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Consideration of uncertain forcings in the global sensitivity analysis and metamodeling of a pesticide transfer model

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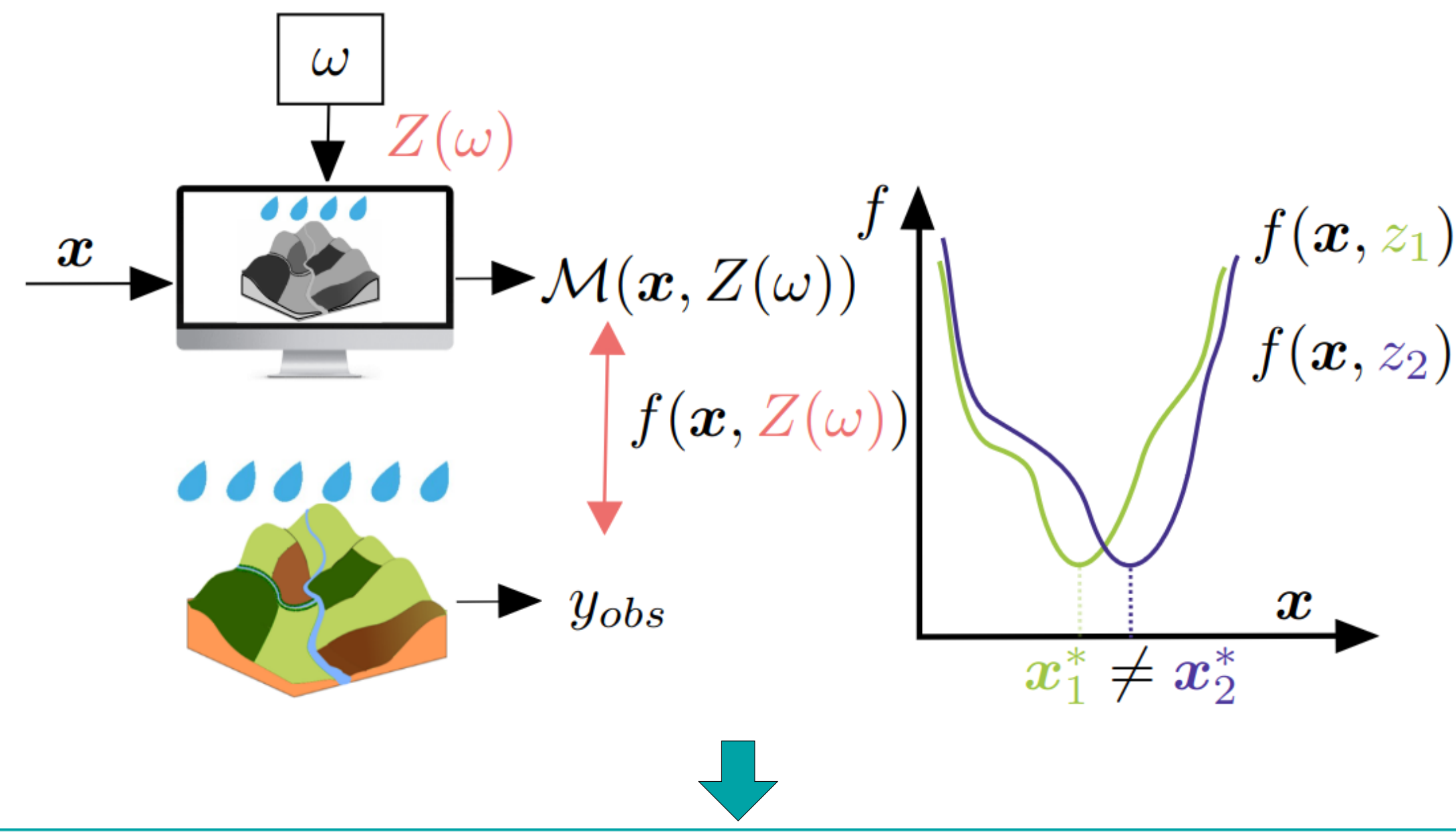
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Uncertainty quantification in decision support for water quality

Pesticide transfer modeling at the catchment scale (e.g. [1]) simulates surface/subsurface hydrology and reactive solute transport:

- based on non linear equations
- need for a large set of spatialized parameters
- many interactive processes not (well) represented

→ **controllable model inputs:** the model parameters
→ **uncontrollable model inputs:** the forcings : rainfall / **pesticide app. dates** (typ. known within a 2/3 day range)



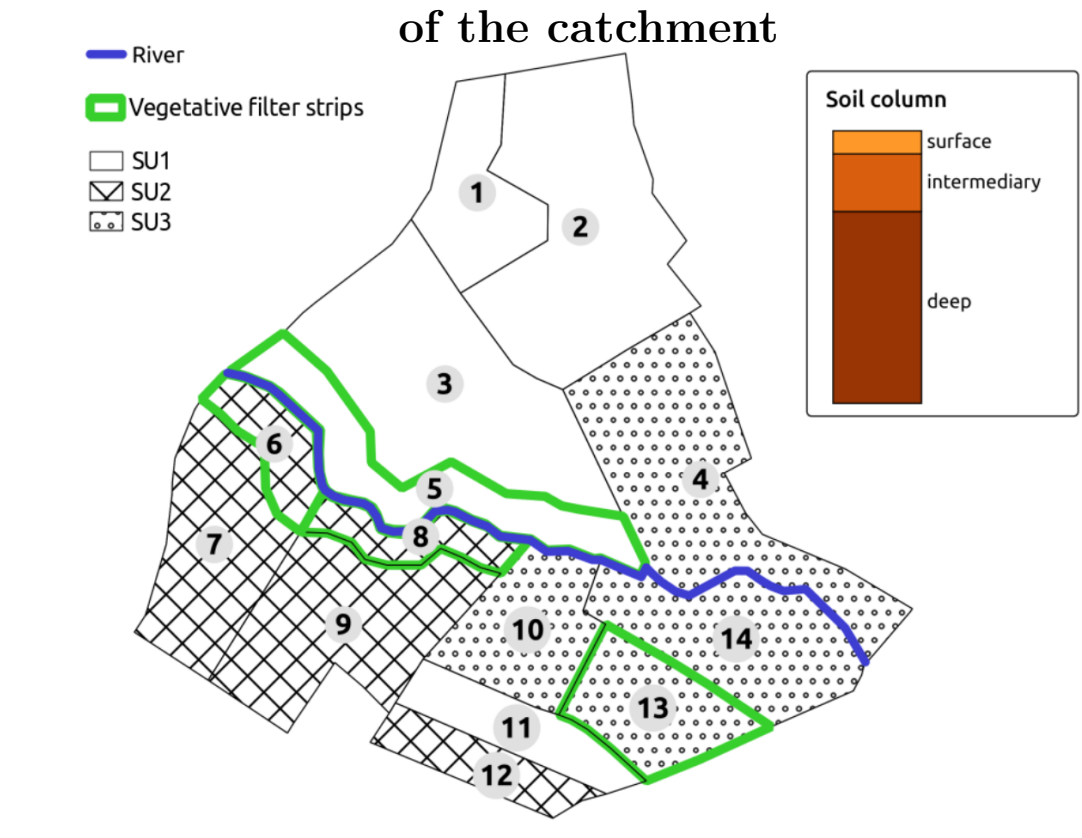
Uncertainty in forcings is propagated to:

- the estimation of the model input parameters
- the **global sensitivity analysis (GSA)** of model outputs: this is generally not taken into account due to the complexity of the models [2,3] ⇒ *this study objectives*

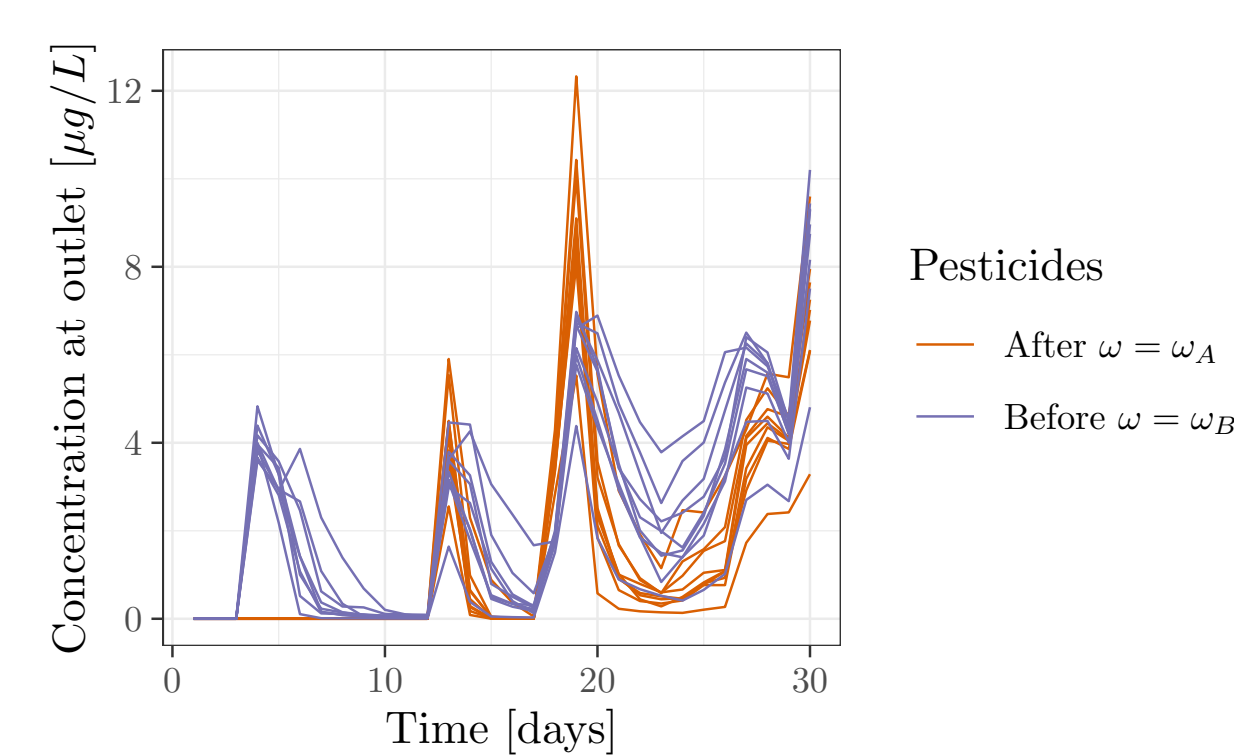
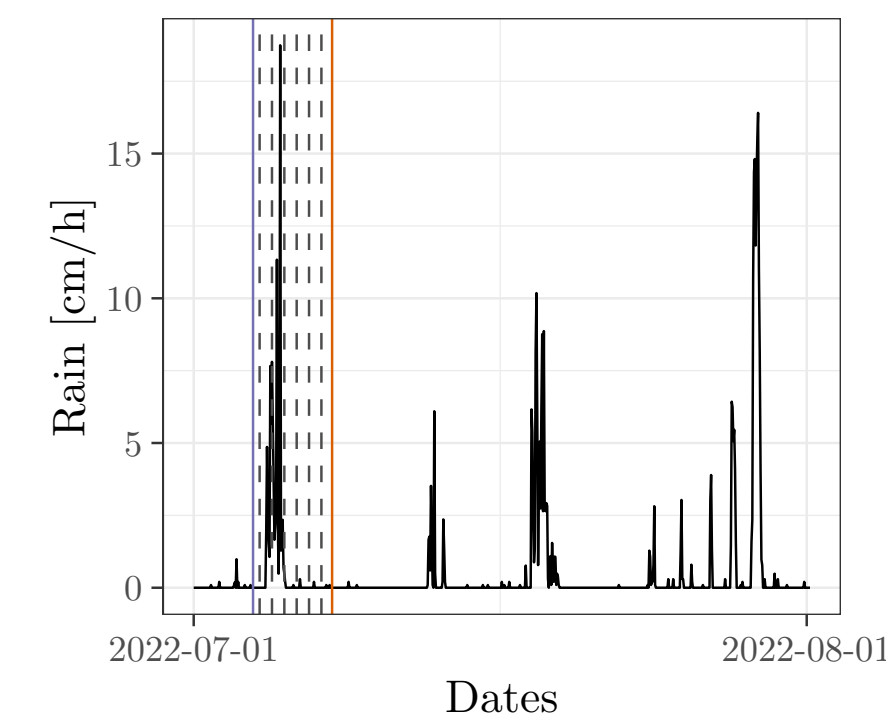
Case study: uncertainty on the pesticide application date



Application of pesticides on the vineyard parcels of the catchment



What if this is uncertain whether pesticide applications occurred before or after a heavy rainfall?



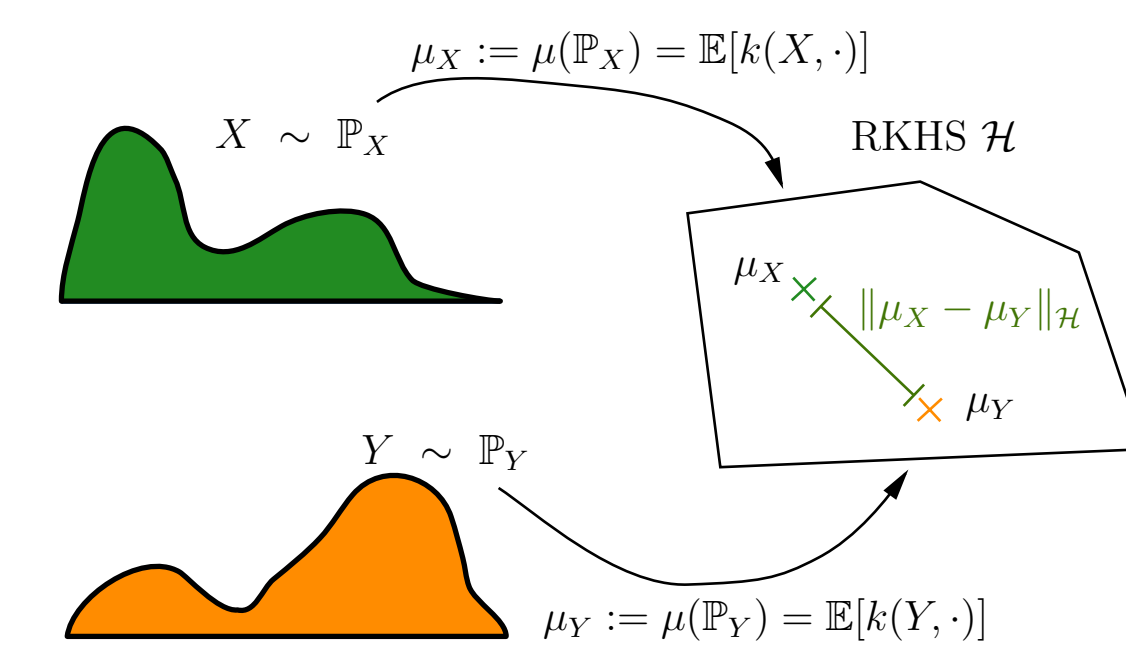
- ✓ pesticides are applied over a small catchment
- ✓ output var. studied: concentration at the outlet
- ✓ simulated pesticide concentrations differ w.r.t. the application date and model parameters
- ⇒ need for a 2-steps global S.A. to investigate [5-6]

2-steps GSA

- Screening with HSIC independence test

$$H_0 : X_i \perp\!\!\!\perp Y \text{ vs. } H_1 : X_i \text{ and } Y \text{ are not independent}$$

$$p_{\text{val}B} = \frac{1}{B} \sum_{b=1}^B \mathbb{1}_{\widehat{HSIC}^{[b]}(X_i, Y) > \widehat{HSIC}(X_i, Y)} \quad (1)$$



HSIC indices, ©Guerlain Lambert

- Sobol' indices with Polynomial Chaos Exp.

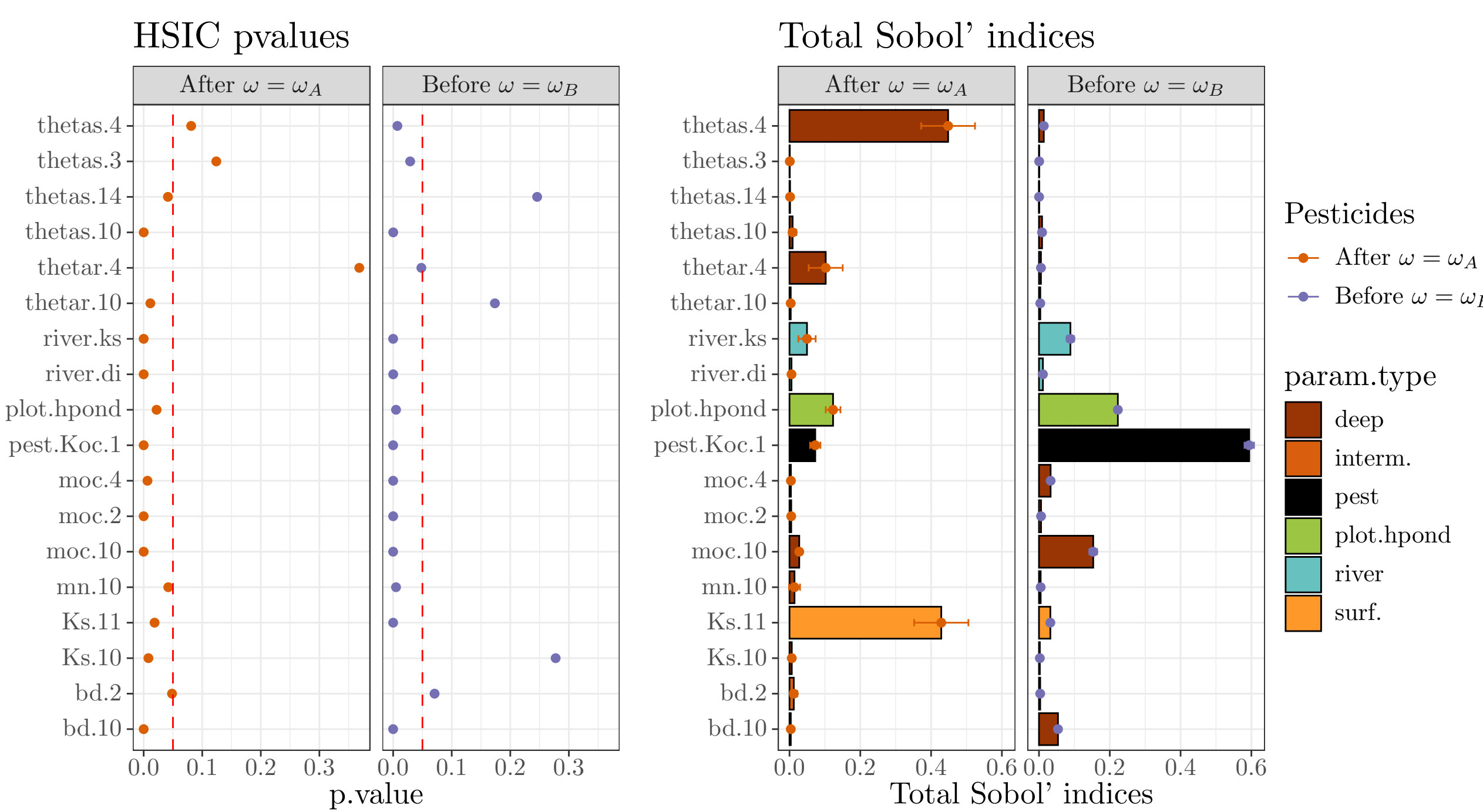
$$Y = f_d(\mathbf{X}) \approx f_{PCE}(\mathbf{X}) = \sum_{\alpha \in \mathcal{A}} c_\alpha \psi_\alpha(\mathbf{X}),$$

$$\hat{S}_i = \frac{\sum_{\alpha \in \mathcal{A}_i} c_\alpha^2 / \hat{D}}{\hat{D}}, \quad \mathcal{A}_i = \{\alpha \in \mathcal{A} : \alpha_i > 0, \alpha_{j \neq i} = 0\},$$

$$\hat{S}_{T_i} = \frac{\sum_{\alpha \in \mathcal{A}_{T_i}} c_\alpha^2 / \hat{D}}{\hat{D}}, \quad \mathcal{A}_{T_i} = \{\alpha \in \mathcal{A} : \alpha_i > 0\},$$

$$\hat{D} = \text{Var} \left[\sum_{\alpha \in \mathcal{A}} c_\alpha \psi_\alpha(\mathbf{X}) \right] = \sum_{\alpha \neq \{0\}} c_\alpha^2 \quad (2)$$

Sensitivity in two contrasting scenarios

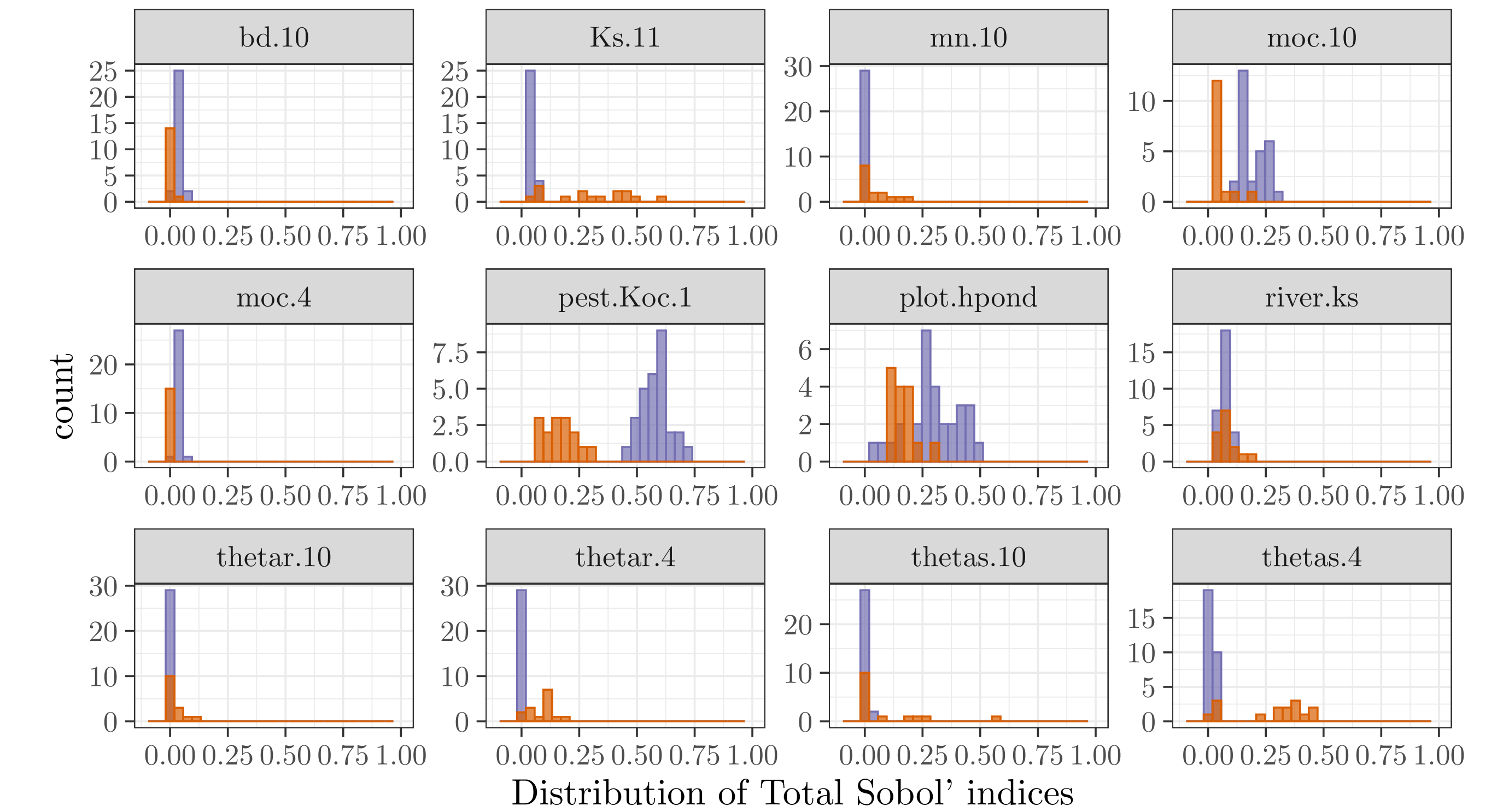


- The HSIC identifies 28 influential parameters on 150
- The Sobol' indices for the 28 parameters are calculated
- **GSA results are different in the two cases**
- ⇒ what about the application dates between ω_A and ω_B ?

References

- [1] Rouzies et al., 2019. 10.1016/j.scitotenv.2019.03.060 [2] Gatel, L. et al., 2019. 10.3390/w12010121 [3] Rouzies et al., 2022. 10.5194/egusphere-egu22-10384 [4] Sudret et al., 2008 10.1016/j.res.2007.04.002 [5] Gretton et al., 2005 10.5555/1046920.1194914 [6] Lüthen et al., 2023 10.1016/j.cma.2022.115875

A more global approach: Sobol' indices as random variables

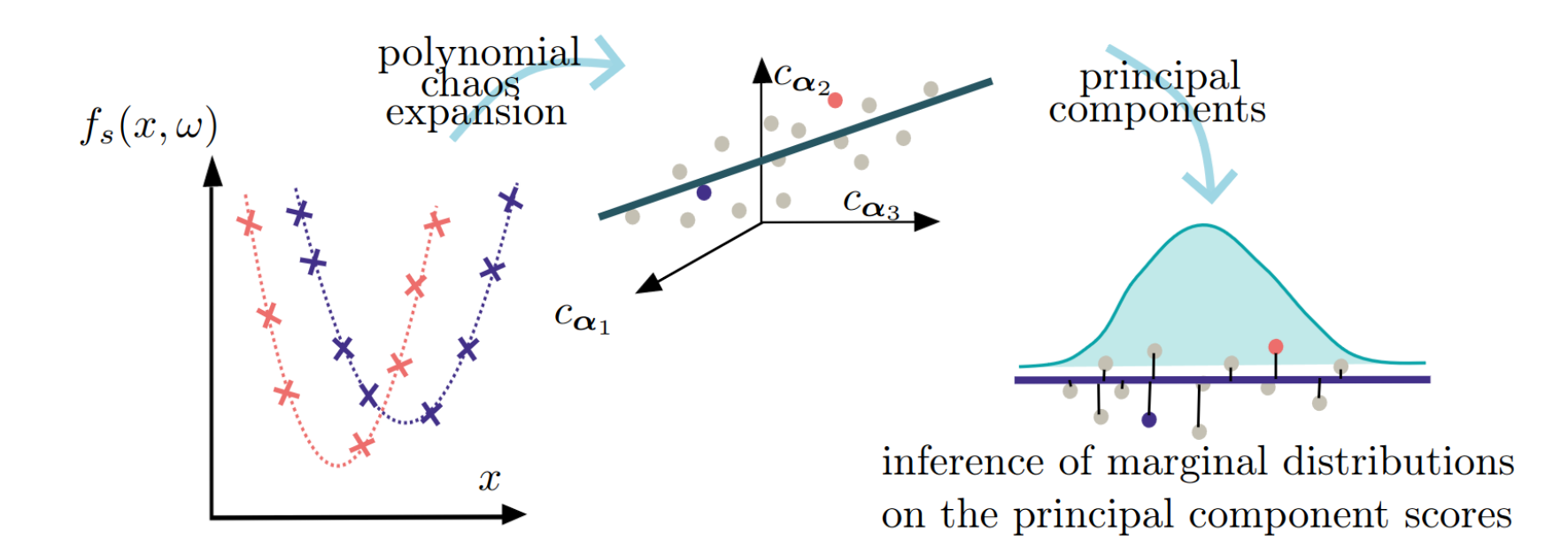


Application Before and during rain After rain

- ✓ Sobol' indices are seen as random variables,
- ✓ Sobol' indices represented as histograms (depending on the application date)
- ✓ the sensitivity of the output on the pest.Koc.1 (pesticide mobility) and others par. differs visibly w.r.t. the application moment

Conclusion / Next steps

- The GSA results lead to contrasting conclusions depending on the uncertain pesticide application date
- Considering Sobol' indices as random variables reveals a difference in the influence of some input factors (pest.mobility Koc, θ_s , K_s of some horizons, hpond, etc.) on the concentration at the outlet.
- Next step : building a **stochastic metamodel** of PESHMELBA by inferring the distributions of the PCE coefficients [6]:



BUT: in our case complex nonlinear interactions between determ. and stochastic inputs ⇒ other methods are tested for inferring distrib. of the coeff. such as KDE, GMM, Principal Curve Analysis in 3D on the PCs

1. Approximate each trajectory with a PCE
 $f_s(x, \omega) \approx f_{PCE}^{(1)}(x) = \sum_{\alpha \in \mathcal{A}} c_\alpha(\omega_1) \psi_\alpha(x)$
 $f_s(x, \omega_2) \approx f_{PCE}^{(2)}(x) = \sum_{\alpha \in \mathcal{A}} c_\alpha(\omega_2) \psi_\alpha(x)$
 $\rightarrow c_\alpha$ is a random vector in \mathbb{R}^{15}
2. Infer the distribution of c_α (out of R_{train} available realizations)
 a) Dimensionality reduction of c_α
 $PC_1 : 80.61\%$
 $PC_2 : 91.61\%$
 $PC_3 : 98.15\%$
 b) Infer a GMM on the PCs
 $f_s(x, \omega) \approx \sum_{\alpha \in \mathcal{A}} c_\alpha^{new} \psi_\alpha(x)$