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A new method for assessing the uncertainty associated with 3D dispersion simulations in variable meteorological conditions

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Introduction – Context

1) Dispersion simulations of "hazmat" released within complex industrial or urbanised sites require 3D models able to take account of the combined influence of the topography and buildings

2) There is an increasing demand for such 3D simulations for assessing precisely and realistically the impact of toxic releases on human health for regulatory purpose and emergency management

3) While the 3D simulations are most often performed with a deterministic set of parameters for the release and meteorological conditions, these quantities are imperfectly known and they are a major source of uncertainties on the flow and dispersion patterns

4) Hence, methods for propagating uncertainties through 3D models are needed, especially for flow and atmospheric dispersion simulations at local scale (from 1×1 up to 50×50 km^2) in the follow-up of previous work (in the references below)

Aguirre Martinez, F., Y. Caniou, C. Duchenne, P. Armand and T. Yalamas, 2016: Probabilistic assessment of danger zones associated with a hypothetical accident in a major French port using a surrogate model of CFD simulations. 17th Int. Conf. on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Harmo'17, May 9-12, 2016, Budapest, Hungary

Armand, P., F. Brocheton, D. Poulet, F. Vendel, V. Dubourg and T. Yalamas, 2014: Probabilistic safety analysis for urgent situations following the accidental release of a pollutant in the atmosphere. Journal of Atmospheric Environment, Vol. 96, pp. 1-10

Problem formalisation (1/2)

1) Here, for the sake of simplicity, only the wind direction and velocity are considered as uncertain!

2) Dispersion simulation following an atmospheric release starts from a meteorological "conjecture" (the "conjecture" is a source of information or "something we believe in about what will happen")
   >> How does the uncertainty on the wind conjecture impact the atmospheric dispersion prediction?

3) As local scale met' ensembles are hard to obtain, we use here a unique WRF wind field conjecture

4) The wind field exhibits limited statistical stationarity which precludes fitting stochastic processes such as ARMA or conditioning simulations with a kriging model; thus, inferring the structure and amplitude of the wind uncertainty solely from available data is not possible here!

5) Yet, a careful inquiry of expert knowledge (and also operational requirements) should allow subduing the arbitrariness to a restricted set of intelligible parameters…

Problem formalisation (2/2)

5) At this stage, four specifications of the (wind) uncertainty simulator can be identified:

   a) Confidence in the conjecture – Uncertain wind simulations should be close to the conjecture and the level of confidence should be explicitly controllable by the user

   b) Physical origin of spatio-temporal structures – Spatio-temporal structures in the conjecture originate from physical phenomena and should be preserved when applying the uncertainty

   c) Link between uncertainty and conjecture variability – Experts in atmospheric dispersion expect the wind conjecture to be more uncertain when it is intrinsically highly variable

   d) Operational constraint – The uncertain simulator should be quite automatic and not require parameter tuning or unconstrained data analysis, but be organized into a preset plan

6) Specifications a) and b) provide a general bearing of the (wind) uncertainty model structure while specification c) and d) constrain the amplitude of the variability and the decision plan

7) Moreover, "equifinality" principle implies that while the diversity of possible uncertainty structures should be largely explored, the resulting probabilistic models can be sieved to achieve a simple and concise formulation (modelling wind field uncertainty is here a means, not the final aim!)

   >> In practice, we frame the probabilistic model as two distinct perturbations of the conjecture

Applicative case study (1/2)

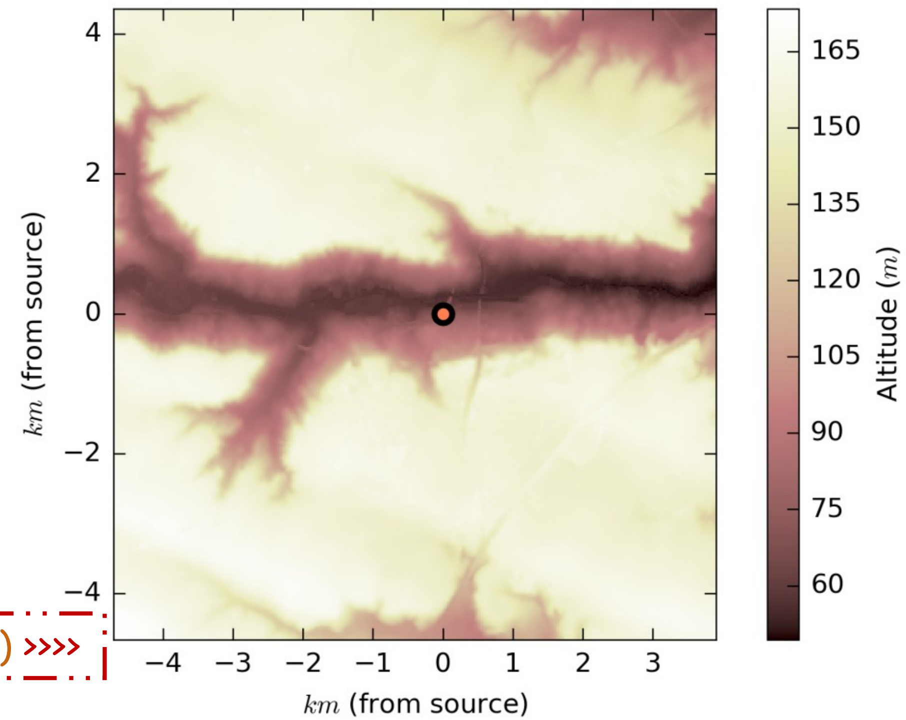
1) We suppose one unit of mass (1 u) of a hazardous (radioactive or chemical) material to be emitted during 10 min within a 3 hrs time frame and dispersed in the atmosphere over an 8×5 km^2 domain
>> The source is hypothetically located in a real and complex terrain (in the talweg of a river)

2) First, the 3D wind field is computed with WRF reconstruction and forecast meso-scale modelling system (resolution = 1 km), then downscaled to the local scale (highest resolution = 1 m to 10 m)

3) The local-scale flow and dispersion is simulated with the PMSS (Parallel-Micro-SWIFT-SPRAY) modelling system developed by the CEA and ARIA Technologies with MOKILI and ARIANET

4) The highly parallelized PMSS comprises PSWIFT, a mass-consistent flow diagnostic model, and PSPRAY, a Lagrangian particle dispersion model (both taking into account topography and buildings)

Map of the real terrain with the source (orange dot) >>>>



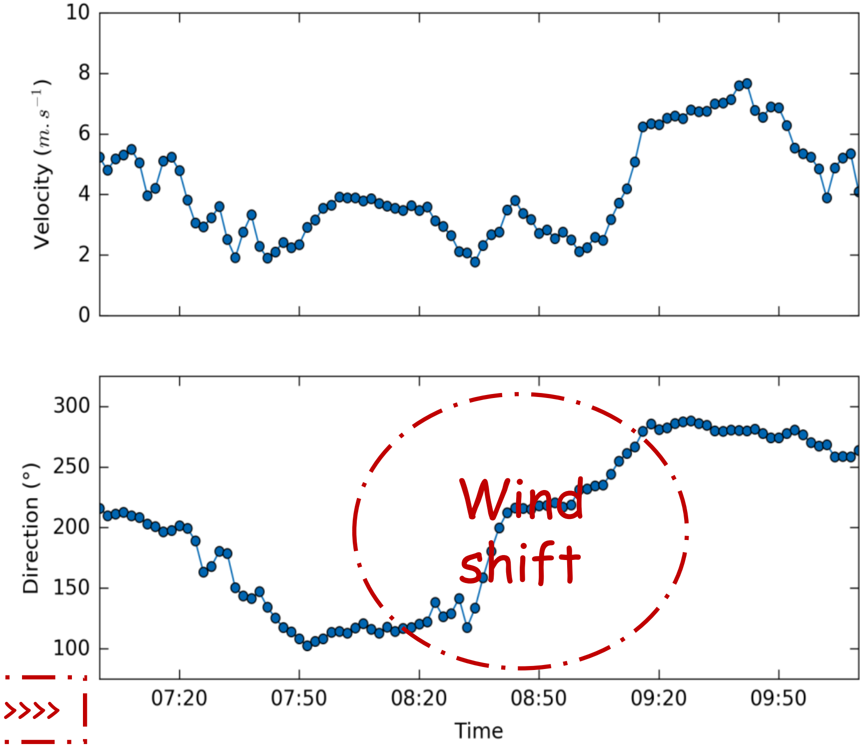
1) Here, the wind conjecture is a set of WRF vertical profiles of the horizontal wind components
   a) As our interest is fluctuating met' conditions, we contracted a 24 h original WRF sequence to 3 h
   b) The spatial resolution in WRF domain centered on the valley is 1 km and there are 31 vertical layers
   c) PMSS computational chain (PSWIFT + PSPRAY) is fed with the resulting 2 min time-step sequence

2) Two probabilistic models whose expectation is the WRF conjecture are devised:
   1) A perturbation of the wind direction and velocity
   2) A time warp of the wind direction and velocity

3) The perturbations are independent of the location, solely dependent on the vertical layer and time

4) Two samples of 100 uncertain PSWIFT wind fields + PSPRAY concentration fields were simulated (300 h with 28 cores of a cluster at CEA computing center)

5) We have compared the variability of the dosage results induced by two kinds of wind perturbations



Time series of WRF wind at 10 m above the ground level >>>>

Additive perturbation of WRF conjecture

$$\underbrace{Z_{constant}(x,h,t)}_{\text{Perturbed field}} = \underbrace{z_0(x,h,t)}_{\text{Conjecture}} + \underbrace{\varepsilon_c\, a\, \sigma_c(h,t)}_{\text{Perturbation}}$$

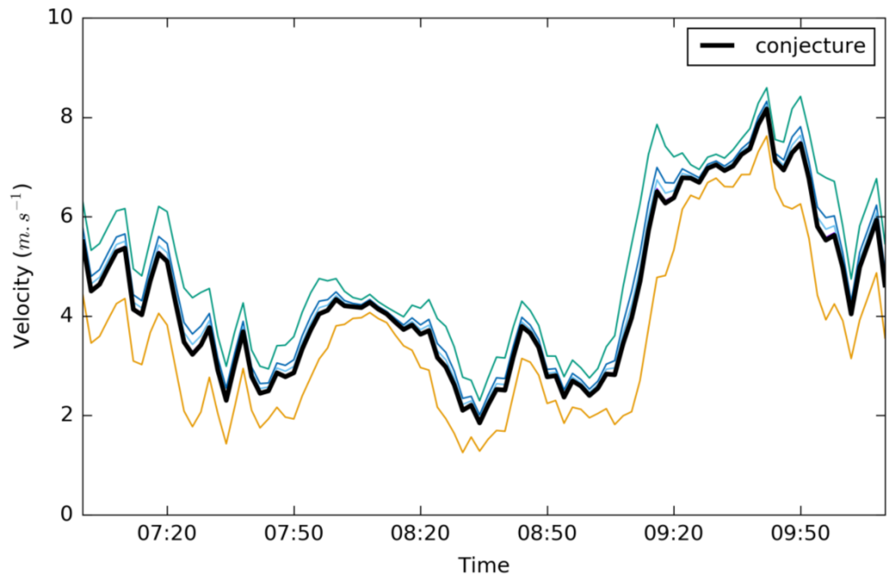
ε_c : Sandard Gaussian noise

a : Confidence factor

$\sigma_c(h,t)$: Rolling standard deviation

1) We apply small perturbations to the conjecture
2) The structure is prescribed beforehand
3) The amplitude is linked to the conjecture local variability and it is tunable depending on the confidence in the conjecture

Five time series of perturbed wind velocity (at 10 m above the ground level)



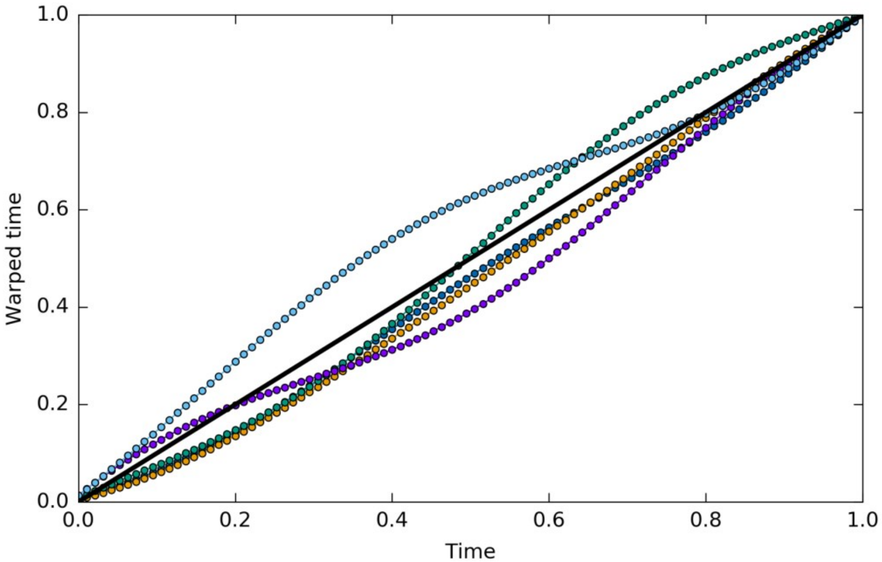
Time warp of WRF conjecture

$$Z_{warp}(x,h,t) = z_0\big(x,h,\Phi(t)\big)$$

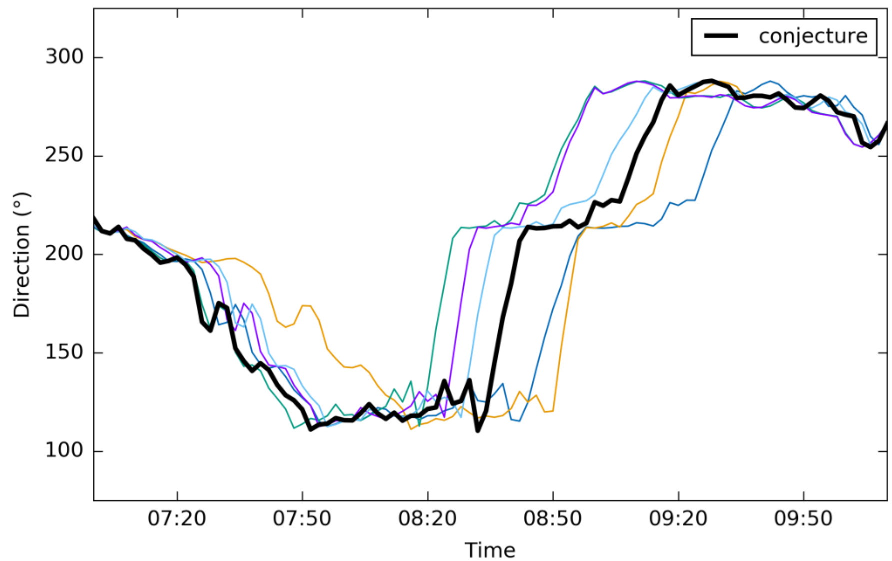
Perturbed field | Conjecture | Time warp function

The time warp function transforms time by using oscillating functions

(time is alternatively accelerated or slowed down)

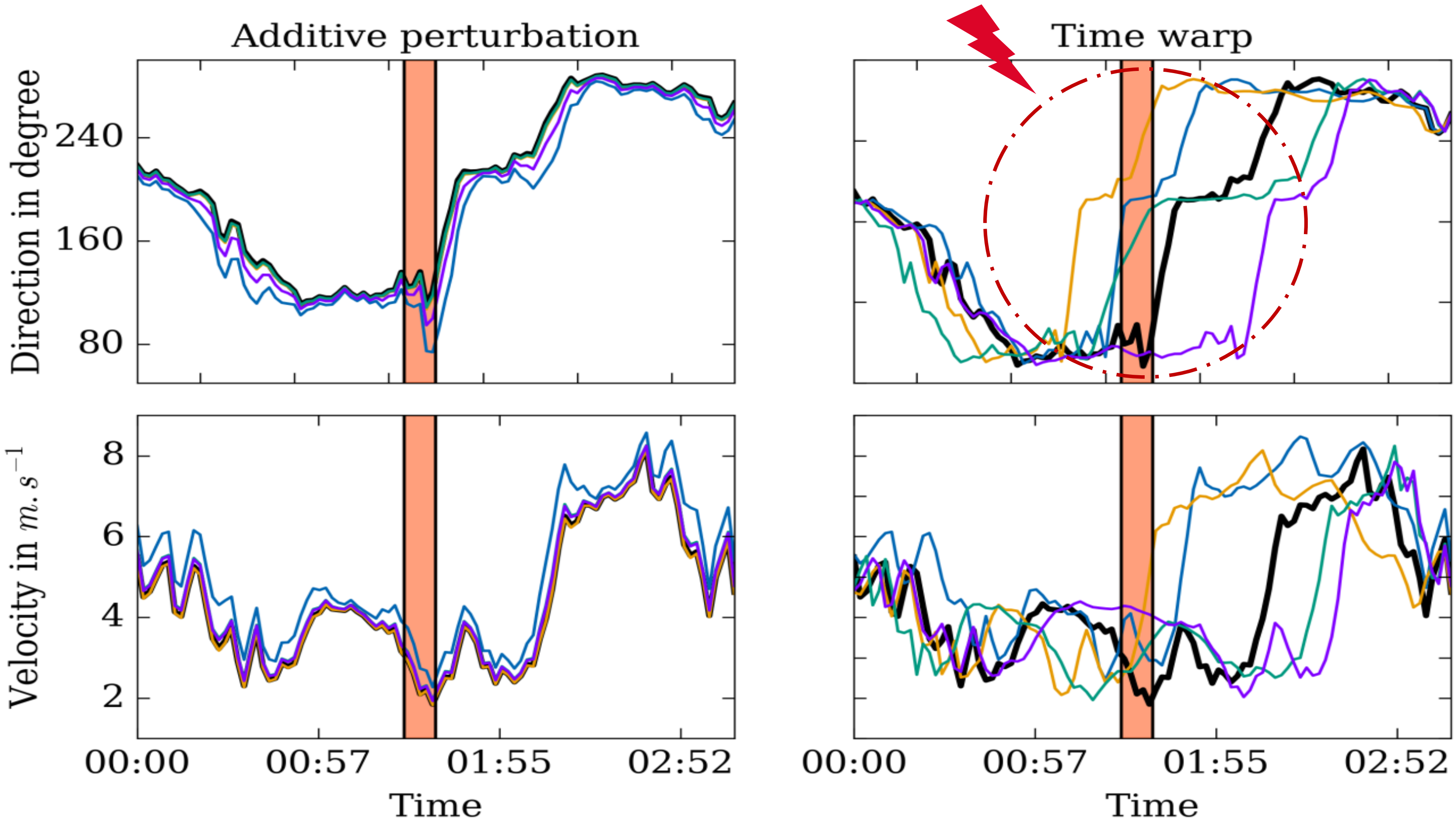


Five time series of warped wind direction (at 10 m above the ground level)



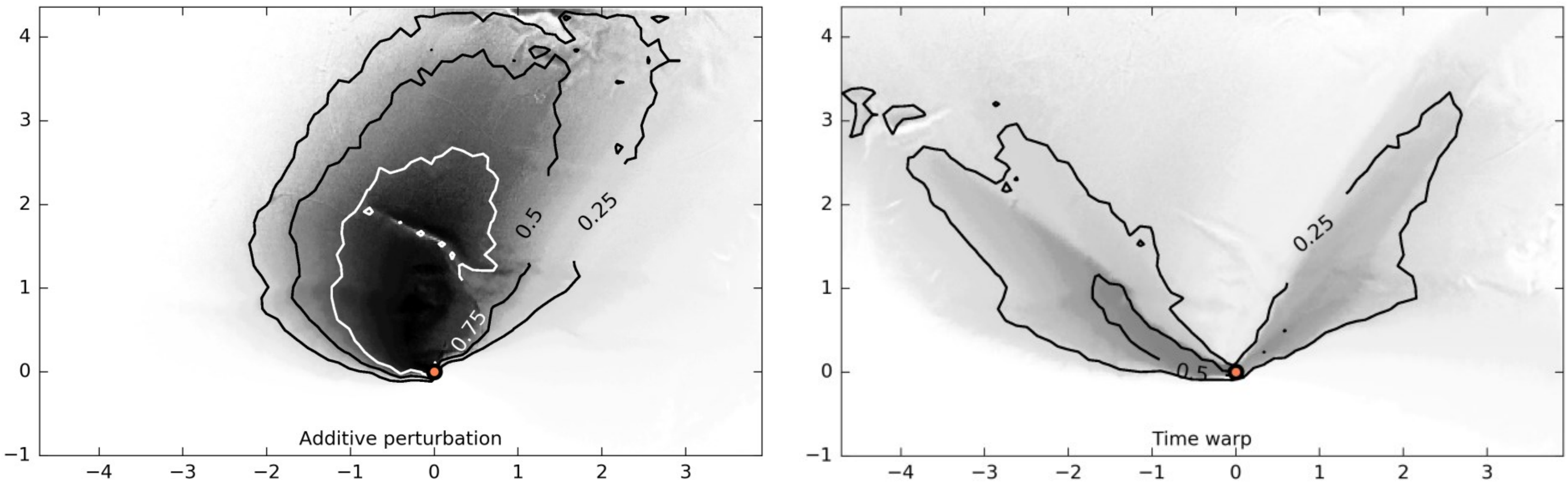
DoE for the two samples of perturbations

The wind shift can be before, during or after the release!



The conjecture is plotted as a thick black line & The orange vertical bar spans the release time frame

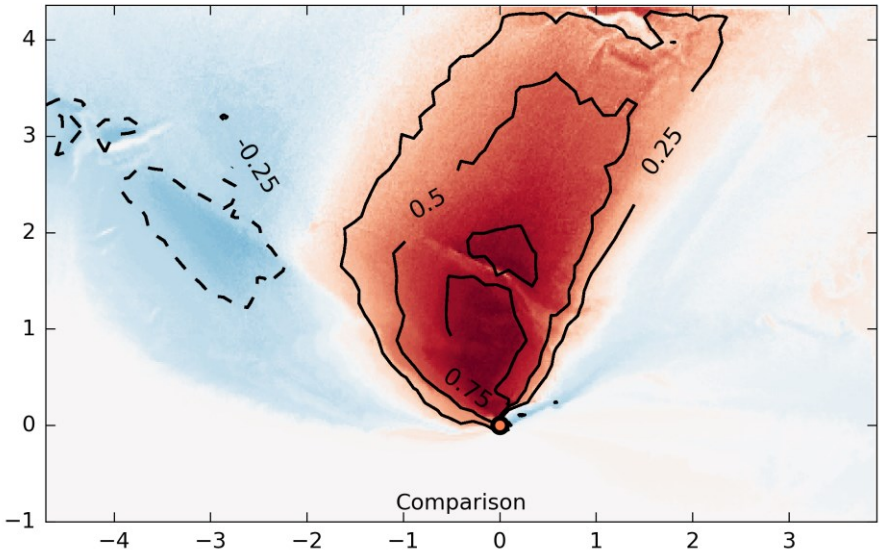
Empirical probabilities of the dosage exceeding (the arbitrary value of) 10^{-7} u.s.m^{-3} under additive perturbation (left) and time warp (right)



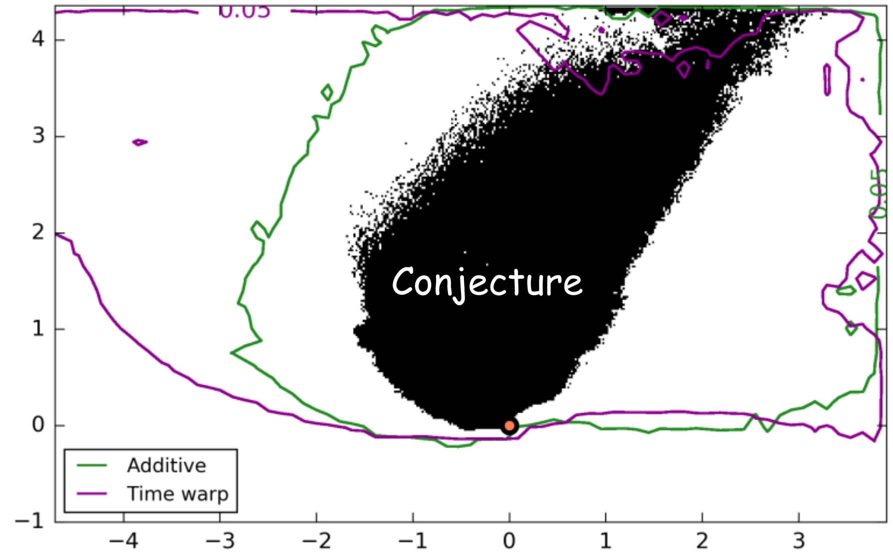
The perturbations lead to significantly differing zones. The probability surface resulting from the additive perturbation assumes the same overall shape as the exceedance region of the conjecture. On the contrary, time warp spreads the simulations all over the northern part of the domain.

Dosage results – Exceedance probability (2/2)

Differences of the dosage exceedance probabilities (additive perturbation – time warp)



Exceedance zone for the conjecture in black and level lines of the 5% exceedance probability for both perturbations



The low probability contour lines displayed over the conjecture are of particular interest for emergency management. With time warp, the delimited zone spans most of the northern plateau, while it is notably smaller with additive perturbation.

Dosage – Principal component analysis (1/2)

1) Principal component analysis seeks uncorrelated linear combinations of the parameters (here, wind direction and wind velocity) that account for most of the overall variance (in the dosage)
   a) The principal components variances are controlled by the confidence in the conjecture parameters
   b) The principal components "directions" enable to analyze the uncertainty model potential equifinality

2) The additive perturbation has two prominent effects:
   a) Rotate the plume within a limited domain of about 45° (40% of the variance)
   b) Concentrate or spread the plume symmetrically on either side of its main axis (20% of the variance)

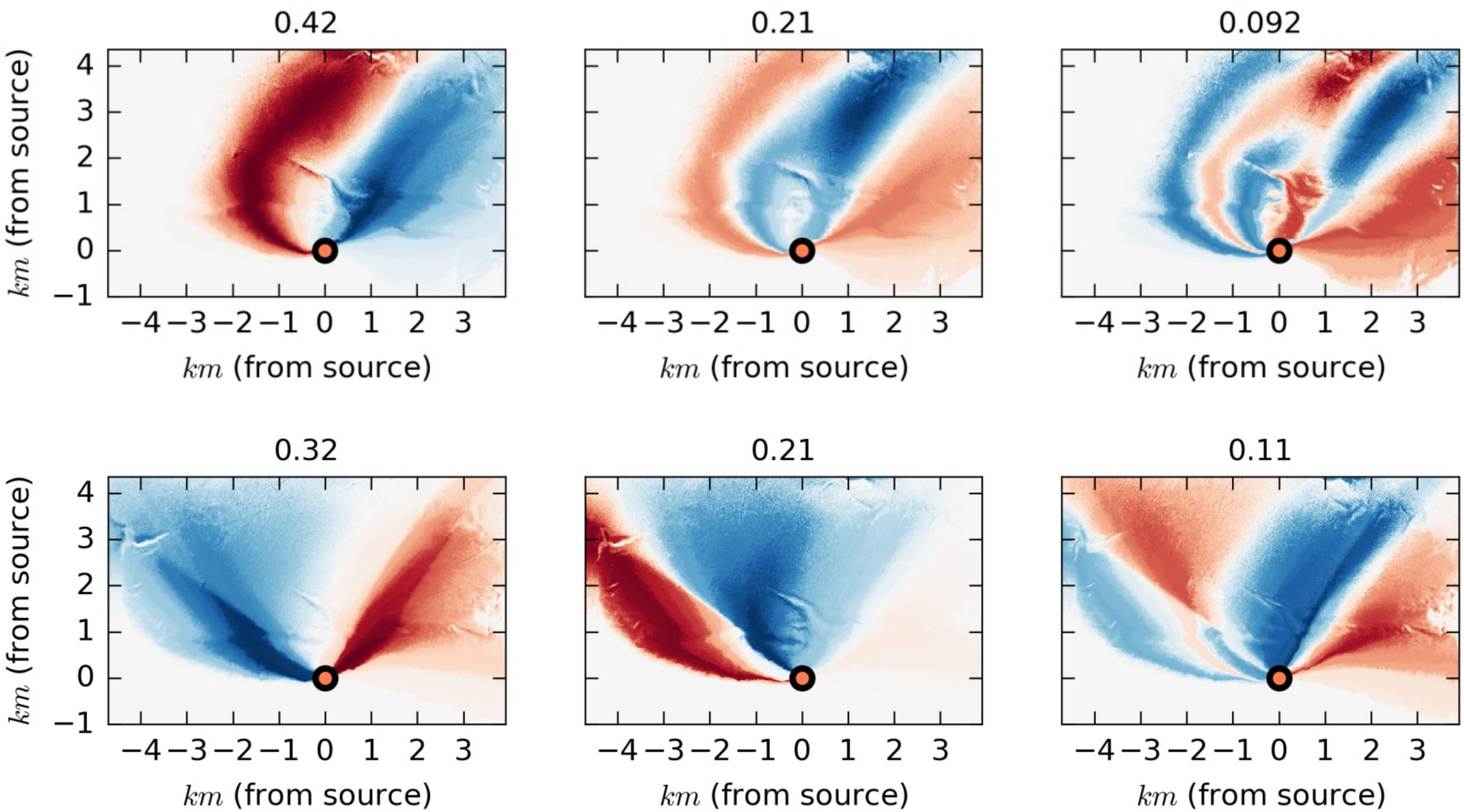
3) The time warp has two main effects:
   a) Select and switch between two prominent directions (30% of the variance)
   b) Refine the plume direction in the western part of the domain (20% of the variance)

Dosage – Principal component analysis (2/2)

Breakdown of the perturbation effects along the three first principal components
(numbers above the figures are the parts of the variance associated with the component)

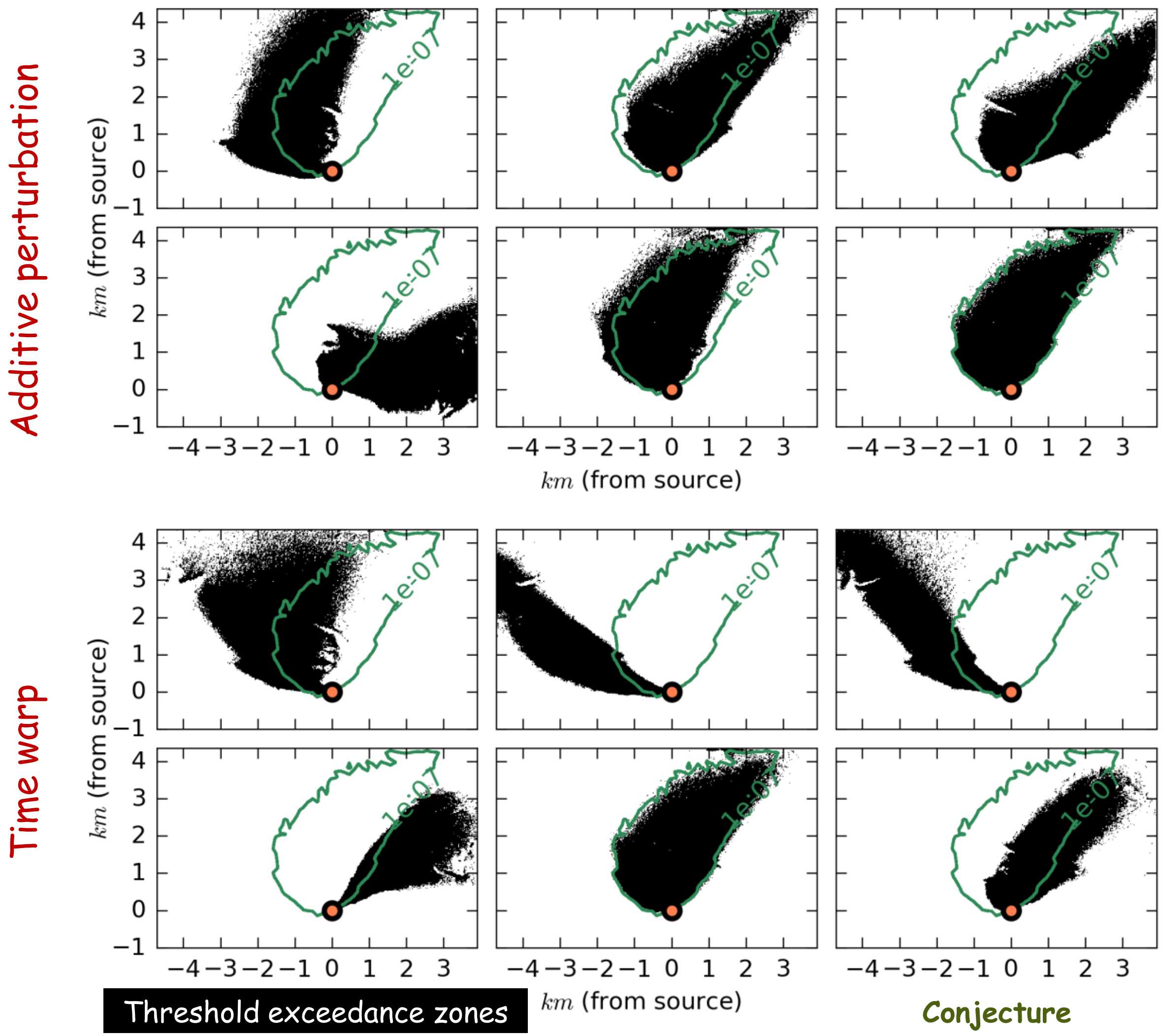
Additive perturbation

Time warp



Dosage results - Archetypes

"p-archetypes" are individual simulations of the most widespread 2*p sized subsamples with p components



With the additive perturbation, the first "direction" of uncertainty can lead to outcomes very different from the conjecture.

With the time warp, the main "direction" of the plume is highly uncertain.

Conclusions and perspectives

1) This research is an attempt to take account of the uncertainty on any meteorological conditions
2) Two uncertainty models are created to introduce perturbations of a pre-computated WRF wind
3) The perturbed WRF wind fields are downscaled with PMSS also used for dispersion simulations
4) For the sake of simplicity, only the wind direction and velocity are considered as uncertain
    a) The uncertainty models are simple, but versatile
    b) They are able to capture some of the diversity of wind field uncertainty
    c) The two models affect the dispersion outcome in complementary "uncertainty directions"
    d) Each has a parameter representing the confidence in the conjecture
5) Our approach can accommodate the diversity of topographic and meteorological conditions
6) The perturbation approach could be transposed to other sources of uncertainties, meteorological (LMO, H, rate of precipitation…) or source term related (location, height and rate of emission)
7) The "uncertainty directions" offer a new viewpoint on sensitivity analysis of multivariate outputs (not focused solely on variance) and on selection of the most relevant sources of uncertainty
8) Further work will calibrate the parameters of the uncertainty models and test the uncertainty propagation in operational contexts: impact assessment, risk studies and simulated emergency

Questions?

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