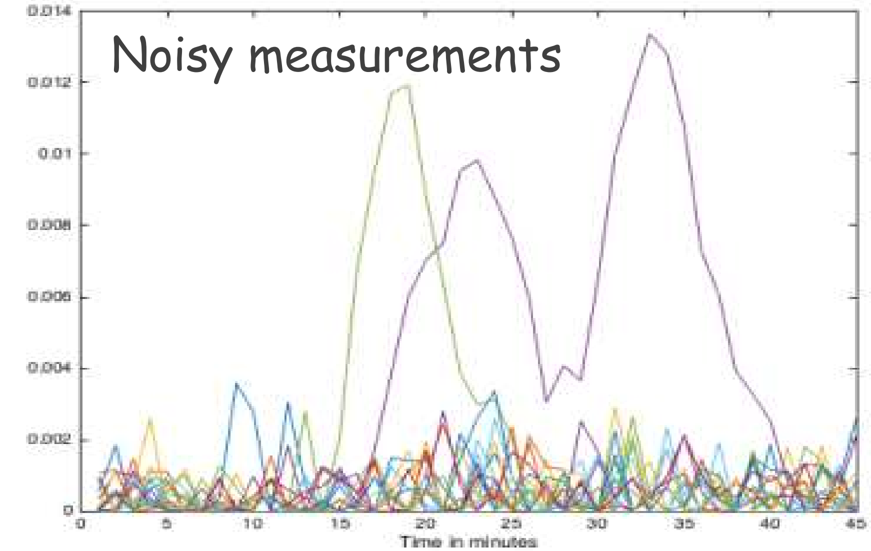
SIMULATIONS AND AMIS RESULTS (1)

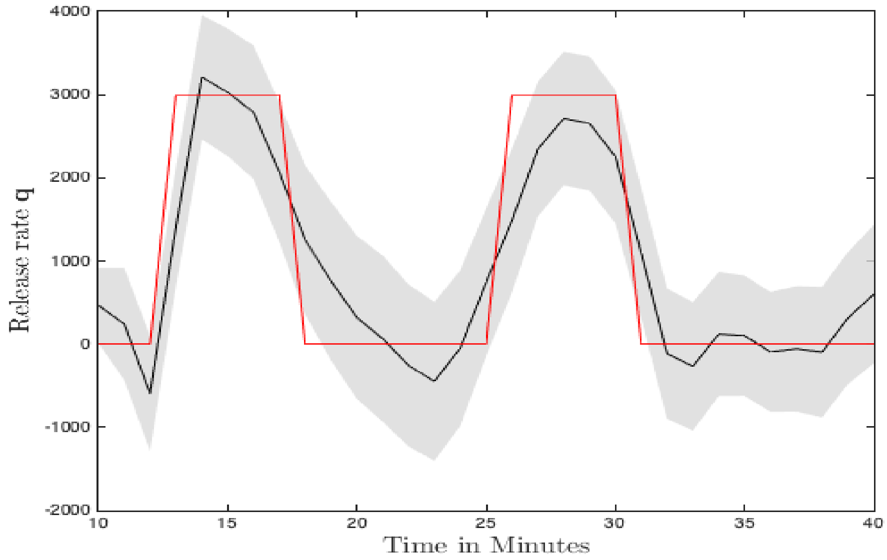
- A synthetic case is carried out in a built-up environment (Paris Opera district)
- Lagrangian Particle Dispersion Model is Parallel-Micro-SWIFT-SPRAY (PMSS)
- Wind speed and wind direction are variable (from west-northwest to north-northeast)
- AMIS features are the following: D = 9 adaptive components in the proposal, $N_p = 100$ particles with $T = 20$ iterations

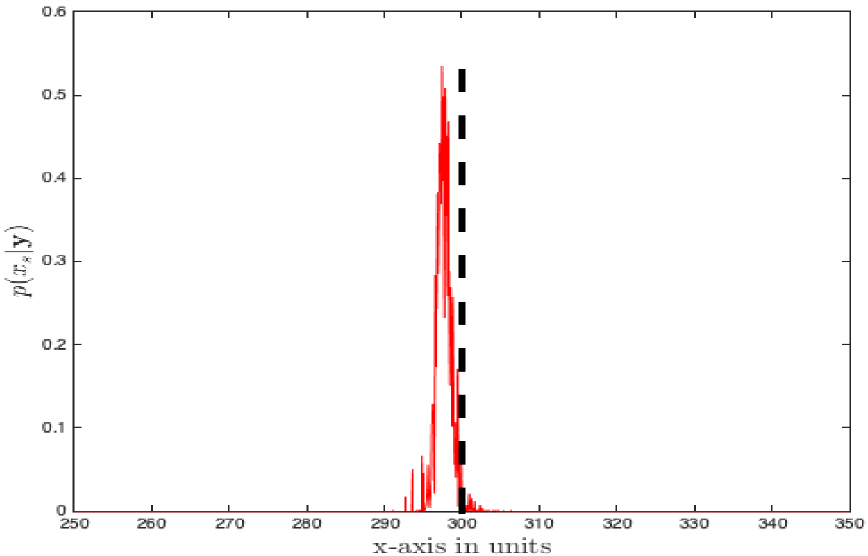


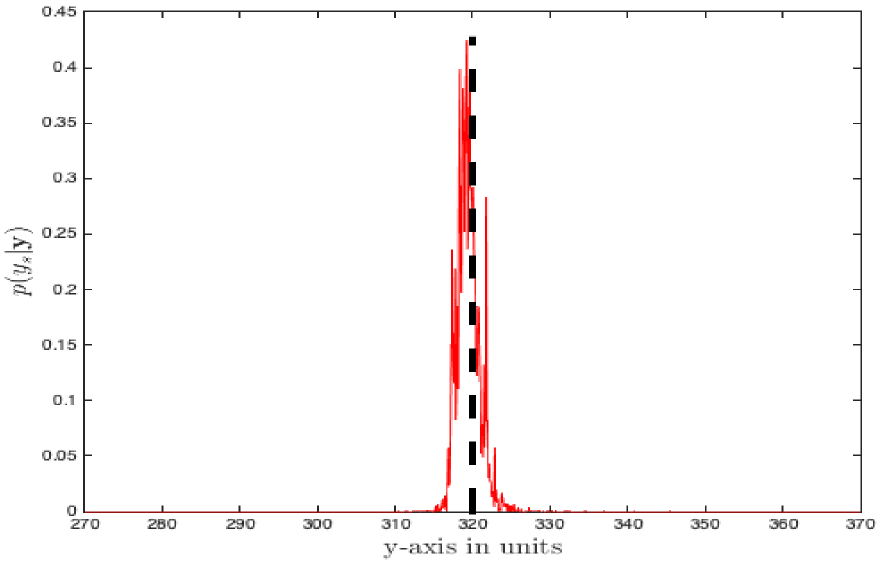
View of the source and the sensors in the urban area of 450 m × 550 m meshed at an horizontal and vertical resolution of 2 meters

SIMULATIONS AND AMIS RESULTS (2)





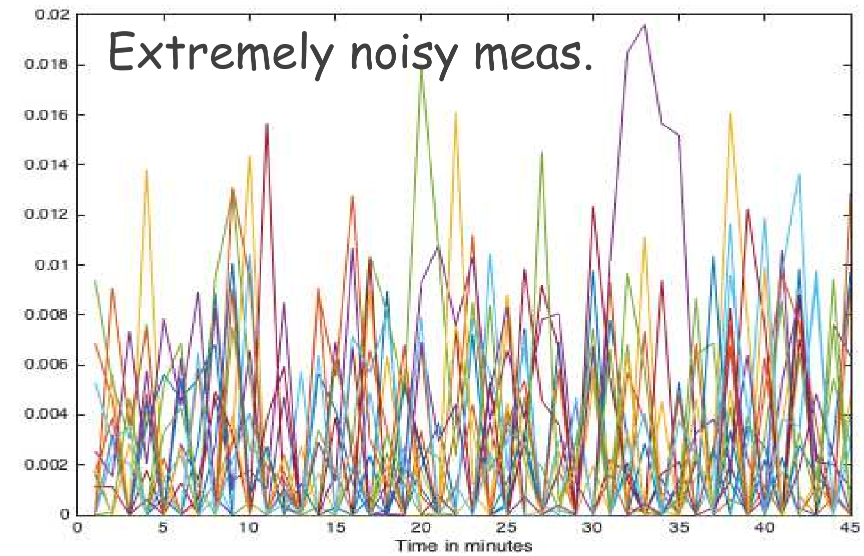


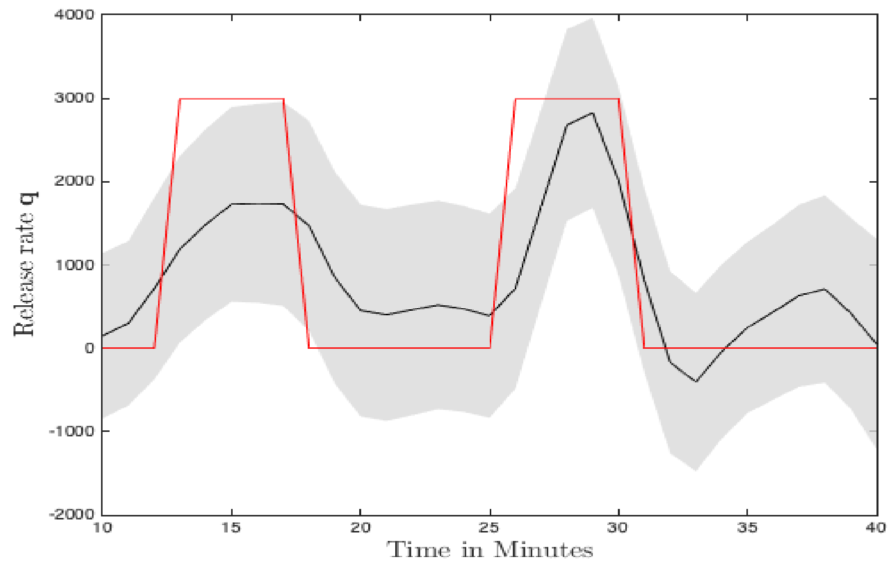


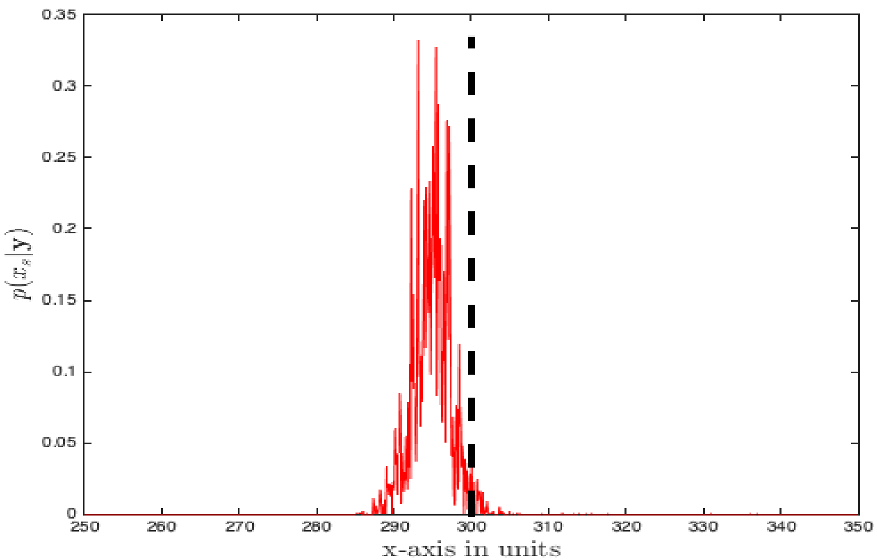
Good estimation of posterior distributions (position and release rate)

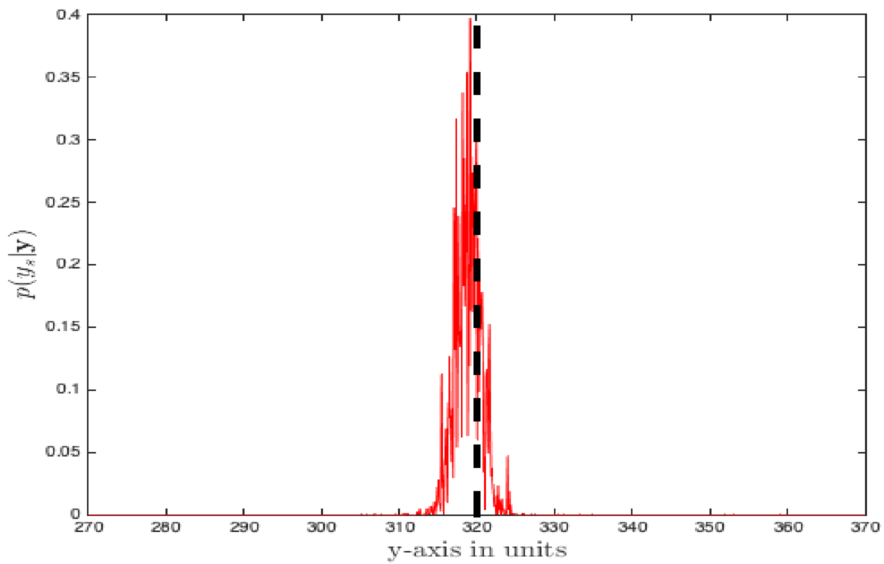
Significant gain of computational time (factor of 100) with retro-dispersion

SIMULATIONS AND AMIS RESULTS (3)



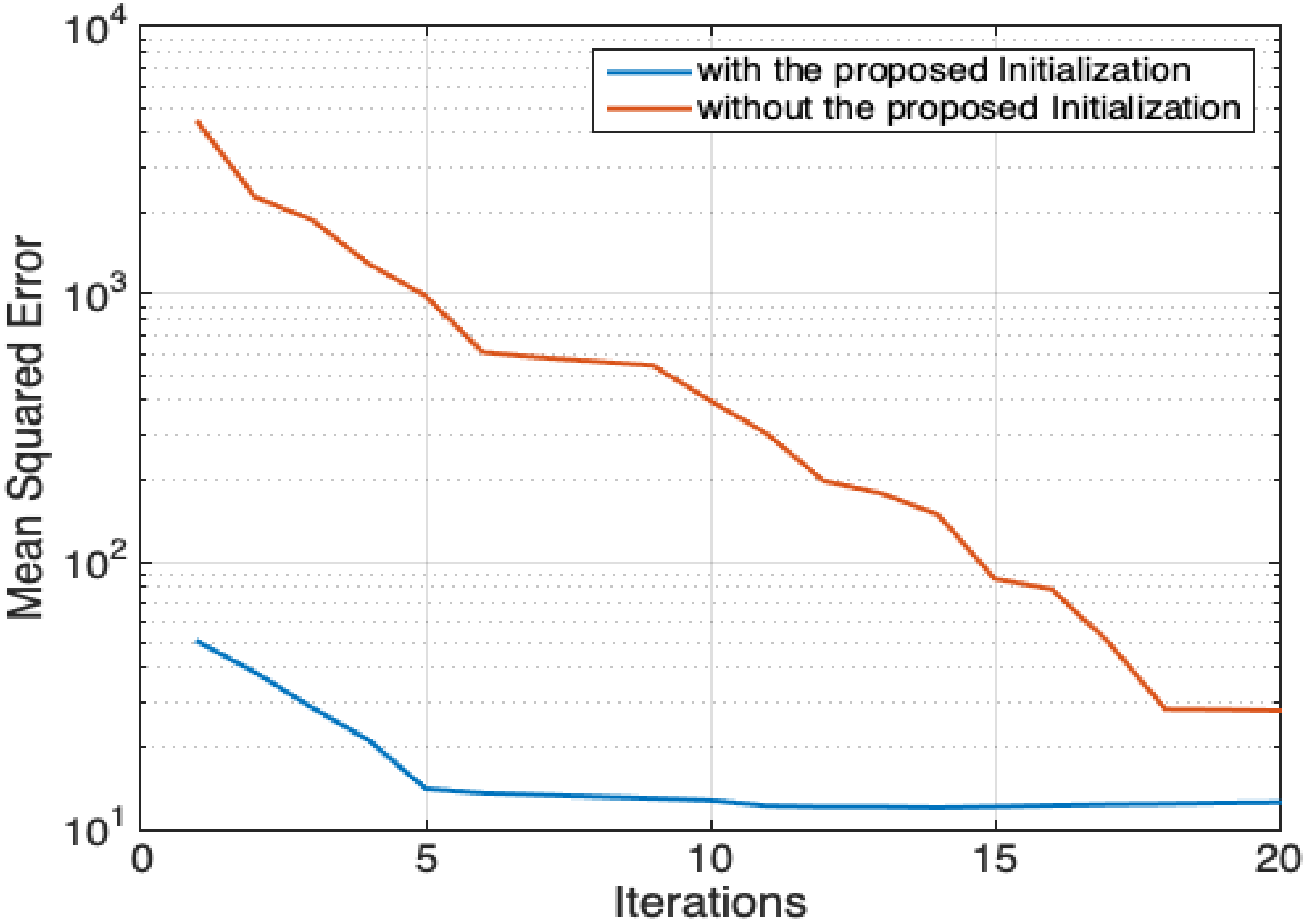






Good estimation of posterior distributions (position and release rate)…

… Even in an extremely noisy environment



Mean squared error on the source position at the different iterations of the AMIS with and without the initialization strategy which uses the backward LPDM

Significant improvement of the convergence speed

CONCLUSIONS AND PERSPECTIVES

- AMIS is an original Bayesian stochastic approach to solve Source Term Estimate for instantaneous or non-instantaneous releases
- Enhancements of the original AMIS were carried out by efficiently using LPDM in backward mode:
  - ✓ To construct the source-receptor matrix $C(x_s)$
    ⇒ Reduction of the computational time!
  - ✓ To initialize the adaptive components of the proposal
    ⇒ Improvement of the convergence speed!
- The first results on synthetic data are very encouraging and more results with experimental data are yet to come to validate the method
- Ongoing research directions:
  - ✓ Taking into account the wind uncertainty into the estimation
  - ✓ Being able to process the measurements sequentially

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Thank you for your attention.

Questions ?

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