A Bayesian approach of the source estimate coupling retro-dispersion computations with a Lagrangian particle dispersion model and the Adaptive Multiple Importance Sampling

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ARIA TECHNOLOGIES

DE LA RECHERCHE À L'INDUSTRIE cea

Direct modeling : the "murderer" point of view

(*) an almost perfect ~~crime~~ model

Inverse modeling: the "investigator" point of view

- A lot of solutions
- What are the clues ?
- More clues, more efficient !

Outline

1- Introduction

2- The Bayesian framework and the AMIS algorithm

3- Optimizing the AMIS by using a retro-dispersion model

4- Two-use cases : open-country and city downtown

5- Conclusion

Introduction

- Goal: estimate the parameters (location and release rate) of a hazardous release, in order to:
  - Give the best term source (where and how much)
  - Enhance the simulation of the resulting plume by giving better input data to the dispersion model ➔ provide the best impact assessment map of the current situation
- Two main approaches are possible and have been investigated in the literature:
  - Optimizatic
    - Variation
    - Genetic a


Inverse modelling of methane fugitive emissions from waste water treatment plant

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  - Bayesian inference and stochastic sampling (find the highest probability)

The Bayesian framework

- Why a probabilistic approach :
  - Taking into account the various uncertainties in the observations and in the dispersion model
  - Dealing with the presence (or also absence) of prior information on the source term parameters
  - Estimating the uncertainty related to the estimation results
- Generative model for the observation data:

$$d = q\, C(\theta) + \varepsilon$$

  - q (t) temporal release profile
  - $C(\theta)$ is a source-receptor matrix obtained by running a dispersion model for a unitary release from a source located at position θ
  - ε is an aggregation of all error sources (model, observation, representativeness) into a single vector
- In the Bayesian context, the objective is to estimate the posterior distribution $p(\theta, q \mid d)$ of the source parameters (location θ and temporal release profile q) given the concentration measurements d provided by a sensor network:

$$p(\theta, q \mid d) = \frac{p(d \mid \theta, q)\, p(\theta, q)}{p(d)}$$

The Bayesian framework

- The posterior distribution of the source parameters can be expressed using its marginal components:

$$\boldsymbol{p(\theta, q \,|d\,) = p(q|\theta, d)p(\theta|d)}$$

- Estimating the marginal posterior $p(q|\theta, d)$ of q can be done analytically :
  - prior distribution $p(q)$ is Gaussian
  - the observation error is also Gaussian centered on measurements

- Estimating the posterior distribution $p(\theta|d)$ of θ :
  - Calls for the application of Bayes rule :

$$\boldsymbol{p(\theta|d) = \frac{p(d|\theta)p(\theta)}{p(d)} \propto p(d|\theta)p(\theta)}$$

  - Requires the use of simulation-based methods (Monte Carlo) because it has no closed form due a highly non-linear likelihood $p(d|\theta)$ that relies on an atmospheric dispersion model run.
  - Can be done using a sequential-based approach **(Markov Chain Monte Carlo -MCMC-)** or a population-sampling approach **(Importance Sampling).**

The AMIS algorithm

- The *Adaptive Multiple Importance Sampling* (AMIS) algorithm is based on an consequent sampling scheme, where a target distribution (namely the posterior distribution) is approximated by weighted samples from a proposition distribution

- The *"Adaptive"* algorithm improves the standard importance sampling procedure by:
  - Allowing the update of the proposal distribution, which can be chosen as a flexible combination of well-known kernels (e.g. a multivariate Gaussian mixture)
  - Optimally recycling the importance weights at each iteration to fully exploit the full available information and accelerate the convergence

First Application restriction

- One release (time dependent / accidental release)
- The source and measurements are at ground level
- No plume rise
- The time of release starting and ending are unknown
- Meteorological data are time dependent

The AMIS algorithm

Iterative scheme of the AMIS algorithm applied to the STE problem:

Sample N_p elements $\theta_k^{(1)}, \theta_k^{(2)}, \dots, \theta_k^{(N_p)}$ from the current proposal distribution

Compute the likelihood $p(d|\theta_k^{(i)})$ and $p(q|\theta_k^{(i)}, d)$ by calling a dispersion model

Compute the current importance weight $w_k^{(i)}$

Loop over all the sampled elements

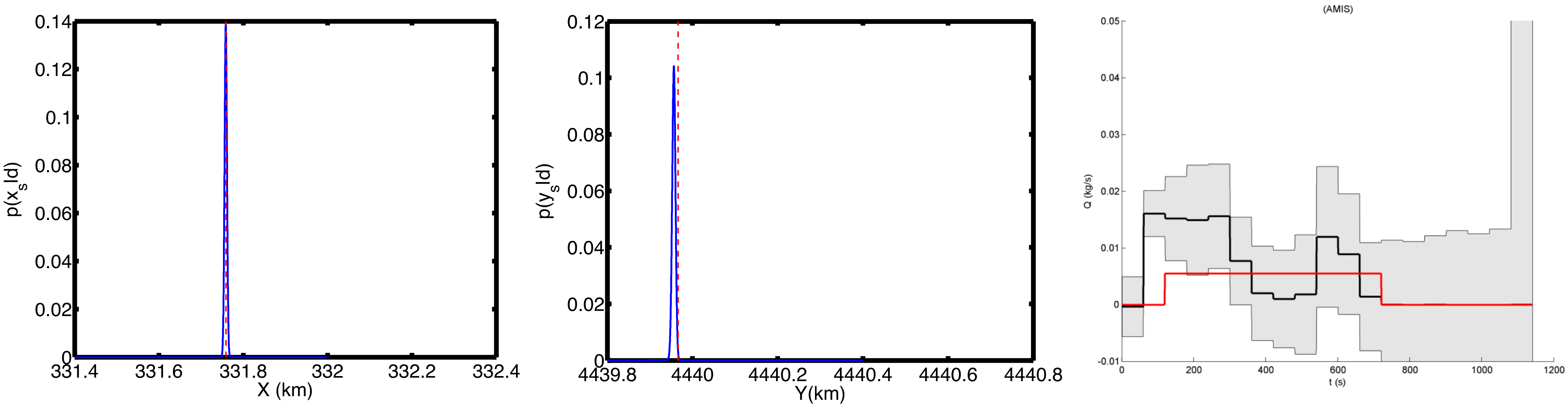
Compute the recycled importance weights over all previous iterations $w_{0:k-1}$

Update the proposal parameters

Need of a very quick dispersion model that does not allow to take benefit of all the 3D available info

The AMIS algorithm

- Preliminary tests applied on an experimental case (FFT07 experiment) showed a good estimation of the source location, but the release rate reconstruction is not as accurate as expected [Rajaona et al, 2015]



Estimation of the source parameters for the trial 7 of FFT07: position in x (left) and y (center) compared to the true location (red), and reconstructed release rate (right) with 95% confidence interval compared to the true emission profile (red). The dispersion model used to compute the likelihood is a simple Gaussian puff model.

[Rajaona et al., 2015] : Rajaona, H., Septier, F., Armand, P., Delignon, Y., Olry, C., Albergel, A., & Moussafir, J. (2015). *An adaptive Bayesian inference algorithm to estimate the parameters of a hazardous atmospheric release.* Atmospheric Environment,122, 748-762.

The AMIS algorithm

- One of the downsides of the stochastic Bayesian approach is the high number of calls to a CPU-time consuming forward model when it comes to iteratively compute the likelihood for each sampled element.

- The model cannot scale efficiently if a more complex dispersion model is needed (e.g. in an urban scenario).

- The AMIS scheme needs to be optimized in order to deal with a more elaborate dispersion model.

Optimizing using a retro-dispersion model

- Solution: use the duality relationship as mentioned in [Keats et al., 2007] to switch to a retro-dispersion model

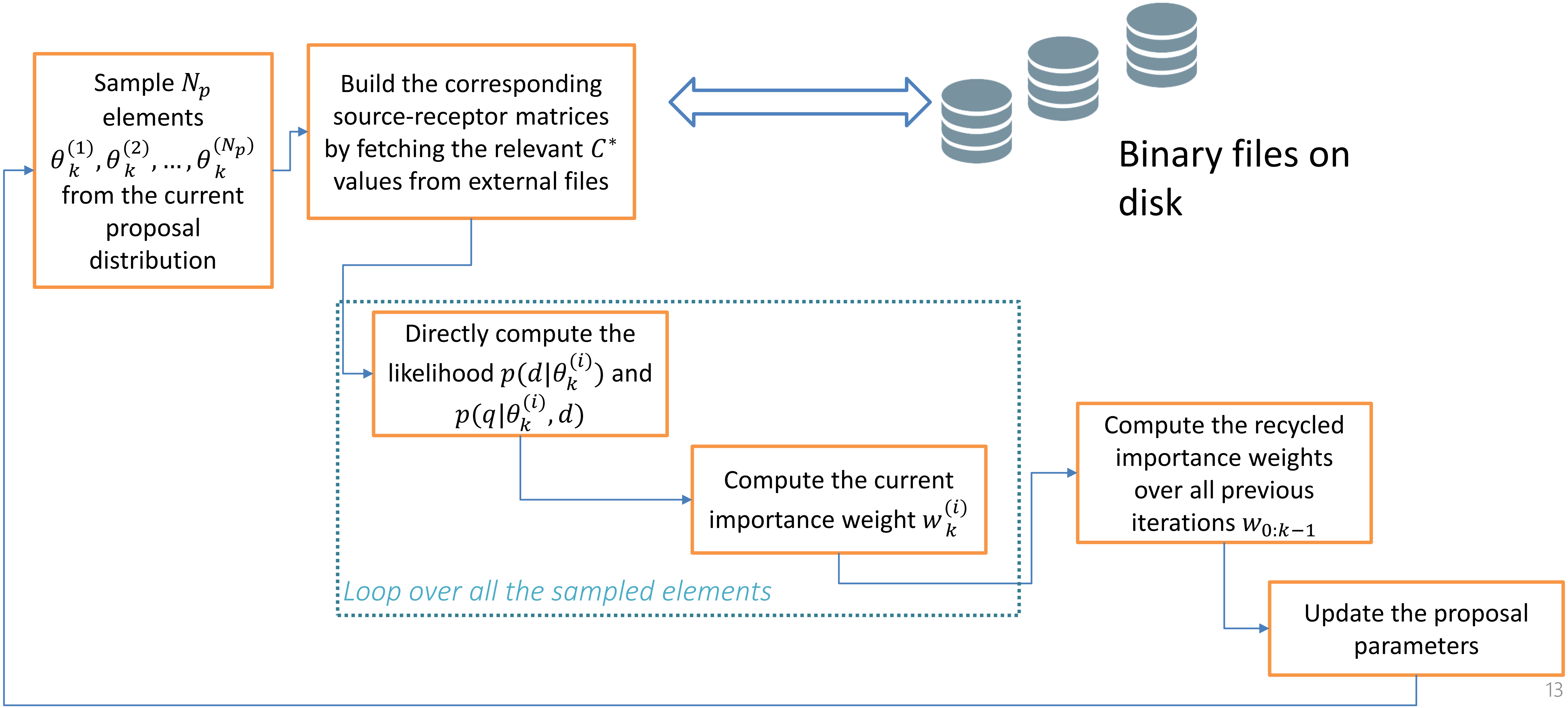
$$C(\theta)=\begin{bmatrix} C(R_1,t_1|\theta,t'_1) & C(R_1,t_1|\theta,t'_2) & \cdots & C(R_1,t_1|\theta,t'_{T_s}) \\ C(R_1,t_2|\theta,t'_1) & C(R_1,t_2|\theta,t'_2) & \cdots & C(R_1,t_2|\theta,t'_{T_s}) \\ \vdots & \vdots & & \vdots \\ C(R_1,t_{T_c}|\theta,t'_1) & C(R_1,t_{T_c}|\theta,t'_2) & \cdots & C(R_1,t_{T_c}|\theta,t'_{T_s}) \\ C(R_2,t_1|\theta,t'_1) & C(R_2,t_1|\theta,t'_2) & \cdots & C(R_2,t_1|\theta,t'_{T_s}) \\ C(R_2,t_2|\theta,t'_1) & C(R_2,t_2|\theta,t'_2) & \cdots & C(R_2,t_2|\theta,t'_{T_s}) \\ \vdots & \vdots & & \vdots \\ C(R_2,t_{T_c}|\theta,t'_1) & C(R_2,t_{T_c}|\theta,t'_2) & \cdots & C(R_2,t_{T_c}|\theta,t'_{T_s}) \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ C(R_{N_c},t_{T_c}|\theta,t'_1) & C(R_{N_c},t_{T_c}|\theta,t'_2) & \cdots & C(R_{N_c},t_{T_c}|\theta,t'_{T_s}) \end{bmatrix} \Longleftrightarrow C^*(\theta)=\begin{bmatrix} C^*(\theta,t'_1|R_1,t_1) & C^*(\theta,t'_2|R_1,t_1) & \cdots & C^*(\theta,t'_{T_s}|R_1,t_1) \\ C^*(\theta,t'_1|R_1,t_2) & C^*(\theta,t'_2|R_1,t_2) & \cdots & C^*(\theta,t'_{T_s}|R_1,t_2) \\ \vdots & \vdots & & \vdots \\ C^*(\theta,t'_1|R_1,t_{T_c}) & C^*(\theta,t'_2|R_1,t_{T_c}) & \cdots & C^*(\theta,t'_{T_s}|R_1,t_{T_c}) \\ C^*(\theta,t'_1|R_2,t_1) & C^*(\theta,t'_2|R_2,t_1) & \cdots & C^*(\theta,t'_{T_s}|R_2,t_1) \\ C^*(\theta,t'_1|R_2,t_2) & C^*(\theta,t'_2|R_2,t_2) & \cdots & C^*(\theta,t'_{T_s}|R_2,t_2) \\ \vdots & \vdots & & \vdots \\ C^*(\theta,t'_1|R_2,t_{T_c}) & C^*(\theta,t'_2|R_2,t_{T_c}) & \cdots & C^*(\theta,t'_{T_s}|R_2,t_{T_c}) \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ C^*(\theta,t'_1|R_{N_c},t_{T_c}) & C^*(\theta,t'_2|R_{N_c},t_{T_c}) & \cdots & C^*(\theta,t'_{T_s}|R_{N_c},t_{T_c}) \end{bmatrix}$$

- The conjugate concentrations C^* is obtained from the retro-model to build the source-receptor matrices.

- By pre-computing the C^* matrix before the AMIS estimation process and store the results on disk, we remove the multiple calls to the forward dispersion model in the loop.

[Keats et al., 2007]: Keats, A., Yee, E., & Lien, F. S. (2007). *Bayesian inference for source determination with applications to a complex urban environment.* Atmospheric environment, 41(3), 465-479.

Optimizing using a retro-dispersion model

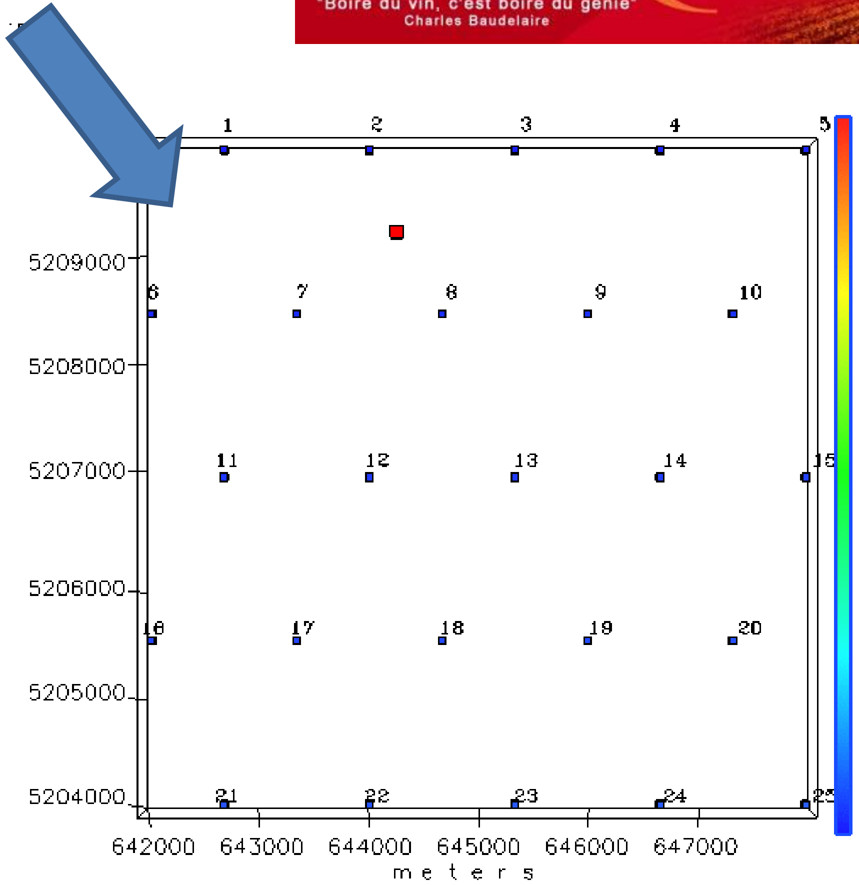


Optimizing using a retro-dispersion model

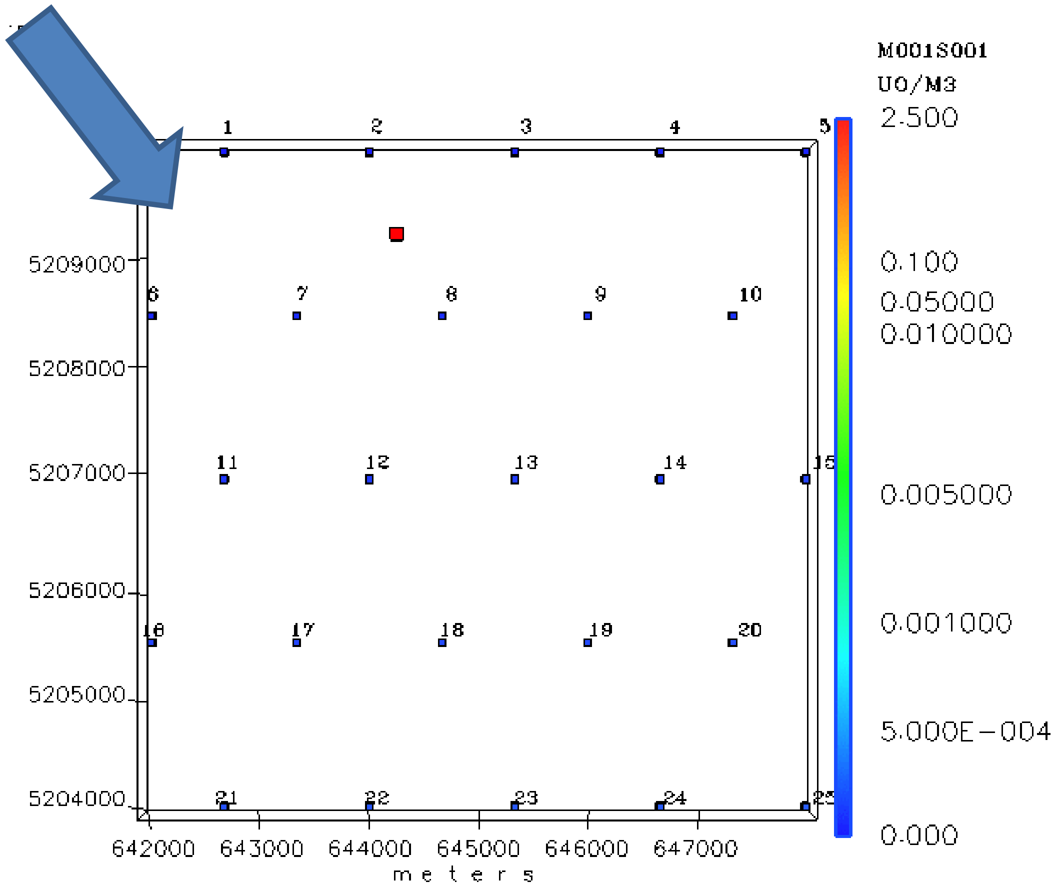
- We use Parallel Micro-SWIFT-SPRAY (PMSS) as dispersion model:
  - SWIFT is a diagnostic model using a mass-conservation principle to build 3D interpolated wind fields
  - SPRAY is a Lagrangian particle dispersion model that is used to generate synthetic concentration observations
  - Retro-SPRAY is the dual of the SPRAY model, and is used to build the C^* retro-dispersion fields

- Validation tests were performed using simulated observation data over realistic terrain characteristics in two cases:
  - 1st use case ("BEAUNE"): in a countryside landscape with a constant wind
  - 2nd use case ("OPERA"): in an urban context (neighborhood in downtown Paris) with a heterogeneous wind field

First use-case “Beaune”



First use-case “Beaune”

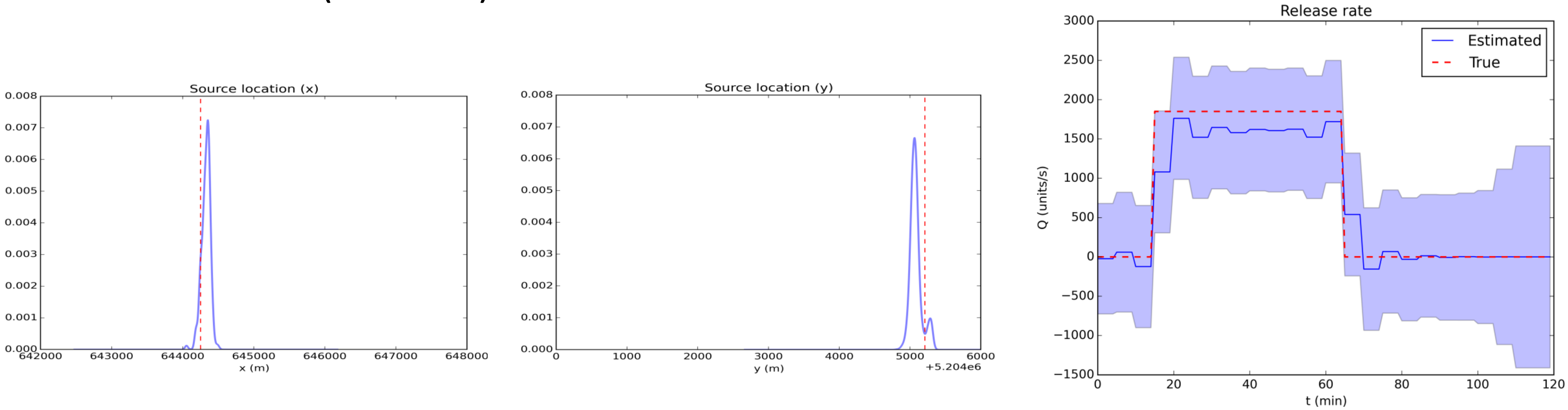


1st use-case (BEAUNE) input data:

SW point coordinates (km)	(642.000; 647.980)
NE point coordinates (km)	(5204.000; 5209.980)
Nb. Of meshes (X,Y)	**(300,300) = 90 000**
Mesh resolution (m)	20
Wind speed	1.5 m/s
Wind direction	330°
Release duration	45 mn (from 10:15 to 11:00 am)
Release rate	1850 units/s
Nb. sensors	**25**
Observation time frame	From 10:05 am to 12:00pm

First use-case "Beaune"

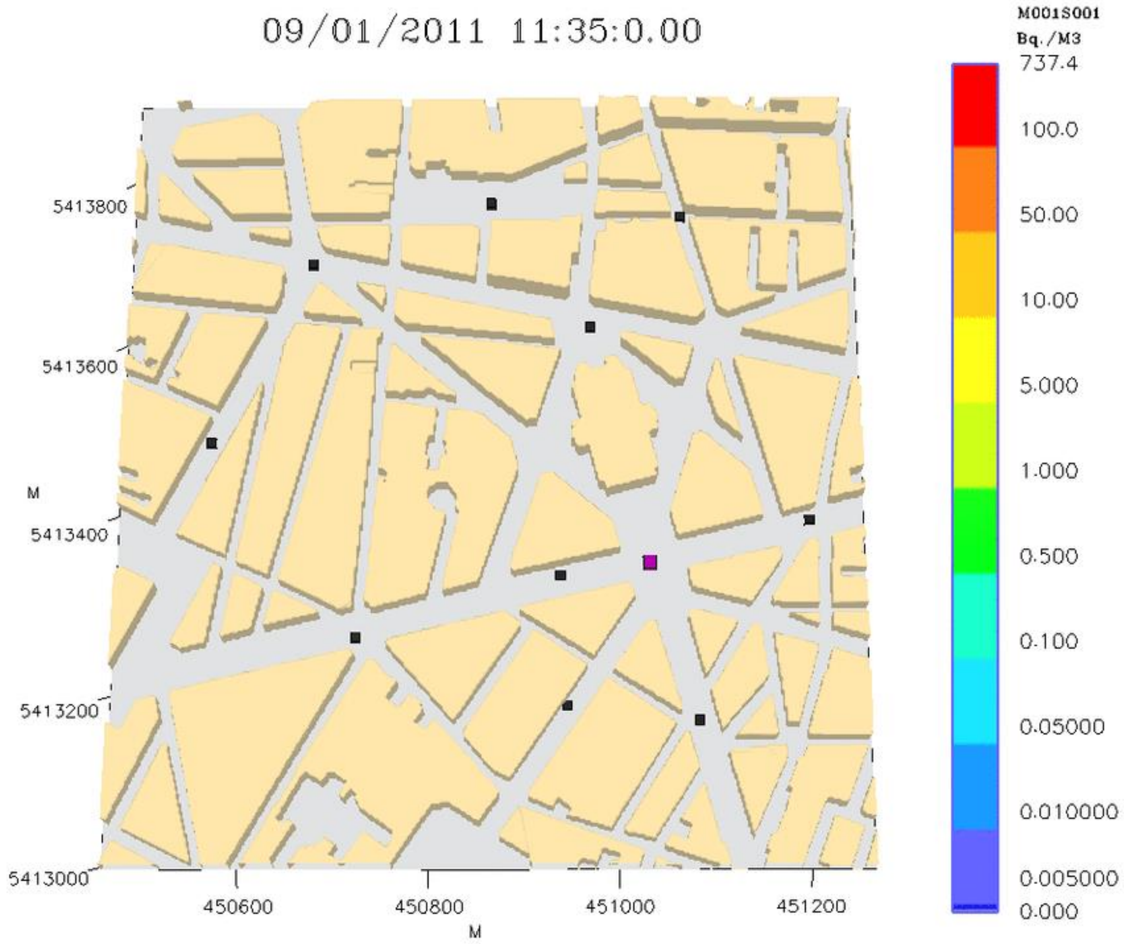
- 1st use case (BEAUNE) results:



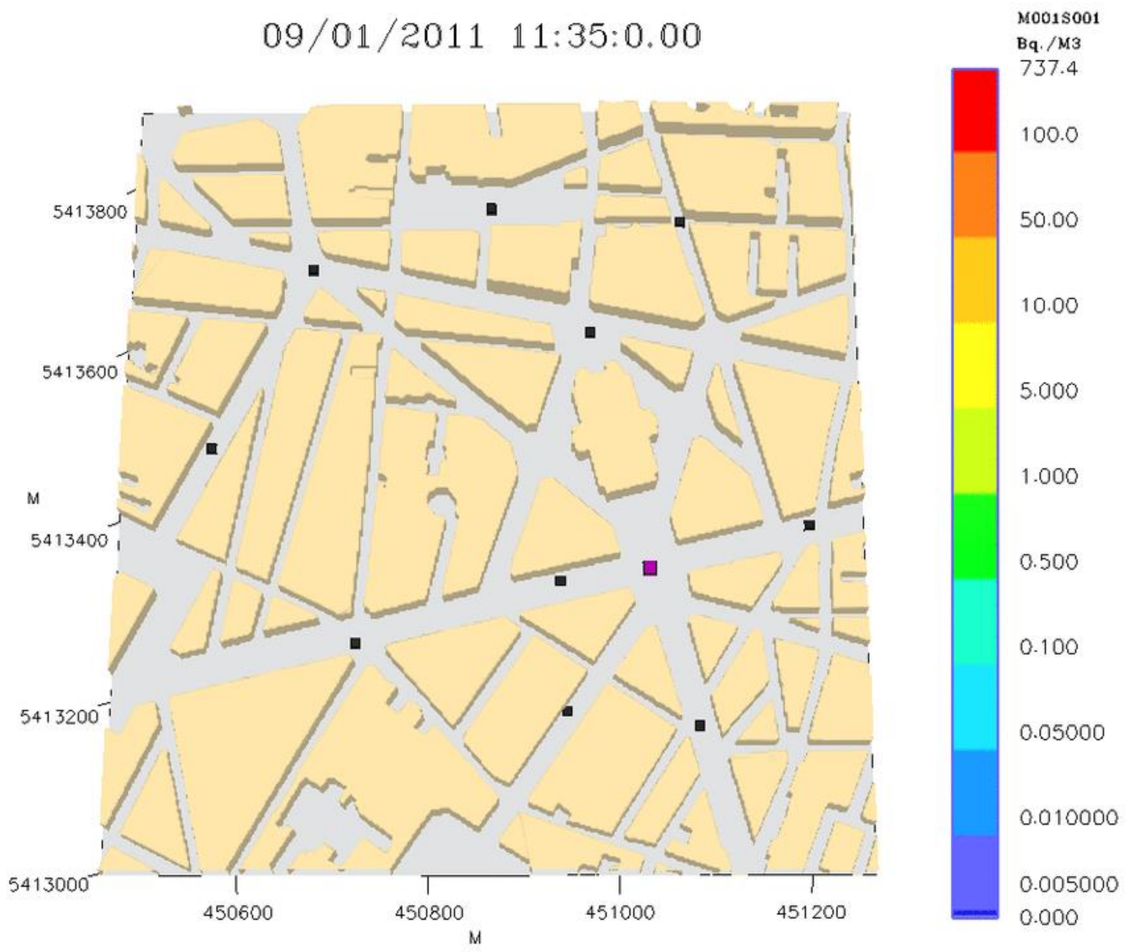
Estimation of the source parameters for the BEAUNE simulation: position in x (left) and y (center) compared to the true location (red), and reconstructed release rate (right) with 95% confidence interval compared to the true emission profile (red).

- Good estimation of the release rate
- The estimated source location is not as good. Cause: differences between C and C^* source-receptor matrices ?

Second use-case “OPERA”



Second use-case "OPERA"

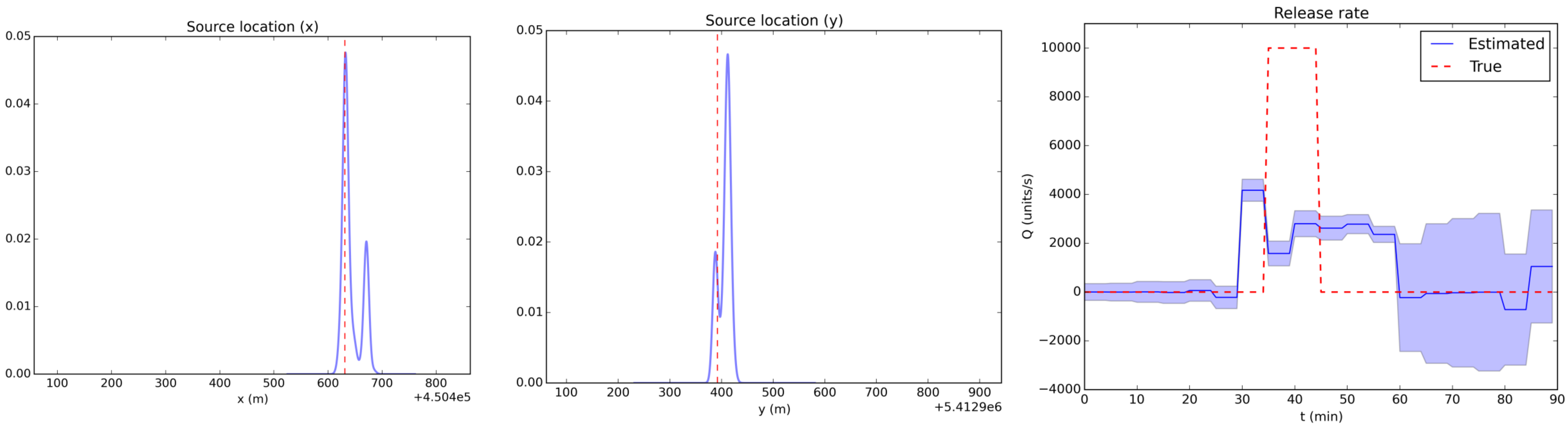


2nd use-case (OPERA) input data :

SW point coordinates (km)	(450.457;451.263)
NE point coordinates (km)	(5412.961;5413.842)
Nb. Of meshes (X,Y)	**(404,441)= 178 164**
Mesh resolution (m)	(2,2)
Wind speed	3m/s
Wind direction	11:00am-12:00 pm: **230°** | 12:00pm-1:00pm: **180°** | 1:00pm-2:00pm: **45°**
Release duration	10 mn (from 12:10 to 12:20 pm)
Release rate	10^4 units/s
Nb. sensors	**10**
Observation time frame	From 11:35 am to 1:00pm

Second use-case "OPERA"

- 2nd use case (OPERA):



Estimation of the source parameters for the OPERA use-case: position in x (left) and y (center) compared to the true location (red), and reconstructed release rate (right) with 95% confidence interval compared to the true emission profile (red).

- Estimation of the source location ➔ OK
- Difficulties to reconstruct the release rate due to the complexity of the use case (wind rotation, obstacles)

Conclusion

- New design of an optimized estimation process relying on Bayesian inference, stochastic modeling and a 3D Lagrangian dispersion model.
- AMIS methods improve MCMC methods efficiently
- The proposed scheme is able to hold the computational load and thus be scalable by using pre-computed retro-dispersion data obtained by the retro-dispersion model.
- The validation tests using this process show that the AMIS algorithm, could be used with any dispersion model and first results in complex situation are encouraging
- Perspectives and improvements:
  - Improve the method and test the estimation process on experimental data in an urban scenario
  - Study the influence of the various parameters in the AMIS algorithm
  - Extension of the method : elevated sources (including plume rises) and multi-sources

Thank you for your attention.

Positive Constraint Procedure